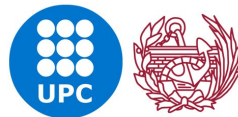


COMPUTATIONAL STRATEGIES FOR TIME-ACCURATE SIMULATION OF PART-SCALE LPBF

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ACRONYMS

AM	Additive Manufacturing
MAM	Metal Additive Manufacturing
DED	Directed Energy Deposition
PDE	Partial Differential Equation
ODE	Ordinary Differential Equation
LPBF	Laser Powder Bed Fusion
LBM	Laser Beam Melting
FSI	Fluid-Structure Interaction
FE	Finite Element
FEM	Finite Element Method
FCM	Finite Cell Method
FDM	Finite Difference Method
FVM	Finite Volume Method
HAZ	Heat Affected Zone
SLM	Selective Laser Melting
SLS	Selective Laser Sintering
EBM	Electron Beam Melting
LENS	Laser Engineered Net Shaping
DOF	Degrees of Freedom
AMR	Adaptive Mesh Refinement
DD	Domain Decomposition
BC	Boundary Condition
GPU	Graphics Processing Unit
CPU	Central Processing Unit
FH	Flash Heating
DN	Dirichlet-Neumann
DR	Dirichlet-Robin
NIST	National Institute of Standards and Technology
CIMNE	International Center for Numerical Methods in Engineering
HTC	Heat Transfer Coefficient
LLNL	Lawrence Livermore National Laboratory
SPD	Symmetric Positive Definite
DN	Dirichlet-Neumann
RR	Robin-Robin
ALE	Arbitrary Lagrangian-Eulerian

ABSTRACT

The qualification of Metal Additive Manufacturing (MAM) processes remains a major challenge due to the complex thermo-mechanical phenomena involved. The process is driven by a small moving heat source that generates highly localized, transient thermal gradients and induces thermal strains. As these strains are constrained by the surrounding material, residual stresses and warpage develop, causing part distortion or even failure.

Accurate modeling is essential for understanding the underlying physics, as well as for reliable process qualification and parameter optimization. However, such simulations are computationally expensive due to the small size of the heat source, which introduces disparate spatial scales, and its continuous motion, which gives rise to equally disparate temporal scales. The need to simultaneously resolve these scales renders high-fidelity part-scale simulations prohibitively expensive.

This thesis contributes to the field of MAM modeling on both the applied and methodological fronts. On the applied side, methods for warpage and stress mitigation are investigated in both Directed Energy Deposition (DED) and Laser Powder Bed Fusion (LPBF) processes, including a novel *substrate design* strategy for DED that significantly reduces residual stresses, and a modeling framework to capture *recoater-induced build failure* in LPBF.

On the methodological front, the thesis focuses on developing efficient strategies for high-fidelity part-scale simulations of LPBF processes, with particular emphasis on overcoming the disparity of temporal scales. While Adaptive Mesh Refinement (AMR) has become a popular approach to address the challenge of disparate spatial scales, uniform time-stepping remains the standard approach in the field. For centimeter-scale parts, this can require hundreds of millions of time-steps, making such simulations computationally unfeasible.

Commonly used strategies to alleviate this issue involve extreme simplifications of the thermal model, such as lumping multiple tracks or layers into a single time-step. Effectively, this eliminates the small scales associated with the moving heat source but compromises the model's predictive accuracy, requiring additional calibration.

Two methods are proposed to address the temporal-scale disparity without eliminating the underlying small scales: the *advected subdomain* and a *Robin-Robin* substepping scheme, both designed to preserve model fidelity while drastically reducing computational cost.

The *advected subdomain* method attaches a moving mesh to the laser. By solving the thermal problem in the reference frame of the heat source, the transient dynamics near the melt pool become quasi-steady, allowing the use of significantly larger time-steps.

Substepping divides the domain into regions that evolve with different time-steps: finer steps are applied locally around the moving heat source, while larger steps are used away from it. The developed Robin-Robin coupling scheme proves robust and ensures mesh-independent convergence between the regions.

These methods and their components are systematically evaluated through numerical analysis, benchmarked against standard approaches, and validated against experimental data. Furthermore, they are combined to compound their respective benefits.

Together, these contributions advance numerical MAM modeling, thereby improving the computational efficiency of high-fidelity simulations and enabling reliable process qualification and optimization.

MOTIVATION

In the 80s and 90s, Additive Manufacturing (AM) was regarded as a rapid prototyping technology: it enabled for a quick workflow from Computer Aided Design (CAD) to 3D printed part, therefore accelerating the development cycle and the time-to-market, but the resulting parts used to be of poor quality [Onuh and Yusuf, 1999]. In recent decades, speed, part accuracy and material properties have improved significantly and AM is now considered a fully-fledged manufacturing technology [Campbell et al., 2012].

Large scale adoption started already in the 2000s in the biomedical field, where the capacity to manufacture complex patient-specific geometries was a game changer for prosthetics [Dalgarno, 2017]. Another advantage is the elimination of tooling dependency: Roscoe et al. [2023] gives as an example an aerospace engine, where “a design change to one component in the combustion system requires cascading changes to the fan, compressors, turbines and shaft”, which in turn require changes to the dedicated molds, dies and fixtures used in traditional manufacturing. AM offers a solution as it both replaces all the dedicated tooling with a single tool, and reduces considerably the amount of individual piece parts in a system.

For example, propellant injectors for rocket engines were traditionally composed of hundreds of subcomponents: AM is now the mainstream manufacturing technique for injectors [Soller et al., 2017], and the part count has been reduced to the single digits [NASA, 2013]. More broadly, AM has become the standard choice for producing many such low-volume, highly specialized parts [Leonor and Wagner, 2024].

To understand the source of these advantages, it is important to examine how Metal Additive Manufacturing MAM works at the process level. MAM is based on the layer-by-layer deposition of molten metal, which then cools and solidifies in place. In DED, metal powder is blown coaxially with the energy source, which is either a laser or an electron beam. In LPBF, the powder is deposited first into a thin layer, then melted. Schematics of both processes are shown in fig. 1.

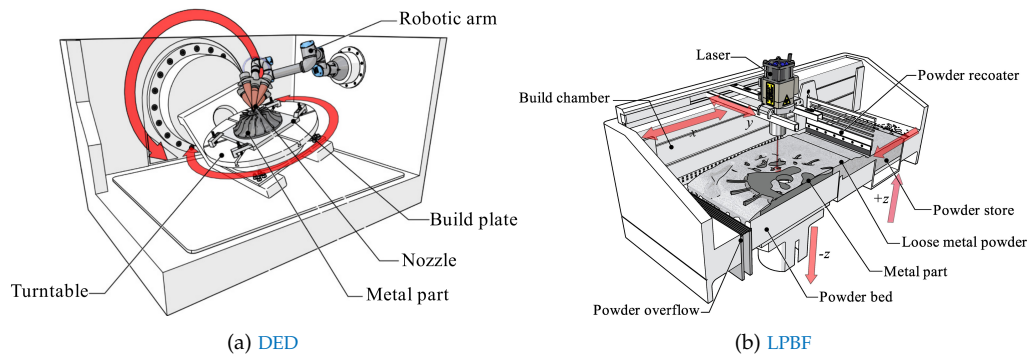


Figure 1: Schematics of DED and LPBF processes [Armstrong et al., 2022].

The progressive nature of the process enables the manufacture of intricate geometries which would require molds or dies, or even, be impossible to produce with subtractive manufacturing. Moreover, complex parts are traditionally made of multiple subcomponents which are then assembled together using fixtures, fasteners and welds. The geometric freedom that AM offers enables the manufacture of single, monolithic parts.

However, the similarity of the technology to welding also means it is prone to the same issues. Driven by the desire of manufacturers to maximize throughput, machines are often operated in regimes of high laser power and high speed. The intense and localized heating induces constrained thermal expansion and contraction, which in turn leads to residual stresses that build up with each additional layer. In excess, these

L	R	V	Minimum number of steps	Net print time
1 cm	1 mm	50 mm s ⁻¹	1 K	20 s
10 cm	1 mm	50 mm s ⁻¹	1 M	5.5 h
1 cm	100 μ m	1000 mm s ⁻¹	1 M	1.6 min
10 cm	100 μ m	1000 mm s ⁻¹	1000 M	27.7 h

Table 1: Minimum number of steps and net printing duration (time laser is turned on) for a cube of size L , with laser radius R and speed V . The first two rows correspond to [DED](#) parameters, while the last two rows correspond to [LPBF](#) parameters.

stresses can lead to build failure, or, worse even, in-service failure, through cracking, warping or poor mechanical properties. Process parameter optimization can help mitigate and avoid these issues.

To tackle this problem, the engineer has three options: repeated experimentation, analytical modeling and numerical modeling. The large design space, combined with the high cost of experimentation, makes trial-and-error impractical. Modeling provides practical means to explore the design space at a fraction of the cost, but analytical modeling is limited to simple cases, while numerical modeling is, put bluntly, too slow.

This computational bottleneck arises because [MAM](#) simulation, and [LPBF](#) in particular, is “extremely multiscale” in nature [[Hodge, 2021](#)]. In [DED](#), the relevant spatial scales range from a beam radius and layer thickness on the order of a millimeter up to part sizes of several decimeters or more. In [LPBF](#), the contrast is even sharper: the beam radius and layer thickness are typically on the order of 20–50 μ m, while part dimensions extend to the centimeter scale.

This disparity of spatial scales manifests itself numerically both in space and time. Spatially, the melt pool must be resolved with elements on the order of the beam radius, while the overall mesh must also cover the full part, leading to a very high number of elements. Temporally, the laser motion prohibits the use of time-steps that advance the laser position by more than one beam radius per step. When compared to the total length of the scan path, which exceeds the part size by a large margin, an exorbitant number of time-steps is required to simulate the full build.

Consider a cubic part of size L processed by a laser with radius R and speed V . Since $R \ll L$, the problem is spatially multiscale and resolving both the fine-scale laser motion and the full part domain requires a high number of elements.

Assuming the layer thickness and the hatch spacing are both equal to R , table 1 lists the minimum number of time-steps required to simulate cubes of varying size. These estimates are presented alongside the net print time (the laser-on time) for both [DED](#) and [LPBF](#) configurations.

Notably, [LPBF](#) simulations for parts of size 1 cm and 10 cm require approximately one million and one billion time-steps, respectively. This is a direct consequence of $R \ll L$, which, when combined with the laser speed V , translates into a severe temporal contrast with respect to the net print time.

On the one hand, time-steps must be on the order of $T_{hs} = R/V$ to accurately capture the motion of the heat source without skipping elements. On the other hand, the length of a single hatch is on the order of L ; the number of hatches per layer is on the order of L/R and the number of layers is also on the order of L/R . Therefore, the net print time is on the order of $T_{print} = L^3/(R^2V)$.

These disparities can be summarized

$$\begin{aligned} \text{Ratio of length scales} &= \mathcal{O}\left(\frac{L}{R}\right) \\ \text{Ratio of time scales} &= \frac{T_{\text{print}}}{T_{\text{hs}}} = \mathcal{O}\left(\left(\frac{L}{R}\right)^3\right) \end{aligned}$$

This cubic relationship is what makes high-fidelity LPBF simulations so computationally expensive.

The combination of spatial and temporal scale disparity is a well-known challenge in the field [Hodge, 2021, Proell et al., 2024]. If one considers volume ratios instead of length ratios, the situation is comparably severe in space and time: resolving a cubic part of size L with elements of size R requires $\mathcal{O}((L/R)^3)$ elements for a uniform mesh. In practice, it would be unthinkable to employ a uniform mesh, and AMR is the standard approach to mitigate this issue. By contrast, uniform time-stepping remains the standard.

Even for DED, which involves a narrower range of scales, the cost of high-fidelity simulation remains prohibitive, particularly when physics beyond heat transfer are included. Mathews et al. [2023] presents simulations of a thin wall, 2 layers thick, using both thermofluidic and thermoplastic models. Using commercial software, they report a simulation time above 2 hours¹ for a build that takes seconds. Similarly, Biegler et al. [2018] reports an 11 hours computation time for their thermoplastic simulation of a 1.2 cm thin wall, while the build takes about 10 minutes. In a later work, Biegler et al. [2022] reports an 80 hour computational time for a similar simulation of a 5 cm tall part. To address this, they proposed “grouping the transient increments”, which reduced simulation time under 10 hours.

Currently, the dominant approach to reduce simulation time is to use simplified models, and in particular, lumped heat sources and coarse time stepping strategies [Chiumenti et al., 2017c, Malmelöv et al., 2019]. These models are typically calibrated to match experimental outcomes such as melt pool size or thermocouple measurements [Lu et al., 2023, Patil et al., 2021], but their accuracy remains limited, as they effectively bypass the fine-scale physics and must be recalibrated for each new configuration.

Since small scale phenomena drive part-scale distortions, accurate representation of the Heat Affected Zone (HAZ) and its steep thermal gradients is essential for reliable prediction of warpage and residual stresses. Yet, capturing these fine-scale features is prohibitively expensive, even for centimeter-scale LPBF parts.

Without new modeling approaches, high-fidelity part-scale simulation of LPBF will remain limited to small builds for the foreseeable future. Ideally, these approaches should be able to reduce computational cost while retaining physical accuracy.

1.1 OBJECTIVES

As the demand for fast, reliable and physically consistent simulations increases, particularly at the part scale, there is a growing need for computational methods that reduce simulation time without sacrificing accuracy.

This thesis addresses this challenge by focusing on the time-scale disparity in MAM, which has received considerably less attention than its spatial counterpart. The aim is to develop methods that reduce the global number of time steps required in high-fidelity simulations, especially LPBF, where fine temporal resolution is needed due to the small size and high speed of the heat source.

The specific objectives of this thesis are:

- To investigate practical MAM cases, assess the feasibility of high-fidelity simulations and quantify time-stepping bottlenecks in simulations of DED and LPBF at the part scale.
- To review and assess existing methods for addressing time-stepping challenges in MAM and related fields, identifying their strengths and limitations.
- To explore novel methods for reducing the number of time-steps required in MAM modeling, with emphasis on LPBF, where temporal resolution constraints are more severe.

¹ For the best accuracy-to-cost refinement level.

- To combine these methods in order to achieve significant reductions in simulation time.
- To validate the proposed methods on realistic test cases and compare their performance with conventional simulation strategies.
- To validate the underlying physical models and numerical methods against experimental data.
- To provide realistic speedup estimates, along with practical guidelines on effectively implementing the proposed methods and variants thereof.
- To ensure open science and reproducibility by releasing the developed methods, input data, and benchmark cases through publicly available repositories, accompanied by Docker images that enable straightforward replication of the reported results.

1.2 THESIS OUTLINE

This thesis is presented as a compendium of 3 articles, included in chapter 5 through chapter 7. Chapter 8 presents the latest work of the author, which is currently under review.

The present chapter motivates this work, outlines the main computational challenges in MAM simulation, and states the objectives and outline of the thesis.

Chapter 2 provides a state-of-the-art on MAM modeling and on current approaches to reduce computational cost.

Chapter 3 presents the finite element models used in this thesis. The thermal model, which is the main focus of the subsequent methodological developments, is described in detail, while the mechanical model is briefly introduced for completeness. Chapter 4 introduces the domain decomposition framework at the core of chapters 7 and 8, providing the relevant theoretical background.

The following two chapters, 5 and 6, present thermomechanical case studies addressing warpage and residual stress mitigation.

Chapter 5 presents a practical DED case study focused on the reduction of residual stresses. In this case, high-fidelity simulation is feasible due to the problem being moderately multiscale. A novel substrate design is proposed to mitigate stress accumulation.

Chapter 6 models a practical LPBF scenario involving recoater-induced part distortion. Due to the severe temporal resolution constraints, the simulation requires substantial model simplification via layer lumping, highlighting the limits of conventional modeling for industrial LPBF problems.

Chapters 7 and 8 constitute the main contributions of the author. They introduce novel methods for computational cost reduction in high-fidelity thermal LPBF simulations, with emphasis on the stringent temporal resolution constraints of the process.

Chapter 7 introduces the advected subdomain method to reduce the number of time-steps in MAM modeling and bypass the conventional constraint on their maximum size. The method is shown to provide improved accuracy in the HAZ compared to standard approaches.

Chapter 8 develops substepping methods for MAM modeling and combines them with the advected subdomain to achieve further reductions in simulation time.

Finally, Chapter 9 closes the thesis by summarizing its main findings, discussing the advantages, limitations, and potential impact of the proposed methods, and providing an outlook on future research directions.

This chapter surveys the evolution of part-scale thermal and thermo-mechanical modeling in [DED](#) and [LPBF](#), with a particular focus on techniques developed to reduce computational cost. The discussion begins by situating part-scale models within the broader context of multiscale [MAM](#) modeling. It then presents a general chronological overview of key contributions to the field, before focusing on works that introduce specific computational simplifications, such as lumped heat sources, inherent strain methods, etc. The end of the chapter focuses on recent contributions that explore new avenues for cost reduction, such as Graphics Processing Unit ([GPU](#))-based frameworks, matrix-free methods and Forward-Euler time-integration.

2.1 DIFFERENT PHYSICS AT DIFFERENT SCALES

[MAM](#) is governed by a multitude of physical phenomena that span multiple spatial and temporal scales [[Meier et al., 2018](#)]. At each scale, a different subset dominates, yet all are fundamentally linked. This interplay poses significant challenges for computational modeling.

- **Microscale** (microstructure): the rapid solidification of molten metal governs the evolution of the microstructure. Grain morphology, phase distribution, and texture are influenced by thermal gradients and solidification rates and can be improved via heat treatment. Conversely, microstructural features impact mechanical behavior at larger scales.
- **Mesoscale** (melt pool): the heating, melt pool dynamics and powder consolidation occur at this scale. Heat transfer is dominated by convection, conduction and radiation, and surface tension effects (Marangoni convection, wetting) drive the fluid flow and govern melt pool shape [[Meier et al., 2018](#), [Zhang et al., 2018b](#)]. Physics at this scale are highly non-linear and transient.
- **Macroscale** (part): residual stresses, distortions and global thermal fields are determined by the cumulative, layer after layer, effects of the aforementioned phenomena. The mechanical response determines the final part shape and residual stresses.

Each of these regimes is governed by different equations (see fig. 2). At present, it is “impossible to simulate all relevant physical phenomena including both the fluid flow and stress evolution at part-scale level” [Bayat et al. \[2021\]](#). Therefore, simplifications are adopted depending on the objective; if the goal is to study melt pool shape and stability, a multiphase thermofluid model is adopted; if the goal is to predict residual stresses, a thermomechanical model is more appropriate.

As mentioned above, it is difficult to decouple these scales since they are not isolated: temperature history computed at the melt pool or part scales informs the microstructure, which in turn influences the constitutive laws at the macroscale. The motion of the [HAZ](#) generates compressive and tensile stresses that accumulate over time, leading to part distortion and residual stresses. The motion of the melt pool directly affects warpage and final residual stresses of the build. One thing remains constant across all scales: heat transfer is the central phenomenon.

The next section presents a chronological overview of part-scale thermal and thermomechanical modeling, highlighting how different assumptions have been employed to balance computational cost and model accuracy.

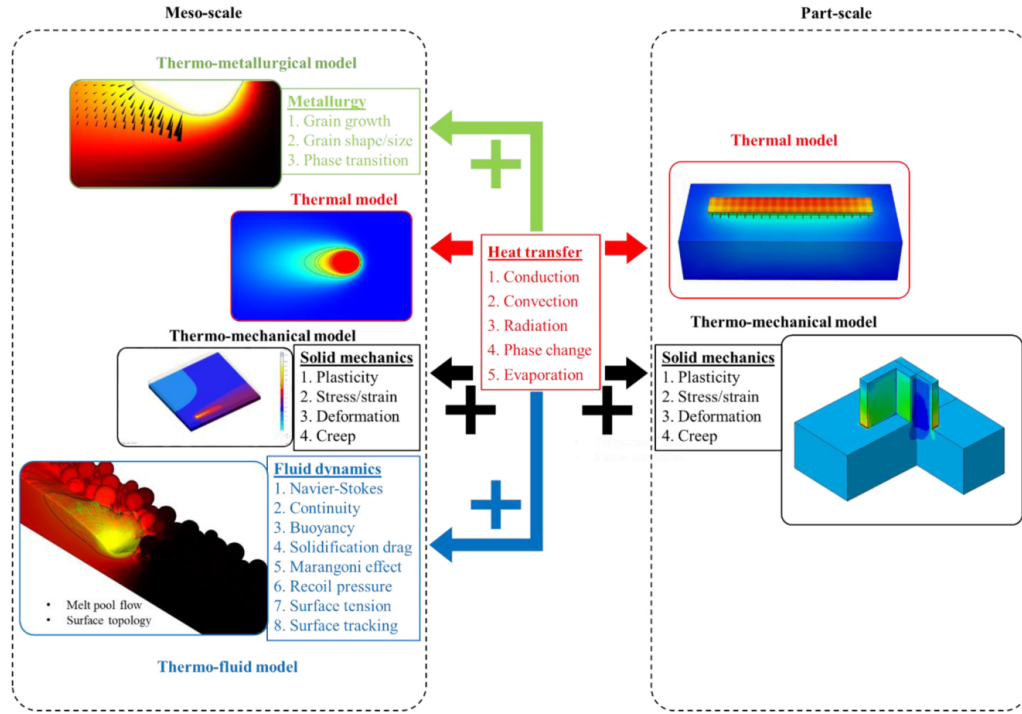


Figure 2: Relevant physics at melt-pool scale and part-scale [Bayat et al., 2021].

2.2 PART-SCALE DED AND LPBF MODELING THROUGHOUT THE YEARS

To understand how part-scale modeling has evolved, it is useful to retrace its origins. This section compiles a non-exhaustive set of foundational works and representative case studies that illustrate the progressive development of part-scale modeling for DED and LPBF to what it is today.

To this end, the following account focuses on impactful studies published between 2000 and the present. The selection of works was informed by several review articles [Bikas et al., 2015, Guan and Zhao, 2020, Meier et al., 2018, Bayat et al., 2021], as well as the author's own browsing. The author also includes a number of studies that, while do not necessarily correspond to the aforementioned criteria, are noteworthy for their originality or being ahead of their time.

The first MAM works were published in the early 2000s. The limited computational capabilities of the time meant most of them were 2D models of single tracks or single layers i.e. practically melt pool scale models. One of the first works to introduce Finite Element Method (FEM) modeling to MAM was carried out by Shiomi et al. [1999], who used a 2D thermal model at the mesoscale to study the solidification process in Selective Laser Sintering (SLS).

Bugeda et al. [1999] developed a 3D thermosintering FEM model to study the HAZ in SLS. While demonstrated on a polymer track, their model is intended for general SLS processes. It fully couples nonlinear heat transfer and sintering kinetics by accounting for the dependence of density and thermal conductivity on local porosity. To enable steady-state simulation, the governing equations are reformulated in a reference frame moving with the laser beam. The model allowed for the direct estimation of sintering depth and material consolidation.

Among the earliest published thermomechanical simulations applied to MAM is the work of Vasinonta et al. [2000]. They used a 2D sequentially coupled thermoplastic FEM formulation with a point source in order to establish process maps for thin walled structures produced via laser cladding, a form of DED. The sequential coupling, also known in the literature as *adiabatic split* [Armero and Simo, 1992], neglects the mechanical

dissipation: the thermal problem is solved first, and the resulting temperature field is used as input for the mechanical analysis.

Dai and Shaw [2001] developed a 3D thermomechanical FEM model to simulate Multi-Materials Laser Densification (MMLD), a Selective Laser Melting (SLM) variant. They investigated the effect of scanning pattern on temperature, residual stresses and distortion in small two-layer builds composed of nickel and porcelain. The simulations were performed in ANSYS using a thermoplastic formulation with transient stresses, temperature-dependent material properties, convection losses, and plastic hardening. Radiation, latent heat are neglected, and no separate material properties are assigned to the powder phase. To mimic the behavior of molten material, the elastic modulus, tangent modulus, and yield strength were assigned very low values above the melting point. The laser beam was modeled by prescribing the temperature of surface nodes along the scan path to a value slightly above the melting point. The authors concluded that transient thermal stresses are negligible under the considered conditions.

The tangent modulus is the slope of the stress-strain curve in the plastic regime. In linear hardening, it corresponds to the hardening/plastic modulus.

Matsumoto et al. [2002] used the plane-stress assumption in their 2D sequentially coupled, thermoelastic FEM model to predict the temperature and stress fields in SLM prints. The latent heat was modeled using the *temperature recovery* method: after the calculation, the temperature field is corrected to account for the latent heat. The laser beam was resolved by no more than five elements, which all received the same power input (fig. 3).

Chen and Zhang [2004] applied a 2D thermal model to study the melt pool of a multi-layer SLS deposition. Phase change was modeled using an apparent heat capacity formulation, and the Finite Volume Method (FVM) was applied in the moving reference frame of the heat source to obtain steady-state solutions.

Dai and Shaw [2004] extended their earlier work [Dai and Shaw, 2001] to consider the powder phase and include radiation losses. Similar two-layer nickel-porcelain depositions were simulated. The authors observed that including the powder phase led to steeper thermal gradients and an asymmetric melt pool shape. While the overall distortion profile remained similar, its magnitude was significantly reduced when the powder phase was omitted.

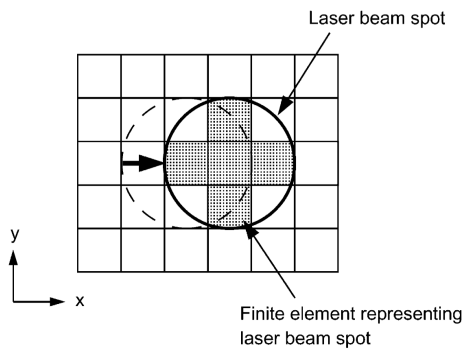


Figure 3: Uniform heat source by Matsumoto et al. [2002].

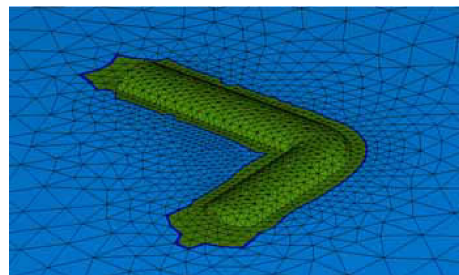


Figure 4: Mesh conforming to deposition geometry in Crespo et al. [2006].

The transition to full 3D modeling was initiated around 2005. One of the earliest examples is the work of Kolossov et al. [2004], who simulated a single layer, multi-track SLS deposition of titanium. Using a thermal model with a surface source, they were able to replicate trends in the experimental thermography data.

Toyserkani et al. [2004] implemented a 3D thermal model in FEMLAB (now COMSOL) to investigate the effects of pulse intensity and frequency in a single track laser cladding application: a pulsating Gaussian was applied as a boundary condition in order to model the laser. The authors presented one of the most comprehensive models of its time, incorporating a wide range of physical effects rarely seen in early AM simulations. The model took into account thermal dependency of parameters, latent

heat of fusion, Marangoni phenomena and the Brewster effect¹, as well as radiation and convection. Furthermore, it dynamically resolved the geometry of the deposition using a two-solves-per-time-step approach. After the first solve, the melt pool boundary was extracted and intersected with the powder jet. The resulting circular area was then used to compute the layer thickness together with the powder feedrate and the time-step size. Finally, elements were inserted over that circular area by remeshing, and a second thermal solve was performed to obtain the temperature in the deposition. Figure 5 shows the numerically predicted clad geometry and a comparison with experimental data².

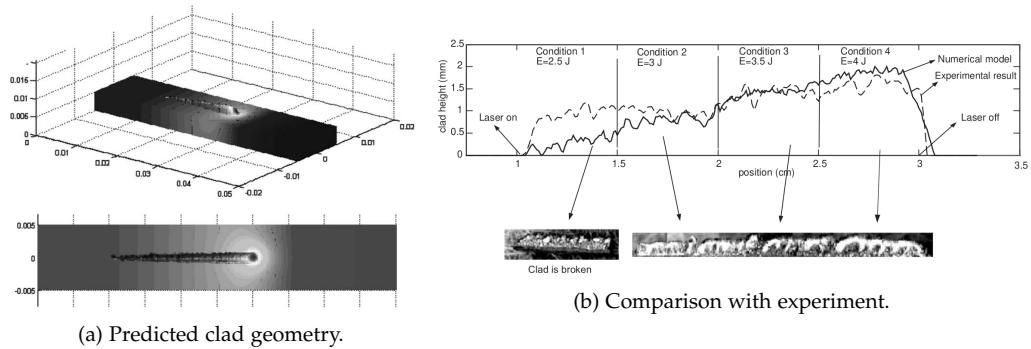


Figure 5: Toyserkani et al. [2004]

Dai and Shaw [2005] extended again their previous work [Dai and Shaw, 2004] to account for volume shrinkage during the phase change. The mechanical model was excluded from the simulation in this work, and a heuristic approach was used to model the shrinkage: upon melting, the top nodes of powder elements were moved downwards in the direction of gravity. Said displacement was computed based on the element's initial porosity, and mass conservation. Additionally, the authors replaced their previous fixed-temperature heat input with a Gaussian volumetric heat source. They found that neglecting volume shrinkage gives reasonable predictions of temperature distribution, but accounting for it improves the prediction of the final solid geometry.

Childs et al. [2005] tested their 3D FEM-based thermal model of SLM against single-track experiments to study the effect of laser power and scan speed on the formation and shape of the resulting solid track, as well as on the occurrence of balling. The study proposed two empirical laws describing the temperature-dependent evolution of powder porosity during sintering.

Around this time, 3D simulations began spanning multiple layers, with the thin wall emerging as the most popular part-scale example. Costa et al. [2005] proposed a 3D sequential thermo-kinematic model for a symmetric, 10-layer thin wall produced by DED to study microstructure and hardness variations during steel part fabrication. Their model, implemented in Abaqus, incorporated latent heat through a sink term in the heat equation and demonstrated good agreement with published experimental data.

Similarly, Crespo et al. [2006] applied a related model, although without latent heat, to a deposition of a few hatches belonging to a single layer. A key feature of this work was the use of meshes that directly represented the geometry of the deposition (fig. 4).

Longuet et al. [2006] applied a thermo-viscoplastic model to the study of a symmetric thin wall deposited through DED. Rather than using a volumetric heat source, they initialized newly deposited nodes at elevated temperatures. This approach enabled the prediction of general trends in both temperature and displacement.

Using a linear thermal model to study a 50 layer thin wall LENS deposition of AISI 316 SS, Ye et al. [2006] was able to determine the order of magnitude of the thermal gradients in the vicinity of the melt pool. Similarly to Longuet et al. [2006], nodes were activated at the liquidus temperature instead of using a volumetric heat source.

¹ Angle dependent absorption.

² Nowadays, deposition shape is predicted using mesoscale thermofluidic models.

Wang et al. [2006] presented a 3D thermal model of a ten-layer Laser Engineered Net Shaping (LENS) thin wall deposition with a conical Gaussian power density profile. Their SYSWELD implementation included convection and radiation and coupled thermal and phase models in order to take the metallurgical transformation into account. The authors reapplied their model in their subsequent works, which focused on both simulation methodology and process parameter optimization [Wang and Felicelli, 2007a,b, Wang et al., 2007, 2008a].

Wang et al. [2008c] added upon their previous work by including a mechanical model to study the residual stresses in the same thin wall. They included “transformation plasticity” in their model, which is caused by the difference of volume between the various phases and the ensuing plastic flow. Good agreement with observed longitudinal residual stresses was reported.

Yin et al. [2008] developed a 2D thermal model with phase change and compared it to 3D results obtained by the model of Wang et al. [2008b]. For a 10-layer LENS thin wall structure, both models obtained similar results, though the 2D model required additional calibration in order to recover the equivalent power level in 3D. The main drawback found by the authors was the inability to predict the heat flow into the substrate, hence the discrepancy between both models was most pronounced in the early layers.

Roberts et al. [2009] developed a 3D thermal FEM-based model for SLM applications in ANSYS. This work was among the first to explicitly refer to the *birth-death* activation technique, where elements in to-be-deposited layers do not contribute to the linear system in any way. Depositions of up to five layers were simulated with a volumetric Gaussian heat source and an enthalpy formulation of the heat equation. Porosity, thermal dependency, convection and radiation were all considered. Good agreement was obtained with previously published infra-red thermography data.

Neela and De [2009] modeled a three-dimensional 25 layer LENS deposition of a thin wall in Abaqus. Using a moving Gaussian surface flux, the authors captured transient thermal histories that agreed with previously published benchmark thermocouple data. By capturing heat-build-up across two dozen layers, the study pushed the state of DED part-scale modeling.

Around this time, attention began shifting from benchmark-scale model validation cases to industrially relevant geometries. Among the first to tackle this complexity was Zaeh and Branner [2009], whose work marked a turning point in part-scale literature by addressing the gap between the complexity of industrial parts produced by SLM at the time (cf. fig. 6) and the case studies available in the literature. The authors employed a sequentially coupled thermo-mechanical simulation in ANSYS to model the SLM fabrication of a T-shaped cantilever with dimensions $70 \times 15 \times 12 \text{ mm}^3$ (fig. 7), i.e. an industrially relevant case. Due to computational limitations, the original $50 \text{ }\mu\text{m}$ layer thickness was replaced by 1 mm thick *meta-layers*, effectively grouping 20 physical layers into one. A lumped heat source was used, distributing power uniformly across each meta-layer. What would later be known as Flash Heating (FH) was also employed, where the input power and on-time of the laser is calibrated against experimental data in order to obtain comparable thermal gradients. Figure 8 showed the final temperature, distortion and residual stresses obtained with the model. While the distortion predictions deviated from experimental measurements, the residual stress magnitudes were within the correct order of magnitude, demonstrating the model’s utility for coarse-grained prediction.

Chiumenti et al. [2010] presented a fully coupled thermo-mechanical Finite Element (FE) framework for the simulation of multi-pass welding and Shaped Metal Deposition (SMD), a process analogous to modern DED. The model solved the heat transfer and mechanical problems in a staggered fashion. The thermal analysis accounted for latent heat through an enthalpy-based approach, and applied a uniform volumetric heat source to newly activated elements, based on the actual arc power and layer geometry. The mechanical model was a temperature-dependent elasto-visco-plastic constitutive law



Figure 6: Typical parts produced by SLM circa 2009.

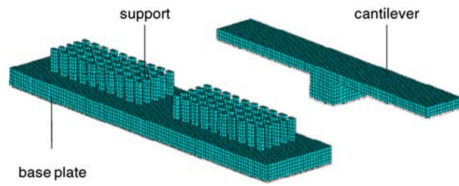


Figure 7: Mesh used by Zaeh and Branner [2009] to model the T-shaped cantilever.

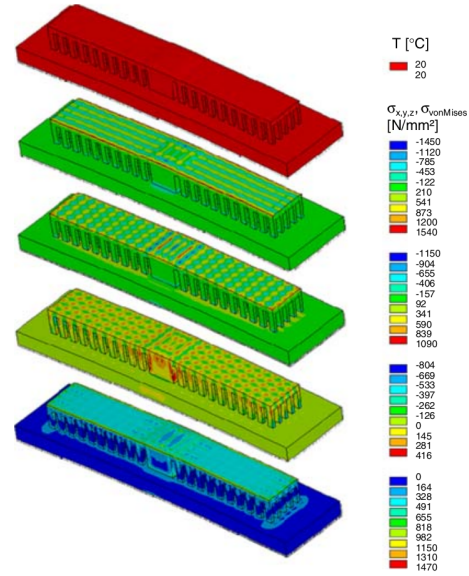


Figure 8: Final temperature, distortion and residual stresses obtained by Zaeh and Branner [2009].

that captured the solid, mushy, and liquid behavior through an evolving solid fraction, allowing a smooth transition from elastic-plastic to viscous flow behavior across the solidus and liquidus temperatures. The model captured solidification and shrinkage, and included a continuum damage formulation in the mushy zone to estimate hot cracking risk, where damage was driven by a combination of thermal strain and intergranular liquation. Their SMD examples were validated against thermocouple, displacement sensor and hole drilling data. Good agreement was obtained in terms of temperature, and reasonable agreement was achieved for the residual stresses and distortion.

Contuzzi et al. [2011] was among the first to explicitly model the powder phase in an SLM thermal simulation. Implemented in ANSYS, their approach switched the material assignment of each element from powder to solid when its temperature exceeded the melting point. Despite the model not accounting for the temperature dependence of material properties, they obtained errors of less than 8% in the melt pool size. The heat source profile was the same as in Matsumoto et al. [2002], see fig. 3.

In the review conducted by Zeng et al. [2012] of thermal modeling in LPBF, 11 numerical models are summarized, the largest of which is $20 \times 20 \times 9 \text{ mm}^3$.

Keller and Ploshikhin [2014] was the first reference to introduce the *inherent strain method* in the context of MAM simulation. Their methodology is described in section 2.3.3.

Denlinger et al. [2014] built upon the industrial-scale focus introduced by Zaeh and Branner [2009] by presenting a 3D sequentially coupled thermoplastic model with a geometric AMR strategy. Using an ellipsoidal heat source profile³, they simulated a DED build consisting of a thin wall made of 107 layers, each 3.175 mm thick (the smallest dimension of the problem). The underlying substrate measured 3810 mm long, 457 mm wide, and 25.4 mm thick. The model was implemented in a software called CUBIC, and symmetry was exploited to reduce the domain to half its size. Remarkably, the simulation completed in approximately 100 hours of Central Processing Unit (CPU) time, compared to over 600 hours required for the actual manufacturing process. The authors suggested that this modeling framework was suitable for parts “on the order of meters”(!), marking a significant advance in part-scale DED simulation. The predicted

³ Wrongly referred to as a double-ellipsoidal Goldak profile

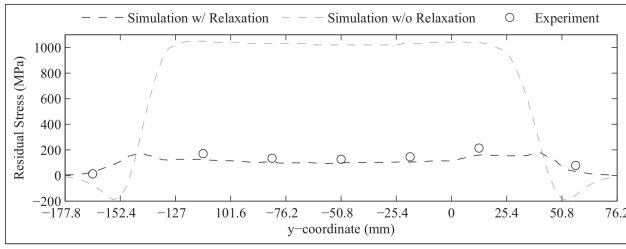


Figure 9: Residual stress along axis of deposition with and without relaxation from Denlinger et al. [2015b]. Omitting stress relaxation leads to large errors.

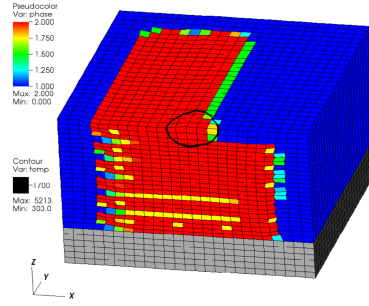


Figure 10: Simulated average phase and melt pool contour from Hodge et al. [2014], showing spatial variation during LPBF.

distortion showed a maximum 29% error relative to the experiment, indicating good agreement despite the scale and complexity of the problem.

Written before Denlinger et al. [2014], but not published until a year later, Denlinger et al. [2015b] was among the first to incorporate residual stress relaxation into MAM thermomechanical modeling. In their model, stress, elastic strain, thermal strain, plastic strain, and equivalent plastic strain were reset to zero when the temperature at all Gauss points exceeded a specified *annealing temperature*. The case study focused on a Electron Beam Melting (EBM) deposition of a sloped thin wall, with displacements and residual stresses measured using Laser Displacement Sensors (LDS) and hole-drilling, respectively. The authors claimed that temperature-induced stress relaxation was crucial for accurate EBM modeling. Comparisons with and without relaxation showed that only the relaxed model achieved good agreement with experimental displacement and residual stress data; neglecting relaxation led to errors as high as 400%, see fig. 9.

Riedlbauer et al. [2014] was also among the first works to employ AMR in MAM simulation. Their study compared two thermo-elastic solution strategies: (i) a monolithic, fully coupled formulation and (ii) the widely used thermal-mechanical sequential solve, or *adiabatic split*, in which the thermal and mechanical subproblems were solved successively, neglecting mechanical heat dissipation. For a small Ti-6Al-4V LPBF test build, the split approach proved 3-5 times faster and essentially as accurate when the problem was linear. For the nonlinear case (temperature-dependent properties), the split scheme required time-steps an order of magnitude smaller to be as accurate, so the authors recommended the monolithic solver whenever strong material non-linearities were present. All results were obtained with Backward-Euler time integration; with Crank-Nicholson they observed displacement oscillations in the nonlinear regime.

Amine et al. published two similar studies in 2014 [Amine et al., 2014a,b] analyzing a 20-layer, single-track, stainless steel wall built by Direct Metal Deposition (DMD). Although described as thermo-mechanical, the model was purely thermal: it consisted of a 3D transient heat equation with latent heat, implemented in ABAQUS via a moving Gaussian surface flux and considered both convective and radiative losses. Validation was performed against thermocouple data, and a maximum error of 20% was reported for an absorptivity of 0.6. Parametric sweeps (600-900 W, 300-450 mm min⁻¹) showed how increased power or reduced speed deepened remelting and raised cooling rates. They also found that alternating scan direction improved fusion in the first few layers.

Hodge et al. [2014] presented the LPBF thermomechanical model implemented in the software DIABLO at Lawrence Livermore National Laboratory (LLNL). The heat source model employed, proposed by Gusarov et al. [2009], was specially tailored for LPBF, as it was derived from the radiation transfer equation considering rays incident on a single, thin powder layer.

The authors distinguished between two phase changes: from powder to consolidated material, where the latter included both solid and liquid phases, and from solid to liquid. For the former, they adopted the heat integration method of Rolph III and Bathe [1982]. As described by Hu and Argyropoulos [1996], this approach imposes a temperature clamp at the melting point; energy added during phase change is stored as a source term until it equals the latent heat of fusion, after which the temperature is allowed to rise. That is, the phase change was implicitly embedded in the energy balance⁴. Similarly, for the solid-liquid phase change, an apparent heat capacity method was used.

The mechanical model was a rate-based thermoplastic formulation that incorporated phase expansion. It was coupled in a staggered fashion to the thermal solver. A 1 mm cube print was presented to illustrate stress and phase evolution (see fig. 10). Among the conclusions, the authors noted that the Rolph algorithm for phase change was computationally intensive and required “extremely small” steps for convergence. The relative size of said time-steps is discussed in section 2.3.4.

Michaleris [2014] compared the two most common approaches to model the growth of the domain: the *quiet element* method and the birth-death method. Both methods start out with a background mesh that covers the final build volume. In the quiet element method (sometimes called dummy material method), the material properties of the elements which are not part of the physical domain are set to very low values so that they do not affect the solution. In the birth-death method, they are simply not assembled. Although the latter is technically more accurate, the former saw early adoption among commercial software users because of its ease of implementation. Michaleris [2014] found that, if the scale-down factors of the quiet elements are chosen correctly, results are “practically identical” using one method or the other. Michaleris [2014] observed that, although the birth-death method reduces the number of Degrees of Freedom (DOF)s early on, it is costlier due to the repeated reallocations. With efficiency in mind, a hybrid approach was proposed, where inactive elements in the current layer are *quiet*, and inactive elements in the remaining layers are *dead*. In this approach, if no AMR is used, matrices are only reallocated upon activating a new layer. Moreover, the study showed that failing to update the convection-radiation boundary when elements are activated leads to significant overheating.

Schilp et al. [2014] compared microscale and macroscale thermal models in the Laser Beam Melting (LBM) deposition of a turbine blade. “On the macroscale level, abstract modeling approaches need to be applied for the virtual process in order to gather numerical results within a computing time which is less than the build time of the part”: layers were subdivided into up to 10 scan areas, which were then time-stepped sequentially, mimicking the original scan-path. The macroscale model deposited layers at a time, and, instead of using a volumetric heat source, prescribed the deposition temperature to the solidus point. The microscale model resolved individual hatches at high spatial and temporal resolution and employed a volumetric Gaussian heat source with exponential attenuation in the depth:

$$Q(x, y, z) = \frac{\eta P}{d} \exp\left(-\frac{z}{d}\right) \exp\left(-2\frac{x^2 + y^2}{2R^2}\right) \quad (1)$$

where x , y , and z are the spatial coordinates centered on the laser spot, P is the laser power, η is the absorptivity, d is the optical penetration depth, and R is the beam radius. Thermographic monitoring was used to validate both models. The study concluded that microscale models are best suited for calibrating macroscale approximations, while the latter are more appropriate for simulation-based process design.

Zeng et al. [2015], from the 3DSIM team, proposed a Representative Volume Element (RVE) workflow to find the effective thermal properties of SLM lattice-like support

⁴ Note that Meier et al. [2018] wrongly assumed in their review article that a volumetric form of the Stefan-Neumann equation was evaluated, since Hodge et al. [2014] wrote out the full Stefan-Neumann phase change problem and state in their text that their method *tracks the volume within which the interface is located*.

structures consisting of solidified material and entrapped powder in the intercellular spaces. Comparison with a parallel spring model showed a close match.

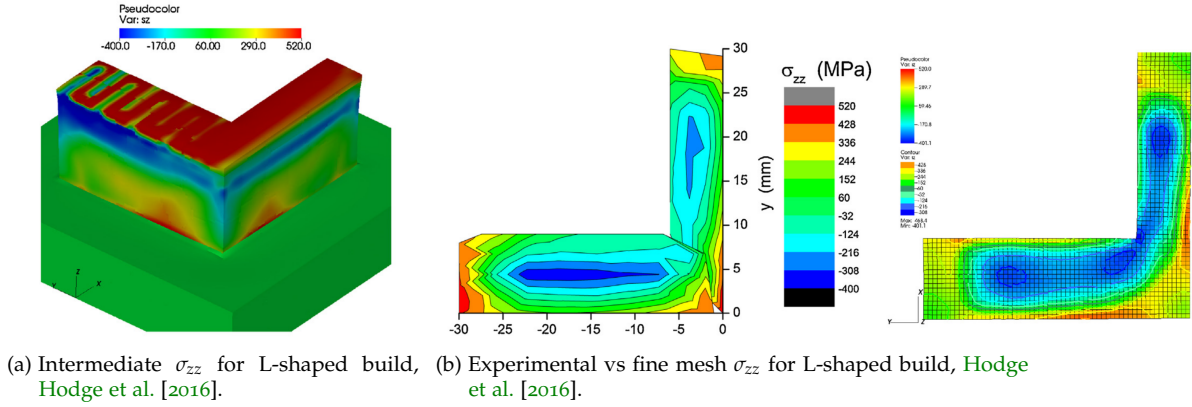


Figure 11: Stresses in build direction for L-shaped build of Hodge et al. [2016].

Hodge et al. [2016] further validated their previously presented LPBF model [Hodge et al., 2014] against experimental data, focusing on the effects of build orientation, infill scan strategy, and preheating on residual stresses and dimensional warping. This updated version omitted the phase contraction effects. Three case studies were presented: a vertical prism, a horizontal prism, and an L-shaped geometry. Displacements and internal stresses were measured using Digital Image Correlation (DIC) and neutron diffraction, respectively. These builds in the centimeter scale represented a significant increase from the millimeter-scale geometries used in their prior work. To keep the simulations tractable, certain simplifications were introduced, including scaling of the heat source and layer thickness, as discussed in section 2.3.1. Figure 11a presents the intermediate σ_{zz} stress field for the L-shaped geometry, while fig. 11b compares the experimental and simulated σ_{zz} stress distributions.

Yang et al. [2016] developed a sequentially coupled thermoplastic FEM model to investigate temperature evolution, distortion, and residual stresses in a 3D thin-walled Ti-6Al-4V structure fabricated via LENS. The thermal analysis neglected phase change and used a double-ellipsoidal heat source model [Goldak et al., 1984]. They compared quasi-static and transient dynamic mechanical simulations, and found that both yielded similar deformation patterns and matched well the 3D scanning distortion data. This supported the widely adopted assumption that quasi-static mechanical analysis was sufficient for simulating residual stress and deformation in DED.

Chiumenti et al. [2016] presented a sequential thermomechanical model for Electron Beam Welding (EBW), a process related to LPBF, implemented in their in-house software COMET. While the thermal model did not explicitly account for phase change, the mechanical formulation thoroughly did. Similar, to their previous work [Chiumenti et al., 2010], an elasto-viscoplastic model with a mixed $\mathbf{u}/p$ formulation was used such that under the solidus temperature the law is elastoplastic, above liquidus the law is purely viscous, and the continuous liquid fraction provides a smooth transition from solid to liquid behavior in the mushy phase. The model was able to recover temperature and vertical distortion data from the experiments and was successfully applied to a thermal case study of an industrial component.

Denlinger et al. [2017] extended their previously developed DED model to LPBF. They simulated a 38-layer, 91 mm³ build, which they described as “significantly larger than anything available in the current literature for a full elastoplastic moving-source model”. Their AMR coarsening workflow helped keep the number of DOFs in check. Motivated by the potential for large deformations arising from the small layer thicknesses typical in LPBF, the mechanical model used a total Lagrangian formulation. Consistent with their prior work, an ellipsoidal heat source profile was used to represent the laser

input⁵. Notably, this study was possibly the first to validate such a model against in-situ distortion measurements. Although the powder bed was excluded from the computational domain, the model achieved strong agreement with the experimental data, with only a 5% error in final peak distortion. Figure 12 presents the resulting residual stress distribution in the σ_{xx} direction.

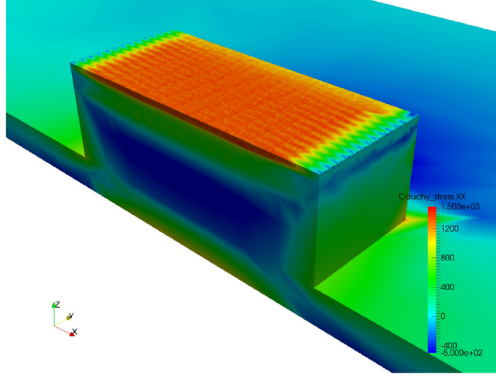


Figure 12: σ_{xx} distribution after completion of build, Denlinger et al. [2017].

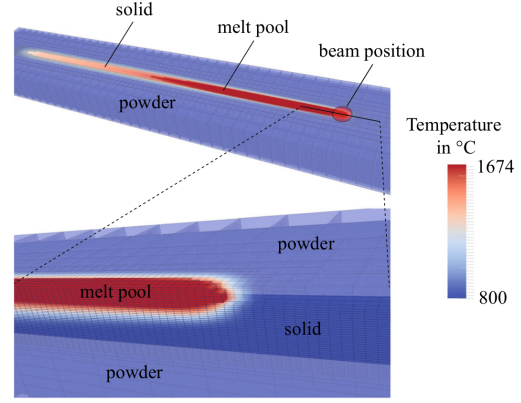


Figure 13: EBM simulation including powder bed and AMR in vicinity of beam, Riedlbauer et al. [2017].

Riedlbauer et al. [2017] restricted their earlier model to a purely thermal analysis to investigate melt pool behavior in thin-walled structures produced by EBM. The simulated walls consisted of 60 layers, and the powder bed was explicitly included in the model (see fig. 13). Phase change was captured through a temperature-dependent specific heat capacity, and three distinct material states were defined: powder, bulk, and melt. The material state of each element was updated after each time step based on its temperature. The thermal problem was solved using an implicit Runge-Kutta time integration scheme, and the heat input was modeled with the semi-empirical, EBM-specific heat source developed by Klassen et al. [2014], which accounts for penetration depth, angle of incidence, and electron backscattering through empirical correlations. Good agreement was found, and the authors established that the lifetime of the melt pool increases linearly with the power, while the dimensions show a nonlinear relationship.

Kollmannsberger et al. [2018] showcased a thermal LPBF model featuring hp-AMR on top of a detailed treatment of powder-to-bulk phase change. Latent heat was handled using a regularized source-based method inspired by Celentano et al. [1994], with a hyperbolic tangent regularization of the liquid fraction function. As in Contuzzi et al. [2011], elements that exceed the melting temperature are flagged and converted from powder to bulk after the thermal solution step. However, a key difference is that Kollmannsberger et al. [2018] use temperature-dependent properties for both powder and bulk phases. Said properties are chosen equal above the melting point, ensuring continuity at and above the melting point. The growing domain was modeled using the Finite Cell Method (FCM), which, like the quiet element method, employs a scale-down factor to deactivate inactive regions. Unlike quiet elements, however, the FCM uses an indicator function that can vary within each element, enabling more precise and flexible geometric representation.

Ganeriwala et al. [2019] present a novel thermomechanical model for predicting residual stresses in LPBF. The thermal model follows the formulation used in their previous work [Hodge et al., 2014], while the mechanical model introduces a temperature-dependent constitutive law: (i) strain rate-independent plasticity for temperatures $T < 0.5T_m$, (ii) viscoplasticity for $0.5T_m \leq T < 0.8T_m$, and (iii) Maxwell-type viscoelasticity for $T \geq 0.8T_m$. The model is implemented in DIABLO, and numerical simulations employ a combined *layer lumping* and *heat source scaling* strategy to reduce computa-

⁵ Again misnamed to a double-ellipsoidal profile in the reference.

tional cost. Validation against synchrotron X-ray diffraction measurements of residual strains in bridge-shaped specimens shows generally good agreement.

Lu et al. [2019] studied a DED deposition of S-shaped and box structures, each composed of 44 layers. The thermo-visco-plastic model of Chiumenti et al. [2017a] was reused in the same software while also considering annealing temperature. Heat transfer coefficients were calibrated against thermocouple data and the model was validated against distortion data. The work then considered the error introduced by neglecting the varying layer thickness in DED, analyzed the benefits of preheating the substrate, and investigated the error introduced by time-stepping four layers at a time. Regarding the latter, the authors found that computational time was greatly reduced, and although the HAZ accuracy was lost, average values of temperature and distortion were still preserved.

Soldner and Mergheim [2019] proposed a computationally efficient framework for part-scale thermal analysis of LPBF, implemented in the deal.ii software library. Notably, it was the first work to introduce substepping to MAM modeling. To further reduce computational cost, the authors employed (i) a lumped line heat source model based on an integrated form of the beam model by Klassen et al. [2014], and (ii) an error-based AMR strategy. The heat input was homogenized to allow longer time steps while preserving energy consistency. The model included phase change via an enthalpy formulation of the heat equation. Numerical examples showed that substepping combined with the line heat input model and AMR achieved substantial cost reductions without compromising temperature field accuracy. The adopted substepping strategy is described in section 2.3.4.

In Dugast et al. [2021] and Olleak et al. [2022], the authors presented a matrix-free GPU-based thermal model for LPBF and obtain very significant speed-ups compared to CPU-based models. The authors claimed that their framework enabled “for the first time, scanwise process simulation of the LPBF process with temperature-dependent thermophysical properties at the part-scale”. These contributions are discussed in section 2.3.5.

Recently, Proell et al. [2024] presented a highly optimized thermal model for LPBF, implemented in deal.II and designed for distributed-memory CPU architectures. Their model neglects latent heat and uses a cylindrical Gaussian heat source. Radiation and evaporation heat losses are considered while convection is neglected. The framework incorporates a wide range of computational optimizations, including Forward Euler time integration, matrix-free FEM, AMR, vectorization, and cache-efficient memory access. To demonstrate its capabilities, the authors perform the first fully resolved (high-fidelity) simulation of the NIST AM Bench 2022 cantilever specimen, as shown in fig. 14. The simulation spans 44 million time steps and resolves up to 8.5 million DOFs. Leveraging 1248 CPUs, the entire simulation completes in under 24 hours, corresponding to just a few milliseconds per time step. The authors also indicate plans to extend the framework to GPU architectures, with the goal of further improving performance and accessibility.

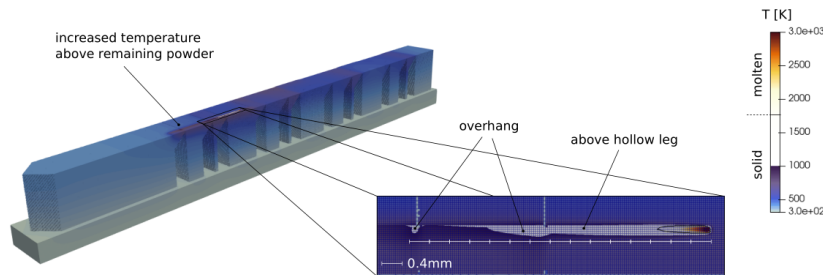


Figure 14: Intermediate step from the high-fidelity simulation of the National Institute of Standards and Technology (NIST) AM Bench 2022 cantilever specimen by Proell et al. [2024].

2.3 OVERVIEW OF COST-SAVING STRATEGIES IN PART-SCALE MAM MODELING

As outlined in the previous section, the need for efficient part-scale modeling strategies has driven the development of cost-saving techniques over the past fifteen years. These methods aim to relax the most restrictive spatial and temporal resolutions while preserving the required physical accuracy. Such advances were essential in enabling simulations of industrially relevant size and complexity.

The most widely adopted strategies are lumped heat-input models and the inherent-strain method, both of which trade-off local fidelity for global efficiency. Another widely used technique is [AMR](#), offering a practical solution to the spatial resolution problem by concentrating elements only where steep gradients occur. Finally, although substepping and other multirate time-integration schemes are less common in the literature, they hold great promise for mitigating the temporal bottleneck.

The remainder of this chapter provides a state-of-the-art overview of these methods and surveys additional cost-saving approaches that fall outside the above categories.

2.3.1 Lumped heat input models

Among the most (if not the most) widely adopted strategies for reducing computational cost in [MAM](#) modeling is the use of *lumped heat sources*. Their use bypasses the need to explicitly resolve the moving laser beam at fine spatial and temporal scales, making them particularly effective at addressing the strong scale separation.

Central to this discussion is the constraint imposed on the time-step by laser's motion. As noted by [Irwin and Michaleris \[2016\]](#), "to accurately model the motion of the heat source, the simulation time increments must be small enough such that the source moves a distance smaller than its radius over the course of an increment. When the source radius is small and its velocity is large, a strict condition is imposed on the size of time increments regardless of any stability criteria".

To formalize this observation, let T_{hs} denote the characteristic timescale of the heat source, defined as the time it takes for the heat source to move by one beam radius R :

$$T_{hs} = \frac{R}{V}$$

where V is the laser scan speed. The aforementioned constraint on Δt can be expressed as:

$$\Delta t \leq T_{hs} \quad (2)$$

Violating this inequality results in the heat source skipping over part of the domain and producing artificial peaks and valleys in the temperature field.

This effect is illustrated in [figs. 15 and 16](#), where time-steps larger than T_{hs} lead to pronounced oscillations, regardless of the time-integration scheme.

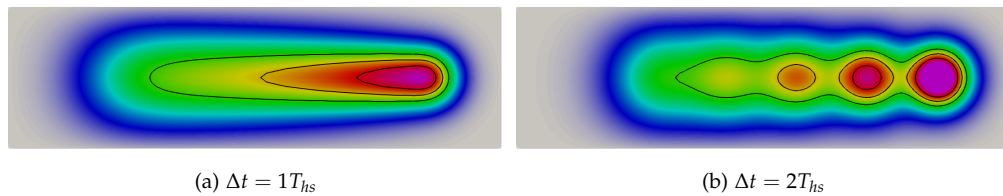


Figure 15: 2D heating track example with admissible and inadmissible time-step sizes according to inequality (2).

Lumped heat source models, sometimes referred to as *temporal reduction techniques* [[Lindwall et al., 2018](#)], alleviate this issue by averaging the heat input along the scan path, effectively decoupling the time step from the laser's radius and speed. This allows

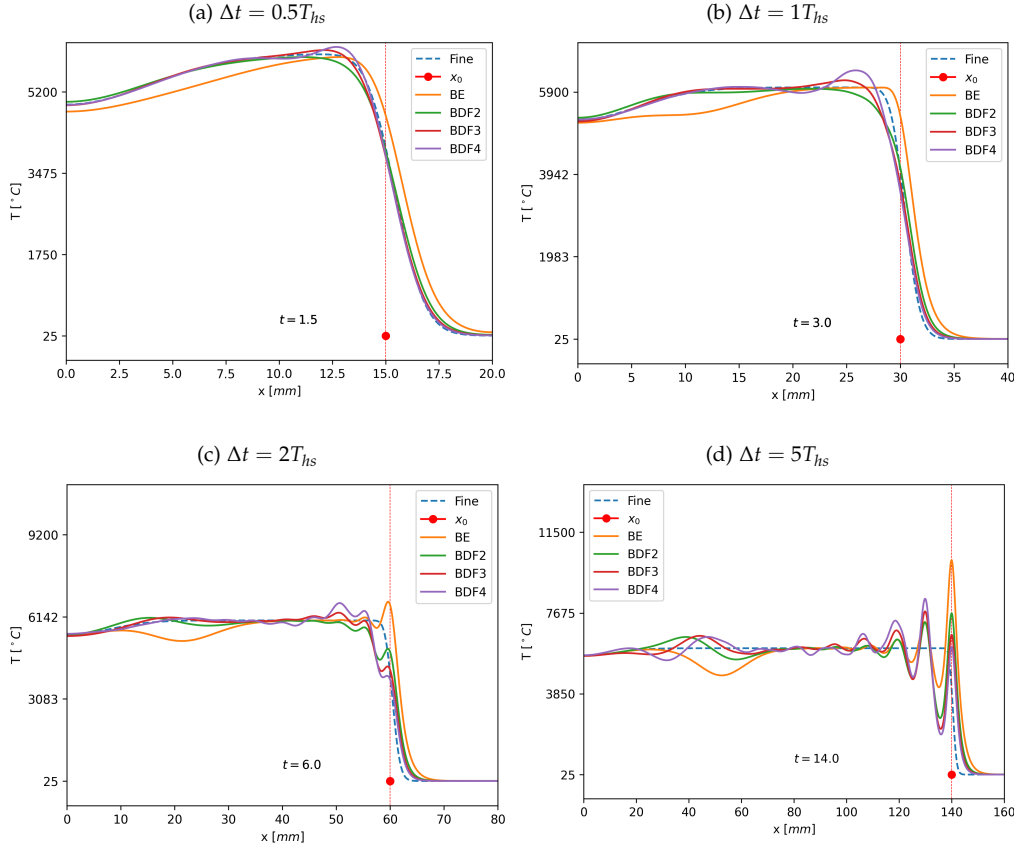


Figure 16: 1D heating track example with admissible and inadmissible time-step sizes according to inequality (2). Various time-integration types are shown but all of them exhibit oscillations above $\Delta t = 1T_{hs}$. BE = Backward Euler, BDF = Backward Differentiation Formula.

significantly larger increments to be used; although local fidelity is sacrificed, overall energy conservation and part-scale accuracy can still be maintained [Van Elsen et al., 2007].

Early references would often simplify the representation of the heat input due to the limited resolution and the absence of consensus on the correct heat source profile⁶. Some studies distributed the laser energy uniformly over a few elements [Matsumoto et al., 2002, Contuzzi et al., 2011], while others circumvented the modeling of the source term entirely by assigning a fixed temperature to newly deposited regions [Dai and Shaw, 2001, Longuet et al., 2006, Ye et al., 2006, Schilp et al., 2014]. These approaches reflect the state of the field at the time, when thermal modeling in additive manufacturing was still emerging and the trade-offs between accuracy and modeling assumptions had not yet been clearly defined.

As mentioned in the previous section, Zaeh and Branner [2009] is recognized as the first work to propose what would later be coined meta-layering and Flash Heating (FH). To make the simulation of an industrially sized part feasible, multiple physical layers are grouped into a single *meta-layer* or *process layer*, over which the heat input for the time-interval is distributed uniformly. Their FH strategy calibrates both laser power and exposure time against experimental data to reproduce representative thermal gradients at the part scale. The only earlier mention of meta-layers the present authors could find appears in Krol et al. [2009], a conference entry available only in German.

⁶ There is arguably still no consensus on the “correct” heat source profile, as present-day models use Gaussian, double-ellipsoidal [Goldak et al., 1984], and more complex profiles [Gusarov et al., 2009, Klassen et al., 2014]. However, surface flux models have largely fallen out of use, and there appears to be general agreement that the source should be volumetric and Gaussian-like.

Papadakis et al. [2014] presented a multiscale FE-based framework for modeling part distortion in an SLM twin-cantilever geometry after support structure removal using SYSWELD. The approach began with a mesoscale thermal simulation using five-layer deposition and a detailed moving heat source profile. The thermal history at a central point was then used to define a uniform hatch-level heat input, which was further homogenized into a layer-level heat input for the part-scale model. The part-scale thermomechanical model used the layer-level heat input and was time-stepped layer-by-layer or in groups of three layers. To capture spring-back effects due to support removal, the corresponding elements were deactivated, and the simulation was restarted using the final state of the previous analysis as the initial condition. A maximum error of approximately 25% in peak deflection was reported for the three-layer stepping case when compared to experimental data. The framework was considered adequate for assessing the influence of total heat input and structural stiffness on distortion behavior.

As discussed previously, Hodge et al. [2016] tackles centimeter-scale LPBF builds with a full thermomechanical model. Despite using 128-512 CPUs, simplifications were necessary to keep simulations tractable. The layer thickness and radius of the heat source were scaled up by a factor of 20, while the scanning speed was preserved and the laser power calibrated to achieve melting.

Irwin and Michaleris [2016] introduces two lumped heat source models. A time-step Δt is selected independently of (2), and the base ellipsoidal profile⁷

$$Q = \frac{6\sqrt{3}P\eta}{abc\pi^{3/2}} \exp\left(-\frac{3x^2}{a^2} - \frac{3y^2}{b^2} - \frac{3(z-Vt)^2}{c^2}\right) \quad (3)$$

is first modified by averaging it over time

$$\bar{Q} = \frac{1}{\Delta t} \int_{t_0}^{t_0+\Delta t} Q(t) dt$$

yielding the *line input* model. Figure 17b shows temperature profiles obtained using this model at various time-step sizes. As illustrated, large time-steps can lead to unphysical staircase artifacts.

To address this, the authors propose the *elongated ellipsoid* model, which increases the effective radius of motion, smoothing out temperature gradients. Figure 17a compares the standard, line input (LI), and elongated ellipse (EE) profiles side by side.

The full sequentially coupled thermoplastic model is implemented in CUBES by Pan Computing. The LI model provides higher accuracy in predicting displacements, whereas the EE model yields smoother and more accurate thermal fields, especially for larger time-steps.

For a time-step of $\Delta t = 10T_{hs}$, the displacement error at a selected node is 1.3% for the LI model and 13.4% for the EE model, relative to a high-fidelity reference solution. Thermal errors are approximately 20% for both.

To generalize the choice of time step across different materials and process parameters, the authors fit a dimensionless correlation to their simulation data, leading to the following expression:

$$\Delta t = \frac{\alpha B}{V^2} \left(\frac{Vc}{\alpha}\right)^A$$

where α is the thermal diffusivity and B and A are fitting parameters specific to the chosen heat source profile.

[Chiumenti et al., 2017c] implement an SLM model in COMET and simulate the joint deposition of a thin and thick wall structures composed of 992 layers. Phase change is neglected, and several lumping strategies are compared, including meta-layers (fig. 18c), layer-by-layer (fig. 18b), hatch-by-hatch (fig. 18a) and a high-fidelity approach. In the hatch-by-hatch strategy, multiple hatches are lumped into one, which is printed in a

⁷ The authors refer to the ellipsoid profile as a Goldak profile, despite it not being a double ellipsoid.

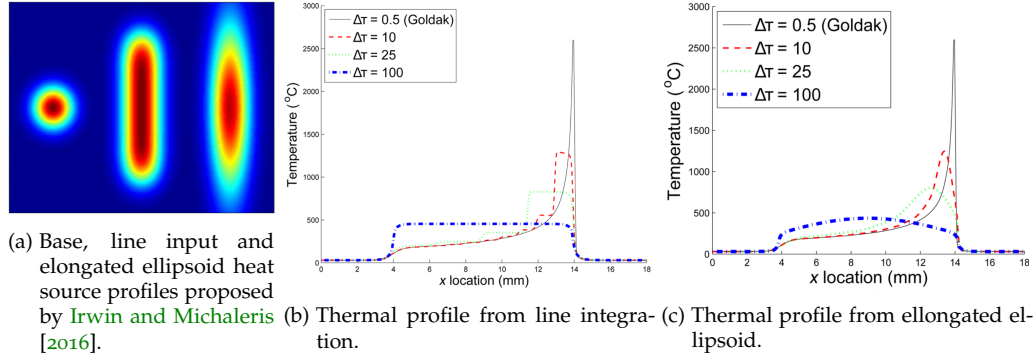


Figure 17: Line input and elongated ellipsoid profiles from Irwin and Michaleris [2016]. $\Delta\tau$ refers to the time-step normalized by T_{hs} .

single time-step ; the high-fidelity approach also lumps multiple hatches, but each time-step traverses a portion of the lumped hatch instead of activating it at once.

An extensive calibration campaign is undertaken to determine the effective heat transfer coefficients and powder porosity. The authors find that the high-fidelity approach best captures the local temperature history, while hatch-by-hatch offers a favorable trade-off between accuracy and computational cost. Note from fig. 18 that temperatures are way below the melting point, since the laser on-time is not calibrated to achieve melting (FH).

The study also evaluates the impact of excluding the powder bed from the domain, showing that while an equivalent heat transfer condition can be calibrated, including the powder bed is recommended when local thermal gradients are of interest.

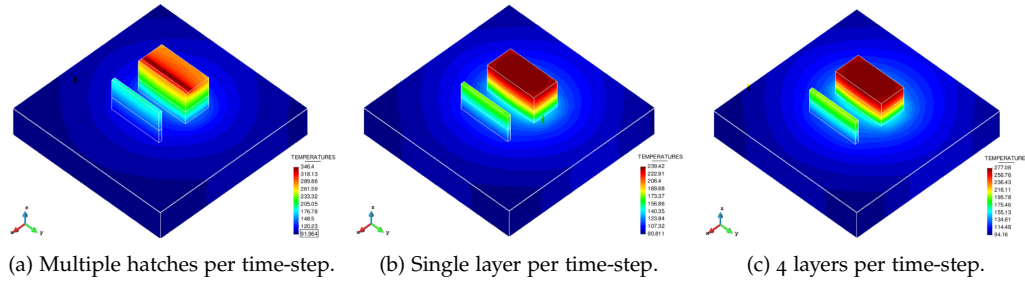


Figure 18: Lumped heat input strategies from Chiumenti et al. [2017c].

Similar to the approach of Chiumenti et al. [2017c], Lindwall et al. [2018] compare a high-resolution thermal model with simplified hatch-by-hatch and layer-by-layer models implemented in MSC.Marc. Their study focuses on LPBF of bulk metallic glass, where the risk of devitrification depends on peak reheating temperature and cooling rate. AMR is used to reduce computational cost. The high-resolution model employs an ellipsoidal heat input profile⁸. In the hatch-by-hatch and layer-by-layer models, a Gaussian distribution is used in the depth direction, while the energy is applied uniformly across the hatch or layer, respectively. The layer-by-layer model adopts a FH approach, where the heating time corresponds to T_{hs} . A critical location is selected four layers below the top surface to assess devitrification risk. Both simplified models significantly reduce computational time while accurately reproducing the temperature history at this location. Notably, the layer-by-layer model is approximately 500 times faster than the high-fidelity simulation and provides a conservative estimate of devitrification risk.

Zhang et al. [2018b] apply the thermal model of Chen et al. [2017] to an 80-layer deposition of an impeller (see fig. 19), using layer-fraction stepping and a mesh of approximately 2 million elements. The simulation takes 17 hours on a 60 core cluster. To

Devitrification is the loss of the amorphous (glassy) structure in a bulk metallic glass, caused by crystallization during reheating. It is an undesirable effect, since crystallization reduces the unique mechanical and physical properties of metallic glasses.

⁸ As in Irwin and Michaleris [2016], the authors refer to this as a Goldak profile, although it is in fact a single ellipsoid.

mitigate thermal diffusion instabilities from sharp temperature gradients at interfaces, the physical heating time is scaled up by a factor of 40. Zhang et al. [2018a] perform a mechanical simulation on a similar 50-layer impeller (see fig. 20), using time steps ranging from 5% to 25% of a layer. With a comparable mesh size, the simulation requires approximately 3.5 days of computation. They estimate that a full part-scale simulation using their mesoscale melt pool model would take over 240 years.

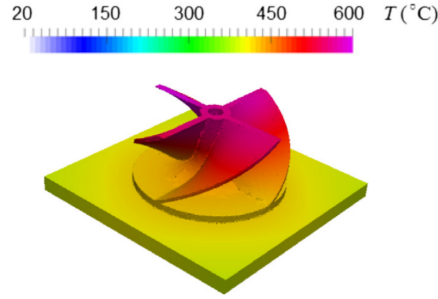


Figure 19: Temperature from impeller build, Zhang et al. [2018b].

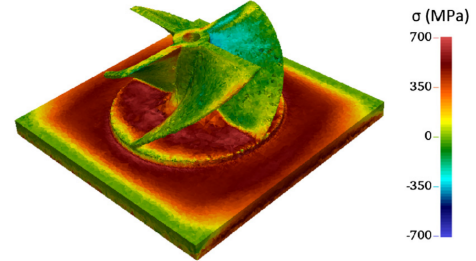


Figure 20: σ_{xx} from impeller build, Zhang et al. [2018a].

Li et al. [2018] presents a multiscale FEM framework for scalable part-scale thermo-mechanical simulation of SLM. At the microscale, a pure thermal analysis of a HAZ using a moving Gaussian heat source is calibrated against the experimentally observed melt pool depth in order to derive the dimensions of an equivalent cuboidal heat source. determines the dimensions of an equivalent cuboidal heat source in order to replicate the experimental melt pool depth. At the mesoscale (hatch level), the power of this cuboidal source is adjusted to ensure effective melting. At the macroscale, the part is built thermomechanically by lumping multiple physical layers into a single block layer. Each block layer is further subdivided into sub-blocks scanned in different sequences to account for the scan pattern effect. They use Abaqus to model an L-shaped deposition and a bridge. The authors find that, in the case of the L-shape, part distortion can still be predicted with reasonable accuracy even when 50 layers are lumped together.

Ganeriwala et al. [2019] use a uniform heat source in combination with various lumping strategies. The authors note that in previous work they had used more detailed heat source models, including the double-ellipsoidal profile [Goldak et al., 1984] and the Gusarov model [Gusarov et al., 2009], but found that “only a minimal difference in the ensuing stress/strain field was noticed when using these other beam types at the agglomerated scale.”

Their main lumping strategy, based on earlier work by Hodge et al. [2016], involves scaling up both the layer thickness and the heat source radius. The laser heat source then follows its scan path over each meta-layer, and the laser power is numerically tuned to ensure complete melting. The authors note that the design of a heat source lumping strategy that produces accurate residual stresses results without requiring calibration remains an open question.

In their LPBF-bridge examples, their main lumping strategy employs meta-layers consisting of 17 physical layers. The beam diameter is scaled up by a factor of approximately 18.5, and the laser power is increased by a factor of 100, while the scan speed is kept constant. The interlayer cooling time is adjusted to maintain consistency with the total physical build time.

This baseline strategy is compared against several alternatives, including: (i) holding the power constant while reducing the scan speed, (ii) increasing the power and simultaneously decreasing the scan speed, and (iii) applying a Flash Heating (FH) approach that deposits heat across the entire layer over a brief time interval. The authors find that both the baseline strategy and the FH approach yield the best agreement with experimental measurements. However, despite simulating the scan path, the baseline method fails to fully capture the scan strategy effects observed in the island scan

experiments. Consequently, they conclude that the FH method is preferable, given its comparable accuracy and significantly lower computational cost.

In the final paragraph, the authors note a renewed interest of commercial software in high-fidelity, full thermomechanical modeling. They also hint at their ongoing work on “temporally adaptive techniques,” which would be published a few years later [Hodge, 2021].

Zhang et al. [2019] investigate various FH configurations involving meta-layers that lump up to 24 physical layers in order to provide guidelines for efficient part-scale LPBF simulation. The powder bed is represented via a convection boundary condition. Their thermal model without latent heat, is monolithically coupled to a thermoplastic mechanical model, since mechanical dissipation is considered. The study finds that layer scaling beyond a factor of 4 introduces significant errors in temperature and stress predictions, even when mesh convergence is achieved. Interlayer cooling time is identified as the key parameter influencing residual stresses and thermal gradients. The authors achieve comparable results when time-stepping 1 or 4 layers at a time, provided that the cooling time for the latter is scaled proportionally. Counterintuitively, the authors conclude that “the heating step time has negligible influence on [...] stress within layer scaling”.

Malmelöv et al. [2020] proposes a novel lumping approach: *lumping of weld passes*, that is, use thicker layers while preserving the original scan path. The proposed approach does not require extra calibration, as the modifications in the process parameters (scan speed, dwell time) are only a function of the lumping factor. The strategy is integrated into a thermomechanical model with a double-ellipsoidal heat source implemented in MSC.Marc. A “fully” staggered coupling is employed: the thermal and mechanical problems are solved iteratively until convergence, with mechanical dissipation included in the thermal analysis, although its contribution is found to be minor. The model is validated against the DED thin-wall experiment published by [Denlinger et al., 2015a]. Lumped simulations reproduce thermocouple readings and vertical distortion measurements, albeit with increasing oscillations as the lumping factor increases. While residual stresses are slightly underestimated compared to the high-fidelity model, the computational cost is significantly reduced.

Bayat et al. [2020] propose a variant of FH referred to as *Sequential Flash Heating* (SFH) for part-scale thermo-mechanical modeling of LPBF. This strategy combines elements from the weld-pass lumping approach of Malmelöv et al. [2020] and the hatch-lumping scheme of Chiumenti et al. [2017c]. Following layer lumping, each meta-layer is subdivided into narrow stripes that are activated sequentially. Heat input is applied homogeneously within each stripe, and, like in conventional FH, the exposure time is calibrated to achieve melting while maintaining the total energy input of the real process.

Both FH and SFH are implemented in Abaqus. The thermal model incorporates phase change via an enthalpy-based formulation and includes convective and radiative boundary conditions. The mechanical analysis is elasto-plastic and accounts for transformation strains. The authors highlight that standard FH yields isotropic, scan-path-insensitive residual stresses and overpredicts deflection by nearly 50% compared to experiments. In contrast, an SFH approach with 20 stripes per meta-layer achieves much lower deflection error of nearly 1%, though at the cost of a 13-fold increase in computational time.

2.3.2 Adaptive Mesh Refinement

Due to the minute size of the moving laser relative to the part and the presence of highly localized, steep thermal gradients, it is prohibitively expensive to finely resolve the entire scan path using a uniformly dense mesh. AMR is well suited to this challenge, as it enables fine spatial resolution only where necessary, while keeping the number of DOFs relatively constant throughout the simulation. In the present, AMR is a well-

established technique in [MAM](#); as discussed in chapter 1, it has become a prerequisite for “high-fidelity” part-scale simulation [[Dugast et al., 2021](#), [Proell et al., 2024](#), [Baiges et al., 2021](#)].

[Patil et al. \[2015\]](#) present the first dedicated [MAM-AMR](#) algorithm, developed for modeling moving thermal loads in the software 3DSIM. The work argues that the thermal field in [SLS](#) is continuously *spatiotemporal periodic* and behaves like a traveling wave i.e. $f(\mathbf{x}, t) = f(\mathbf{x} + \mathbf{V}T, t + T)$, $T \rightarrow 0$, where $\mathbf{V}$ is the velocity of the laser and T is the period. Unlike conventional [AMR](#) schemes, the proposed algorithm uses a moving fine-mesh subdomain that replaces a region of the coarser background mesh as it follows the heat source. The motion of the fine mesh is constrained such that the fine and coarse meshes always conform at their shared interface i.e. element facets align (see fig. 21). In the companion work [Pal et al. \[2016\]](#), the model is extended to include phase change and microstructural evolution. The framework is then applied to simulate melt pool evolution and phase fractions in Ti-6Al-4V, showing close agreement with thermal imaging and microstructural observations. Notably, [Patil et al. \[2015\]](#) also point to the development of “new quasi-static formulations and algorithms for moving waves” as a promising direction for future research, relevant to the scope of the present manuscript.

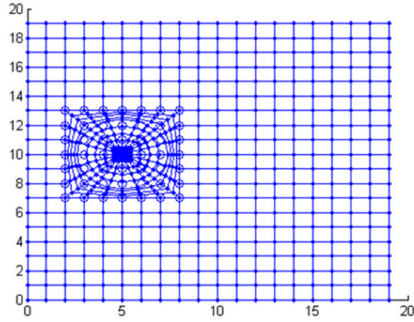


Figure 21: Moving mesh [AMR](#) from [Pal et al. \[2016\]](#).

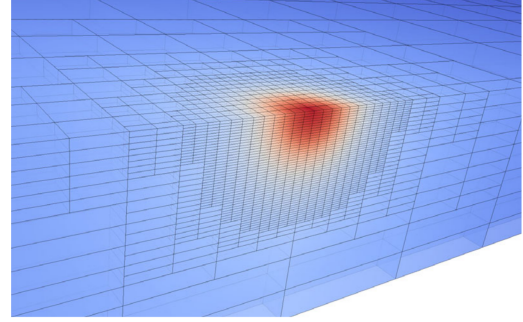


Figure 22: Adaptive mesh refinement in [LPBF](#) case using [deal.II](#), [Riedlbauer et al. \[2014\]](#).

[Denlinger et al. \[2014\]](#) is among the first to use [AMR](#) for coarsening purposes. Their geometric criterion coarsens previously deposited layers to reduce the global number of [DOFs](#) while preserving accuracy in the active deposition region. Around the same time, [Riedlbauer et al. \[2014\]](#) take a similar approach, refining the mesh in the [HAZ](#) and coarsening it far away, see fig. 22.

[Soldner and Mergheim \[2019\]](#) employ an [AMR](#) strategy based on the Kelly error estimator [[Kelly et al., 1983](#)], which considers the jumps of the gradients of the solution along element facets. To further resolve phase change, elements close to the melting point are refined.

[Kollmannsberger et al. \[2018\]](#) use separate meshes for the thermal field and material state. This distinction is motivated by the observation that, while the thermal gradients diffuse outward from the [HAZ](#), the material state remains unchanged in time. By decoupling these two fields, different [AMR](#) strategies can be applied to optimize computational cost and resolution for each. Moreover, this is the first work to employ *p*-refinement (change polynomial order) in [MAM](#) on top of *h*-refinement (change mesh size). Through their validation cases, the authors demonstrate that the framework is well suited for accurate, efficient simulation of thermal fields in [LPBF](#); the separation of the temperature and material state meshes allows the reduction of the number of [DOFs](#) throughout the simulation.

[Baiges et al. \[2021\]](#) addresses the challenges of mesh coarsening in in [MAM](#) simulations. The work identifies two related issues: (i) the loss of mechanical information when transferring state variables from a fine to a coarse mesh, and (ii) the potential instability introduced by coarsening. In contrast to the thermal problem, which is largely local (a spot heats and cools, often returning close to its initial state), the mechanical

problem is global in nature: each heating/cooling cycle leaves behind plastic strains that accumulate, making coarsening far more sensitive.

To address these issues, the authors propose stress and force correction terms to be applied during coarsening; the first preserves the sharp local stress variations that would otherwise be smoothed out by coarsening, and the second restores global force equilibrium after coarsening. The framework is implemented in Femuss software developed at CIMNE and showcased in SLM examples using the *inherent strain* method (section 2.3.3). The correction terms are shown to be vital in ensuring accuracy.

Moreira et al. [2024] present a thermomechanical model with AMR for part-scale DED simulations, implemented in the Femuss. The AMR strategy relies on the work of Baiges and Bayona [2017] to break from the usual 2:1 refinement ratio constraint, enabling a more flexible and efficient AMR mesh structure. The refinement algorithm combines both geometric and error-based criteria, with a gradient-based error estimator [Zienkiewicz and Zhu, 1987] applied to the displacement field. To mitigate information loss during coarsening, correction terms based on the work of Baiges et al. [2021] are introduced and found to be essential for achieving convergence. The framework demonstrates strong scalability, achieving 71% parallel efficiency on 2048 CPU cores for a gear demonstrator case, consisting of 20 layers deposited 1 by 1, and up to 15 million nodes, that is, 45 million displacement DOFs.

The octree-based AMR strategy employed by Proell et al. [2024] is inspired by the approach of Neiva et al. [2019]. It relies exclusively on geometric criteria. All elements in the top layer are deposited at the finest mesh resolution: while this may temporarily increase the number of DOFs, it avoids the need for additional AMR cycles during laser scanning. Cells located four layers below the top are allowed to coarsen, provided that none of their neighboring cells are still unsolidified.

2.3.3 Inherent strain method

In the last decade, as part-scale simulations grew more ambitious, full thermomechanical models became increasingly limited by their computational expense⁹. In response, researchers began adapting simplifications originally developed in welding mechanics to MAM. The inherent-strain concept, originally formulated by Ueda et al. [1975] for welded structures, was first applied to large welding structures by Deng et al. [2007] and to LPBF modeling by Keller and Ploshikhin [2014]. In this approach the total strain is decomposed as

$$\varepsilon = \varepsilon_{el} + \varepsilon_{pl} + \varepsilon_{th} + \dots = \varepsilon_{el} + \varepsilon_{inh} \quad (4)$$

where the inherent strain ε_{inh} collects all non-elastic contributions (plasticity, thermal strain, etc.). These inherent strains are estimated a priori and prescribed as eigenstrains in the subsequent mechanical analysis, which therefore remains purely elastic and computationally inexpensive.

Keller and Ploshikhin [2014] proposes a three-stage, multiscale strategy for predicting part-scale distortion. (i) They first calibrate a thermal model restricted to the HAZ against measured melt-pool geometries, thereby identifying key heat source parameters (radii, absorptivity). (ii) Next, they perform a detailed thermo-mechanical simulation of a representative scan segment to capture path-dependent effects and to extract the corresponding inherent-strain tensor. (iii) Those inherent strains are then imposed as eigenstrains in a purely elastic, layer-by-layer analysis, enabling rapid prediction of global distortion. They apply this workflow to the geometric compensation of an industrial LBM part, an LPBF variant. They conclude that the method can reduce computational time by two or more orders of magnitude compared to a full analysis.

It is important to note that while this method has proven effective for LPBF, its underlying assumptions do not hold for DED, where scales are less disparate and plastic strains are more broadly distributed.

Keller et al. highlight the close analogy between welding and MAM, noting: “[...] AM processes for metallic parts [...] can also be understood as a series of micro-welding processes; therefore the theory of welding can also be applied. However, the direct simulation of the AM process is not feasible, since the process consists thousands to millions of weld seams”.

⁹ For instance, for a high number of DOFs, Moreira et al. [2024] report a cost approximately 6 times higher for the mechanical analysis compared to the joint cost of the thermal analysis and the deposition.

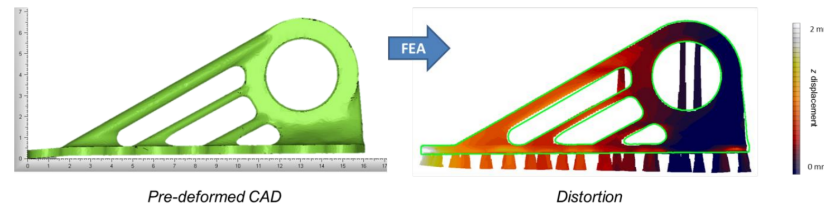


Figure 23: Geometric compensation of LBM print using the inherent strain method [Keller and Ploshikhin, 2014].

Alvarez et al. [2016] apply the inherent strain method in combination with layer lumping to investigate the effect of the lumping factor (the number of layers grouped into one) and to compare isotropic and orthotropic thermal expansion coefficients in the context of SLM cantilever builds with 400 layers of Inconel 718. For their case study, they find that lumping up to eight layers yields accurate distortion predictions. The use of isotropic versus orthotropic coefficients produces similar results, with each performing better depending on the specific scanning strategy.

Li et al. [2016] propose a multiscale SLM simulation framework similar in structure to that of Keller and Ploshikhin [2014], but replace the use of inherent strain with an inherent stress approach. At the microscale, a thermal melt-pool level model is used to derive an equivalent lumped heat source, which captures the thermal gradient effects of laser scanning. This equivalent source is then applied to a thermoplastic mesoscale model representing a single powder layer on a substrate, which is time-stepped hatch-by-hatch. The resulting residual stress field from the mesoscale is mapped to the part-scale model, which is solved layer-by-layer. The parts considered are such that the scan path only varies by a rotation from layer to layer; the derived residual stress is rotated accordingly. The methodology is validated against experimental deflection data, and residual stress distributions are compared across different scanning strategies.

Liang et al. [2018] propose a modified inherent strain method in which the inherent strain is defined as the difference between the maximum compressive strain and the residual elastic strain after cooling. The authors argue that an elastic component must be included in the inherent strain, as the original method assumes that elastic strains induced during processing fully relax. The method is validated for vertical distortion data of small DED builds.

Setien et al. [2019] were among the first to propose an experimental approach for the determination of the inherent strains. The authors use twin-cantilever beam coupons fabricated with various scanning strategies and focus on predicting vertical distortion after baseplate removal. A subset of the coupons is used for calibration, while the remainder serves for validation. Despite lumping 20 layers into a single meta-layer, the model achieves good agreement, with a maximum deviation of 10%.

2.3.4 Substepping

In all the aforementioned works, spatial discretization using FEM leads to a matrix Ordinary Differential Equation (ODE), which is integrated in time using a separate time-marching scheme, typically based on Finite Difference Method (FDM).

In multiscale problems, certain subdomains may exhibit significantly smaller characteristic spatial or temporal scales than the rest of the domain. As discussed in section 2.3.2, a smaller characteristic spatial length in a subdomain can often be addressed via AMR. However, handling disparate time-scales is more complex.

Small time-steps are required in the vicinity of the heat source, which is typically a small fraction of the entire domain. However, in the conventional approaches offered by most commercial softwares, a uniform time integration scheme is applied across the entire domain. This leads to the global time-step being constrained by the smallest characteristic time-scale in the domain. As a result, regions of the solution far away

from the heat source are forced to adopt unnecessarily small time-steps, reducing computational efficiency. In LPBF applications, where radii of 100 μm and velocities of 1000 mm s^{-1} are typical, this results in a significant computational burden.

To overcome this inefficiency, it is necessary to integrate different subdomains using distinct time-steps and/or time integration schemes, and to couple their solutions appropriately. These methods appear in the literature under various names, including multirate, multi-timestep, subcycling, and mixed time integration. In this thesis, they will be referred to as *substepping* methods.

Early substepping research focused on **structural dynamics**, employing explicit integration schemes in stiff regions and implicit schemes elsewhere. These approaches, referred to as mixed time integration, were introduced by Belytschko and Mullen [1977], who proposed an implicit-explicit method for second-order Partial Differential Equations (PDEs) based on nodal partitioning. The stability of such schemes was further investigated in Belytschko and Mullen [1978] and Park [1980]. Subsequently, Hughes and Liu [1978a,b] proposed similar methods based on element partitions rather than nodal ones.

“Proper” substepping was first introduced by Belytschko et al. [1979], who referred to it as subcycling. Their method applied explicit schemes to both fast and slow subdomains. The slow subdomain was integrated first, and its interface values were linearly interpolated in time to serve as Dirichlet boundary condition for the fast subdomain.

Several variations of this algorithm were later proposed to simplify its implementation [Belytschko et al., 1979], and to allow for time-steps that are not integer multiples of each other [Neal and Belytschko, 1989, Smolinski, 1996]. Daniel [1997] proposed a further refinement using second-order temporal interpolation, that is, assuming constant acceleration rather than constant velocity at the interface.

Progressively, substepping methods started incorporating Domain Decomposition (DD) strategies. Farhat et al. [1995] proposed a Fluid-Structure Interaction (FSI) method in which the fluid domain is subcycled using an explicit scheme, while the solid domain is integrated with an implicit scheme. The fluid receives a velocity Boundary Condition (BC) from the solid, which receives a force BC from the fluid. Both BCs are enforced through Lagrange multipliers at the interface¹⁰. Gravouil and Combescure [2001] introduced a substepping method for non-linear structural dynamics, enabling the coupling of subdomains integrated with arbitrary Newmark schemes through an interface problem formulated using a dual Schur DD approach. As in the FSI context, velocity continuity at the interface is enforced using Lagrange multipliers. The authors showcase the coupling of subdomains with time-step ratios of the order of 100. A year later, Combescure and Gravouil [2002] propose a similar FETI-based method.

Despite its relevance to MAM and LPBF modeling in particular, substepping has not been widely adopted in the field. To date, only a handful of relatively recent substepping applications to MAM exist. The first reference in the field was Soldner and Mergheim [2019], who propose a substepping strategy for LPBF that is based on the scheme of Nakshatrala et al. [2009].

In Soldner and Mergheim [2019], the computational domain Ω is divided into two non-overlapping partitions: a fast subdomain (Ω_f) and a slow subdomain (Ω_s). The time step in Ω_s , denoted Δt_s , is an integer multiple of the time step in Ω_f , denoted Δt_f , such that $t^{n+1} = t^n + \Delta t_s = t^n + k\Delta t_f$, where $k \in \mathbb{N}$. A Nitsche-based DD strategy is used to couple the two subdomains at their interface Γ . The novelty introduced by Nakshatrala et al. [2009] is the explicit evaluation of the interface terms at t^n . Consequently, in Soldner and Mergheim [2019], all terms in the weak form are advanced using a second order Runge-Kutta scheme, except for the interface terms which are treated explicitly using Forward Euler.

This approach enables efficient independent solves of each subdomain. However, the explicit treatment of the interface introduces a stability constraint on Δt_s . Nakshatrala

¹⁰ Note that Farhat is the co-inventor of FETI (Finite Element Tearing and Interconnecting)

et al. [2009] provide an analytical estimate of the critical time-step size based on mesh size, thermal properties, and penalty parameters. Notably, the critical time step size decreases with increasing thermal conductivity.

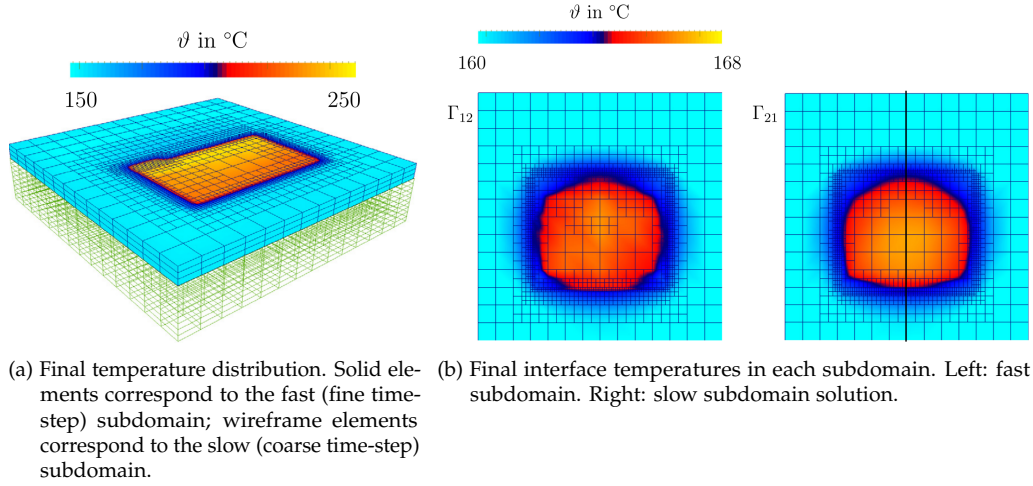


Figure 24: Substepping simulation of a 5-layer PA12 SLS build from Soldner and Mergheim [2019].

The 3D numerical example presented is a SLS polymer deposition (fig. 24). The lumped line heat source model mentioned in the previous section allows for $\Delta t_f = 5T_{hs}$. Results are shown for $\Delta t_s = 10\Delta t_f = 50T_{hs}$. The last 3 layers belong to the fast partition. No numerical or experimental validation is provided. Because each subdomain is advanced independently, two separate temperature fields are obtained at the interface (cf. fig. 24b). The discrepancy is small, in the order of a few degrees.

The authors note that applying the method to metallic materials would require smaller time steps due to higher thermal conductivity. In the conclusion of their work, the authors call for further research on an **implicit** approach in order to increase the benefits of the DD.

A few years later, Hodge [2021] proposed such a scheme. The author states his method is based on the works of Sandu et al. [Roberts et al., 2021, Günther and Sandu, 2022], which developed multirate Runge-Kutta methods. Paraphrasing the author, the calculation of the fast DOFs can be interpreted as stages in the Runge-Kutta method that is integrating the slow degrees of freedom, and the scheme is nominally identical to the *compound-fast* method described by Roberts et al. [2021]. The scheme is described here using the same notation as in the previous paragraphs ($\Omega_s, \Omega_f, \Delta t_s, \Delta t_f, k$). It consists of three steps:

1. Global *predictor step*, which time-steps the entire domain using Δt_s
2. $k - 1$ micro-steps in the fast subdomain which receive a Dirichlet BC from the global predictor step
3. Global *corrector step*, which couples the last micro-step on Ω_f to the slow time-step on Ω_s .

In the abstract, Hodge reports a speed-up of up to 100x compared to uniform time-stepping. This must be contextualized by noting that the baseline model has a particularly fine temporal resolution.

The phase change is modeled using both an apparent heat capacity model and the heat integration algorithm of Rolph III and Bathe [1982]. This results in challenging nonlinear convergence, necessitating extremely small time-steps, even when using the trapezoidal rule for time integration. In one numerical example of Hodge et al. [2014], time-steps of approximately 7×10^{-7} s are used, which corresponds to $0.0014T_{hs}$, or about 3% of the element size. These prohibitively small time-steps were attributed in part to the Rolph algorithm.

The model used in Hodge [2021] is described in detail in Hodge et al. [2014], reviewed in section 2.2.

However, in Hodge [2021], the Rolph algorithm is not used, leaving only the apparent heat capacity approach. But the time-step size remains very small, with the largest Δt_f value being $1.7 \times 10^{-6} \text{ s} = 0.0165 T_{hs}$, or roughly 10% of the element size. Using $k = 180$ ($\Delta t_s \approx 3 T_{hs}$), Hodge achieves small errors¹¹ in their 2D welding example and reports a hundredfold speed-up compared to uniform time-stepping at $\Delta t = 1.7 \times 10^{-6} \text{ s}$.

In their follow-up work [Puso and Hodge, 2023], the authors apply the substepping method to 3D LPBF simulations in conjunction with AMR. Figure 25 illustrates the steps of the substepping algorithm as previously described. The authors employ Backward Euler time integration, motivated by observations of non-physical oscillations when using the trapezoidal rule.

Two numerical examples are presented: one involving LPBF cubes of increasing size, and another featuring a complex bridge structure from the AM-BENCH 2018 challenge problem. In both cases, errors are evaluated relative to reference solutions obtained with uniform time-stepping.

The cube simulations are used to evaluate the method's performance and demonstrate convergence. First, a fast time-step of $\Delta t_f = 1 \times 10^{-5} \text{ s} = 0.2 T_{hs}$ is used, with k values reaching into the thousands to evaluate computational speed-up, which can be as high as 100x. However, errors are not reported for these cases. Convergence tests are then conducted, first without phase change, using a fixed $\Delta t_f = 1 \times 10^{-6} \text{ s} = 0.02 T_{hs}$ and varying k . For the phase change convergence test, Δt_f is set a few orders of magnitude smaller.

The bridge structure from AM-Bench 2018 is used as a more complex/practical example. $\Delta t_f = 6 \times 10^{-6} \text{ s} = 0.0384 T_{hs}$ is used, corresponding to approximately 4% of the element size per time-step. With a substepping factor of $k = 200$, this yields a slow time-step of $\Delta t_s = 7.68 T_{hs}$. Using two different configurations of the fast domain Ω_f , the authors report speed-ups of 22.8 and 15.6 compared to a uniform time-stepping strategy.

Viguerie et al. [2022] propose a scheme structurally similar to that of Hodge [2021], consisting of a global predictor step, $k - 1$ micro-steps, and a final micro-step coupled with the macro-step. Their method builds on a fully overlapping DD framework proposed by the authors [Viguerie and Auricchio, 2022, Carraturo et al., 2022], which allows the use of two separate meshes for the fast and slow subdomains. These are coupled through interface terms inserted directly into the “slow” PDE.

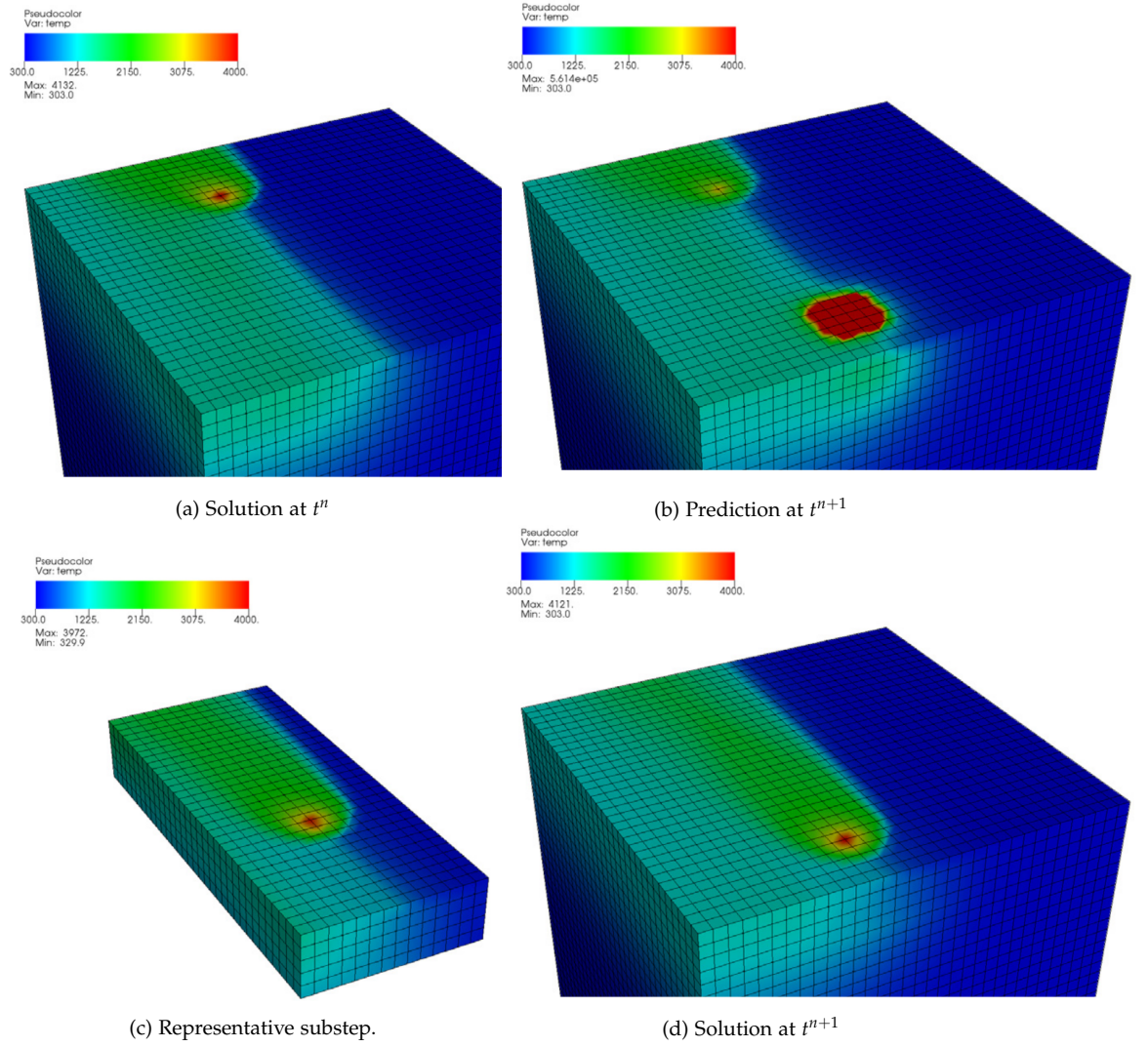
Latent heat effects are included only in the fast problem, using the enthalpy formulation of Kollmannsberger et al. [2018]. A Gaussian heat source is applied in the fast domain, while the slow domain receives uniform heating. The coupled, or “corrector”, step is solved in a staggered manner.

The authors demonstrate their method on 2D and 3D welding simulations, including a final case involving 50 laser scan tracks over an IN625 substrate. Figure 26 shows an intermediate micro-step from the latter.

For this example, the fast time-step is set to $\Delta t_f = 1 \times 10^{-4} \text{ s} \approx 0.94 T_{hs}$, corresponding to roughly one element traversed by the laser per micro-step. A value of $k = 4$ is chosen based on prior numerical tests to strike a balance between accuracy and efficiency. The authors report a speed-up of 2.44x compared to uniform time integration. This result is modest if compared to the speed-ups claimed by Hodge [2021] and Puso and Hodge [2023], but this work employs a much coarser base time-step, which results in a similarly sized Δt_s .

Although not strictly a substepping reference, Kopp et al. [2022] present a space-time FEM method for thermal LPBF modeling. Using an apparent heat-capacity approach for phase change, their hp-AMR framework captures the multiscale nature of the process by locally refining the space-time mesh along the laser path, as illustrated in fig. 27. Close to the HAZ, the element duration and size are reduced through temporal and spatial

¹¹ Note: Error estimates are based on temperature histories at two spatial points, and convergence is assessed using only two values of the time step, limiting generality.

Figure 25: Depiction of all substepping changes, [Puso and Hodge \[2023\]](#)

h-refinement, respectively. The polynomial degree in time is decreased (p-coarsening) away from the [HAZ](#).

At the time of publication, their open-source implementation supported only shared-memory parallelism, limiting its scalability for large part-scale simulations. While no explicit speed-up results are reported, the method is demonstrated on a 3D welding example with [LPBF](#)-like parameters: a 102 mm long scan path on a $10 \times 10 \text{ mm}^2$ substrate is simulated in 7 hours on a single [CPU](#).

[Cheng and Wagner \[2021\]](#) build on the earlier work of [Roux \[2008\]](#), [Roux and Garaud \[2009\]](#), who showed that the stability of Dirichlet-Neumann (DN) schemes depends sensitively on the contrast of material parameters across the interface and may require strong relaxation, whereas Dirichlet-Robin (DR) coupling is unconditionally stable for the Poisson problem when the augmented Robin matrix equals the Schur complement. Cheng and Wagner apply the DR scheme to the linear heat equation and derive a practical algorithm that approximates the Schur complement from a 1D analytical estimate. Moreover, they propose the following substepping strategy:

1. Macro-step: Without performing a predictor step, Ω_s is advanced directly to t^{n+1} , using the fast-domain temperature at t^n as a Dirichlet [BC](#).

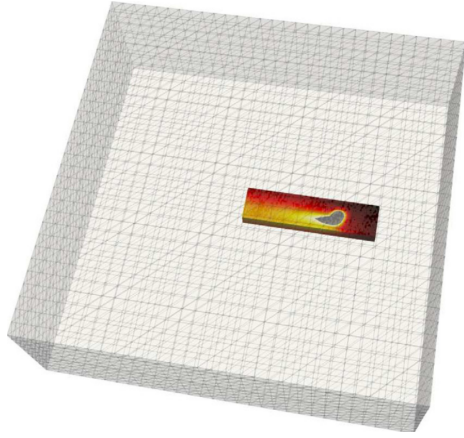


Figure 26: Generic micro-step in 3D welding example from [Viguerie et al. \[2022\]](#).

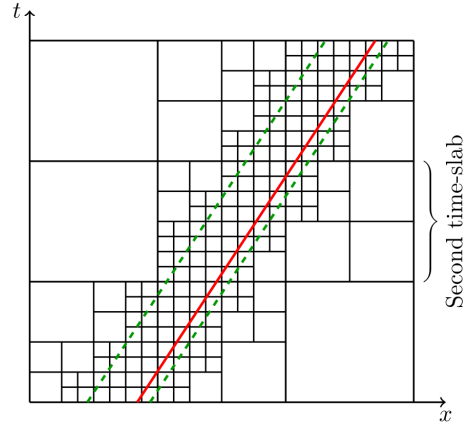


Figure 27: Schematic of locally refined space-time FEs in one-dimensional problem from [Kopp et al. \[2022\]](#). Source path in red, refinement region in dashed green.

2. Micro-steps: The fast subdomain Ω_f is then advanced through k micro-steps to t^{n+1} , receiving a constant Robin BC supplied by Ω_s . Interface temperature is set from the fast solution.

Their final numerical test, a 2D welding example with Ti64-like linear properties, uses Forward and Backward Euler to advance the fast and slow subdomains, respectively. Δt_f is set to the maximum stable time-step size of 6.5625×10^{-6} seconds, or $0.065625 T_{hs}$. Accurate results are obtained with $k = 100$, which the authors use to claim a speed-up of 100x without providing CPU times. Results are compared to uniform time-stepping using the line heat source model of [Irwin and Michaleris \[2016\]](#), which performs well up to $\Delta t = 20T_{hs}$ but underpredicts temperature peaks for larger values.

A recent work by [Moreira et al. \[2025\]](#) investigates mechanical substepping for DED thermo-mechanical simulations, referring to the approach as local-global coupling. The thermal problem is solved uniformly using Backward Euler, whereas the mechanical problem is solved with substepping, with the particularity that the fast partition is redefined at each substep: it consists of a small region of elements surrounding the heat source. No predictor step is used and the fast subdomain is supplied with a Robin BC from the slow solution at t^n , effectively assuming that the slow solution remains constant over the macro-step far enough from the heat source. The derivation of the Robin condition is based on [Neiva et al. \[2020\]](#).

The underlying thermomechanical model employs a lumped heat source and a small-strain thermo-viscoplastic constitutive law. To prevent volumetric locking in nearly incompressible plastic flow, $\bar{B}$ -formulated elements are used. The study includes both academic and industrial examples to assess the accuracy and computational performance of the method. Results demonstrate that the approach achieves substantial speed-ups without a significant loss of accuracy compared to uniform time-stepping. The authors also note that parallel scalability could be improved by incorporating a load-rebalancing strategy tailored to the moving local domain.

[Neiva et al. \[2020\]](#) is discussed at the end of this chapter.

2.3.5 Other cost-saving strategies

Section section 2.3 has presented several established computational strategies that significantly reduce the computational cost of part-scale modeling. However, these methods are still not sufficient to allow for high-fidelity part-scale thermal simulation, let alone thermomechanical.

Recent works in the literature explore a multitude of additional avenues to further reduce the cost. This section briefly reviews these alternative techniques, highlighting their advantages.

In recent years, GPUs have become increasingly popular in scientific computing due to their high computational power and relatively low cost compared to CPUs, which often require dedicated cluster infrastructure to achieve similar throughput. Dugast et al. [2021] present a GPU-based, matrix-free, part-scale thermal LPBF model.

Matrix-free methods circumvent the assembly of the global linear system by relying on iterative solvers that only require matrix-vector product evaluations. In matrix-free FEM, local element matrices are not assembled into a global matrix, but instead used directly during the matrix-vector product computation.

Dugast et al. compare their matrix-free algorithm against a conventional full linear system solve, both executed on GPUs. The latter is implemented using AMGX (NVIDIA) in combination with PETSc. In their block example, the authors report a speed-up of 23x, from 210 seconds to 8 seconds. They also observe a 1.8x speed-up over ANSYS when both are run on a single CPU. When comparing their GPU implementation to ANSYS on a single CPU, they report a speed-up of 300x, from 50 min to 8 seconds.

Voxel grids are used in combination with AMR to coarsen previously deposited layers, in order to further decrease cost. The authors estimate a 5x speed-up from the AMR, and a 2x speed-up when not transferring inactive element data to the GPU. Using a meta-layering approach, the authors are able to simulate a large 150 mm $\times$ 150 mm $\times$ 150 mm build (see fig. 28).

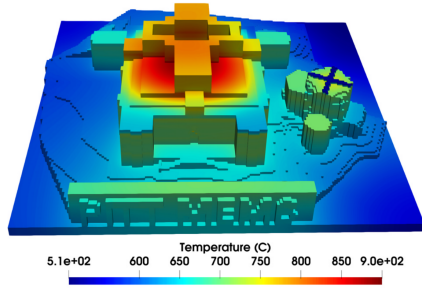


Figure 28: Intermediate temperature snapshot of Cathedral of learning example from Dugast et al. [2021].

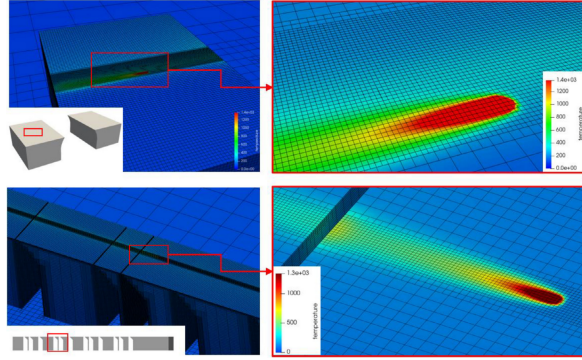


Figure 29: Temperature distributions of bridge example from Olleak et al. [2022].

In the follow-up work, Olleak et al. [2022] present a high fidelity model based on the same framework matrix-free GPU framework introduced by Dugast et al. [2021]. The authors report a speed-up of over 10000x compared to ANSYS running on 10 CPUs, demonstrated on a centimeter-scale bridge structure example (see fig. 29). The example involves several hundred thousand elements and about five million time steps.

The idea that Forward Euler can outperform Backward Euler in LPBF thermal simulations has circulated in the community for some time [Cheng and Wagner, 2021, Mozaffar et al., 2019, Moran et al., 2021]. Essongue et al. [2022] present a thorough benchmark of an in-house Forward Euler implementation against Abaqus, which uses Backward Euler¹². They are compared in an experimental validation case proposed by [An et al., 2021]. The study employs a Goldak double-ellipsoid heat source with a relatively large heat source radius (around 800 μ m), an apparent specific heat capacity model for latent heat and a lumped mass matrix. The Abaqus simulation is constrained to time-steps of around 6.5μ s = $0.005T_{hs}$ to ensure convergence. The in-house implementation obtains speed-ups of 20-95 times with time-steps 1-5 times larger, respectively, with no loss of accuracy. The authors observe that, for the relatively coarse mesh sizes often used in the literature, the explicit scheme's stability limit is of the same order as the constraint (2).

¹² The authors note that softwares like Abaqus or LS-Dyna don't offer Forward Euler as an option

In light of their observation that “accurate modeling of PBF processes demands time step sizes close to that imposed by the explicit scheme” they conclude that Forward Euler is a highly advantageous choice. Furthermore, they demonstrate that the classical stability criterion based on the smallest element size is overly conservative and propose a practical alternative.

In their follow-up work [Essongue et al., 2024], the authors extend their analysis to DED. Due to the larger and slower moving heat source, the stability limit is lower compared to T_{hs} , and the authors report a speed-up of 2-4 times.

As mentioned Proell et al. [2024], previously introduced in section 2.2, Proell et al. [2024] combine a wide range of cost-saving strategies to develop a highly efficient high fidelity thermal simulation framework for LPBF for CPU-based architectures. Their implementation leaves no low-hanging fruit unpicked. The authors employ Forward Euler time integration during laser exposure steps and switch to Backward Euler for cooling phases. Reaffirming the findings of Essongue et al. [2022], they report that the Forward Euler stability constraint is 5-10 times more restrictive than (2) in their numerical examples. The authors not only circumvent the linear system solve, but also its assembly by using a matrix-free approach.

They note that on modern CPUs, the main performance bottleneck often lies in memory access rather than arithmetic operations. To mitigate this, Proell et al. employ several compiler-level optimizations, including instruction vectorization over batches of cells, to improve cache utilization and reduce memory latency. As described in section 2.2, the full capacity of their cluster is utilized in order to fully resolve the NIST AM-Bench 2022 cantilever benchmark. In their conclusions, the authors express plans to extend the framework to GPU architectures, with the goal of further improving performance and making the framework more widely available.

As discussed in section 2.2, many authors choose to exclude the powder bed from their LPBF simulations to reduce computational cost. Neiva et al. [2020] presents a framework for determining surrogate Robin/Dirichlet boundary conditions that approximate heat transfer between the solid and powder domains; this method is referred to as the *Virtual Domain Approximation* (VDA).

The 3D powder-bulk conduction problem is reduced to a 1D heat conduction problem orthogonal to the solid-powder interface. The coefficients of the surrogate BC are then determined through calibration against the “high-fidelity” model or experimental data.

The thermal model considered in Neiva et al. [2020] employs a lumped heat input and neglects latent heat effects; bulk and powder elements are preassigned during preprocessing. The model is validated against experimental data for builds on the centimeter scale, with simulations performed on a computing cluster using layer-by-layer deposition. It is reported that the VDA approach noticeably impacts accuracy while considerably reducing computational cost. The work also examines excluding the build plate but dismisses this option due to the excessive loss of accuracy.

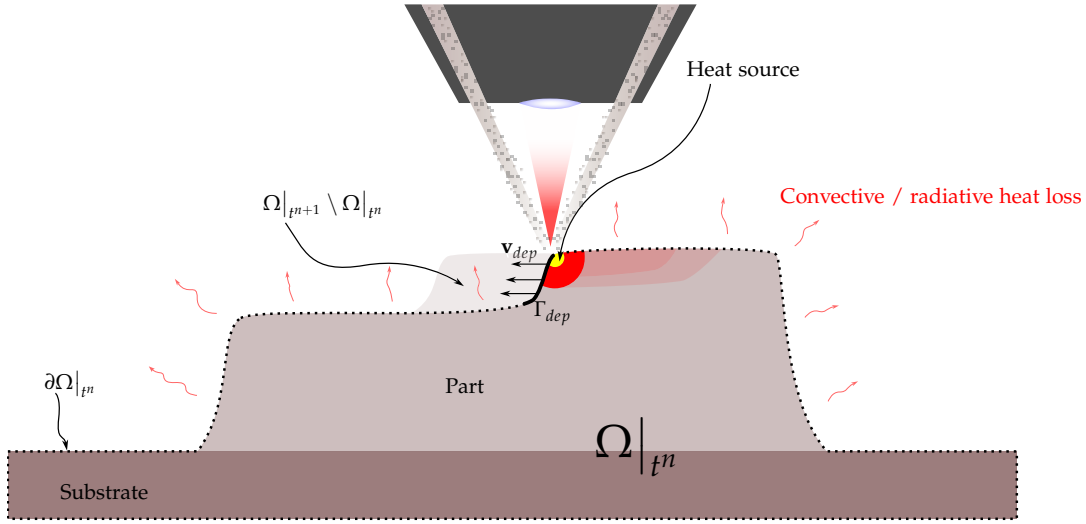


Figure 30: Schematic of **DED** process. The domain $\Omega(t)$ evolves in time due to the progressive addition of material at the deposition front Γ_{dep} . The boundary $\partial\Omega(t)$ exchanges heat with the environment and the heat source (laser or electron beam) provides localized volumetric heating.

3.1 THERMAL PROBLEM

Following the discussion in the previous chapter, it is clear that the energy balance is at the core of **MAM** modeling. The present section derives the heat equation in detail, using **DED** as a reference process. The same formulation applies to **LPBF**, but the continuous feed characteristic of **DED** requires a slightly more subtle treatment of domain growth than the discrete, layer-wise domain growth in **LPBF**.

Figure 30 shows a schematic of the **DED** process from a continuum mechanics perspective. Let $\Omega(t)$ denote a time-dependent control volume that encloses both the growing part and the substrate. Neglecting kinetic and potential energy, the conservation of energy for the material in $\Omega(t)$ reads

$$\frac{D}{Dt} \int_{\Omega(t)} \rho h = - \int_{\partial\Omega(t)} \mathbf{q} \cdot \hat{\mathbf{n}} + \int_{\Omega(t)} r + \int_{\Omega(t)} \dot{D}_{\text{mech}} \quad (5)$$

where h is the specific enthalpy, ρ the density, $\dot{D}_{\text{mech}}$ the mechanical dissipation, r the volumetric heat source, and $\mathbf{q}$ the heat loss through conduction, convection and radiation.

Applying the Reynolds transport theorem to account for the evolving domain results in

$$\frac{D}{Dt} \int_{\Omega(t)} \rho h = \int_{\Omega(t)} \partial_t (\rho h) + \int_{\partial\Omega(t)} \rho h (\mathbf{v}_{\text{mat}} - \mathbf{v}_{\text{dom}}) \cdot \hat{\mathbf{n}} \quad (6)$$

where $\mathbf{v}$ denotes speed, and the suffixes *mat* and *dom* correspond to *material* and *domain*, respectively. Because the material is stationary ($\mathbf{v}_{\text{mat}} = 0$), and the mass influx happens

The substrate undergoes significant heating and deformation; it is therefore necessary to include it in the computational domain (chapter 5).

at the deposition front Γ_{dep} , $\mathbf{v}_{dom} = \mathbf{v}_{dep} \mathbf{v}_{dom}|_{\Gamma_{dep}} = \mathbf{v}_{dep}$ while it is null elsewhere. The surface integral ~~reduces to in (6)~~ reduces to

$$\int_{\partial\Omega(t)} \rho h (\mathbf{v}_{mat} - \mathbf{v}_{dom}) \cdot \hat{\mathbf{n}} = -(\rho h) \Big|_{T_{dep}} \int_{\Gamma_{dep}} \mathbf{v}_{dep} \cdot \hat{\mathbf{n}} \quad (7)$$

where T_{dep} is the deposition temperature. ~~Substituting in:~~ it typically corresponds to the ambient temperature T_{env} or a prescribed preheating temperature. Substituting (6) and (7) into the energy balance (5) and neglecting both the mechanical dissipation and the slow variation of the density ($\partial_t \rho \approx 0$), the equation becomes

$$\int_{\Omega(t)} \rho \partial_t h = +(\rho h) \Big|_{T_{dep}} \int_{\Gamma_{dep}} \mathbf{v}_{dep} \cdot \hat{\mathbf{n}} - \int_{\partial\Omega(t)} (\mathbf{q}_{cond} + \mathbf{q}_{conv} + \mathbf{q}_{rad}) \cdot \hat{\mathbf{n}} + \int_{\Omega(t)} r \quad (8)$$

Using Fourier's law $\mathbf{q}_{cond} = -k \nabla T$ and expanding the enthalpy into $h = c_p T + L f_l$ (with c_p the specific heat capacity, L the latent heat of fusion and f_l the liquid fraction), one obtains the energy balance

$$\int_{\Omega(t)} \rho \partial_t (c_p T + L f_l) = +(\rho h) \Big|_{T_{dep}} \int_{\Gamma_{dep}} \mathbf{v}_{dep} \cdot \hat{\mathbf{n}} + \int_{\Omega(t)} k \Delta T + - \int_{\partial\Omega(t)} (\mathbf{q}_{conv} + \mathbf{q}_{rad}) \cdot \hat{\mathbf{n}} + \int_{\Omega(t)} r \quad (9)$$

where the divergence theorem was applied to the conductive term.

The convective and radiative boundary fluxes follow Newton's and Stefan-Boltzmann's laws, respectively:

$$\mathbf{q}_{conv} \cdot \hat{\mathbf{n}} = h_{conv} (T - T_{env}), \quad \mathbf{q}_{rad} \cdot \hat{\mathbf{n}} = \varepsilon \sigma (T^4 - T_{env}^4)$$

where h_{conv} is the convective Heat Transfer Coefficient (HTC), T_{env} the ambient temperature, ε the emissivity, and σ the Stefan-Boltzmann constant.

3.1.1 Strong form

~~After localization of eq. (9), the governing system defines a temperature field $T(\mathbf{x}, t) : \Omega(t) \times \mathbb{R}^+ \rightarrow \mathbb{R}$. Let t_{final} denote the end time of the simulation. To circumvent mathematical difficulties associated with taking temporal derivatives on previously nonexistent points, the extension functions $T_e : \bar{\Omega}(t_{final}) \times [0, t_{final}] \rightarrow \mathbb{R}$ and $f_{l,e}$ are defined as follows:~~

$$T_e(\mathbf{x}, t) = \begin{cases} T(\mathbf{x}, t) & \mathbf{x} \in \bar{\Omega}(t) \\ T_{dep} & \mathbf{x} \in \bar{\Omega}(t_{final}) \setminus \bar{\Omega}(t) \end{cases} \quad f_{l,e}(\mathbf{x}, t) = f_l(T_e(\mathbf{x}, t)) \quad (10)$$

~~so that T_e and $f_{l,e}$ coincide with T and f_l on $\Omega(t)$, while material that has not yet been deposited is mathematically present and held at T_{dep} .~~

~~The strong form of the thermal problem follows from localizing eq. (9)~~

$$\rho c_p \partial_t T_e + \rho L \partial_t f_{l,e} - k \Delta T = r(\mathbf{x}, t) \quad \forall \mathbf{x} \in \Omega(t) \quad (11)$$

$$-k \partial_n T = h_{conv} (T - T_{env}) + \varepsilon \sigma (T^4 - T_{env}^4) \quad \forall \mathbf{x} \in \partial\Omega(t) \quad (12)$$

$$T(\mathbf{x}, 0) = T_0 \quad \forall \mathbf{x} \in \Omega(0) \quad (13)$$

where $\partial_n = \hat{\mathbf{n}} \cdot \nabla$ and eq. (13) ~~specifies a constant~~ prescribes a uniform initial temperature T_0 , typically equal to T_{env} . The deposition energy is implicitly taken into account ~~in the growth condition ??~~. Numerically, when a new element joins the computational domain, it carries the energy of the deposited material. ~~Remark the limit from the left notation in ??, which indicates that new material is added at the~~

deposition temperature T_{dep} and heated immediately afterward: if point $\mathbf{x}_{new}$ was just added at time t , then $T(\mathbf{x}_{new}, t^-) = T_{dep}$ and $T(\mathbf{x}_{new}, t^+)$ results from the solution of the heat equation by the growth of the domain and the numerical activation of new elements in the computational mesh.

Mathematically, this introduces a discontinuity in the temperature field, which translates into The use of the extended fields T_e and $f_{l,e}$ ensures that time derivatives are well-defined for points that have just joined the domain. Mathematically, T_{dep} fulfills the role of an initial condition for newly deposited regions. Physically, however, the material never resides at T_{dep} : upon deposition, it is immediately exposed to the laser and the surrounding thermal field. Note that T_e exhibits a jump across the deposition front Γ_{dep} : Kollmannsberger and Kopp [2021] showed that this discontinuous behavior leads to slower convergence and numerical oscillations, as demonstrated by Kollmannsberger and Kopp [2021]. This discontinuity is arguably the main difference between and welding models. Compared to As discussed in chapter 7, LPBF models are closer to welding, as domain growth (recoating) occurs only at the end of each more closely resembles welding than DED, since domain growth occurs only once per layer during the cooling phase. Hence, the scanning of each layer is very much akin to welding LPBF layer is akin to a sequence of welding passes, whereas each DED pass involves continuous domain growth. This jump discontinuity is arguably the key distinction between MAM and welding models.

For clarity, the subscript e is omitted in the remainder of this manuscript.

3.1.2 Melting and latent-heat treatment

Liquid-solid phase change

The latent heat term in eq. (11) is negligible in DED compared to the heat source power [Chiumenti et al., 2017b], whereas in LPBF, the lower powers and higher scan speeds make its contribution non-negligible [Umantsev, 2023].

In theory, phase change is governed by the Stefan-Neumann problem. For an isothermal transition, the interface Γ_m between the solid and liquid phases satisfies

$$\begin{aligned} T(\mathbf{x}, t) &= T_m & \forall \mathbf{x} \in \Gamma_m \\ (k_1 \nabla T_1 - k_2 \nabla T_2) \cdot \hat{\mathbf{n}} &= L \rho v_n & \forall \mathbf{x} \in \Gamma_m \end{aligned} \quad (14)$$

with T_m the melting temperature and v_n the normal velocity of the interface. The numbered subscripts refer to the opposite sides of the interface. According to the classification of Hu and Argyropoulos [1996], methods that track Γ_m explicitly are termed *strong solutions*.

In practice, the computational cost of solving eq. (14) scales poorly at part-scale, and a common alternative is to incorporate the latent heat in the heat equation, as done in eq. (11). These are called *weak solutions*.

The first step is to express the liquid-fraction f_l as a function of temperature. For a pure material with isothermal phase change, $f_l(T) = H(T - T_m)$, where H is the Heaviside step function. For alloys, a smoother transition is required. Following Kollmannsberger et al. [2018], Kopp et al. [2022], a hyperbolic-tangent regularization can be employed

$$f_l(T) = \frac{1}{2} \left[\tanh \left(S \frac{2}{T_l - T_s} \left(T - \frac{T_s + T_l}{2} \right) \right) + 1 \right] \quad (15)$$

where T_s and T_l are the solidus and liquidus temperatures, respectively, and $S > 0$ is a dimensionless sharpness parameter. Figure 31 shows f_l together with its first and second derivatives for several values of S ; as S increases, the transition zone narrows and f_l approaches the step function, while retaining differentiability for numerical purposes. Thus, this regularization is also suitable for isothermal phase change.

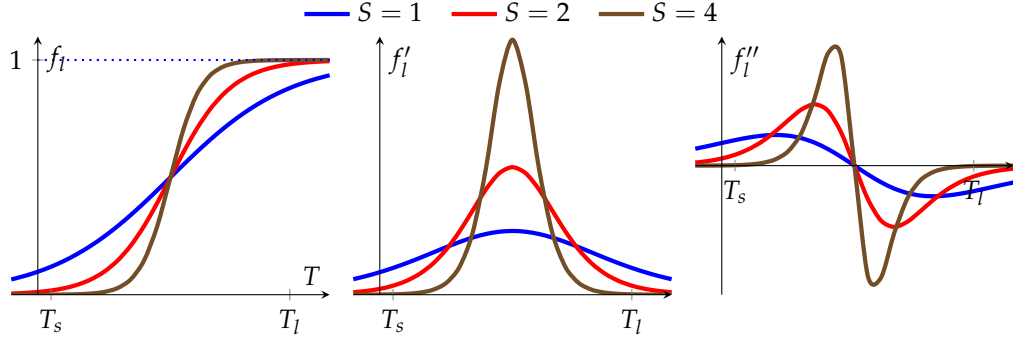


Figure 31: Liquid fraction and derivatives. The latter is used in section 4.2.

A widely used weak solution approach that requires no modifications to standard heat solvers is the *apparent heat capacity* method. Here, the latent heat term is absorbed into a temperature-dependent specific heat by applying the chain rule to the liquid fraction in eq. (11):

$$c_{app} = c_p + Lf'_l$$

so that the PDE simplifies to

$$\rho c_{app} \partial_t T - k \Delta T = r(\mathbf{x}, t)$$

This approach effectively incorporates latent heat into the thermal dependency of the specific heat. Since most solvers support temperature-dependent or piecewise-linear material properties, the latent heat can be modeled by adjusting the specific heat accordingly.

An alternative is the *enthalpy-based* method proposed by Celentano et al. [1994], in which a regularization of f_l is directly inserted into the heat equation (11) and derived with respect to time, so that the transient terms correspond to the time derivative of the enthalpy.

Celentano uses a piecewise linear approximation of the liquid fraction and discusses several strategies for approximating the Jacobian matrix. Kollmannsberger et al. [2018] replaces the piecewise linear approximation with a hyperbolic tangent interpolation, which is more suitable for a full Newton-Raphson strategy and an exact Jacobian computation.

The appendix of chapter 8 compares both methods on a model 1D melting problem with an analytical solution. The enthalpy-based method is found to be significantly more robust and will therefore be adopted in this work, specifically in chapter 8. The effect of latent heat is neglected in chapters 5 to 7.

Powder-bulk phase change

In LPBF simulations, the powder bed may either be included in [Hodge et al., 2014, Riedlbauer et al., 2014] or excluded from the computational domain [Chiumenti et al., 2017c, Denlinger et al., 2017, Neiva et al., 2020]. When excluded, heat loss through the surrounding powder is typically replaced by a surrogate, calibrated, convection-like BC (see chapter 6 or Neiva et al. [2020]).

When included, the powder is usually modeled as the same base material with a reduced thermal conductivity, as in chapters 7 and 8. Some authors even simulate the surrounding air [Kollmannsberger et al., 2018], although this remains uncommon.

The inclusion of powder needs to be accompanied by an irreversible powder-to-bulk phase change treatment. In practice, as for the liquid-solid phase change, the Stefan-Neumann problem is not solved explicitly and approximate methods are used instead.

Chapter 7 adopts an ad-hoc method: powder elements that intersect a bounding box around the deposited hatch (fig. 32a) are converted to the bulk material before the calculation step. In chapter 8, the approach of Kollmannsberger et al. [2018] is implemented, which combines (i) temperature-dependent material properties that make powder and bulk indistinguishable above the melting temperature, and (ii) a post-calculation step in which powder elements whose average temperature exceeds the melting point are converted to bulk (fig. 32b).

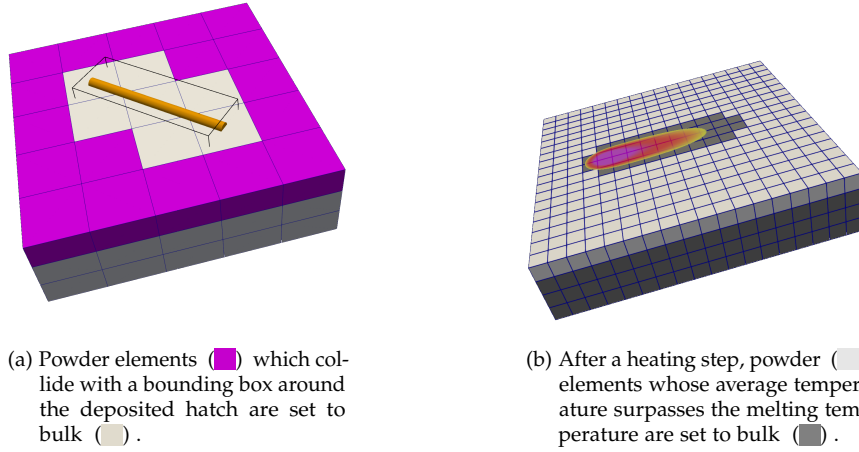


Figure 32: Powder bed melting methodologies employed respectively in chapters 7 and 8.

3.1.3 Volumetric heat source

As discussed in the previous chapter, early MAM models would adopt surface heating terms or directly impose a deposition temperature at the newly activated nodes. Nowadays, volumetric heating is standard practice in the literature.

There is a broad consensus in the literature that the heat source profile $r(x,t)$ is Gaussian-like. High-fidelity references in the DED literature generally use ellipsoidal or double-ellipsoidal Gaussian profiles, see fig. 33. The latter was developed based on the Goldak's observation that gradients obtained from the former profile are too flat ahead of the heat source and too steep behind it, hence the introduction of a shorter ellipsoid in the front and a longer one in the back. Since most heat sources are symmetric in practice, the Goldak profile is considered an artificial construct that attempts to capture the effect of the heat source's motion [Van Elsen et al., 2007]. This point will be revisited in chapters 4 and 7.

In LPBF, many authors augment the aforementioned profiles with an exponential decay in the depth direction, see eq. (1). As mentioned in the previous chapter, Gusarov et al. [2009] proposed an LPBF-specific profile that, although not widely adopted, is used by the LLNL team, see Hodge et al. [2014].

At the part-scale, however, the most common approach is to use a lumped heat source: this is the profile used in chapters 5 and 6, which tackle practical cases. The algorithm is detailed in Chiumenti et al. [2017b]: bounding boxes are defined around the hatches during each time interval $[t^n, t^n + \Delta t]$ and elements colliding these boxes (fig. 34a) are uniformly heated (fig. 34b).

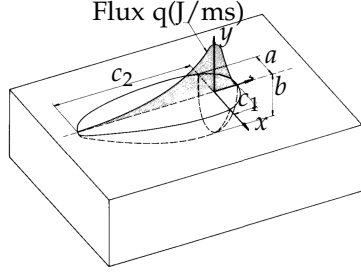


Figure 33: Double ellipsoidal profile [Goldak et al., 1984]. ξ is the welding direction.

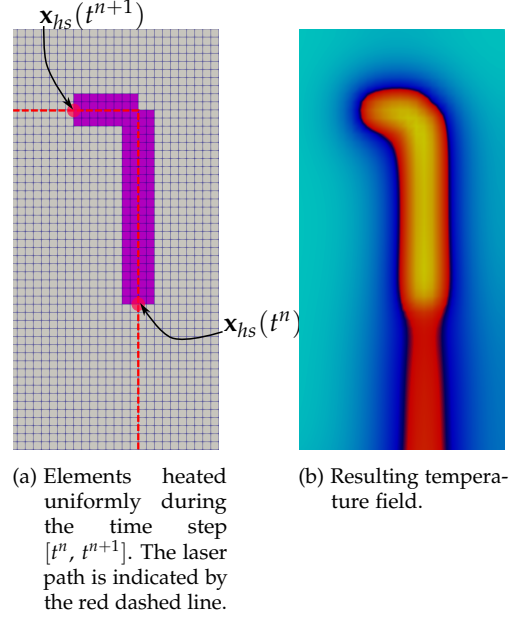


Figure 34: Schematic of a lumped heat source algorithm.

While chapters 5 and 6 focus on applied, part-scale studies and therefore employ a lumped heat source, chapters 7 and 8 aim to develop techniques for high-fidelity MAM modeling without sacrificing accuracy in the HAZ, for which lumped heat input is not suitable. Accordingly, Gaussian-like profiles are used in these works.

3.1.4 Weak form

The weak form of the heat equation eq. (11) is obtained by multiplying the PDE by an arbitrary test function $\phi \in V_T(t) = H^1(\Omega(t))$. After integrating over the computational domain $\Omega(t)$, applying integration by parts on the diffusion term and inserting BCs, the weak form reads

$$\begin{aligned} \int_{\Omega} \phi \rho (c_p \partial_t T + L \partial_t f_l) + \int_{\Omega} \nabla \phi \cdot (k \nabla T) &= \int_{\Omega} \phi r \\ \forall \phi \in V_T(t) &+ \int_{\partial\Omega} \phi \left(h_{\text{conv}} (T - T_{\text{env}}) + \varepsilon \sigma (T^4 - T_{\text{env}}^4) \right) \end{aligned} \quad (16)$$

3.2 MECHANICAL PROBLEM

3.2.1 Strong form

The mechanical problem is governed by Cauchy's first law of motion. As shown by Yang et al. [2016], inertial effects can be neglected in favor of the quasi-static assumption. The ensuing balance of momentum equation defines a boundary-value problem for the displacement field $\mathbf{u}_{(\mathbf{x},t)} : \Omega(t) \times \mathbb{R}^+ \rightarrow \mathbb{R}^3$

$$\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}) + \mathbf{b} = 0 \quad \forall \mathbf{x} \in \Omega(t) \quad (17)$$

where $\boldsymbol{\sigma}$ and $\mathbf{b}$ stand respectively for the Cauchy stress tensor and the body forces. $\boldsymbol{\sigma}$ is symmetric due to the balance of angular momentum.

To properly account for the nearly incompressible behavior of the material when melted, the problem is recast in a mixed $\mathbf{u}$ - p formulation. Let p denote the pressure and $\mathbf{s}$ the deviatoric stress tensor

$$\begin{aligned}\boldsymbol{\sigma} &= \mathbf{s} + p\mathbf{I} \\ p &= \frac{1}{3} \text{tr } \boldsymbol{\sigma}\end{aligned}\tag{18}$$

Note that $\mathbf{s}$ is symmetric and trace-free by construction. The decomposition (18) is substituted into eq. (17). Together with the continuity equation, this yields the mixed formulation

$$\nabla \cdot \mathbf{s} + \nabla p + \mathbf{b} = 0 \quad \forall \mathbf{x} \in \Omega(t) \tag{19}$$

$$(\nabla \cdot \mathbf{u} - \text{tr } \boldsymbol{\varepsilon}_{th}) - \frac{p}{K} = 0 \quad \forall \mathbf{x} \in \Omega(t) \tag{20}$$

with unknowns $\mathbf{u}$ and p . K and $\boldsymbol{\varepsilon}_{th}$ are the bulk modulus and the thermal strain tensor, respectively. The latter is the main driver of the problem and is defined as

$$\boldsymbol{\varepsilon}_{th}(T) = \left[\alpha(T) (T - T_{ref}) - \alpha(T_0) (T_0 - T_{ref}) \right] \mathbf{I} \tag{21}$$

where $\alpha(T)$ is the secant thermal expansion coefficient, T_0 is the initial temperature and T_{ref} is the strain-free reference temperature. Heating and cooling generate thermal strains. External and internal mechanical constraints restrict these deformations, giving rise to elastic strains and, consequently, to stresses.

The problem statement is complemented by Dirichlet and Neumann BCs

$$\begin{aligned}\mathbf{u}(\mathbf{x}, t) &= \mathbf{u}_d & \forall \mathbf{x} \in \partial\Omega_d \\ \boldsymbol{\sigma}(\mathbf{x}, t) \cdot \mathbf{n} &= \mathbf{t} & \forall \mathbf{x} \in \partial\Omega_n\end{aligned}$$

with $\partial\Omega_d \cup \partial\Omega_n = \partial\Omega$ and $\partial\Omega_d \cap \partial\Omega_n = \emptyset$. The Dirichlet and Neumann boundaries generally prescribe zero displacement and zero traction, respectively i.e. surfaces are either clamped or free.

Under the small strain assumption

$$\boldsymbol{\varepsilon} = \nabla^S \mathbf{u} := \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

where ∇^S is the symmetric gradient operator. The total strain is additively decomposed into elastic, inelastic (plastic or viscous), and thermal parts. Let T_{anneal} denote the annealing temperature introduced in chapter 2. Above this temperature, the material is assumed to behave like a liquid, and thus cannot store elastic energy. Accordingly, the yield stress is approximately zero for $T \geq T_{\text{anneal}}$, and the total strain reads

$$\boldsymbol{\varepsilon} = \begin{cases} \boldsymbol{\varepsilon}_{el} + \boldsymbol{\varepsilon}_{vp} + \boldsymbol{\varepsilon}_{th} & \text{for } T < T_{\text{anneal}} \\ \boldsymbol{\varepsilon}_{vp} + \boldsymbol{\varepsilon}_{th} & \text{for } T \geq T_{\text{anneal}} \end{cases} \tag{22}$$

To close eq. (19), constitutive laws relate the Cauchy stress $\boldsymbol{\sigma}$ to $\mathbf{u}$.

3.2.2 Constitutive laws

Hooke's law relates the elastic strain to the total stress tensor

$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}_{el} \tag{23}$$

where $\mathbf{C}$ is the fourth-order stiffness tensor. For isotropic materials, it is determined by two scalar parameters, usually the Young modulus E and the Poisson ratio ν , which

govern the material's stiffness and lateral expansion/contraction, respectively. Both parameters are considered temperature-dependent: in the liquid state, the material loses stiffness ($E \rightarrow 0$) and approaches the incompressible limit ($\nu \rightarrow 0.5$). In chapters 5 and 6, ν is capped at 0.43 to avoid volumetric locking [Chiumenti et al., 2021].

The bulk and shear moduli, K and G , are related to E and ν by

$$K = \frac{E}{3(1-2\nu)} \quad G = \frac{E}{2(1+\nu)}$$

COMET, the software employed in chapters 5 and 6, adopts this convention.

They dictate the material's resistance to volumetric and shear deformation, respectively. K and G may be used instead of E and ν as independent parameters.

Below the annealing temperature, the onset of viscoplastic flow is governed by a yield function Φ :

$$\Phi(\sigma, \text{hardening variables}, T) \begin{cases} \leq 0 & \text{elastic regime} \\ = 0 & \text{plastic/viscous regime} \\ > 0 & \text{inadmissible state} \end{cases}$$

In this work, the von Mises yield criterion with isotropic hardening is adopted

$$\Phi(\mathbf{s}, q_h, T) = \|\mathbf{s}\| - \sqrt{\frac{2}{3}} [\sigma_Y(T) - q_h] \quad (24)$$

where $\sigma_Y(T)$ is the temperature-dependent yield stress, $\|\mathbf{s}\| = \sqrt{\mathbf{s} : \mathbf{s}}$ is the Frobenius norm of the deviatoric stress tensor and q_h is the isotropic hardening stress

$$q_h(\xi, T) = -[\sigma_\infty(T) - \sigma_Y(T)] \left(1 - e^{-\delta(T)\xi}\right) - H(T)\xi$$

with ξ the hardening variable, $\sigma_\infty(T)$ the saturation stress, $\delta(T)$ the saturation exponent and $H(T)$ the linear hardening modulus. The evolution laws of the hardening variable ξ and the viscoplastic strain ε_{vp} are defined as follows

$$\begin{aligned} \dot{\varepsilon}_{vp} &= \dot{\gamma}^{vp} \mathbf{n} \\ \dot{\xi} &= \dot{\gamma}^{vp} \frac{\partial \Phi}{\partial q_h} = \sqrt{\frac{2}{3}} \dot{\gamma}^{vp} \\ \mathbf{n} &:= \frac{\partial \Phi}{\partial \mathbf{s}} = \frac{\mathbf{s}}{\|\mathbf{s}\|} \\ \dot{\gamma}^{vp} &:= \left\langle \frac{\Phi}{\eta(T)} \right\rangle^{\frac{1}{m(T)}} \end{aligned}$$

where $\mathbf{n}$ is the outward normal to the yield surface, $\dot{\gamma}^{vp}$ is the viscoplastic multiplier, η is the plastic viscosity, $\langle \cdot \rangle$ denotes the Macauley brackets and m is a rate sensitivity parameter.

3.2.3 Weak form

Similarly to the thermal problem, the weak form of the mechanical problem is obtained by multiplying the strong forms (19) by arbitrary test functions $\delta \mathbf{u} \in V_u(t)$ and $\delta p \in V_p(t)$

$$\begin{aligned} V_u(t) &:= \{\delta \mathbf{w} \in H^1(\Omega(t))^3 \mid \delta \mathbf{w} = \mathbf{0} \text{ on } \partial\Omega_d\} \\ V_p(t) &:= \{\delta q \in L^2(\Omega(t))\} \end{aligned}$$

and integrating over the domain $\Omega(t)$

$$\begin{aligned} \int_{\Omega} \delta \mathbf{u} \cdot (\nabla \cdot \mathbf{s} + \nabla p + \mathbf{b}) &= 0 \quad \forall \delta \mathbf{u} \in V_u(t) \\ \int_{\Omega} \delta p \left(\nabla \cdot \mathbf{u} - \text{tr} \boldsymbol{\varepsilon}_{th} - \frac{p}{K} \right) &= 0 \quad \forall \delta p \in V_p(t) \end{aligned} \quad (25)$$

Integration by parts of the first term in (25) yields the weak form of the mechanical problem

$$\begin{aligned} \int_{\Omega} \nabla^S \delta \mathbf{u} : \mathbf{s} + \int_{\Omega} (\nabla \cdot \delta \mathbf{u}) p &= \int_{\partial \Omega_n} \delta \mathbf{u} \cdot \mathbf{t} + \int_{\Omega} \delta \mathbf{u} \cdot \mathbf{b} \quad \forall \delta \mathbf{u} \in V_u(t) \\ \int_{\Omega} \delta p \left(\nabla \cdot \mathbf{u} - \text{tr} \boldsymbol{\varepsilon}_{th} - \frac{p}{K} \right) &= 0 \quad \forall \delta p \in V_p(t) \end{aligned} \quad (26)$$

Because $\mathbf{s}$ is symmetric, $\nabla \delta \mathbf{u} : \mathbf{s} = \nabla^S \delta \mathbf{u} : \mathbf{s}$. Note that V_u and V_p must satisfy an inf-sup condition to ensure the stability of the mixed formulation [Codina, 2000].

Recall that the symmetric part of $\nabla \mathbf{u}$ corresponds to expansion and shear, while the antisymmetric part corresponds to rigid body rotation.

3.3 DISCRETIZATION

The governing equations eqs. (11) and (17) are solved numerically by discretizing the spatial and temporal domains with FEM and FDM, respectively. Throughout chapters 5 to 8, first-order hexahedral and tetrahedral elements are used together with Backward Euler time integration.

The time-step Δt varies depending on whether the laser is *on* or *off*. During scanning, Δt is chosen smaller than T_{hs} , ensuring that the heat source does not skip any element. This is in the order of milli- to micro-seconds in DED and LPBF, respectively, while cooling steps are generally in the order of seconds. Hence,

$$t^{n+1} = \sum_{i=0}^n \Delta t_i$$

where Δt_i is the time step at the i -th step.

3.3.1 Domain growth: birth-death method

At times t^n and t^{n+1} , the computational domain is represented by the meshes $\mathcal{T}(t^n)$ and $\mathcal{T}(t^{n+1})$, respectively. They differ by a few elements corresponding to the deposition. These are incorporated before each calculation step through the *birth-death method* [Roberts et al., 2009], explained below.

At each time step, an *active* mesh is defined by a subset of elements of a background mesh $\mathcal{T}_{bg}$ that covers the final extent of the computational domain: at time t^n , each element is either *active* or *inactive*, depending on whether it belongs to the current domain $\Omega(t^n)$. Only active elements contribute to the system assembly and solution. Consequently, the underlying linear algebra data structures are reallocated each time new elements are activated. These new elements are identified through a spatial search over the background mesh, and once activated, their nodal temperatures are initialized to the deposition temperature T_{dep} .

In high-fidelity DED models, elements to be activated are identified via collision detection: Oriented Bounding Boxes (OBBs) are defined along the laser path during the time interval $[t^n, t^{n+1}]$, and elements colliding with these OBBs are activated. For 3D hexahedral elements, this may involve up to 15 projections along various testing planes [Moreira et al., 2022]. To reduce computational cost, a preliminary broad-phase search is performed to discard elements that are too far from the laser path, and only potential collisions are tested in detail in the subsequent narrow-phase.

A decade ago, repeated reallocation of the global matrices was considered a drawback of the birth-death method in comparison to the quiet element method [Michaleris, 2014]. Nowadays, with the widespread adoption of AMR, frequent reallocations are standard and no longer a significant concern. Moreover, the quiet element method requires special treatment of plastic strains to avoid spurious stresses [Lindgren and Hedblom, 2001].

The broad-phase generally relies on hierarchical space partitioning, and concretely, bounding box trees. Elements correspond to the leaves of the tree data structure, and each parent node corresponds to a bounding box that contains all its children. For each element, collision tests are performed top-down, starting from the root node. If a parent node does not collide with an element, all its children can be discarded.

The spatial search is comparatively simpler in LPBF models. Since entire powder layers are activated simultaneously during recoating steps, all elements lying below the current build height are activated. Naturally, a broad-phase search can still be used to accelerate the process.

3.3.2 Discretized problem

Let $V_{h,T}^{n+1}$, $V_{h,u}^{n+1}$ and $V_{h,p}^{n+1}$ be the FE spaces of the temperature, displacement and pressure fields, respectively, with

$$\{\phi_{i,T}\}, \{\phi_{i,u}\}, \{\phi_{i,p}\} \quad i = 1, \dots, n_{adofs}$$

their corresponding sets of scalar shape functions, with n_{adofs} the number of active DOFs at time t^{n+1} . The FEM approximations of the temperature, displacement and pressure fields are given by linear combinations of the basis functions

$$T_h(\mathbf{x}, t^{n+1}) = \sum_{i=1}^{n_{adofs}} T_i(t^{n+1}) \phi_{i,T}(\mathbf{x}) \quad (27)$$

$$\mathbf{u}_h(\mathbf{x}, t^{n+1}) = \sum_{i=1}^{n_{adofs}} \mathbf{u}_i(t^{n+1}) \phi_{i,u}(\mathbf{x}) \quad (28)$$

$$p_h(\mathbf{x}, t^{n+1}) = \sum_{i=1}^{n_{adofs}} p_i(t^{n+1}) \phi_{i,p}(\mathbf{x}) \quad (29)$$

Let the superscript n denote evaluation at time t^n . After inserting T_h into the weak form (16) and approximating the time derivative with Backward Euler time integration, the discretized residual weak form of the thermal problem defines an integral equation whose root is the solution $T_h^{n+1} \in V_{h,T}^{n+1}$:

$$\begin{aligned} \mathcal{R}^{n+1} = & \int_{\Omega(t)} \phi_{i,T} \rho \overbrace{\left(c_p \frac{T_h^{n+1} - T_h^n}{\Delta t} + L \frac{f_l(T_h^{n+1}) - f_l(T_h^n)}{\Delta t} \right)}^{\text{enthalpy } h} \\ & + \int_{\Omega(t)} \nabla \phi_{i,T} \cdot (k \nabla T_h^{n+1}) - \int_{\Omega(t)} \phi_{i,T} r^{n+1} \\ & - \int_{\partial\Omega(t)} \phi_{i,T} \left(h_{\text{conv}} (T_h^{n+1} - T_{\text{env}}) + \varepsilon \sigma (T_h^{n+1,4} - T_{\text{env}}^4) \right) = 0 \quad \forall \phi_{i,T} \in V_{h,T}^{n+1} \end{aligned}$$

The root-finding problem can be solved using Picard or Newton-Raphson iterations. In chapters 5 and 6, it is solved with the former. Chapter 7 considers a linear system, which can be solved directly. Chapter 8 uses Newton-Raphson, which is more suitable when considering the latent heat term.

A Newton-Raphson iteration is performed as follows: given a current guess $T_h^{n+1,k} \in V_{h,T}^{n+1}$, find $\delta T \in V_{h,T}^{n+1}$ such that

$$\left. \frac{\partial \mathcal{R}^{n+1}}{\partial T_h^{n+1}} \right|_{T_h^{n+1,k}} \delta T = -\mathcal{R}^{n+1}(T_h^{n+1,k})$$

The solution is updated as $T_h^{n+1,k+1} \leftarrow T_h^{n+1,k} + \delta T$ until convergence is reached when either the residual norm is small or the norm of the increment is small.

The discretization procedure above applies to the thermal problem. For the mechanical problem, a similar finite element discretization is employed at each time level t^{n+1} . After solving the thermal problem, the temperature field T_h^{n+1} is used to compute the thermal strain ε_{th} , resulting in one-way coupling, and the quasi-static mechanical problem described in section 3.2 is solved. The detailed formulation of the mechanical problem is omitted here for brevity; the reader is referred to [Moreira \[2022\]](#).

Both cost-saving methods developed in this thesis (Chimera and substepping) share the same core idea of modifying the formulation of the thermal problem in the [HAZ](#) to achieve computational advantages. Consequently, an appropriate [DD](#) strategy is required to ensure consistent coupling of the resulting subproblems.

While these two methods differ in their specific [DD](#) strategies (same-mesh, multi-mesh), they rely on the same **transmission conditions** to enforce physical continuity between subdomains.

The first half of this chapter introduces classical non-overlapping [DD](#) to provide the necessary background to understand both the [DD](#) principles of chapters 7 and 8. The second half presents the Chimera method, which will later be used in both chapters 7 and 8.

4.1 BASICS OF NON-OVERLAPPING DOMAIN DECOMPOSITION

For the sake of simplicity, consider the linear heat equation with Dirichlet boundary conditions

$$\begin{cases} \partial_t T - \alpha \Delta T = r & \forall \mathbf{x} \in \Omega \\ T(\mathbf{x}, t) = T_d & \forall \mathbf{x} \in \partial\Omega_D \end{cases} \quad (30)$$

Let Ω_1 and Ω_2 be a non-overlapping decomposition of the domain $\Omega = \Omega_1 \sqcup \Omega_2$ such that

$$\overline{\Omega}_1 \cup \overline{\Omega}_2 = \overline{\Omega} \quad \Omega_1 \cap \Omega_2 = \emptyset \quad \Gamma = \partial\overline{\Omega}_1 \cap \partial\overline{\Omega}_2$$

where Γ is the interface between the two subdomains. Let χ_1 and χ_2 form a partition of unity

$$\begin{cases} \chi_i(\mathbf{x}) \geq 0, & \forall \mathbf{x} \in \overline{\Omega}_i \\ \chi_i(\mathbf{x}) = 0, & \forall \mathbf{x} \in \Omega \setminus \overline{\Omega}_i \\ \chi_1(\mathbf{x}) + \chi_2(\mathbf{x}) = 1, & \forall \mathbf{x} \in \Omega \end{cases}$$

A hybrid system of [PDEs](#) can be defined such that the solution T_i in each subdomain Ω_i satisfies

$$\begin{cases} \partial_t T_i - \alpha \Delta T_i = r & \forall \mathbf{x} \in \Omega_i \\ T_i(\mathbf{x}, t) = T_d & \forall \mathbf{x} \in \partial\Omega_{D,i} \\ \mathcal{I}_i(T_i, T_j) = 0 & \forall \mathbf{x} \in \Gamma, i \neq j \end{cases} \quad (31)$$

where $\mathcal{I}_i$ denotes a boundary operator which enforces Dirichlet, Neumann or Robin conditions on Γ . Then, a global solution T can be reconstructed as

$$T(\mathbf{x}, t) = \chi_1(\mathbf{x})T_1(\mathbf{x}, t) + \chi_2(\mathbf{x})T_2(\mathbf{x}, t)$$

The hybrid system is equivalent to the original problem provided the solutions are smooth enough and the *transmission conditions*

$$T_1 = T_2 \quad \forall \mathbf{x} \in \Gamma \quad (32)$$

$$k_1 \partial_n T_1 = k_2 \partial_n T_2 \quad \forall \mathbf{x} \in \Gamma \quad (33)$$

are satisfied [[Mathew, 2008](#)]. Equations (32) and (33) require the continuity of the solution and its normal flux, respectively. Both conditions are necessary to ensure

energy conservation across Γ . The normal direction in (33) corresponds to either $\hat{n}_1$ or $\hat{n}_2$.

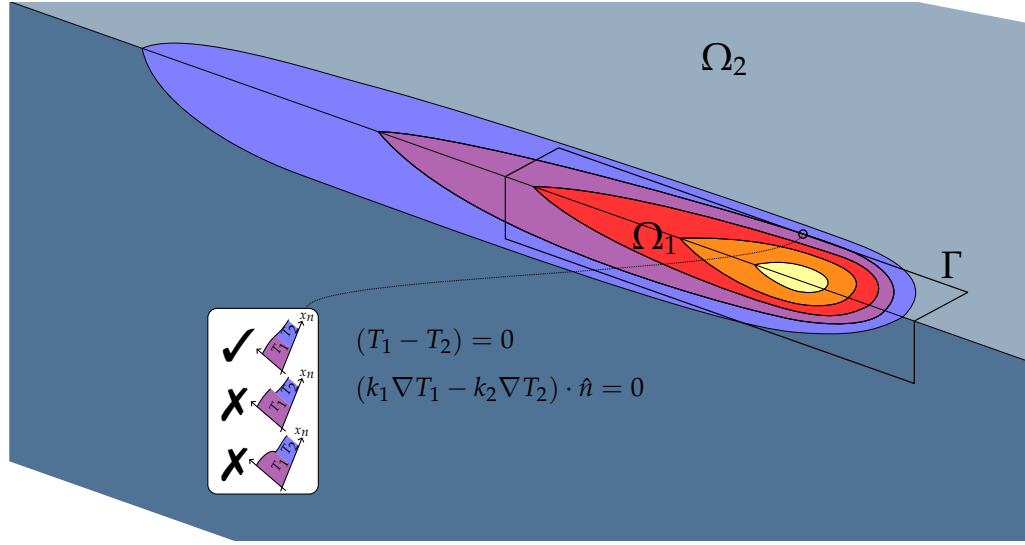


Figure 35: Non-overlapping DD schematic for a welding problem. Ω_1 and Ω_2 cover the HAZ and underlying substrate, respectively. Transmission conditions must be satisfied at the interface $\Gamma = \partial\Omega_1 \cap \partial\Omega_2$. Admissible and inadmissible transmission conditions are shown in the miniature plots, which represent temperature fields across Γ .

Figure 35 shows a non-overlapping decomposition $\Omega = \Omega_1 \sqcup \Omega_2$ for a moving heat source problem. Ω_1 covers the HAZ and Ω_2 the underlying substrate. The problem in Ω_1 can be reformulated: in chapter 7, it will be posed in the reference frame of the heat source, and, in chapter 8, it will be integrated with a finer time step.

Equations (32) and (33) must be satisfied at Γ . In terms of interface operators,

$$\begin{cases} \mathcal{I}_1(T_1, T_2) = 0 \\ \mathcal{I}_2(T_1, T_2) = 0 \end{cases} \iff \begin{cases} T_1 = T_2 \\ k_1 \partial_n T_1 = k_2 \partial_n T_2 \end{cases} \quad \forall \mathbf{x} \in \Gamma \quad (34)$$

Condition (34) renders the hybrid system mathematically equivalent to the original problem [Mathew, 2008]. Admissible and inadmissible temperature fields across Γ are shown in the miniature plots: jumps in the temperature or its normal flux across Γ are not allowed to ensure physical consistency. By linearly combining eqs. (32) and (33)

$$\begin{pmatrix} \mathcal{I}_1 \\ \mathcal{I}_2 \end{pmatrix} = \underbrace{\begin{pmatrix} \gamma_1 & \eta_1 \\ \gamma_2 & -\eta_2 \end{pmatrix}}_{\text{Coefficient matrix}^1} \begin{pmatrix} T_1 - T_2 \\ k_1 \partial_{n_1} T_1 - k_2 \partial_{n_1} T_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \forall \mathbf{x} \in \Gamma \quad (35)$$

one can construct valid pairs of local problems

$$\begin{cases} \rho c_p \partial_t T_1 - k \Delta T_1 = r & \text{in } \Omega_1 \\ T_1 = T_d & \text{in } \partial\Omega_{D,1} \\ \gamma_1 T_1 + \eta_1 k_1 \frac{\partial T_1}{\partial n_1} = \gamma_1 T_2 + \eta_1 k_2 \frac{\partial T_2}{\partial n_1} & \text{in } \Gamma \end{cases} \quad (36)$$

$$\begin{cases} \rho c_p \partial_t T_2 - k \Delta T_2 = r & \text{in } \Omega_2 \\ T_2 = T_d & \text{in } \partial\Omega_{D,2} \\ \gamma_2 T_2 + \eta_2 k_2 \frac{\partial T_2}{\partial n_2} = \gamma_2 T_2 + \eta_2 k_2 \frac{\partial T_2}{\partial n_2} & \text{in } \Gamma \end{cases} \quad (37)$$

as long as the coefficient matrix is invertible. In particular, the choices:

- $\gamma_1 = \eta_2 \neq 0$ and $\gamma_2 = \eta_1 = 0$ results in DN coupling.

¹ Typically, the η coefficients are set to 1, resulting in two Robin conditions, such that very low or very high γ values tend to Neumann and Dirichlet conditions, respectively.

- $\gamma_i \neq 0$ and $\eta_i \neq 0$ results in Robin-Robin (RR) coupling. Equal weights $\gamma_i = \eta_i \neq 0$ yield “standard” RR coupling.
- $\gamma_1 \neq 0, \eta_1 = 0, \gamma_2 \neq 0$ and $\eta_2 \neq 0$ results in Dirichlet-Robin coupling, [Cheng and Wagner, 2021, see].

Specific values of the coefficients can prove advantageous, as discussed later in this chapter.

4.1.1 Solution strategies: monolithic and staggered approaches

Once a pair of compatible local problems (36) and (37) has been defined, the coupled system must be solved. In the two subdomain case, one can either solve the two subproblems simultaneously as part of a single global system, or solve them sequentially and iteratively until convergence. The former is known as a **monolithic** approach, while the latter is known as a **staggered**/partitioned or partitioned approach.

To illustrate both approaches, consider the steady-state version of (30), which leads to a Poisson problem on $\Omega = \Omega_1 \sqcup \Omega_2$. After FEM discretization, the system of equations takes the form

$$\begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{1\Gamma_1} & \cdot & \cdot \\ \mathbf{A}_{\Gamma_1 1} & \mathbf{A}_{\Gamma_1 \Gamma_1} + \mathbf{R}_{11} & \cdot & \mathbf{R}_{12} \\ \cdot & \cdot & \mathbf{A}_{22} & \mathbf{A}_{2\Gamma_2} \\ \cdot & \mathbf{R}_{21} & \mathbf{A}_{\Gamma_2 2} & \mathbf{A}_{\Gamma_2 \Gamma_2} + \mathbf{R}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{T}_1 \\ \mathbf{T}_{\Gamma_1} \\ \mathbf{T}_2 \\ \mathbf{T}_{\Gamma_2} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_1 \\ \mathbf{F}_{\Gamma_1} \\ \mathbf{F}_2 \\ \mathbf{F}_{\Gamma_2} \end{pmatrix} \quad (38)$$

where the matrices $\mathbf{A}$, $\mathbf{R}$ and $\mathbf{F}$ correspond each to the following terms in the weak form:

$$\underbrace{\int_{\Omega_i} \nabla v_i \cdot k \nabla T_i}_{\mathbf{A}} - \underbrace{\int_{\Gamma} v_i \gamma_i T_i}_{\mathbf{R}_{ii}} = \underbrace{\int_{\Omega_i} r v_i}_{\mathbf{F}} - \underbrace{\int_{\Gamma} v_i (\gamma_i T_j + \eta_i k \partial_n T_j)}_{\mathbf{R}_{ij}}$$

Directly solving eq. (38) corresponds to the monolithic approach. In contrast, the staggered approach involves solving the local problems iteratively: at iteration $k+1$, the first subproblem is solved using interface data from the k -th iteration of the second subproblem

$$\begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{1\Gamma_1} \\ \mathbf{A}_{\Gamma_1 1} & \mathbf{A}_{\Gamma_1 \Gamma_1} + \mathbf{R}_{11} \end{pmatrix} \begin{pmatrix} \mathbf{T}_1^{k+1} \\ \mathbf{T}_{\Gamma_1}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_1 \\ \mathbf{F}_{\Gamma_1} - \mathbf{R}_{12} \mathbf{T}_{\Gamma_2}^k \end{pmatrix} \quad (39)$$

The newly computed interface value $\mathbf{T}_{\Gamma_1}^{k+1}$ is then used to solve the second subproblem

$$\begin{pmatrix} \mathbf{A}_{22} & \mathbf{A}_{2\Gamma_2} \\ \mathbf{A}_{\Gamma_2 2} & \mathbf{A}_{\Gamma_2 \Gamma_2} + \mathbf{R}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{T}_2^{k+1} \\ \mathbf{T}_{\Gamma_2}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_2 \\ \mathbf{F}_{\Gamma_2} - \mathbf{R}_{21} \mathbf{T}_{\Gamma_1}^{k+1} \end{pmatrix} \quad (40)$$

This variant of the staggered approach is known as *multiplicative/Gauss-Seidel*. In the *additive/Jacobi* counterpart, $\mathbf{T}_{\Gamma_1}^k$ is used instead of $\mathbf{T}_{\Gamma_1}^{k+1}$ in (40), that is, there is no intermediate update of the interface value. Jacobi iterations are more suitable for parallel computing: although they exhibit slower convergence than Gauss-Seidel iterations, the subproblems can be solved independently. In this manuscript, only the Gauss-Seidel variant is considered,

Staggered iterations are performed until changes in each local solution fall below a specified convergence threshold. Although a single staggered iteration is computationally cheaper than the monolithic solve, the total number of iterations ultimately determines the relative cost of the staggered versus monolithic approaches, and this is problem dependent. Additional considerations include

- Relative cost between assembly and solution of the linear systems: If assembly is significantly more expensive than solving, the monolithic approach will be more efficient.
- Localization of non-linearities within a single subdomain, which can favor the staggered method.
- Different PDEs may govern each subdomain (e.g., diffusion vs. advection-diffusion), making tailored solvers advantageous.

4.1.2 Staggered iterations: DN and RR coupling

The choice of interface conditions plays a crucial role in ensuring rapid convergence of staggered iterations. For instance, in the AM literature, [Cheng and Wagner \[2021\]](#) obtains convergence in a single iteration using an analytically derived Robin coefficient in their Dirichlet-Robin coupling. In the FSI literature, Dirichlet-Neumann coupling is often used, with the fluid subdomain receiving the Dirichlet condition and the solid subdomain receiving the Neumann condition.

However, it is well known that the unrelaxed version exhibits slow convergence, [[Yu et al., 2020](#), see]. Moreover, for advection problems, DN is not guaranteed to converge, without relaxation, as opposed to RR coupling, [[Canuto and Lo Giudice, 2019](#), see]. Contributions by [Gander and Halpern \[2007\]](#), [Chen et al. \[2014\]](#) propose optimized Robin coefficients to improve convergence of RR schemes.

In this section, the number of staggered iterations required for convergence of DN and RR schemes is compared using a simple example: a Poisson problem on the unit square, $\Omega =]0, 1[\times]0, 1[$, with a manufactured polynomial solution $T(x, y) = 1 - x^2 - y^2$. The two subdomains correspond to the right and left halves of the unit square:

$$\Omega_1 =]0.5, 1.0[\times]0, 1[\quad \Omega_2 =]0, 0.5[\times]0, 1[$$

The left and right subdomains are discretized using Q1 and P1 meshes, respectively, with 8 elements per side. Unit material properties are assumed: $\rho = 1$, $c_p = 1$, and $k = 1$. Following eq. (30), Dirichlet boundary conditions are applied on the external boundaries.

For all examples, a zero initial guess is used, i.e., $T_1^0 = T_2^0 = 0$. Staggered iterations are performed until the following convergence criterion is satisfied

$$\frac{\|T_{\Gamma_2}^{k+1} - T_{\Gamma_2}^k\|_2}{\|T_{\Gamma_2}^k\|_2} \leq 10^{-6}$$

First, DN coupling is presented. Left and right correspond respectively to the Neumann and Dirichlet subproblems. The first iteration is shown in detail in fig. 36, while iterations 5, 10, 15, and 20 are displayed in fig. 37.

Here, the DN coupling requires 49 iterations to converge. The error contours in figs. 36 and 37 show that the iterates oscillate around the exact solution, so that the error from one iteration to the next decreases in one subdomain and increases in the other.

To reduce the number of iterations, one can relax the Dirichlet condition:

$$T_1^{k+1} = (1 - \theta)T_2^k + \theta T_1^k$$

Using a constant relaxation coefficient of $\theta = 0.5$, the number of iterations required for convergence is reduced to 18. With a more sophisticated scheme, such as Aitken's method [[Aitken, 1926](#), [Yu et al., 2020](#)], convergence can be achieved in only 11 iterations.

RR coupling is now considered: fig. 38 shows the first iteration in detail using standard RR coupling. Figure 39 presents iterations 5 and 10; convergence is achieved in only 11 iterations.

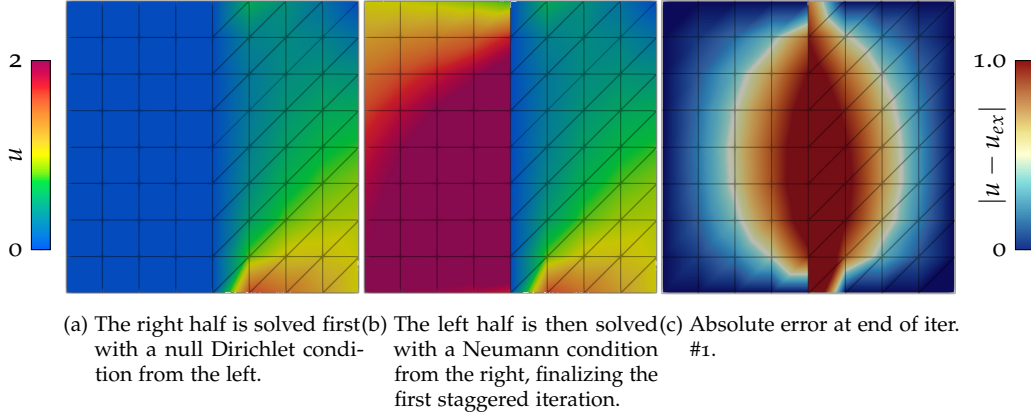


Figure 36: Steps of the first staggered DN iteration.

The Robin coefficients can be tuned in order to improve convergence. A relatively recent contribution by [Chen et al. \[2014\]](#) proposes an “optimal choice” of the Robin coefficients to achieve a convergence rate independent of the mesh size, namely $\gamma_1 = \mathcal{O}(1)$ and $\gamma_2 = \mathcal{O}(1/h)$, where h is the mesh size. The reference also recommends relaxing the Robin condition in the first subdomain

$$T_1^{k+1} + k_1 \partial_n T_1^{k+1} = (1 - \theta) \left(T_2^k + k_2 \partial_n T_2^{k+1} \right) + \theta \left(T_1^k + k_1 \partial_n T_1^k \right)$$

In this example, following the guidelines of [Chen et al. \[2014\]](#), $\gamma_1 = 1$, $\gamma_2 = 1/h$, and $\theta = 1/3$ are set. However, the number of iterations required for convergence is still 11.

The coefficient values proposed by [Gander and Halpern \[2007\]](#) work better in this case: convergence is achieved in 5 iterations with $\gamma_1 = \gamma_2 = 1/\sqrt{h}$ and no relaxation.

Table 2 shows the number of staggered iterations required for the aforementioned DN and RR variants for decreasing mesh sizes (the previously discussed results correspond to the second row). The unrelaxed DN scheme performs the worst, while RR coupling without tuning performs fairly well, as observed e.g. by [Canuto and Lo Giudice \[2019\]](#). Both methods tend to require more iterations as the mesh size decreases. DN with Aitken relaxation seems appears particularly robust to mesh refinement; however, in this case, RR with coefficients proposed by [Gander and Halpern \[2007\]](#) still outperforms it. Notably, the mesh independency predicted by [Chen et al. \[2014\]](#) is not observed here.

Mesh size	Dirichlet–Neumann			Robin–Robin		
	$\theta = 0.5$	Aitken [1926]		Gander and Halpern [2007]	Chen et al. [2014]	
1/4	24	16	10	7	4	8
1/8	49	18	11	8	5	11
1/16	99	21	11	10	6	13
1/32	197	19	11	14	7	15
1/64	394	21	11	18	9	16

Table 2: Number of staggered iterations required for DN and RR coupling schemes across mesh refinements.

Overall, these results illustrate the advantage of tuned RR coupling strategies over standard DN approaches in staggered iterations. The next section corroborates this finding with a more representative example.

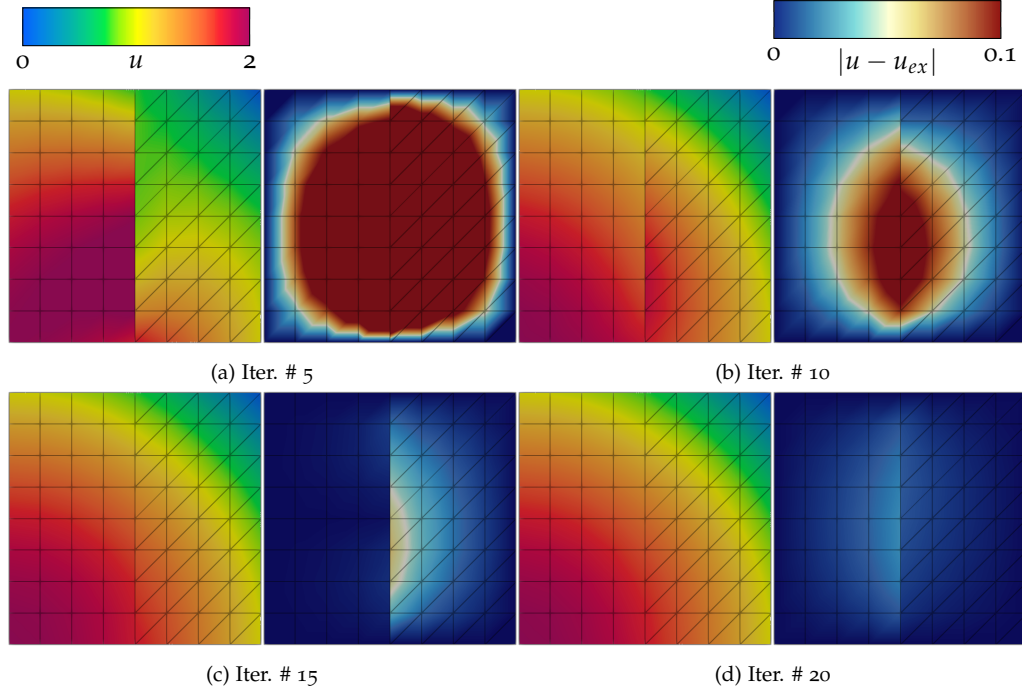


Figure 37: Staggered DN coupling example at iters. #5, 10, 15, and 20.

4.2 CHIMERA METHOD AND MOVING HEAT SOURCE

The term *Chimera* generally refers to DD approaches employing overlapping or overset grids, which may be in relative motion. In this thesis, the term is used more loosely to refer to *multi-mesh* methods, including the non-overlapping case.

In the authors' work, the Chimera method is employed as a means to an end. The goal is to solve the heat equation with a moving heat source whose HAZ represents only a small fraction of the domain. The problem is therefore decomposed into two subproblems: one defined in the HAZ and another in the remainder of the domain, and the Chimera method serves as a tool for coupling the resulting subproblems.

In particular, a moving mesh is attached to the heat source, allowing the problem in the HAZ to be posed in a reference frame where the heat source is stationary. This formulation makes the HAZ subproblem significantly steadier. Pros and cons of this approach are discussed in chapters 7 and 8.

The domain Ω is decomposed into two, possibly overlapping, open subdomains

$$\begin{aligned}\overline{\Omega} &= \overline{\Omega}_m(t) \cup \overline{\Omega}_f(t) & \Omega_m(t) \cap \Omega_f(t) &\neq \emptyset \\ \partial\Omega_m \cap \Omega &= \Gamma_m & \partial\Omega_f \cap \Omega &= \Gamma_f\end{aligned}$$

where the subscripts m and f stand for *moving* and *fixed*, respectively. The time dependence of the subdomains arises from the motion of Ω_m . Figure 40 shows a schematic illustration of the decomposition.

Let $\chi_m(\mathbf{x}, t)$ and $\chi_f(\mathbf{x}, t)$ be a partition of unity such that

$$T(\mathbf{x}, t) = \chi_m(\mathbf{x}, t)T^m(\boldsymbol{\xi}(\mathbf{x}), t) + \chi_f(\mathbf{x}, t)T^f(\mathbf{x}, t)$$

with $T^m : \Omega_m \rightarrow \mathbb{R}$ and $T^f : \Omega_f \rightarrow \mathbb{R}$ the temperature fields in the moving and fixed domains, respectively. In particular, on $\Omega_f \cap \Omega_m$, one can either set a linear combination of both functions or one of them as the solution.

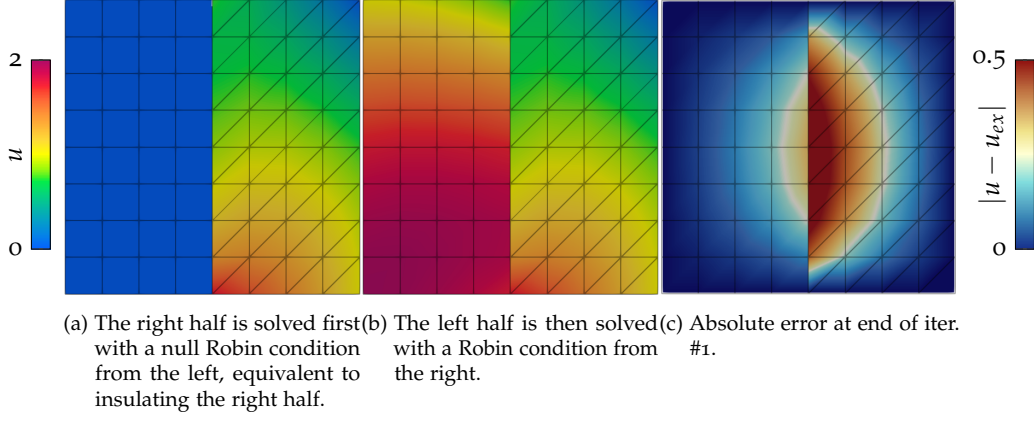


Figure 38: Steps of the first staggered RR iteration.

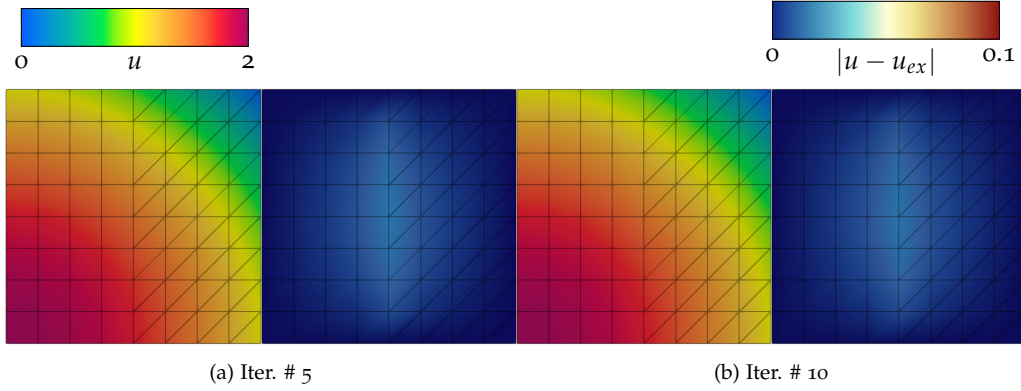


Figure 39: Staggered RR coupling example at iters. # 5 and 10.

The linear heat equation (30) remains unchanged in the fixed subdomain Ω_f , while a transformed version is posed in the moving subdomain Ω_m . Let $\mathbf{v} = \frac{d\mathbf{x}_{hs}}{dt}$, denote the speed of the heat source, where $\mathbf{x}_{hs}$ is its position. The change of reference frame is performed as follows:

$$(\mathbf{x}, t) \longrightarrow (\xi, \eta), \begin{cases} \xi = \mathbf{x} - \int_0^t \mathbf{v}(t) dt \\ \eta = t \end{cases} \implies \begin{cases} \partial_{x_i} = \partial_{\xi_i} \Rightarrow \nabla_{\mathbf{x}} = \nabla_{\xi} \\ \partial_t = \partial_{\eta} - v_i \partial_{\xi_i} = \partial_{\eta} - \mathbf{v}(t) \cdot \nabla_{\xi} \end{cases}$$

resulting in an extra advection term in the PDE governing the moving subdomain:

$$\rho c_p \left(\partial_t T^m(\xi, t) - \mathbf{v} \cdot \nabla T^m(\xi, t) \right) - \nabla \cdot (k \nabla T^m(\xi, t)) = r(\xi) \quad \xi \in \Omega_m \quad (41)$$

To connect T_f and T_m at their respective interfaces Γ_f and Γ_m , transmission conditions-based coupling is employed:

$$\gamma_m T_m + \eta_m k_m \partial_n T_m = \gamma_m T_f + \eta_m k_f \partial_n T_f \quad x \in \Gamma_m \quad (42)$$

$$\gamma_f T_f + \eta_f k_f \partial_n T_f = \gamma_f T_m + \eta_f k_m \partial_n T_m \quad x \in \Gamma_f \quad (43)$$

As discussed in section 4.1, these conditions are typically used in non-overlapping DD. However, Houzeaux [2002], Houzeaux and Codina [2003] demonstrated their validity in the presence of an overlap, which is often unavoidable in practice, as explained in chapter 7.

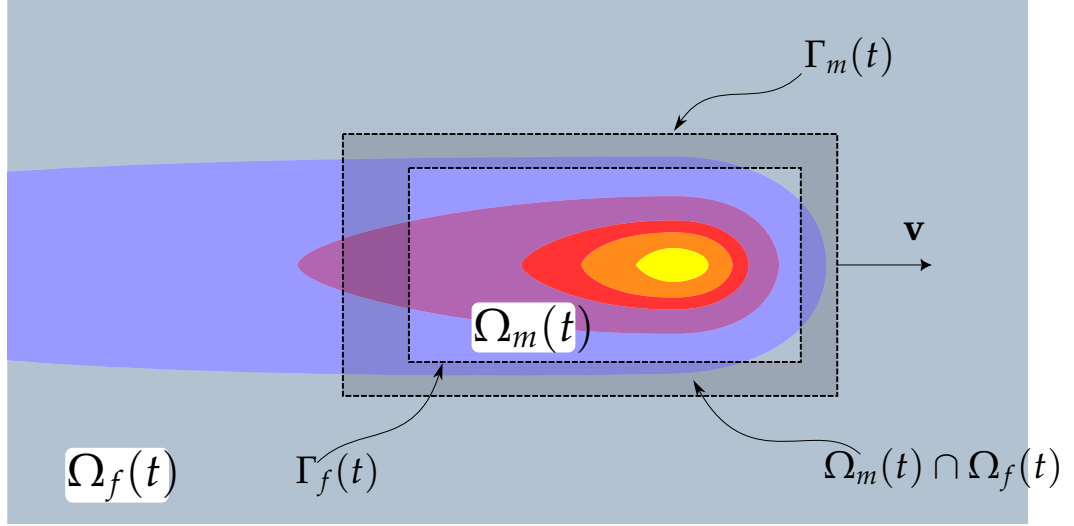


Figure 40: Schematic of Chimera approach illustrating overlapping subdomains $\Omega_m(t)$ and $\Omega_f(t)$.

Both subproblems are discretized using [FEM](#) and Backward Euler time integration. The weak forms of the local problems can be found in chapters 7 and 8, while details on the stabilization of the advection term are provided in the appendix of chapter 8. Using lumped mass matrices, the resulting monolithic system resembles (38).

$$\begin{pmatrix} \frac{\mathbf{M}_m}{\Delta t} + \mathbf{A}_{mm} & \mathbf{A}_{m\Gamma_m} & \cdot & \cdot \\ \mathbf{A}_{\Gamma_m m} & \frac{\mathbf{M}_{\Gamma_m}}{\Delta t} + \mathbf{A}_{\Gamma_m \Gamma_m} + \mathbf{R}_{mm} & \cdot & \mathbf{R}_{mf} \\ \cdot & \cdot & \frac{\mathbf{M}_f}{\Delta t} + \mathbf{A}_{ff} & \mathbf{A}_{f\Gamma_f} \\ \cdot & \mathbf{R}_{fm} & \mathbf{A}_{\Gamma_f f} & \frac{\mathbf{M}_{\Gamma_f}}{\Delta t} + \mathbf{A}_{\Gamma_f \Gamma_f} + \mathbf{R}_{ff} \end{pmatrix} \begin{pmatrix} \mathbf{T}_m \\ \mathbf{T}_{\Gamma_m} \\ \mathbf{T}_f \\ \mathbf{T}_{\Gamma_f} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_m \\ \mathbf{F}_{\Gamma_m} \\ \mathbf{F}_f \\ \mathbf{F}_{\Gamma_f} \end{pmatrix} \quad (44)$$

where $\mathbf{M}$, $\mathbf{A}$ and $\mathbf{F}$ correspond to the mass, stiffness and source terms, respectively, and $\mathbf{R}$ represents the interface conditions in (42) and (43). If either (42) or (43) is a Dirichlet condition, the corresponding row and column will be altered or removed according to the chosen method of enforcing the condition.

Note that the stiffness matrices of Ω_m include an advection term, making the system non-Symmetric Positive Definite (SPD), whereas the original formulation without the moving frame yields an SPD system. As mentioned in section 4.1.2, a staggered approach might be advantageous for isolating the SPD and non-SPD components. Specifically, at the $(k+1)$ -th iteration, one can, for instance, solve the moving subproblem first using data from the fixed subproblem at the k -th iteration

$$\begin{pmatrix} \frac{\mathbf{M}_m}{\Delta t} + \mathbf{A}_{mm} & \mathbf{A}_{m\Gamma_m} \\ \mathbf{A}_{\Gamma_m m} & \frac{\mathbf{M}_{\Gamma_m}}{\Delta t} + \mathbf{A}_{\Gamma_m \Gamma_m} + \mathbf{R}_{mm} \end{pmatrix} \begin{pmatrix} \mathbf{T}_m^{k+1} \\ \mathbf{T}_{\Gamma_m}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_m \\ \mathbf{F}_{\Gamma_m} - \mathbf{R}_{mf} \mathbf{T}_f^k \end{pmatrix} \quad (45)$$

then use the newly computed interface value to solve the fixed subproblem

$$\begin{pmatrix} \frac{\mathbf{M}_f}{\Delta t} + \mathbf{A}_{ff} & \mathbf{A}_{f\Gamma_f} \\ \mathbf{A}_{\Gamma_f f} & \frac{\mathbf{M}_{\Gamma_f}}{\Delta t} + \mathbf{A}_{\Gamma_f \Gamma_f} + \mathbf{R}_{ff} \end{pmatrix} \begin{pmatrix} \mathbf{T}_f^{k+1} \\ \mathbf{T}_{\Gamma_f}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_f \\ \mathbf{F}_{\Gamma_f} - \mathbf{R}_{fm} \mathbf{T}_m^{k+1} \end{pmatrix} \quad (46)$$

where (46), with appropriate treatment in the nonlinear case, is SPD, whereas (45) is not.

In order to evaluate whether the staggered approach is more efficient than the monolithic one, the former must converge in a few iterations at most. This evaluation is performed in the context of a welding problem involving a heat source moving straight ahead and heating a two-dimensional domain Ω . Figure 41 shows the temperature

field at $t = 17T_{hs}$ using monolithic [RR](#) coupling, and the parameters for the problem are summarized in table 3. Linear Ti-6Al-4V-type material properties are used.

The domain $\Omega = (-10R, 20R) \times (-4R, 4R)$ is a rectangular region with a heat source moving along the x -axis. The subdomain Ω_m surrounds the heat source and moves with it, while the fixed subdomain Ω_f remains stationary.

Both subdomains are discretized using separate Q1 meshes, and time integration is performed with the Backward Euler method. At each time-step, the mesh of Ω_m cuts a hole (*Chimera hole cutting*) in the mesh of Ω_f to produce the decomposition, as explained in more detail in chapter 7. Due to the chosen parameters, the decomposition happens to be non-overlapping: the mesh size h exactly divides the distance traveled by the heat source in one time-step: $v\Delta t \mid h$. As indicated in table 3, Δt starts at $0.5T_{hs}$ during the initial heating time-steps and increases to $2T_{hs}$ in the later time steps.

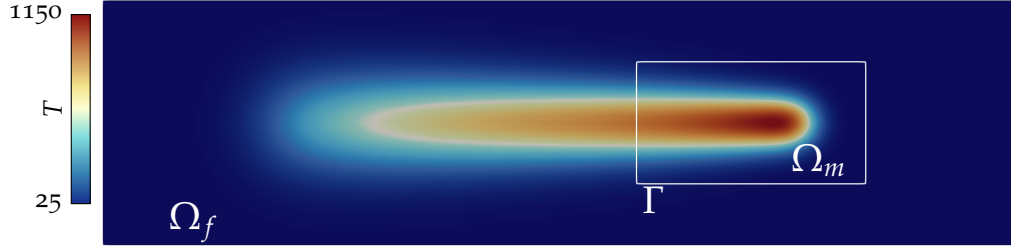


Figure 41: Temperature field and non-overlapping domain decomposition at $t = 17T_{hs}$ using monolithic [RR](#) coupling. The [HAZ](#) is represented by Ω_m , the fixed domain by Ω_f , and the interface by Γ .

Parameter	Value	Parameter	Value	Parameter	Value
ρ	4300 kg m^{-3}	Radius R	0.1 mm	Element size h	$\in [0.125 R, 0.5 R]$
c_p	$700 \text{ J kg}^{-1} \text{ K}^{-1}$	Speed	1 m s^{-1}	Δt	$\in [0.5 T_{hs}, 2 T_{hs}]$
k	$10 \text{ W m}^{-1} \text{ K}^{-1}$	Net power	500 W		
		$\mathbf{x}_{hs}(0)$	$(-4R, 0)$		

Table 3: Material properties, heat source parameters, and numerical settings for the welding example.

Mesh size	Dirichlet–Neumann		Robin–Robin		
	Aitken [1926]		Gander and Halpern [2007]	Chen et al. [2014]	
$0.5 R$	10-34	6-9	5-9	3-6	3-5
$0.25 R$	-	7-12	5-9	5-8	4-5
$0.125 R$	-	8-15	5-8	6-9	4-5

Table 4: Number of staggered iterations required for various coupling methods in the welding example with a moving heat source. The first and second numbers correspond to $\Delta t = 0.5T_{hs}$ and $\Delta t = 2T_{hs}$, respectively.

Table 4 summarizes the number of staggered iterations required for convergence of the [DN](#) and [RR](#) coupling schemes across various mesh sizes. The number of iterations generally increases with mesh refinement and larger time step sizes.

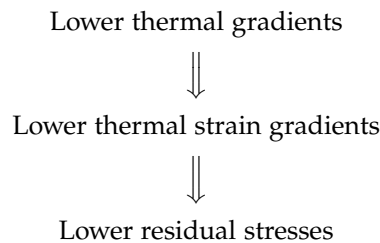
As expected, the unrelaxed [DN](#) coupling performs the worst: it already requires 34 iterations to converge with the coarsest mesh, and fails to converge for finer meshes. Adding Aitken relaxation significantly reduces the number of iterations, but even bare [RR](#) coupling outperforms it in this case. By setting $\gamma_1 = \gamma_2 = k/\sqrt{h}$, according to the recommendations of [Gander and Halpern \[2007\]](#), the number of iterations is further reduced. The lowest number of iterations is achieved by tuning around the values

proposed by [Chen et al. \[2014\]](#). $\gamma_1 = 1/2$, $\gamma_2 = k/h$ and $\theta = 0$ yield less than 5 iterations for all mesh sizes and time-steps.

In conclusion, staggered [RR](#) iterations perform best in this example, in comparison to other staggered coupling methods. However, monolithic coupling remains preferred in practice: as explained in chapters [7](#) and [8](#), the assembly of the system matrix is significantly more expensive than its solution for thermal problem. In this example, for the finest mesh size, the monolithic solve is only about two-thirds more expensive than a single staggered iteration on the author's machine, resulting in approximately twice the overall speed compared to the staggered approach once convergence is achieved. Hence, monolithic [DN](#) and [RR](#) couplings strategies are employed in chapters [7](#) and [8](#), respectively. Staggered iterations will be used in the next chapter.

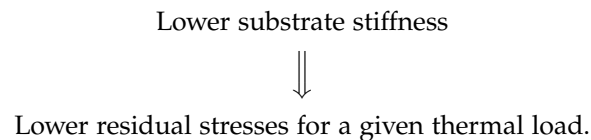
INTRODUCTION

This chapter investigates an alternative approach for residual stress mitigation in DED, based not on thermal management but on the mechanical response of the substrate. Most existing stress-control strategies to date rely on thermal management i.e. controlling the thermal field to reduce the Maximum Temperature Gradient (MTG) [Fu and Guo, 2014]:



Such thermal approaches are typically implemented by decreasing the power input, preheating the substrate or designing tailored scan strategies [Magana-Carranza et al., 2021, Sun et al., 2021, Wu et al., 2019]. While effective, these strategies often have drawbacks such as reduced productivity, or the alteration of other process outcomes, most notably the microstructure.

In contrast, this work explores a mechanical strategy. The underlying idea is that the substrate constrains the part's shrinkage, leading to stress accumulation near the part-substrate interface. By reducing the substrate's effective stiffness, the same thermal strains produce a lower mechanical response:



Previous studies investigated hollowed substrates [Jing et al., 2022, Lu et al., 2021], but these designs risk overheating due to the reduced thermal mass. Here, intermediate solutions are proposed in the form of grooves and slots in the upper portion of the substrate. This concept, referred to as *Smart-substrate*, aims to decouple residual stress mitigation from thermal management, thereby preserving the process window for microstructure control.

SUMMARY & CONCLUSIONS

The *Smart-substrate* concept was tested numerically and experimentally on parts of increasing complexity, from single walls to hollowed blocks. The results show that, while grooves were mildly effective, slotted substrates can significantly reduce residual stresses and warpage without altering the thermal field or microstructure. Contrarily, MTG-based methods inevitably couple stress mitigation with the thermal history and microstructural evolution.

Limitations remain: the reduction in the part's constraint promote warpage, which is detrimental to dimensional accuracy. Future works should explore the combination

of the *Smart-substrate* with geometric compensation techniques, and the application of the concept to more complex, possibly curvilinear, geometries.

From the perspective of this thesis, it is worth emphasizing that all thermo-mechanical simulations in this study remained computationally tractable, with wall clock times of only a few days for the most complex cases. This was achieved using uniform time-stepping at $\Delta t = 0.8T_{hs}$, reflecting the less pronounced multiscale nature of DED compared to LPBF (see chapter 6).

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Smart-substrate: a novel structural design to avert residual stress accretion in directed energy deposition additive manufacturing

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ABSTRACT

Residual stresses, related distortions and cracks are detrimental in metallic Additive Manufacturing (AM). Previously developed stress-control strategies based on reducing thermal gradients hardly diminish the stress concentrations at the built basement and easily affect other physical phenomena involved in AM. To overcome this, a novel strategy, named as Smart-Substrate, consisting of optimising the inner structure and local stiffness of the substrate is proposed to avert stress accretion and related part deformations. To demonstrate its advantages, a coupled thermomechanical finite element model for AM, experimentally calibrated with in-situ temperature and displacement measurements, is employed to analyse the thermal and mechanical behaviour of three groups of different structures with increasing geometrical complexity (single-wall, rectangular and block parts) fabricated by Directed Energy Deposit (DED) on the standard and smart substrates, respectively. Through using Smart-Substrate, the generation of residual stresses, especially the stress concentrations at the bottom corner of DED-builds being highly sensitive to cracks, and the induced deflections, are fundamentally throttled, and contrariwise for the standard substrate. More importantly, the use of Smart-Substrate is almost without prejudice to the temperature field, metallurgy and resulting mechanical hardness. This provides a possibility for addressing different physical problems individually, enlarging the AM process window.

ARTICLE HISTORY

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KEYWORDS

Additive manufacturing; structural design; residual stresses; multi-physics; thermomechanical simulation

1. Introduction

Metallic Additive Manufacturing (AM) is an advanced industrial technology to layer-by-layer fabricate complex parts and repair large components through using a focused high-energy heat source (e.g. laser, electron beam or arc) [1]. To date, several metallic AM techniques, like Directed Energy Deposition (DED) and Powder Bed Fusion (PBF), have been developed to meet the need of manufacturing a variety of products in industry [2,3]. Nevertheless, the AM process always is accompanied by high temperature gradients around the Heat Affected Zone (HAZ) as the printing proceeds. Due to the strong mechanical constraints from the cold substrate or previously deposited layers, the heated metal deposition cannot expand freely. As a consequence, residual stress are induced. Furthermore, the large number of heating and cooling cycles involved in the AM process exacerbates the accretion of residual

stresses in AM-parts [4,5]. Once the magnitude of these stresses reaches the yield strength of the printed materials, plastic deformations or even cracks develop to release them [6,7]. Such defects easily cause the failure of 3D printing and significantly deteriorate the mechanical properties and performance of AM-parts.

To avert stress accretion during the deposition process, many strategies based on the principle of lowering the Maximum Temperature Gradient (MTG) have been developed, such as optimising AM variables and scanning patterns, and preheating substrate before or during AM process [8–11]. Nevertheless, their effectiveness is fairly limited due to the use of a high-energy heat source in metallic AM, which directly causes high MTG. In detail, the optimisation of processing parameters and printing path certainly narrows the process window of metallic AM, especially considered concurrently defect avoidance and microstructure design. Although

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This article has been corrected with minor changes. These changes do not impact the academic content of the article.

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preheating substrate can lower MTG and induced residual stresses, a higher preheating temperature easily leads to remarkable heat accumulation, which may accelerate the formation of harmful phases and microstructural coarsening, deteriorating the mechanical properties of AM deposits [2,12]. In addition, the minimisation of residual stresses in AM-builds can also be achieved by adopting auxiliary equipment (e.g. rolling) [13] or by post-process heat and mechanical treatments (e.g. high-temperature annealing or laser shock peening) [14–16]. However, these substantially increase both manufacturing cost and time and fail to rectify distortions and cracks induced by large residual stresses before being released. Therefore, the critical objective of this work is to seek an optimal solution to prevent stress accretion and related part deformations during the AM printing process but without prejudice to other physical processes (e.g. thermal field and metallurgy).

Residual stresses and part distortions essentially are mechanical outcomes from the repeated heating–cooling cycles during AM. Hence, more attention needs to be paid to the structure and stiffness of the components involved in AM because they markedly influence the mechanical response of the built parts.

For clarity, the formation mechanism of residual stresses during AM is visualised using a typical bar model including a central bar and two lateral bars with the same lengths [17], corresponding to the HAZ and the substrate in AM, respectively, as shown in Figure 1(a). The yielding of the middle bar in the thermal cycle is determined by the yield temperature, $T_Y = \left(\frac{S_{dep}}{S_{sub}} + 1 \right) \frac{\sigma_Y}{\alpha \cdot E}$ where the physical significance of the included terms is present in Figure 1(a) and more details can be found in [17]. When the central

bar experiences thermal cycling, its mechanical response (e.g. stress evolution) closely depends on the maximum heating temperature, T_{max} , responsible for MTG. In detail, three cases are involved and shown in Figure 1(b): (i) When $T_{max} \leq T_Y$ (along loading path OAO), no residual stresses develop; (ii) When $T_Y < T_{max} < 2T_Y$ (along path OABC), the residual stresses increase to the magnitude of the line segment |OC|; and (iii) When $2T_Y \leq T_{max}$ (along path OABDEF), the residual stresses rise to the yield stress. From this bar model, two core factors responsible for the stress generations in AM can be summarised: (i) MTG and (ii) yield temperature, T_Y . In the AM community, the former is well known, but this is not the case with the latter, related to the mechanical constraints during thermal deformations. As mentioned above, reducing MTG is very challenging, but it is possible to minimise residual stresses by increasing T_Y through adjusting S_{dep} and S_{sub} (Figure 1(b)), which correspond to the sizes of HAZ and substrate in AM, respectively. Typically, S_{dep} is very small and almost fixed, while it is feasible to decrease S_{sub} by substrate design to elevate T_Y .

Recently, some researchers [18,19] attempted using hollow substrate structures with some strip holes to control residual stresses in DED-parts. The results showed that the residual stress can be minimised by lowering the substrate stiffness. Yet, using such hollow substrates probably causes overheating due to the poor heat dissipation through the hollow structures, and negatively impact the metallurgical evolution as well as the performance of the final part [20,21]. To address this challenge, this work is focused on designing an optimal internal structure for the substrate to avoid the accretion of both residual stresses and deflections as well as heat accumulation in AM-parts, as shown in Figure 1(c). When adopting thick

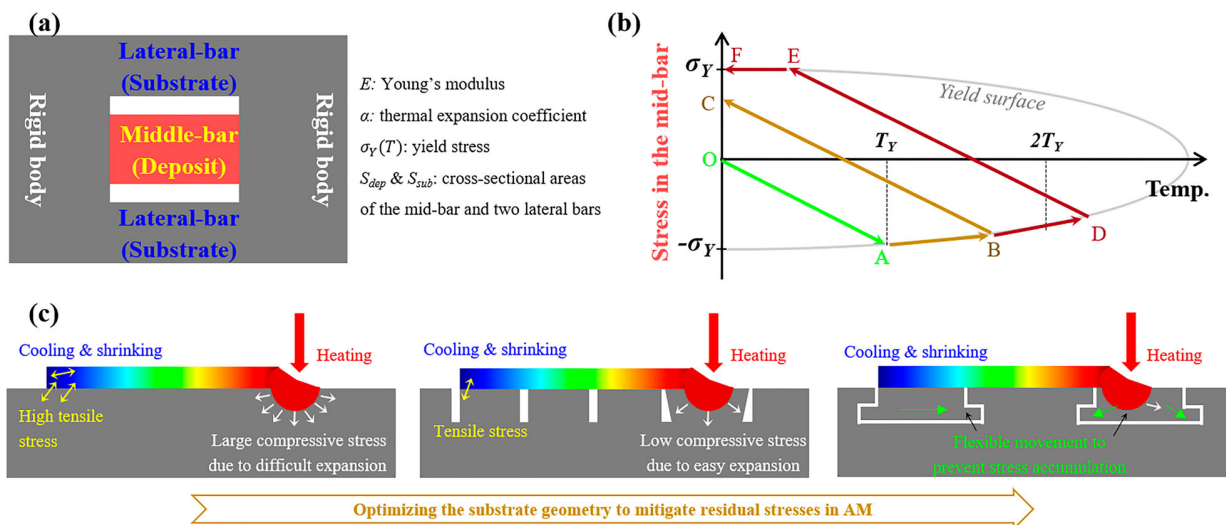


Figure 1. Residual stress formation in AM: (a) three bar model; (b) thermo-mechanical response of the central bar during thermal cycling; (c) residual stress control through the potential structural optimisation of the thick substrates.

substrates (e.g. > 10 mm) with a large horizontal cross-section, high tensile stresses and potential cracks are easily developed because of the strong mechanical constraint from the substrate even though it beneficially prevents part warpages [22–24]. Alternatively, if the local structural stiffness of the substrate is lowered by adding grooves or setting movable components in the base plate to reduce S_{sub} (see Figure 1(c)), T_Y is dramatically elevated. In this case, the stress accretion and the potential plastic strains transformed from the thermal deformations can be efficiently avoided because the metal deposition is allowed to freely expand/contract in an enlarged elastic range during thermal cycles in AM. Favourably, this small change in the structure of the substrate hardly affects the heat conduction from the build to the substrate and workbench. In this work, such modified substrate is named as ‘Smart-Substrate’, as it can automatically defuse thermal stresses induced by the AM process while cutting down the risk of overheating. Smart-substrate is intended as a new concept to enhance AM technology, particularly DED. The main advantage is the self-adjustable stiffness of the proposed substrate design to mitigate the residual stresses independently of AM-build. Thus, the proposed idea resembles the definition of smart materials [25,26].

To this end, a coupled thermo-mechanical Finite Element (FE) model for AM firstly is calibrated with in-situ experimental measurements from three groups of geometries: single-walls, rectangular and block parts fabricated by DED. Next, the validated model is used to study the influence of different substrate designs on the thermo-mechanical response. Finally, the advantage of the proposed Smart-Substrate approach is shown and its potential effect on the thermal evolution, metallurgy and mechanical hardness is also discussed.

2. Materials and experimental procedure

2.1. Laser-based DED process

Three sets of samples consisting of three single-walls, two rectangular structures and two blocks are additively manufactured by DED technique on seven annealed Ti6Al4 V substrates with a thickness of 11 mm, respectively, as shown in Figure 2. Noticeably, the design concept for the substrate structure is based on the thermo-mechanics in AM, which has been illustrated based on Figure 1 above. For the single-wall structures, three different substrates are used: a standard plate, and two plates with vertical grooves and with moveable trapezoidal tenons, corresponding to Wall-1, Wall-2 and Wall-3, respectively. For the rectangular geometries, two types of substrates are included: the standard one for Rectangle-1 and the plate with two moveable trapezoidal chunks for Rectangle-2. Similarly, a standard

substrate and a modified plate assembled by several small tenons are used to build the Block-1 and Block-2 DED parts, respectively (see Figure 2). In detail, Figure 3 displays the design of the Smart-Substrate for building the block parts. Different from the standard substrate, the Smart-Substrate consists of two parts: (i) the basic structural framework and (ii) 16 separate and movable tenons inserted in the substrate framework. It can be seen from Figure 3(a) that the AM deposition region is composed of one central square table surrounded by 8 movable tenons; thereby, only the central small table may provide strong mechanical constraint to the AM-build, while the neighbouring tenons can flexibly adjust in the designed tip clearance to the expansion or shrinkage of the deposited layers during the AM process.

All the cutting patterns within the modified substrates are carried out by the electric discharge machining with a wire diameter of 0.25 mm. In addition, the movement of the tenons inserted in the substrate, driven by the thermal deformations induced by the DED process, just happens in the designed tip clearance (e.g. 0.25 mm).

The used DED machine is equipped with an *IPG YLS-10000-S2 T* ytterbium fibre laser with a wavelength of 1070 ± 5 nm and a maximum power of 10 kW, a five-axis numerical control workbench, a DPSF-2 high-accuracy adjustable automatic power feeder system, and an argon purged fabricating chamber with very low oxygen content (<0.8%). The metal powder used in this work is spherical Ti6Al4 V powder with a diameter range of 53~325 μm and low oxygen content. The powder is produced by a plasma electrode process and dried in a vacuum oven at 130°C for 2 h before AM.

A reciprocating scan strategy is used to build the single-walls, while two kinds of scan patterns defined by 4 different sequences repeated every 4-layers are adopted for the fabrication of the rectangular and block parts, respectively, as shown in Figure 4. Table 1 lists the process parameters used for the DED process and the corresponding size of the deposited workpieces shown in Figure 2.

A chemical solution composed of 1 ml HF, 3 ml HNO₃ and 46 ml H₂O is used as etching agent and the observation of the deposited microstructures is performed by optical microscopy. In addition, the Vickers hardness of the as-built block samples is tested; fifteen different points are selected to measure in each building position. The hardness tests are carried out with a load of 500 g and a load time of 15 s.

2.2. In-situ thermomechanical measurements

To acquire the in-situ measurements in terms of temperatures and displacements during DED process, one

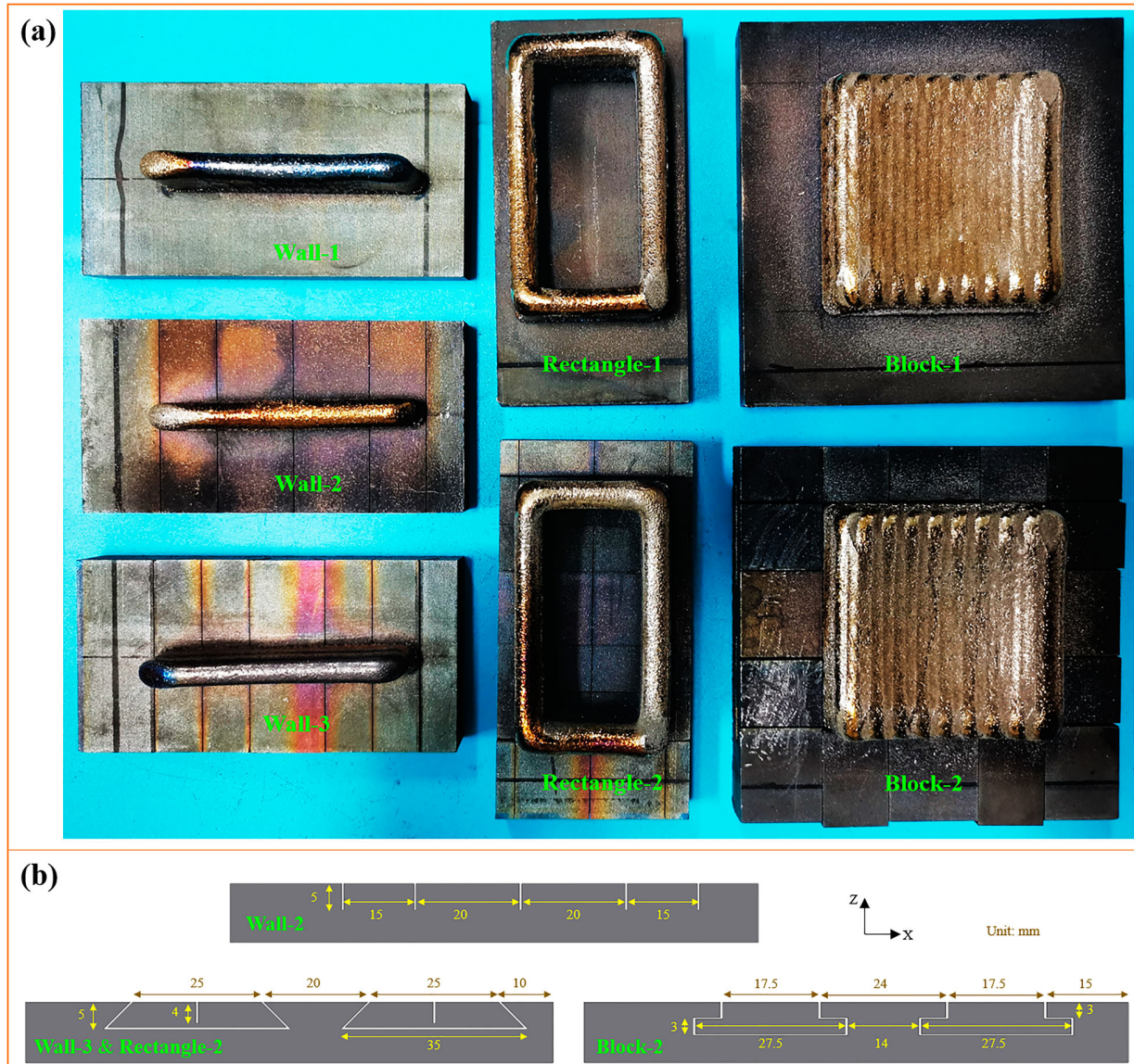


Figure 2. (a) Single-wall, rectangular and block parts printed on different substrates; (b) The sized details of the modified substrates with grooves or including several moveable components.

end of the substrate for all cases is clamped while the opposite end is allowed to freely deflect when new metal powder are deposited, as shown in Figure 5.

Figure 6 shows the dimension of the substrates and the locations of both the thermocouples (TC1~TC9) and the displacement sensors (DS1~DS3) to measure the temperature histories and the displacement evolutions of the lower surface of the substrates, respectively. Nine *Omega* GG-K-30 type thermocouples with a measurement uncertainty of 2.2°C ($\pm 7.5\%$) and three WXXY PM11-R1-20L displacement sensors with a maximum range of 20.00 mm and an accuracy of 0.01% are adopted. A *Graphtec* GL-900 high-speed data-logger with 8 receiver channels is employed to

record all the displacement and temperature signals during the DED process.

3. FE modelling method

3.1. Thermomechanical simulation of DED

An in-house thermo-mechanical FE software, *COMET* [27,28], is employed to carry out the transient analysis during AM process. A time-marching scheme is adopted to advance in time and a staggered solution performs the thermal and mechanical analyses at each time-step, sequentially. Consequently, a coupled thermal-mechanical analysis is achieved including a transient heat transfer analysis of the thermal loading

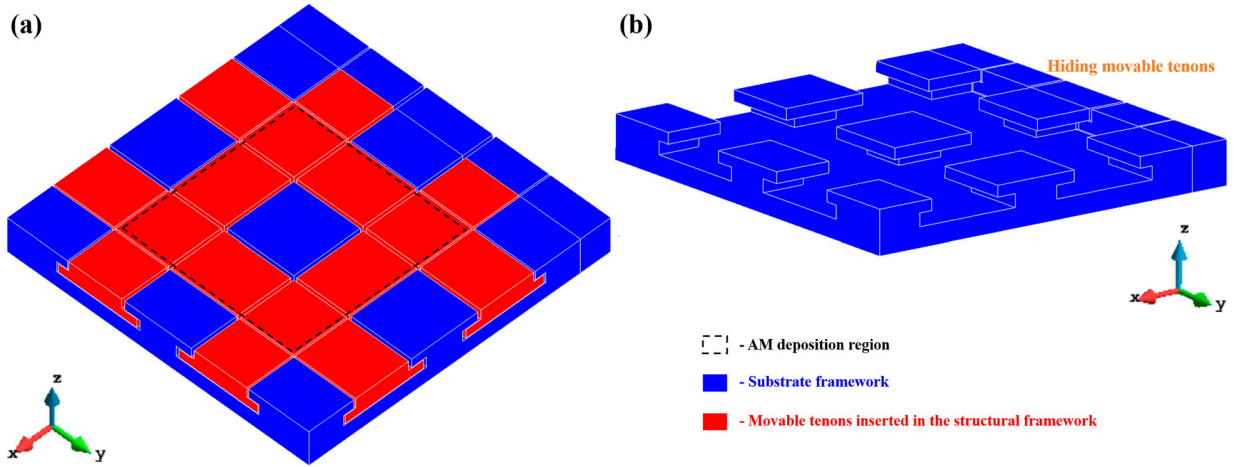


Figure 3. Smart-substrate for building the large-scale block part: (a) whole assembly structure; (b) basic structural framework.

induced by the DED process, followed by a stress analysis which is driven by the temperature field results from the thermal analysis. Because the laser energy input is much higher than the plastic dissipation, the thermo-mechanical problems are weakly coupled (single-way coupling). To simulate the DED process, the *birth-death-element* activation technique [29,30] is used to activate the elements belonging to each new deposition layer according to the user-defined building sequence.

In the simulation for DED, three assumptions are made: (i) A volumetric heat source is used because this study is focused on the macro-scale thermo-mechanical response rather than the melt flow in the molten-pool scale (small). At the global level, it is critical to properly consider the amount of energy introduced in the HAZ. (ii) The effect of the latent heat is negligible since the heat absorption during solid-liquid melting and the heat release during solidification are equal. (iii) The heat generated by plastic deformation is neglected in front of the laser input.

3.2. Governing equations

In the AM process, the heating and cooling are governed by the balance of energy equation:

$$\dot{H} = -\nabla \cdot \mathbf{q} + \dot{Q} \quad (1)$$

where $\dot{H}$ is the enthalpy rate, and $\dot{Q}$ is the heat source, which is defined by the laser input power ($\dot{P}$), the molten-pool volume (V_{pool}), and the laser absorption efficiency (η):

$$\dot{Q} = \frac{\dot{P}\eta}{V_{pool}} \quad (2)$$

In this work, the molten-pool volume is defined as:

$$V_{pool} = D^2(T_l + h) \quad (3)$$

where D is the diameter of the laser beam, T_l and h are the layer thickness and the re-melting depth, respectively. For all simulations, $h = T_l$ and a uniform volumetric heat source is adopted, since the current research is

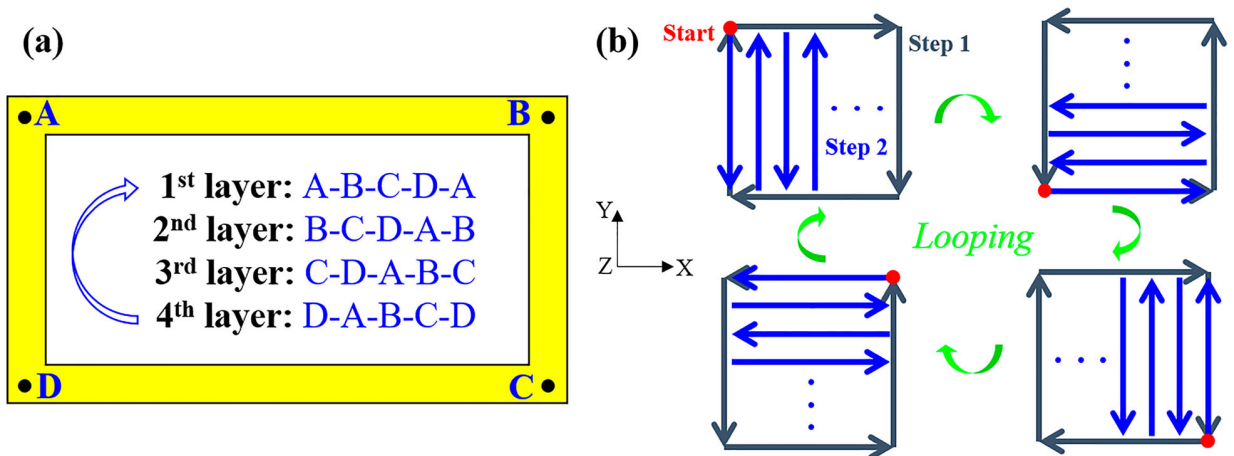


Figure 4. Scanning strategies used to print the (a) rectangular and (b) block parts.

Table 1. Process parameters utilised for DED and the size of different deposits.

	Laser power (W)	Scan speed (mm/s)	Up-lift height (mm)	Beam diameter (mm)	Hatch distance (mm)	Interval between adjacent layers (s)	Feeding rate (g/min)	Layer number (n)	Deposit sizes (mm ³)
Wall-1	4000	20.0	0.4	5.0	-	0	15.0	48	70 × 7 × 17.5
Wall-2	4000	20.0	0.4	5.0	-	0	15.0	40	70 × 7 × 12
Wall-3	4000	20.0	0.4	5.0	-	0	15.0	48	70 × 7 × 17.5
Rectangle-1	4000	20.0	0.4	5.0	-	0	15.0	40	70 × 40 × 14
Rectangle-2	4000	20.0	0.4	5.0	-	0	15.0	40	70 × 40 × 14
Block-1	4000	20.0	0.6	5.0	3.0	200	15.0	20	60 × 60 × 11.6
Block-2	4000	20.0	0.6	5.0	3.0	200	15.0	20	60 × 60 × 13.2

focused on the macro thermal-mechanical response rather than the convective flow within the molten pool.

The heat flux q is expressed via Fourier's law:

$$q = -k\nabla T \quad (4)$$

where $k(T)$ and ∇T are the (temperature-dependent) thermal conductivity coefficient and the temperature gradient, respectively.

The heat loss due to convection is described via Newton's law:

$$q_{conv} = h_{conv}(T - T_{room}) \quad (5)$$

where h_{conv} is the Heat Transfer Coefficient (HTC) through convection, T is the surface temperature of the part and T_{room} corresponds to the ambient temperature.

The radiation heat flux is computed through Stefan-Boltzmann's law:

$$q_{rad} = \varepsilon_{rad}\sigma_{rad}(T^4 - T_{room}^4) \quad (6)$$

where ε_{rad} and σ_{rad} are the emissivity of the radiating surface and the Stefan-Boltzmann constant, respectively.

The stress analysis is performed in sequential thermal load steps adopting the temperature field obtained to solve the mechanical response. The governing equation for the stress analysis is the balance of momentum and the continuity equations written as:

$$\nabla \cdot s + \nabla p + b = 0 \quad (7)$$

$$(\nabla \cdot u - e^T) - \frac{p}{K} = 0 \quad (8)$$

where the Cauchy stress tensor σ is split into its spherical (pressure), p , and deviatoric, s , parts, respectively, as:

$$\sigma = pl + s(u) \quad (9)$$

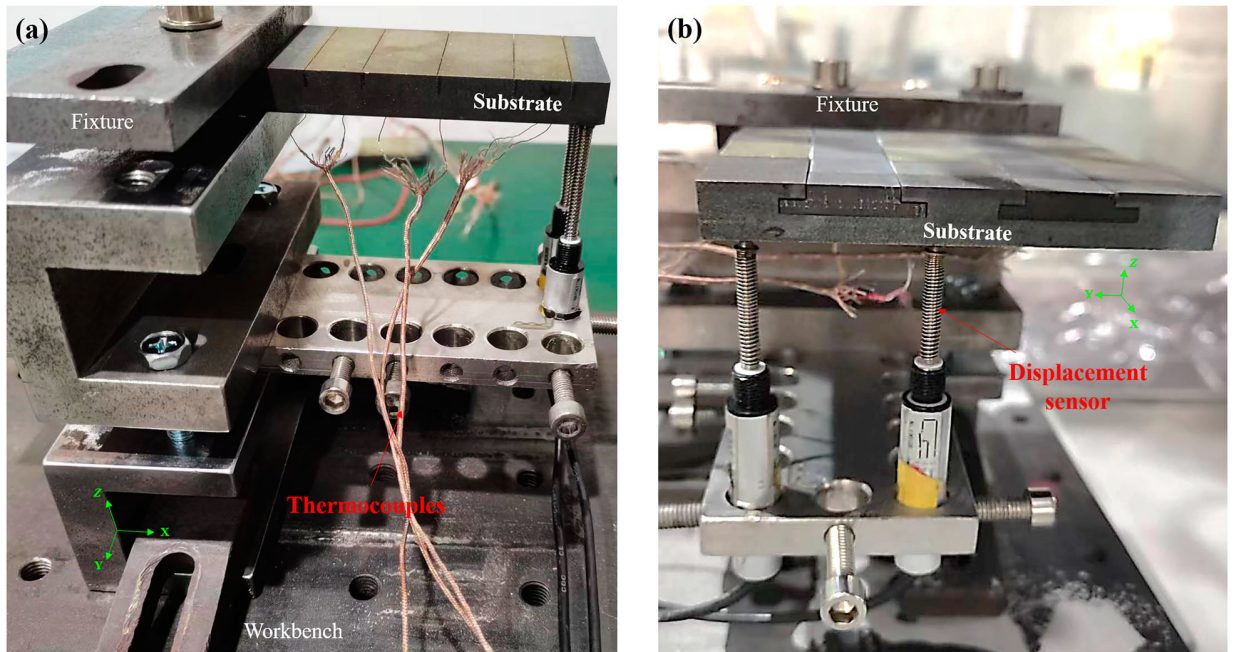


Figure 5. Experimental setup to monitor the temperature and vertical displacement of the bottom surface of the substrates used for building (a) single-walls and (b) block parts during DED.

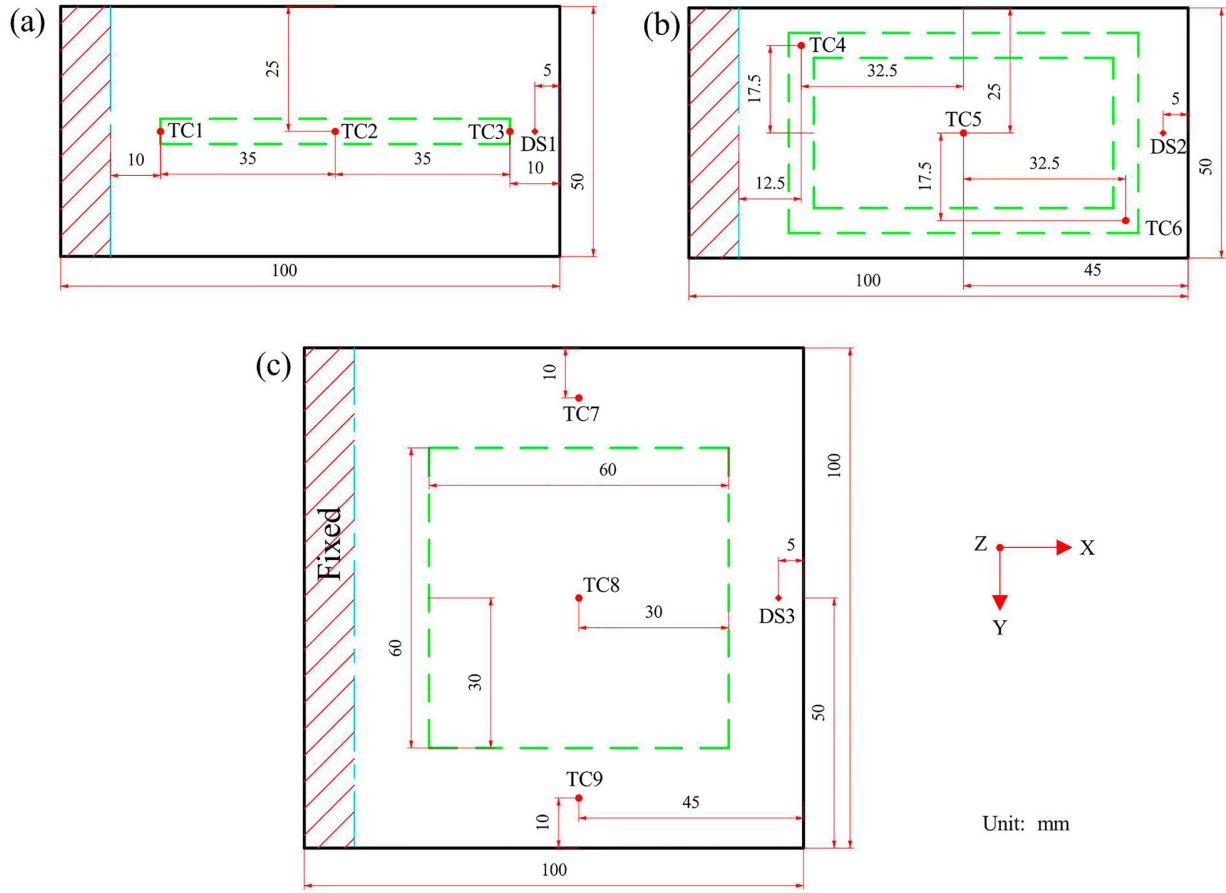


Figure 6. Substrate dimensions and the locations of the nine thermocouples (TC1~TC9) and the three displacement sensors (DS1~DS3) on the bottom surface of the substrates used for fabricating (a) single-wall, (b) rectangular and (c) block builds.

b denotes the body force (per unit of volume), and $K(T)$ are the (temperature-dependent) bulk modulus. The thermal deformation, e^T , is written as:

$$e^T(T, f_s) = e^{cool}(T) + e^{pc}(f_s) \quad (10)$$

where $e^{cool}(T)$ and $e^{pc}(f_s)$ are the thermal expansion and thermal contraction during the liquid/solid phase transformation, described as:

$$e^{cool}(T) = \alpha(T)(T - T_0) \quad (11)$$

$$e^{pc}(f_s) = \beta f_s \quad (12)$$

where α and β are the (temperature-dependent) coefficients of the thermal expansion and shrinkage, respectively, and T_0 and f_s are the initial temperature and the solid fraction, respectively.

In this work, a J2-thermo-elasto-visco-plastic model is used and the von-Mises yield-surface is defined as:

$$\Phi(s, q_h, T) = \|s\| - \sqrt{\frac{2}{3}}[\sigma_y - q_h] \quad (13)$$

where $\sigma_y(T)$ is the (temperature-dependent) yield stress allowing for the thermal softening while q_h is

the stress-like variable controlling the isotropic strain-hardening.

The deviatoric counterpart of Cauchy's stress tensor is expressed as:

$$s = 2G(e - e^{vp}) \quad (14)$$

where G denotes the (temperature-dependent) shear modulus, while e and e^{vp} stand for the total (deviatoric) strain and the visco-plastic strain, respectively.

Ti6Al4 V titanium alloy is characterised by a solid-state phase transformation (SSPT), affecting the total strain. To consider the stress relaxation due to the alpha-beta phase transformation of Ti6Al4 V, Denlinger et al. [31] proposed using an annealing temperature of 690°C in the thermal-induced stress analysis of DED and achieved good agreement with the experimental data. Differently, Chen, Ye, and Xu [32] developed a thermo-mechanical model for wire-fed electron-beam freeform to investigate the SSPT temperature of Ti6Al4 V, and finally determined the annealing temperature as 850°C via variable temperature XRD measurements. The non-unique annealing temperature settings result from the difference in the definition of the

material constitutive laws used to simulate the mechanical behaviour of Ti6Al4 V in AM. For this reason, in-situ displacement measurement during DED is used in this work to seek the most suitable annealing temperature. In detail, the annealing temperature is set at $T_{ann} = 760^\circ\text{C}$ to consider the SSPT-induced stress relief. Once the temperature approaches T_{ann} , $\sigma_y \rightarrow 0$. Thereby, the deviatoric Cauchy stress reduces to:

$$s = \eta_{vp} \dot{\epsilon}^{vp} \quad (15)$$

where η_{vp} is the visco-plastic coefficient. Therefore, the material is featured by a purely viscous law when $T \geq T_{ann}$.

For a more detailed introduction of the governing equations and the constitutive laws implemented in this thermomechanical model, the reader may refer to previous works [33, 34].

3.3. Mesh model, material properties and boundary conditions

Figure 7 shows the FE meshes of seven different DED-components with increasing geometrical complexity from single-walls, rectangular parts to multi-pass multi-layer blocks. Table 2 presents the corresponding numbers of elements and nodes of all the geometries shown in Figure 7. The mesh size is set to $1.0 \times 1.0 \times t \text{ mm}^3$ (where t is equal to the layer thickness) for all the AM-parts based on a mesh convergence study [35], while coarser meshes are utilised for the substrates, balancing the prediction accuracy and the computational cost.

To ensure the computational accuracy of high-fidelity simulations, the step length is set as 4 mm (80% of the laser spot of 5 mm) and the time step size is $\Delta t = 0.2 \text{ s}$. All the simulations are performed using a

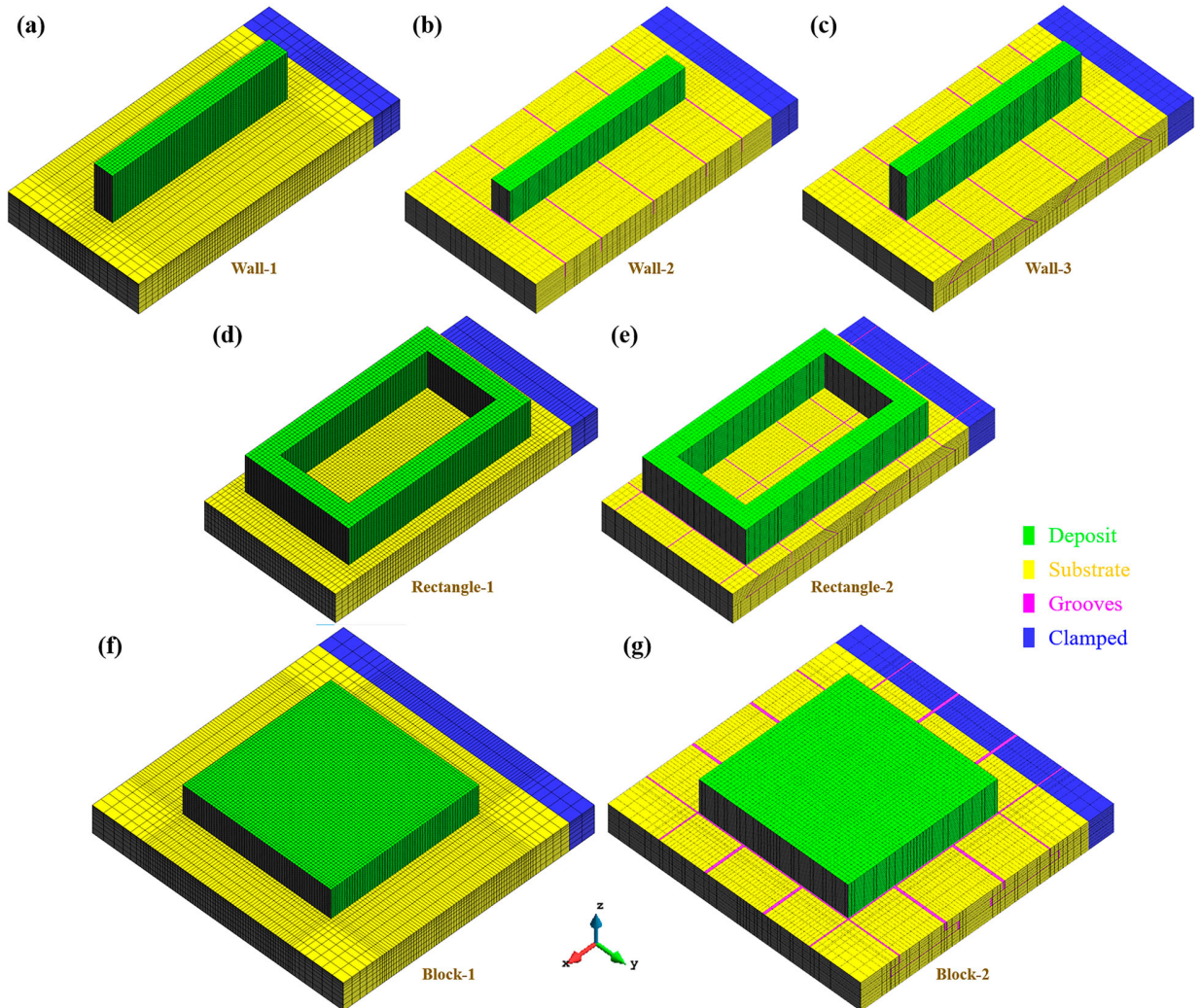


Figure 7. 3D FE meshes: (a) the standard substrate and the substrates (b) with vertical grooves and (c) with moveable trapezoidal tenons used for fabricating single-wall parts; (d) the standard substrate and (e) the substrate with moveable trapezoidal tenons for printing rectangular parts; (f) the standard substrate and (g) the substrate assembled by several small tenons for building block builds.

Table 2. Numbers of FE elements and nodes.

Samples	Number of hexahedral elements	Number of nodes
Wall-1	41,938	48,672
Wall-2	44,160	50,792
Wall-3	46,709	53,952
Rectangle-1	75,000	87,416
Rectangle-2	89,460	102,312
Block-1	116,992	126,395
Block-2	116,640	125,505

personal computer incorporating an Intel core i7-9700, 3.0 GHz processor and 16.0 GB of RAM. The total computational time takes 2.7, 14.2 and 150.4 h, corresponding to 433, 3045 and 16,777 steps, for the single-wall, rectangular and block parts, respectively.

Table 3 presents the temperature-dependent thermo-physical properties of Ti6Al4V titanium alloy [10] adopted for both the printed workpieces and the substrates in the computational simulations. Note that once the temperatures reach the melting point, the heat conductivity is increased to 83.5 W/(m·°C) to account for the convective flow inside the molten pool [36]. For the elements corresponding to the grooves (marked by fuchsia in Figure 6) within the modified substrates, the thermal and mechanical properties of Ti6Al4V are set to 10% and 0.01% of the solids, respectively.

In the simulation of the DED process, the heat dissipation through both the convection and radiation mechanisms is considered for all the free surfaces of the built parts and the substrates. The calibrated emissivity and convective HTC are $\varepsilon_{rad} = 0.6$ and $h_{conv} = 10 \text{ W}/(\text{m}^2 \cdot ^\circ\text{C})$, respectively. Also, the heat loss from the fixed surfaces of the substrate to the clamp system is approximated using an increased HTC of $100 \text{ W}/(\text{m}^2 \cdot ^\circ\text{C})$. The room temperature is assumed as $T_{room} = 25^\circ\text{C}$ for all thermal analyses. The laser efficiency during DED is fixed at $\eta = 0.28$. An initial temperature of 800°C is set to the new elements in the deposition layers to account for the laser pre-heating to the fed powder before arriving at the molten pool.

In the mechanical simulations, the interfaces between the substrate and the fixture are fixed following the actual DED experimental setups. All the model

parameters involved are obtained through comparing the numerical prediction with the in-situ thermo-mechanical measurements as presented in the following section.

4. Results and discussions

In this section, the thermally induced mechanical response of three types of printed geometries is analysed and discussed sequentially: (i) the simple single-wall structures; (ii) the complex hollow rectangular components; and (iii) the large-scale block parts. To achieve this, the coupled thermomechanical FE model applied in this research firstly is calibrated by comparing the in-situ measurement results of all the samples to guarantee the prediction accuracy, although it has been validated in previous works for optimising both the processing and material parameters [10,28]. Next, the mechanical results obtained from the dependable simulations are used to demonstrate the innovation and advantages of the proposed Smart-Substrate solution on controlling both the residual stresses and part warpages.

4.1. Single-wall components

Figure 8 compares the simulated and measured thermal histories and vertical displacements at different positions of the bottom of the substrate (Figure 6), used to fabricate the three single-wall parts. The agreement between the predicted curves (dash lines) and experimental evidence (solid lines) is noteworthy, especially for the temperature predictions. The small discrepancies are mainly attributed to the simplification of the boundary conditions (i.g. the effect of the clamp on the heat conduction is equivalent to an approximate HTC).

It can be seen from Figure 8(b,d,f) that during the printing process the substrate deflects downwards due to the thermal expansion of the deposited layers with a higher temperature than the base plate. Once the DED fabrication is finished, the free end of the substrate sharply warps upwards, especially for the cases of Wall-1

Table 3. Temperature-dependent material properties of Ti-6Al-4V.

Temperature (°C)	Density (kg/m ³)	Thermal Conductivity (W/(m·°C))	Heat Capacity (J/(kg·°C))	Poisson's Ratio	Thermal Expansion Coefficient (μm/(m·°C))	Young's Modulus (GPa)	Elastic Limit (MPa)
20	4420	7	546	0.345	8.78	110	850
205	4395	8.75	584	0.35	10	100	630
500	4350	12.6	651	0.37	11.2	76	470
995	4282	22.7	753	0.43	12.3	15	13
1100	4267	19.3	641	0.43	12.4	5	5
1200	4252	21	660	0.43	12.42	4	1
1600	4198	25.8	732	0.43	12.5	1	0.5
1650	3886	83.5	831	0.43	12.5	0.1	0.1
2000	3818	83.5	831	0.43	12.5	0.01	0.01

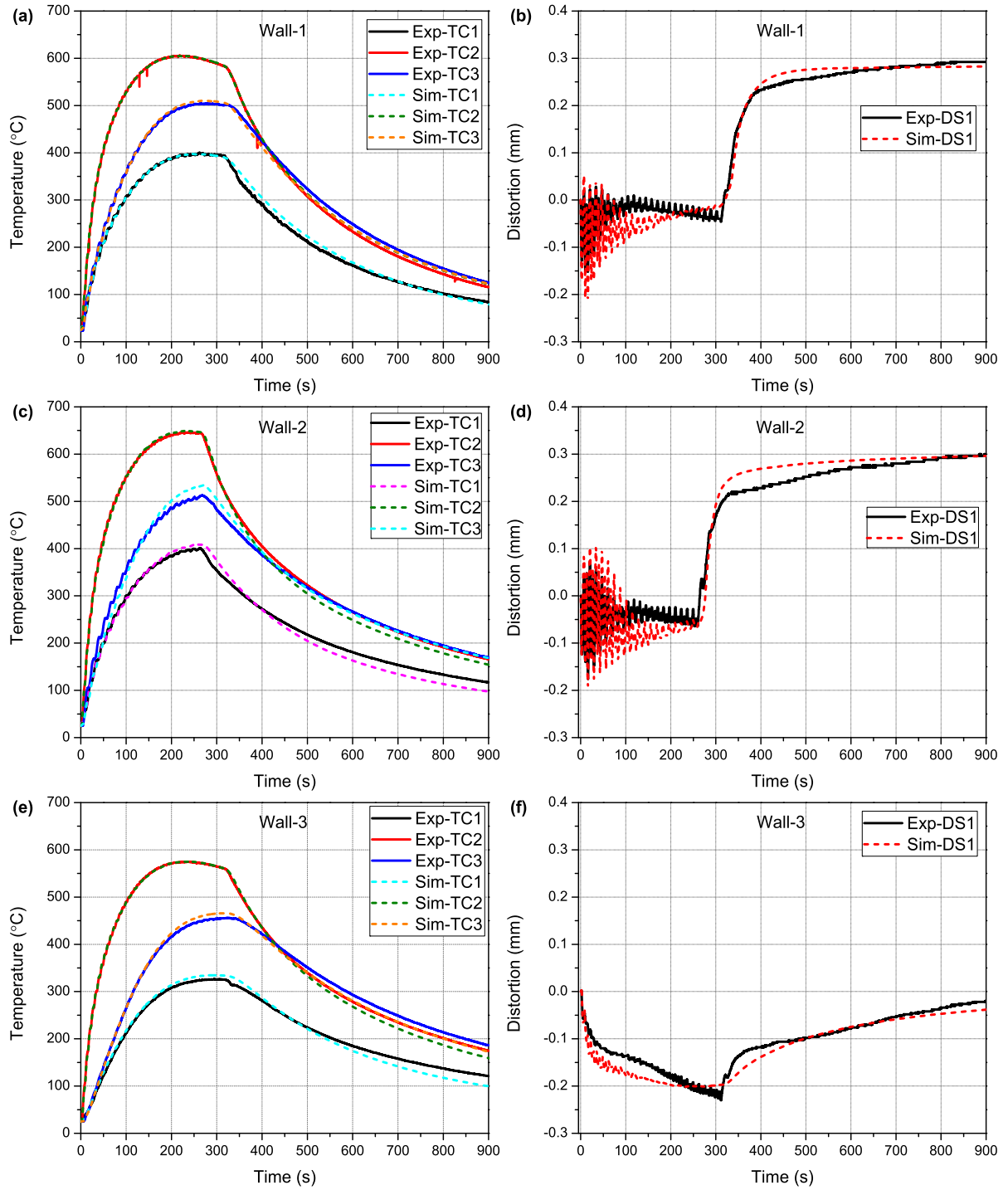


Figure 8. Single-walls: the evolutions of (a,c,e) the temperature histories and (b,d,f) the vertical displacement at the bottom surface of the substrates.

and Wall-2, because of the rapid cooling and contraction of the hot metal depositions. The comparison of the distortion evolution of three different single-wall samples illustrates that using the Smart-Substrate with an optimised inner structure significantly mitigates the final thermal deformations (only -0.02 mm) induced by the fabrication process (Figure 8(f)), compared to another

two cases (up to 0.3 mm). These results are attributed to the evolution of the stress field, determined by the geometrical structures involved in the DED process.

Usually, the larger residual stresses are mainly in the direction of the scan line [37,38]; thereby, the contour-fills of the longitudinal stresses (σ_{xx}) and von Mises stresses of the three single-walls are computationally

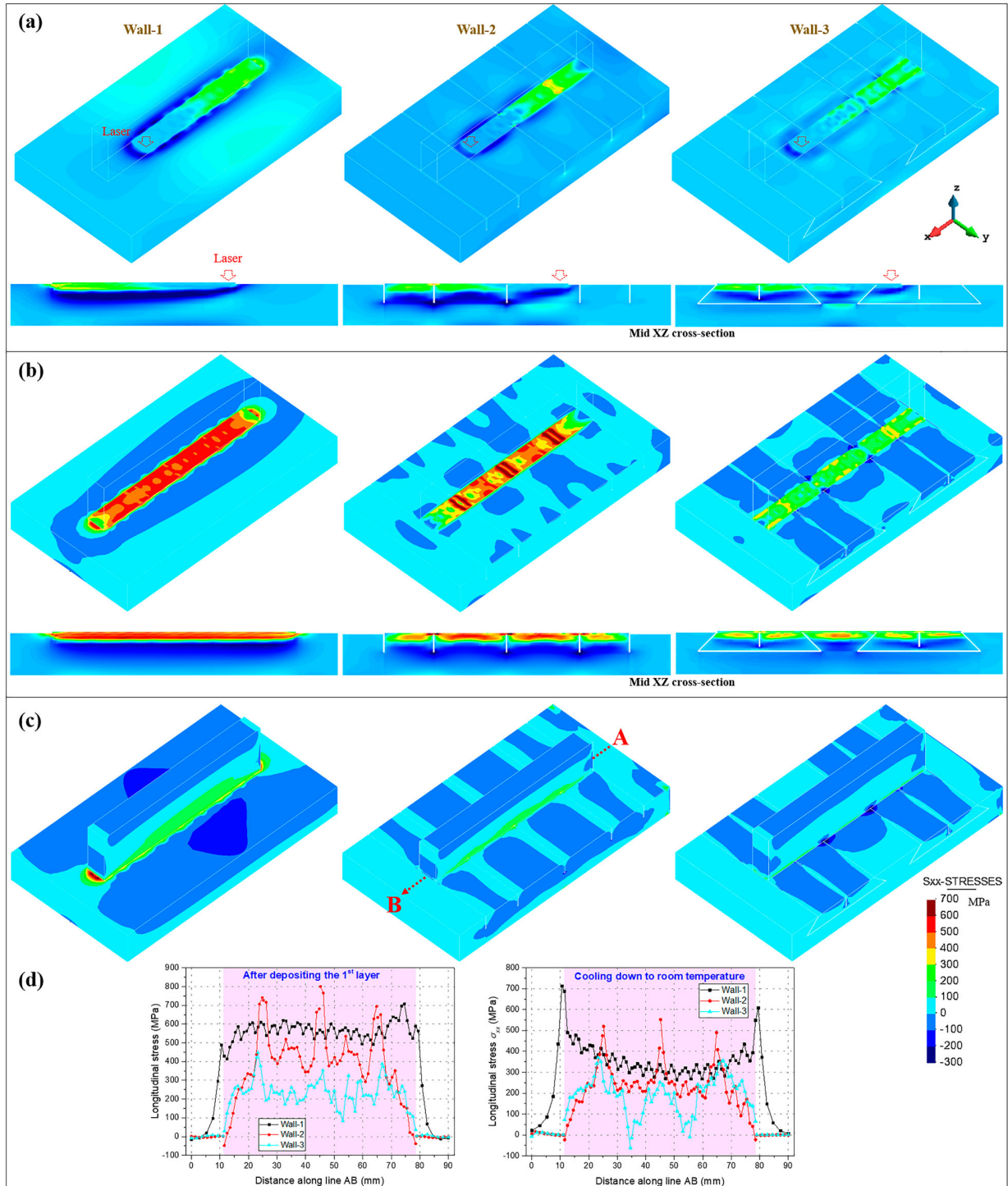


Figure 9. Single-walls: contour-fill of the longitudinal S_{xx} stresses (a) during the printing of the 1st layer; (b) after the deposition of the 1st layer; (c) after cooling down to room temperature; (d) the longitudinal stress distribution at the build-substrate surface (line AB).

simulated using the calibrated model and shown in Figures 9 and 10, respectively. It can be seen from Figure 9(a) and Figure 10(a) that during the printing of the 1st layer, a low stress is produced in the HAZ for the three substrate cases because the high-temperature molten pool softens the metal deposition, promoting

stress relaxation through visco-plastic flow. As the heat source moves forward for the printing of the 1st layer, the metal depositions cool down and shrink quickly, leading to a tensile stress in the upper part of the substrate (corresponding to the past HAZ), while a compressive stress develops beneath the HAZ. Notably, the

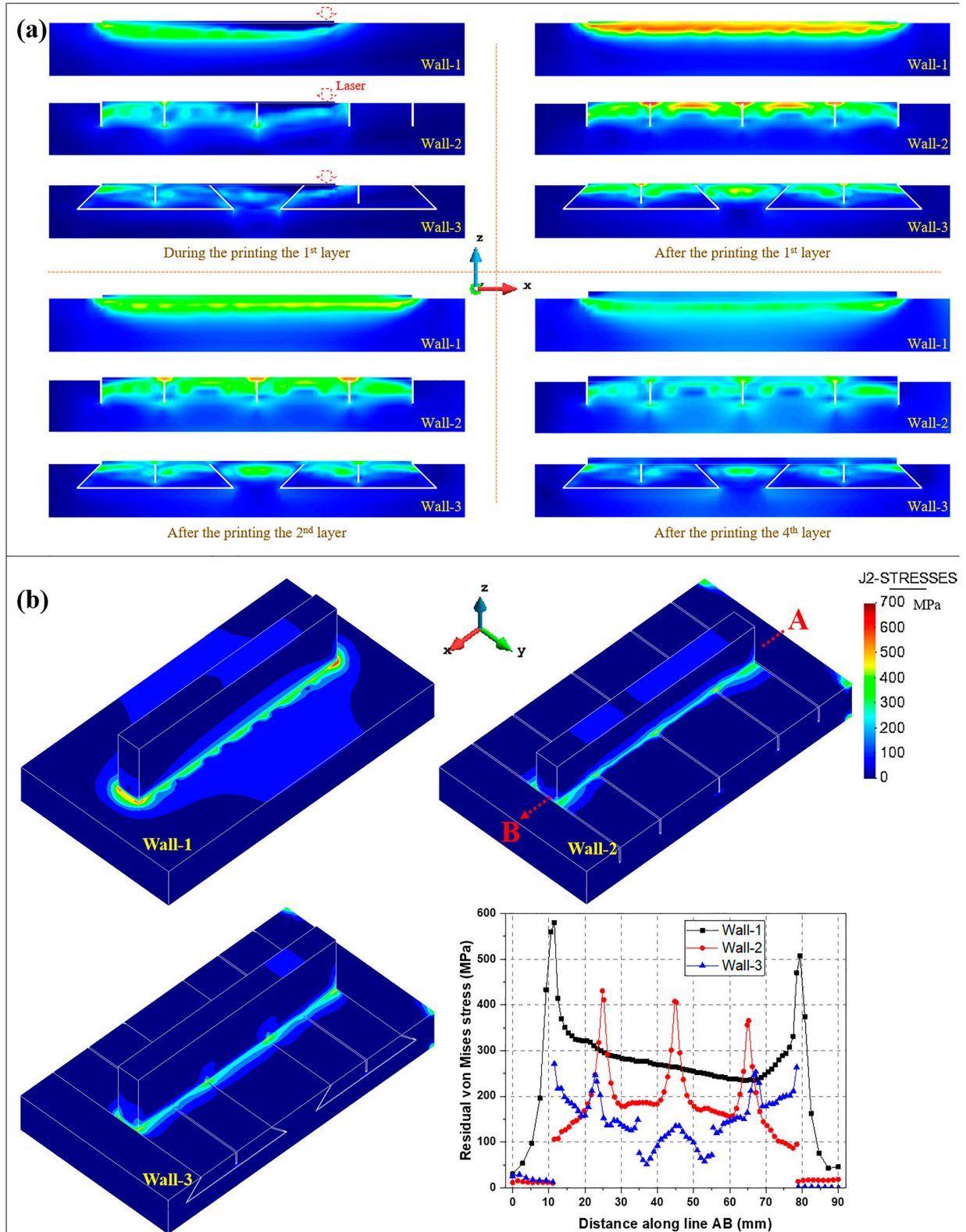


Figure 10. Single-walls: (a) evolution of the von Mises stress field at the mid XZ cross-section for different substrate samples; (b) contour-fill of the von Mises stresses and the stress distribution at the build-substrate surface.

magnitude of both tensile and compressive stresses in the Wall-1 case is pronouncedly higher than that in the other two samples, as shown in Figures 9(b, d) and 10

(a). Note that after building the 1st layer, the Wall-1 and Wall-2 samples show very high tensile stresses (up to 700 MPa). This is not the case for Wall-3 where the

stress level is much lower (about 350 MPa). The reason for this is that although the use of an intact substrate in the Wall-1 case ensures an overall structural stiffness, it also yields strong mechanical restraint to the deposited layer and, thus, high residual stresses. Differently, the substrate with vertical grooves in the Wall-2 case provides the clearance to allow the expanding of the heated material, reducing the development of plastic strains; also, it breaks the continuity of the stress distribution, reducing the stress accretion. The design of the moveable tenon inserted in the Wall-3 substrate further mitigates the generation of residual stresses, due to the significant freedom for thermal deformation during the DED process accompanying the repeated expanding/shrinking cycles.

It can be seen from Figure 10(a) that as the deposited layers increase, the stress level is lowered for all three cases. This is because the very short interval time (about 2 s) between adjacent layers and the high energy-input density (200 J/mm) allow the rapid accumulation of heat in the single-wall builds, functioning as in-situ heat treatment to release the residual stresses induced in the fabrication of the 1st layer. In addition, as the building wall grows, the lower printed material functions as a 'substrate' with an effectively reduced horizontal area (and reduced degree of mechanical constraint if compared to the original large substrate), reducing the formation of residual stresses. However, the magnitude of the residual stresses consistently ranks in the order of Wall-1 > Wall-2 > Wall-3. When the AM buildup is completed and cooling down to room temperature, a large tensile residual stress (700 MPa) is visible at the bottom end of the Wall-1 build, where cracks easily initiate and propagate, as shown in Figure 9(c,d) and Figure 10(b). Similar results are also reported in references [24,39–41]. Nevertheless, the Wall-2 and Wall-3 samples successfully prevent such stress concentrations (Figure 10(b)), especially for the latter (less than 280 MPa), because the tip clearance designed in the Smart-Substrate allows for a freer thermal expansion/contraction of materials during the AM process.

4.2. Rectangular components

Following the simple single-wall structures, in this section, the thermal and mechanical behaviour of the more complex rectangular parts is analysed. Figure 11 compares the calculated and experimental temperature and displacement histories at the lower surface of the substrates (see Figure 6) used to build the rectangular parts. The simulated results agree well with the experimental evidence.

The mechanical response of the rectangular parts is similar to the single-wall, as shown in Figure 11(b) and (d). In detail, the distortion evolution of the standard (Rectangle-1) and smart (Rectangle-2) substrates is different during the printing process. The displacement curve for the Rectangle-1 displays a more dramatic oscillation due to its stronger entire stiffness. However, both cases yield similar displacement values (about -0.22 mm) at the end of the deposition. Moreover, the Rectangle-1 case produces a sharp substrate bending upwards in the final cooling phase, leading to a remarkable residual deformation of approximate 0.28 mm, while a value of only 0.065 mm results for the Rectangle-2 case.

Noticeably, the deformation of the standard substrate for the Rectangle-1 case produces more dramatic fluctuations during the printing process as compared to the Wall-1 case (see Figure 8(b) and Figure 10(b)). This is due to the existence of the four orthogonal thin walls in the rectangular structure, which yields a complex scanning process (Figure 4(a)) and, thus, a more complicated mechanical response during DED. For example, longitudinal bending of the substrate easily happens (deforms upwards) due to the contraction of the metal deposition when the printed long walls (along X-direction) cool down. To the contrary, the fabrication of the short-walls (along Y-direction) yields the transverse shrinkage of the upper part of the substrate, with a downward deflection. However, no obvious deformation fluctuation is found in both the Wall-3 and Rectangle-2 cases (see Figure 8(f) and Figure 11(d)) on account of the flexibility of the Smart-Substrate to avoid stress accretion.

Figures 12 and 13 show the evolution of von Mises stress field and the residual stresses in three orthogonal directions for both cases, respectively. In detail, Figure 12(a) shows the von Mises stress response at different scanning times when depositing the 1st layer. Note that when printing the second long track (corresponding to the scan-line 3) in the Rectangle-1 case, the first long track (scan-line 1) cools down and produces high tensile stress. At the same time, the printed first short track (scan-line 2) starts cooling, and high residual stresses are formed as the laser heat source moves forward to deposit the last short track (scan-line 4). When the 1st layer is completed, high residual stresses, more than 600 MPa, appear at the part-substrate interface region in the case of the standard substrate, similar to the Wall-1 case (see Figure 9(b)). Undoubtedly, such high stress level also is responsible for the large part deflection (Figure 11(b)). However, the Rectangle-2 case successfully avoids the generation of residual stresses in both the long and short tracks, even if their perpendicular geometrical relation increases the challenge of overcoming the stress problem.

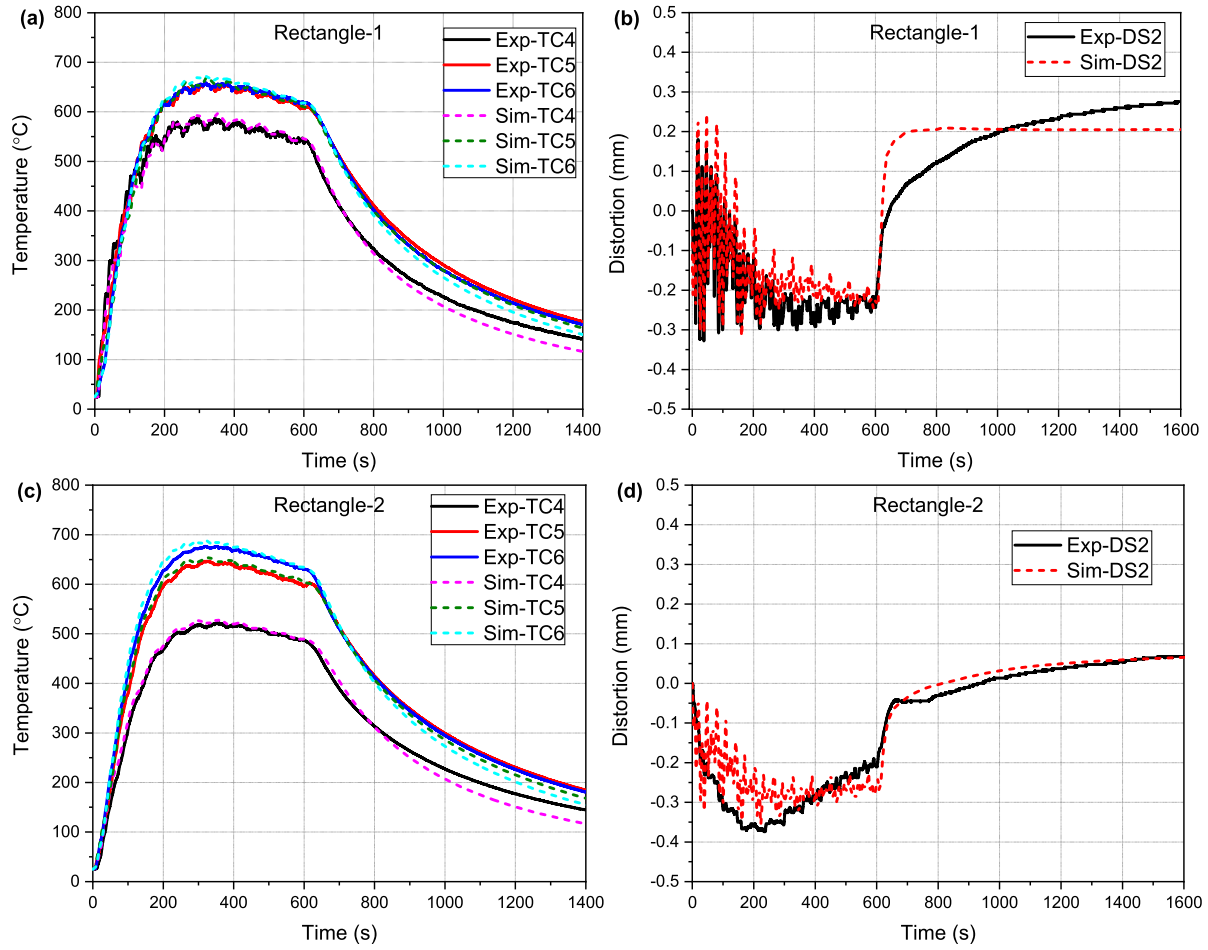


Figure 11. Rectangular part: the evolutions of (a,c) the temperature histories and (b,d) the vertical displacement at the free end of the substrates.

With the increase of the deposited layers, the standard and smart substrates still yield a high and lower stress level, respectively, as shown in Figure 12(b). This illustrates the effectiveness of using the Smart-Substrate on controlling residual stresses. Also, like in the single-wall parts, continuous printing causes an in-situ thermal annealing effect under high temperature (Figure 11), lowering the residual stresses in both the rectangular builds. Nevertheless, the stress concentrations at the bottom corners of the Rectangle-1 deposit are maintained until the build-up is finished, similar to the results reported by Yang et al. [42], while very lower stresses are accumulated in the Rectangle-2 case, as presented in Figures 12 and 13(c), thanks to the Smart-Substrate utilised in the deposition process, curbing the development of plastic deformations.

4.3. Block components

To ulteriorly verify the effectiveness of the proposed Smart-Substrate strategy on mitigating the residual

stresses and deformations of industry-level AM components, two large-scale blocks are printed on the standard and smart substrates, respectively (Figure 2(a)).

As shown in Figure 14, the comparison of the numerically predicted and experimentally measured results in terms of the temperature and displacement histories at the bottom of the substrates for the two block samples, once again exemplifies the remarkable simulation precision of the thermo-mechanical model used.

It can be seen from Figure 14(b) that when the 1st layer of the Block-1 part is fabricated, the free end of the substrate displays a sharp increase in the vertical displacement, up to 1.1 mm (approximately equal to two layer-thicknesses), which is usually unacceptable during DED because it seriously impairs the geometrical precision of the built part. Furthermore, the displacement curve presents a pronounced fluctuation during the subsequent building process while the average value gradually increases to 1.64 mm until completing the whole build-up. Nevertheless, the final displacement is only 0.8 mm for the Block-2 sample (see Figure 14(d)),

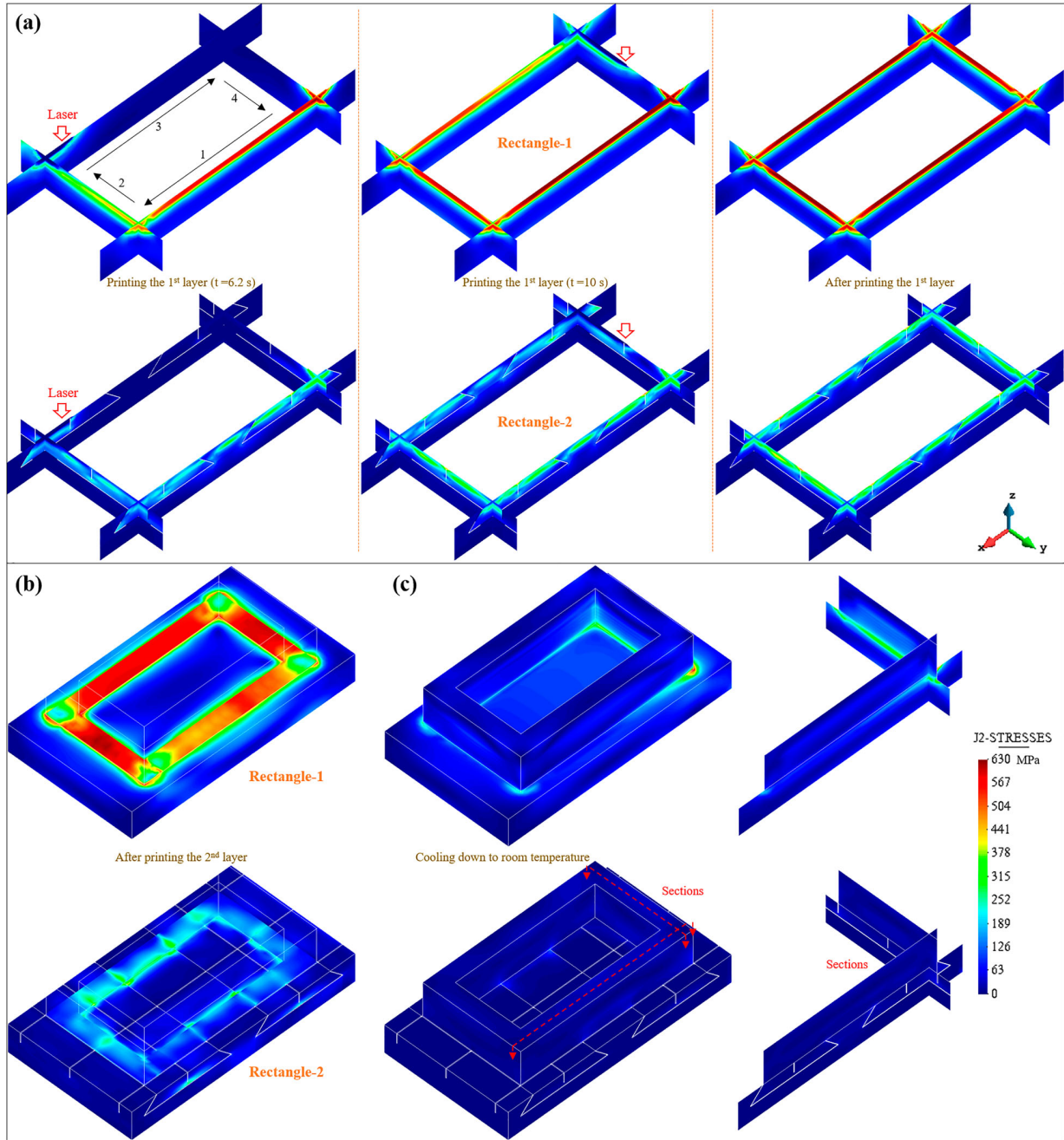


Figure 12. Rectangular parts: contour-fill of von Mises stress field: (a) cross-sections in the mid-line of the thin-walls at different printing times when depositing the 1st layer; (b) after the building of the 2nd layer; (c) cooling down to room temperature.

which is slowly accumulated during DED even if the structural stiffness of the Smart-Substrate is significantly weaker than the standard one.

Figures 15 and 16 show the evolution of von Mises stress field and the residual stresses in three orthogonal directions for the two block components, respectively. Observe that high residual stresses (up to 700 MPa) are induced after depositing the 1st layer for the standard case. However, unlike for the simple single-wall and rectangular samples (Figures 9 and 11(a)), the use of a 40%

overrate (calculated from the beam diameter and hatch distance in Table 1) in the successive hatch-by-hatch scanning within one layer of the block samples yields smaller average stresses, since the tensile stresses formed in the current track are eliminated when depositing the following track. With the increase of the deposition layers, the thermally induced residual stresses gradually decrease due to the development of plastic deformation (Figure 14(b)) and the intrinsic high-temperature heat treatment (Figure 14(a)) facilitating stress

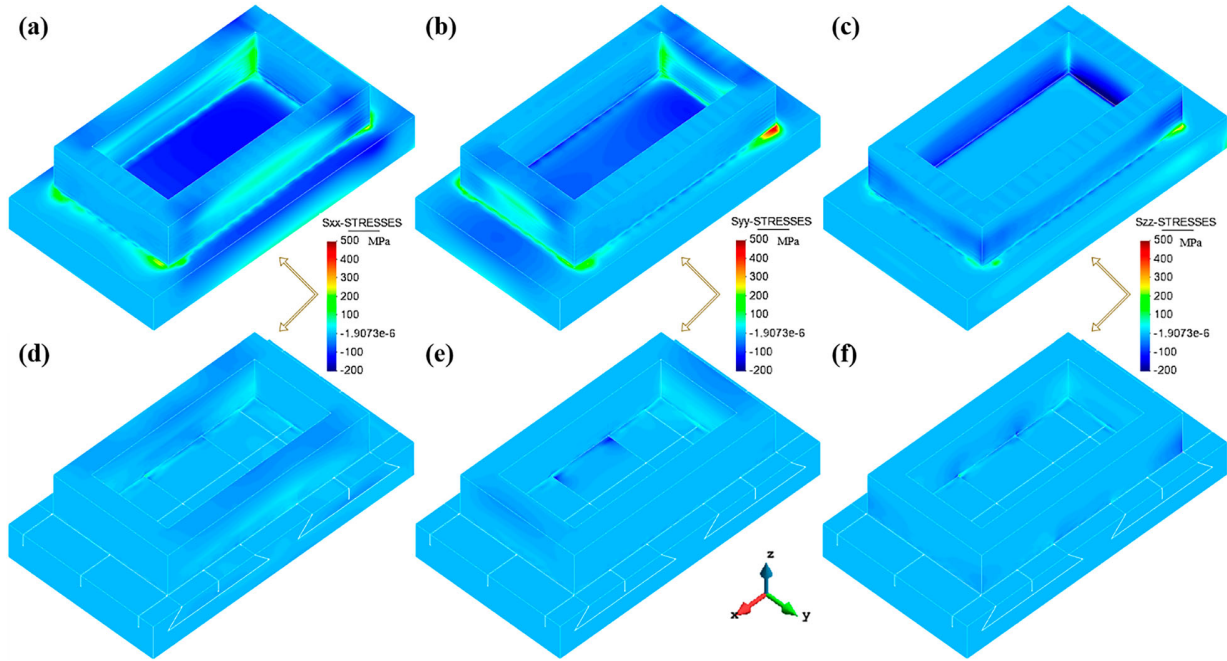


Figure 13. Rectangular parts: contour-fill of the residual stresses in three orthogonal directions (S_{xx} , S_{yy} and S_{zz} for X, Y and Z directions, respectively): (a–c) standard substrate; (d–f) Smart-Substrate.

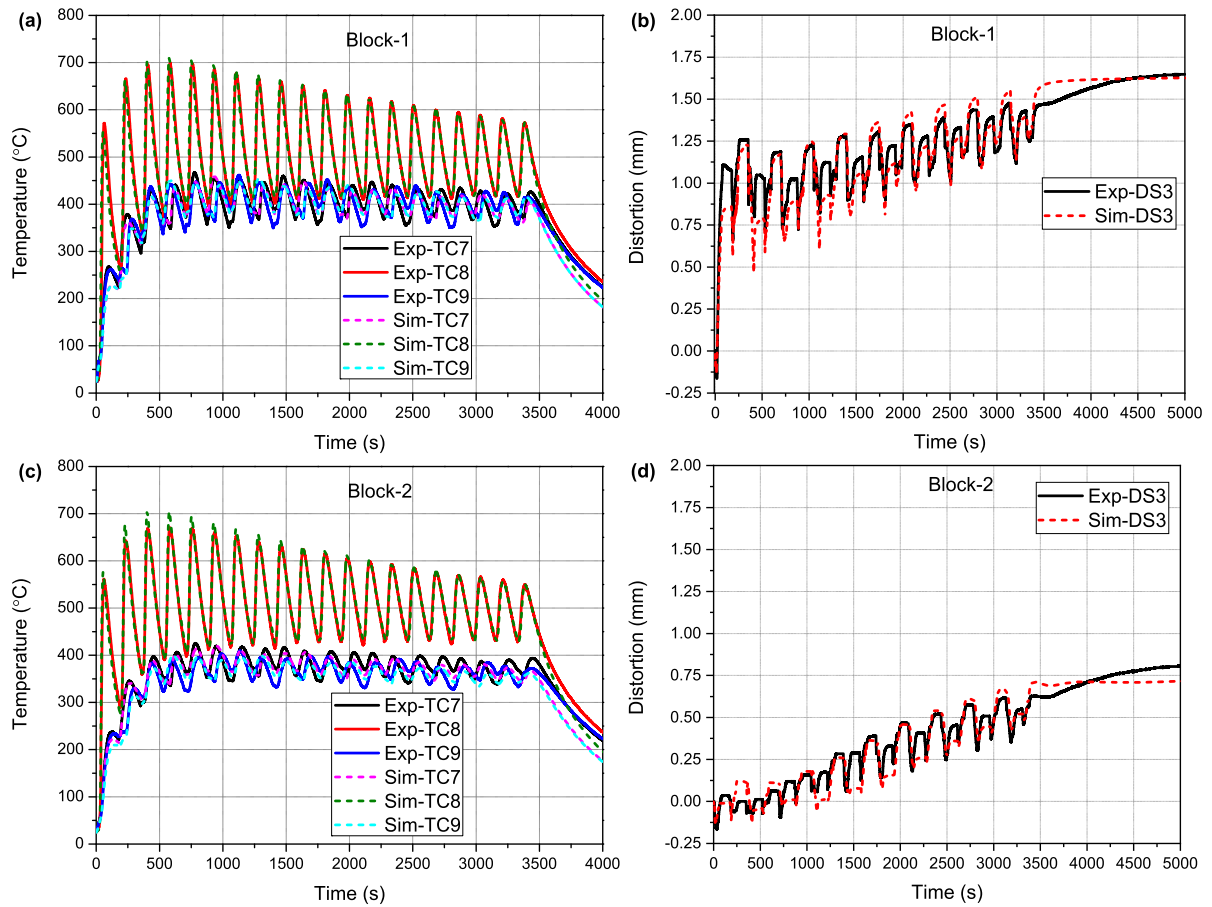


Figure 14. Block parts: the evolutions of (a,c) the temperature histories and (b,d) the vertical displacement at the free end of the substrates.

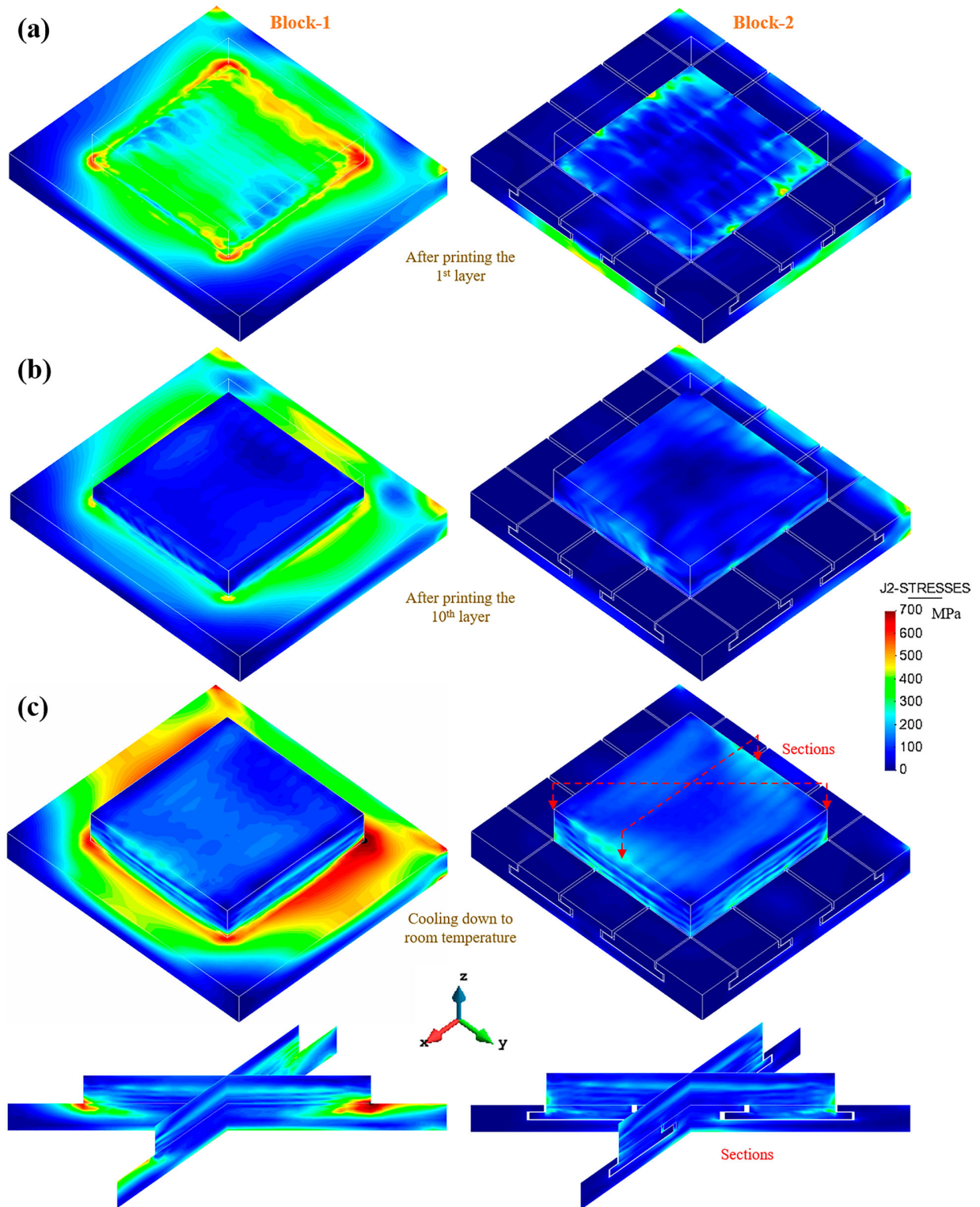


Figure 15. Block parts: the von Mises stress field after building the (a) 1st and (b) 10th layer; (c) cooling down to room temperature.

relief, but the stress concentrations still hold at the base-ment of the builds, especially in the corners (Figures 15 and 16). However, by using the protective Smart-Sub-strate strategy, the residual stresses can be effectively

reduced. Thus, a lower stress level (less than 300 MPa) is achieved during the whole DED printing process, and distortion is also minimised by roughly 50% (Figure 14(d)). In addition, although the use of a long

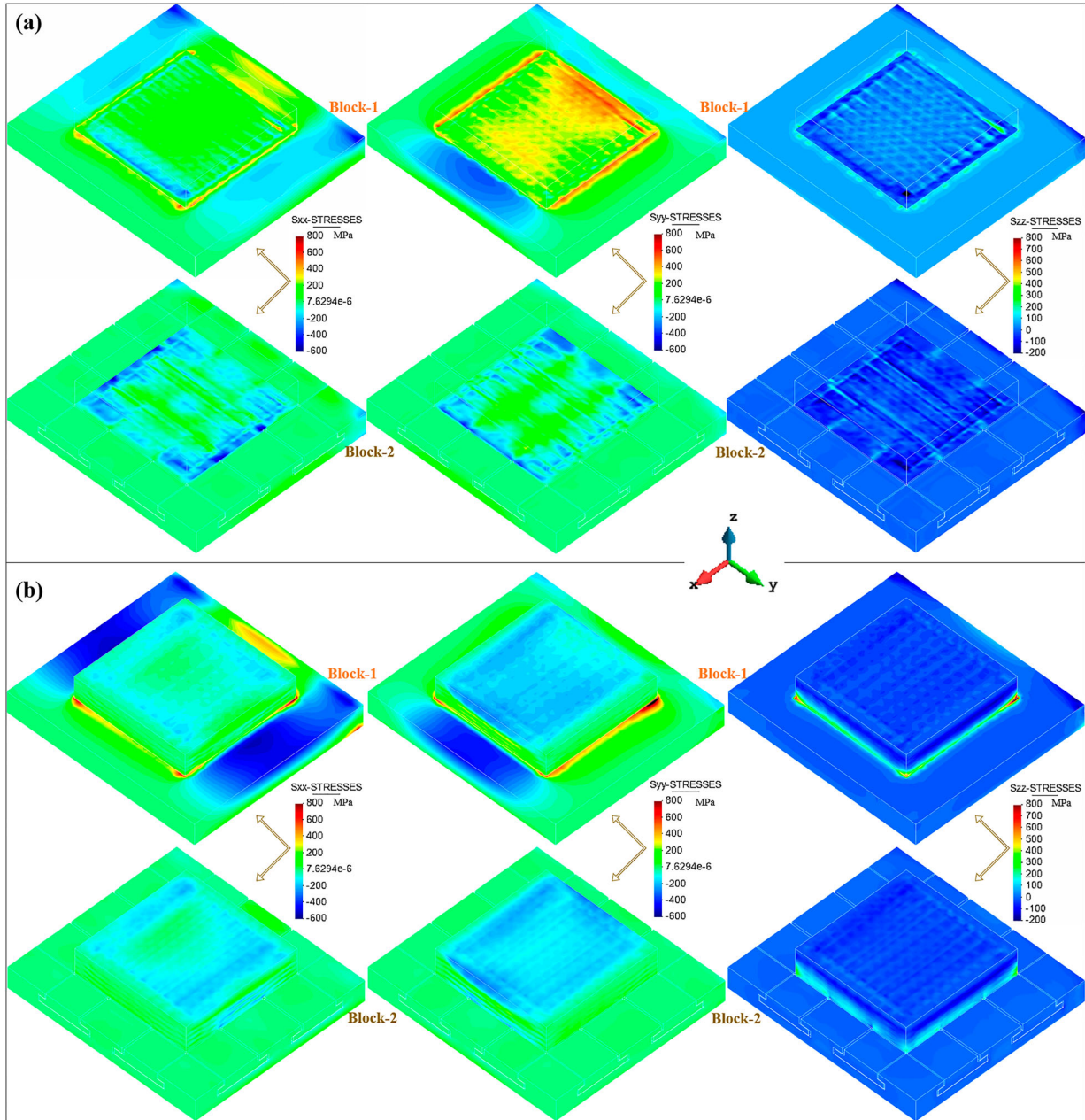


Figure 16. Block parts: the stress fields in three orthogonal directions (S_{xx} , S_{yy} and S_{zz} for X, Y and Z directions, respectively): (a) after the building of the 1st layer; (b) after the build-up and cooling down to room temperature.

dwel time of 200 s during the building the block parts favours stress accretion [31], this disadvantage is completely avoided by applying Smart-Substrate.

4.4. Influence of applying smart-substrate on other physical fields

As mentioned, most of in-situ stress-control strategies developed and based on mitigating MTG inevitably affect the thermal distribution, related metallurgical evolution and potential defect formation. Also, they

fail to diminish the stress concentrations at the deposit-substrate interface, especially the corners [43–45], because where large MTG and strong mechanical constraints coexist. Differently, the Smart-Substrate strategy proposed is designed to increase the yield temperature (by lowering the local mechanical constraint of the substrate) instead of reducing MTG to avert the generation of residual stresses during DED process. As known, AM is a complex multi-physics multi-scale interaction including a large number of input parameters, non-uniform thermal field,

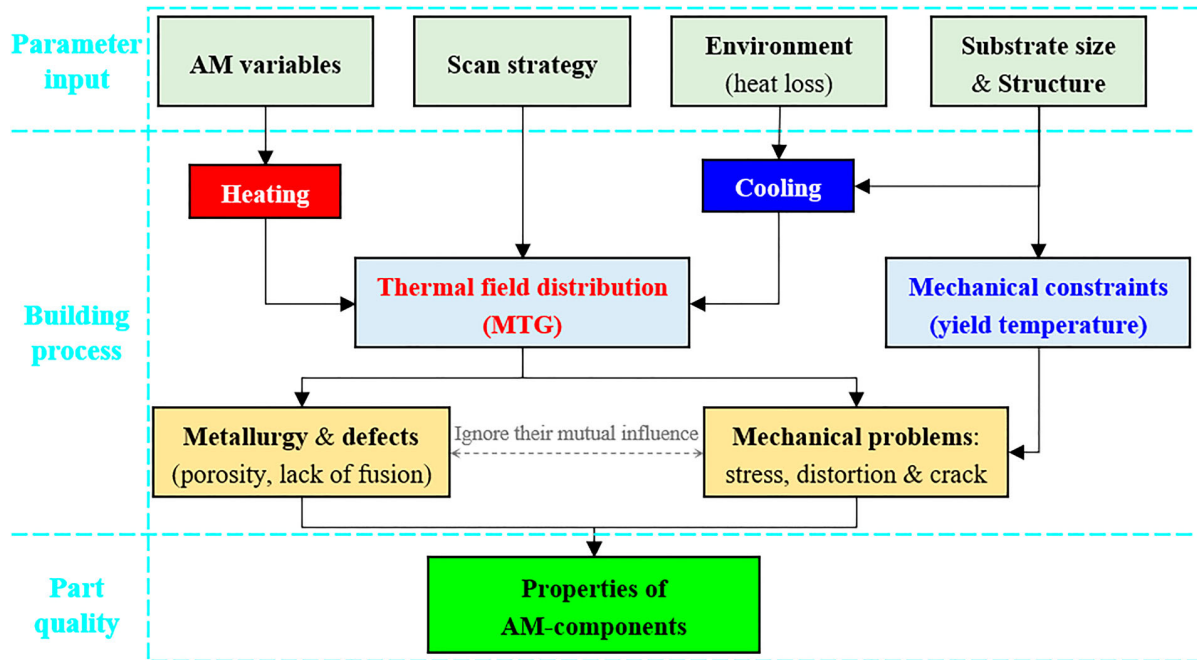


Figure 17. Complex interactions between different physical fields involved in AM.

mechanical response, metallurgical evolution and defect formation, all of which affect the final part properties, as shown in Figure 17. Thereby, the potential impact of using the Smart-Substrate approach to other physical processes must be assessed.

The thermal histories, the deposited macro/micro-structures, the corresponding size of the β -grains and α laths, as well as the microhardness, at the centre and different heights of the block parts manufactured on the standard and smart substrates, respectively, are extracted and compared in Figures 18–21, respectively. Note that both cases present similar temperature histories and resulted macro/microstructures and microhardness for different building positions. This illustrates the independence of the Smart-Substrate strategy in controlling residual stresses and deflections during AM process without compromising other physical phenomena. This makes it unnecessary to consider the stress problem when optimally determining AM variables for achieving superior microstructure and avoiding defect formation. This is beneficial for widening the process window of metallic AM.

4.5. Advantages and limitations of the smart-substrate strategy

According to the stress results presented in this work (see Figures 9, 11, and 15) and the residual stress distribution in AM-parts reported in previous papers [23,35,46,47], it is found that large residual stresses

(or stress concentrations) typically appear at the part-substrate interface, especially at the bottom end or corners of the build. Such phenomenon is explained as follows. When the first layers of the metallic material are deposited on the cold substrate, a large MTG and strong mechanical constraint from the substrate inevitably yield high residual stresses and related part deformations and/or cracks. As the building height increases, the high stresses yielded in the deposition of the first layers are slightly decreased due to the gradually increased heat accumulation (favouring stress annealing) and the weakened mechanical constraint provided by the previously deposited layers, but cannot be erased because of the use of stiff substrates. For this reason, the Smart-Substrate solution is based on the thermo-mechanics of AM and efficiently averts stress accretion by allowing the development of thermal deformations while preserving the overall structural stiffness of the substrate. Although the Smart-Substrate works at the built basement, it also guarantees a pronounced reduction (by more than 60%) of residual stresses in the whole build even with an increased height. This can be proven by comparing the predicted residual stress fields of two single-wall parts with an increased height of 50 mm fabricated on the standard and smart substrates respectively, as shown in Figure 22.

In addition to the typical rectangular structures presented in this work, many other components with curved shapes can also use the smart substrate to

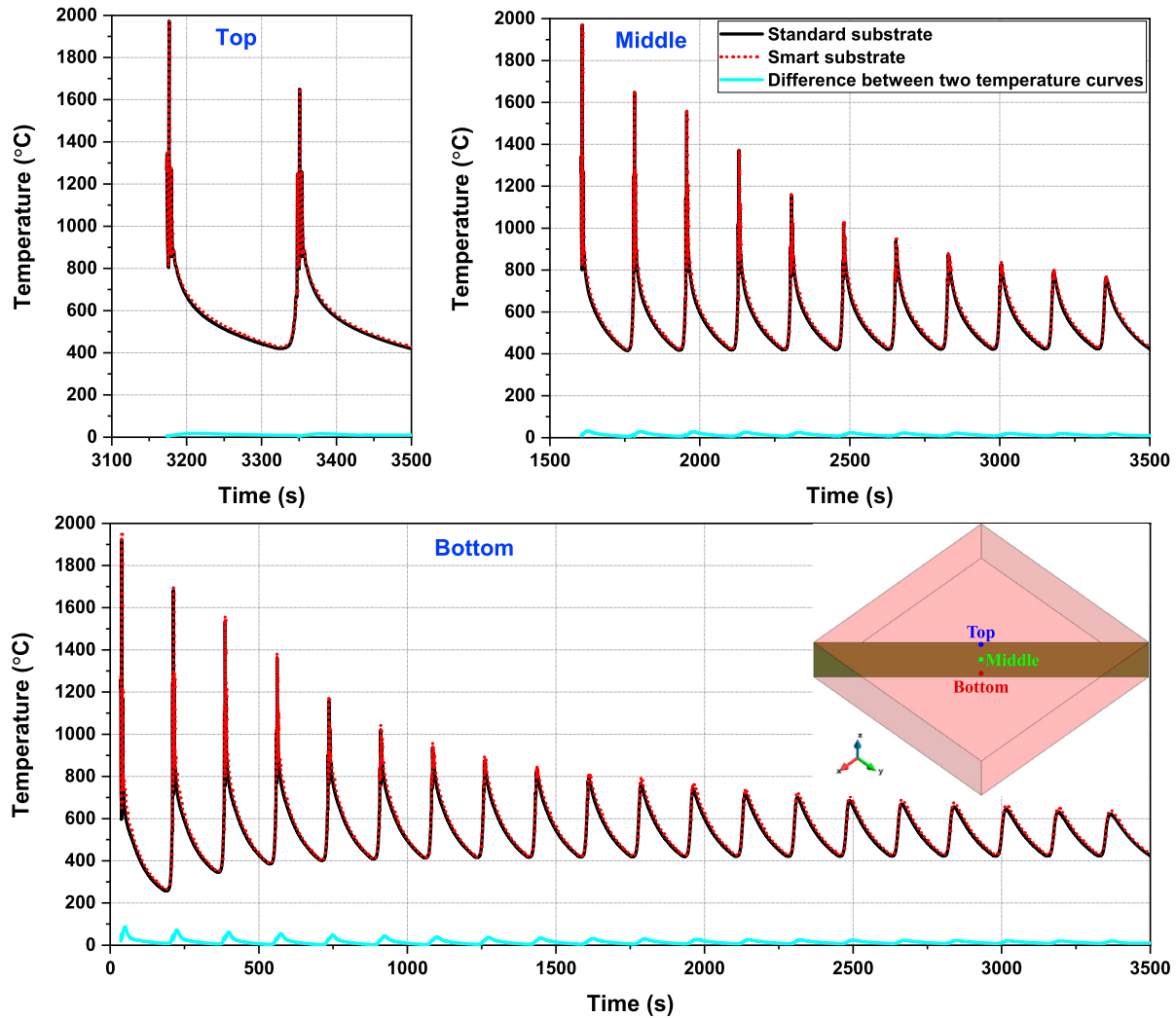


Figure 18. Comparison of the predicted temperature evolution at the building centre and different heights of the block parts fabricated on the standard and smart substrates.

avoid stress accretion during DED. The key is to design the proper moveable tenons (e.g. a clearance of 0.2–1.0 mm, depending on the material properties and the structural size) in the substrate to lower its strong mechanical constraining parallel to the scanning paths as it curbs the thermal deformation, generating residual stresses.

The basis of the Smart-Substrate approach is to avoid the accretion of residual stresses by allowing thermal strains to develop fully in the part. This allows a relatively larger shrinkage of the metal deposition, particularly in the horizontal direction, slightly lowering the geometrical precision of the printed components. This should be considered when designing the part using geometrical compensation.

While the application of Smart-Substrate barely affects the metallurgical microstructure and the mechanical hardness, its influence on other potential AM

defects (e.g. surface roughness, lack of fusion, and porosities) and the fatigue performance of AM-components needs to be investigated in the future study, taking into account that fatigue life is closely related to these intrinsic defects, especially the residual stresses remaining in the builds [48].

5. Conclusions

In this study, an innovative structural design approach, called Smart-Substrate, is proposed to yield lower residual stresses and part deflections in DED process. The major findings are as follows:

- (1) In AM, apart from MTG, the yield temperature, related to the constraint forces during AM thermal deformation, also plays a prominent role in the formation of residual stresses. Based on this, a novel

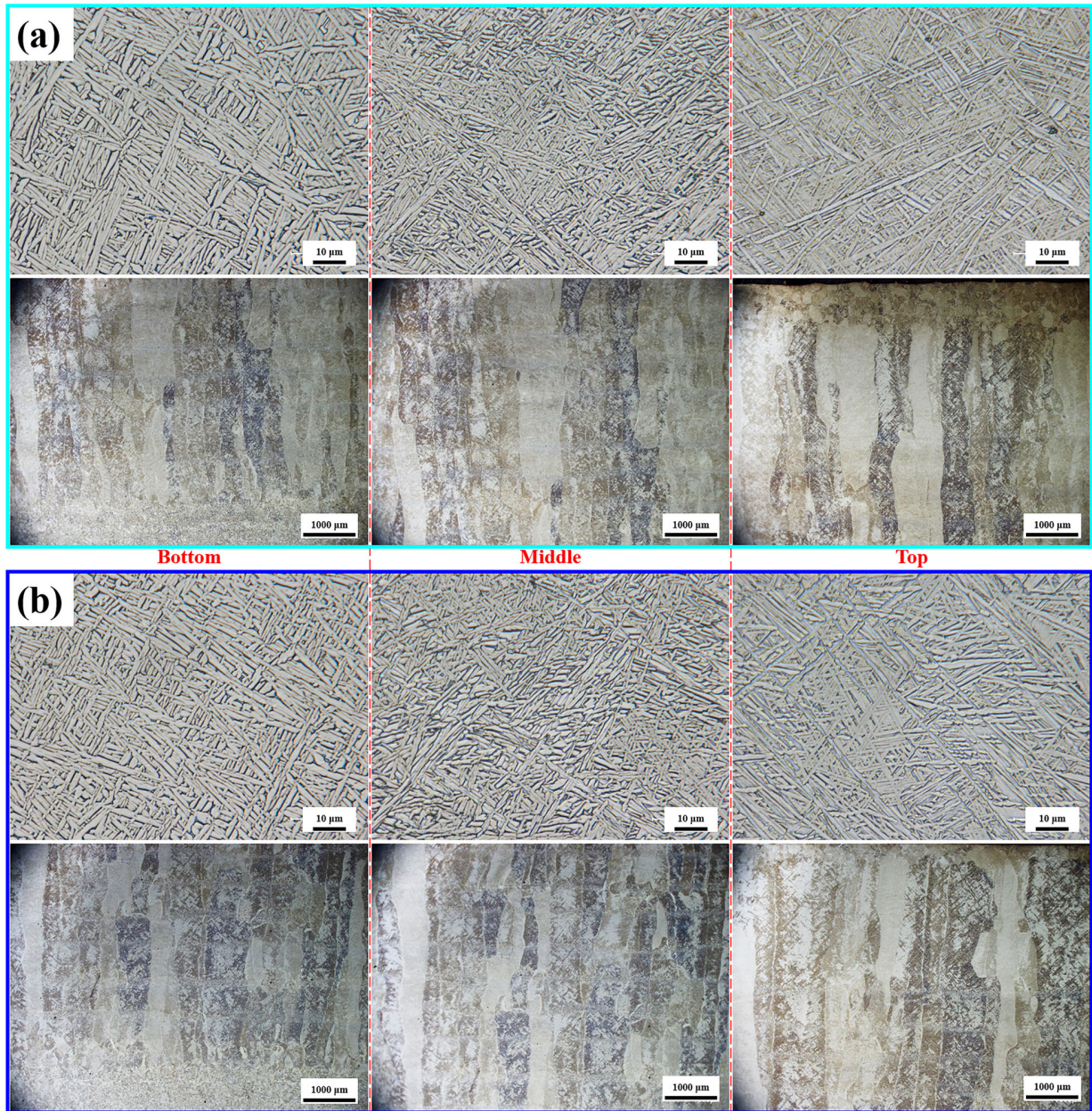


Figure 19. Comparison of the deposited macro/microstructures at the building centre and different heights of the block parts, corresponding to the thermal histories shown in Figure 17: (a) standard substrate; (b) Smart-Substrate.

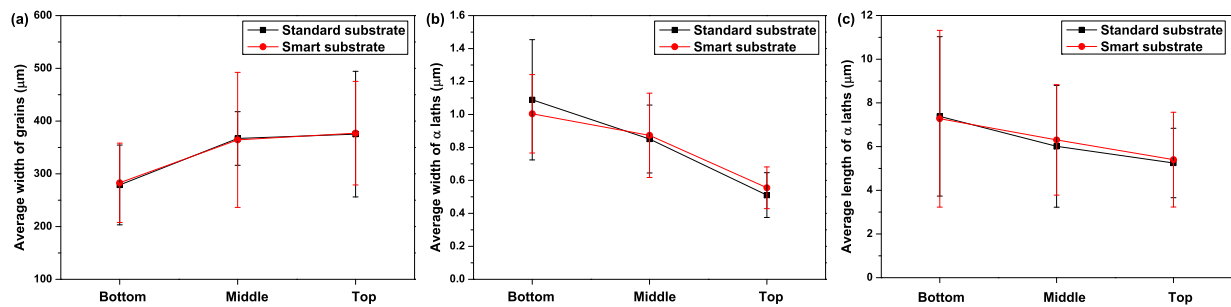


Figure 20. Comparison of the macro/microstructure size shown in Figure 19: (a) the average width of the β -grains; (b) the average width of the α laths; the average length of the α laths.

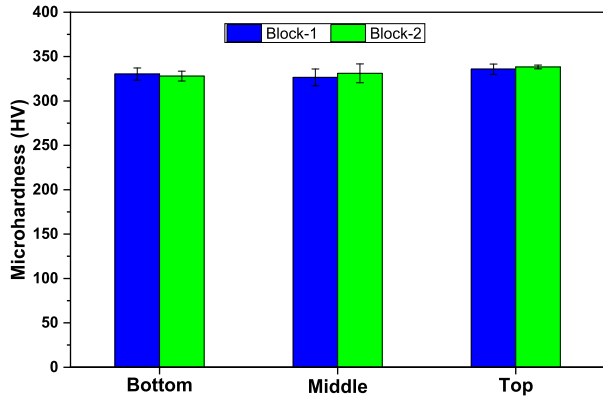


Figure 21. Comparison of the microhardness at the building centre and different heights of the two block parts.

Smart-Substrate strategy to avert stress accretion in DED is developed, different from MTG-based stress-control methods.

- (2) Three groups of different DED structures with increasing geometrical complexity (single-wall, rectangular and block parts) are used to demonstrate the effectiveness of Smart-Substrate. It is found that using the standard substrate easily produces remarkable part deflections and large residual stresses, especially stress concentrations at the corner of the builds, but this is not the case for the Smart-Substrate samples.
- (3) The key physical mechanism of applying the Smart-Substrate approach is to diminish the local mechanical stiffness of the upper part of the substrate to allow strains in the metal deposition to develop fully in an increased elastic range. Thus, the formation of residual stresses and plastic strains is curbed at the cost of slightly lowering the geometric precision of the build due to its freer volumetric contractions. This may be corrected in the design of the part by geometrical compensation.

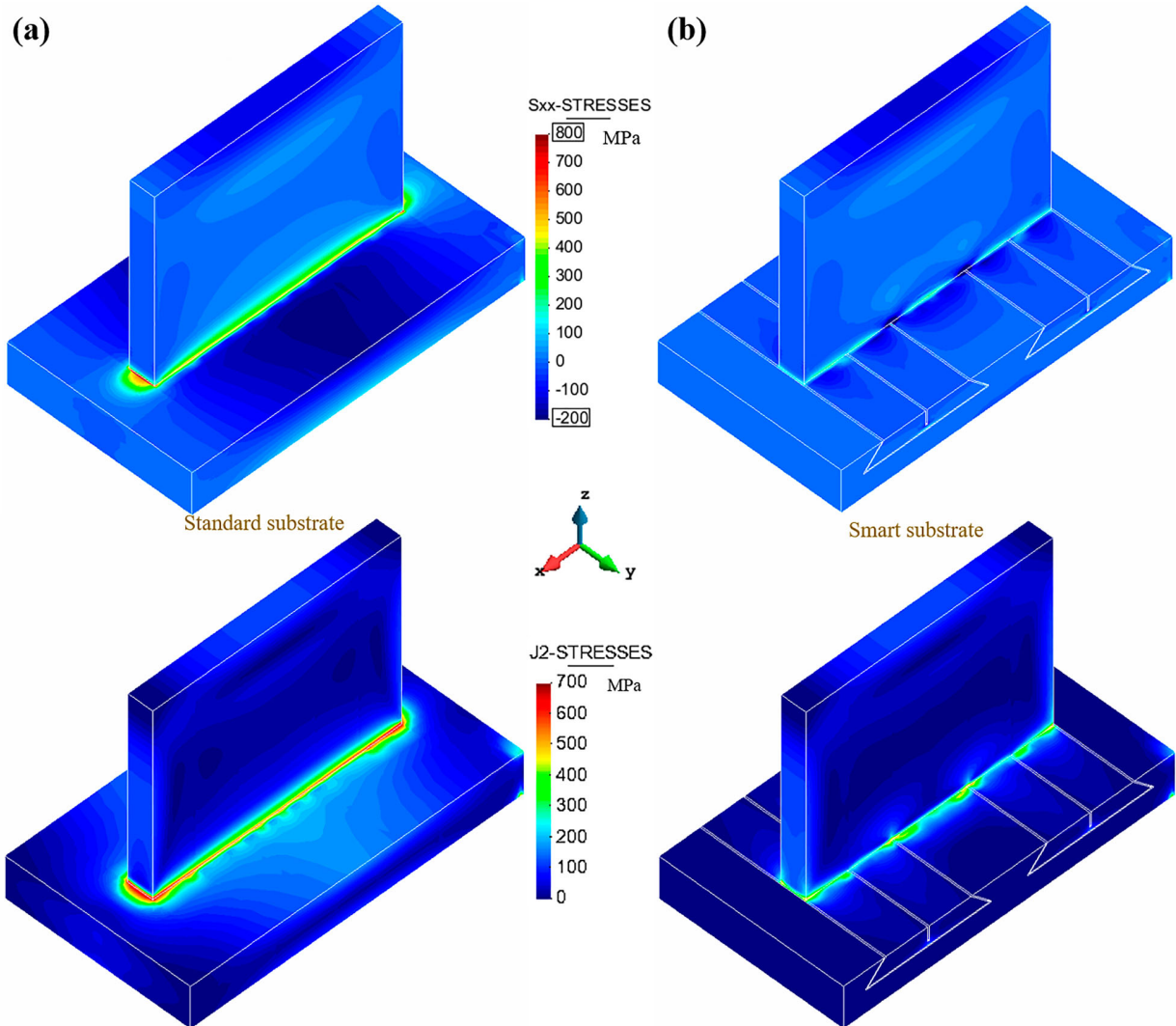


Figure 22. Residual longitudinal (S_{xx}) and von Mises stresses of two single-walls with an increased height of 50 mm built on (a) the standard and (b) the smart substrate.

- (4) Unlike MTG-based strategies, the Smart-Substrate strategy shows an unimportant influence on the thermal and metallurgical evolution as well as the resulting mechanical hardness because it preserves an effective heat conduction channel. This provides the possibility to address the stress problems, the microstructure design and the defect prevention, separately, for obtaining superior mechanical properties of AM-parts.

Disclosure statement

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APPLIED LPBF CASE: RECOATER INDUCED DISTORTION

INTRODUCTION

This chapter investigates recoater-induced distortions and build failures in LPBF, focusing on thin-walled Ti6Al4V parts. The study was motivated by repeated build failures observed in lightweight, thin-wall geometries. It was observed that the warpage consistently aligned with the recoater motion, indicating mechanical interference between the recoater blade and the part.

Recoater-related issues are a well-documented challenge [Yavari et al., 2021, Kayacan et al., 2019], particularly for thin-walled parts. These structures offer weight savings but their reduced stiffness makes them prone to distortion. When vertical warpage at the top of the build exceeds the nominal layer thickness, the recoater blade collides with the part, leading to *recoater crash* and, ultimately, build failure.

SUMMARY & CONCLUSIONS

The case study concerned the simultaneous fabrication of multiple thin-walled geometries, both open and closed. The recoater action was modeled as a distributed volumetric load applied to the top layers of the part. Numerical results were compared to 3D-scanned measurements and showed good agreement with the observed warpage patterns.

The analysis revealed that open-walled geometries were especially vulnerable due to the absence of lateral support, and that orientation relative to the recoater path strongly influenced the magnitude of the distortion: walls facing the recoater were more prone to failure than those aligned along its path.

Possible remedies include geometrical compensation to pre-warp the part in the opposite direction, and component agglomeration to provide mutual support and increase the effective stiffness of the build.

In the context of this thesis, it is worth noting that at the outset of the study, a full high-fidelity thermo-mechanical simulation of the simultaneous build of all the parts was attempted. However, after several unsuccessful runs due to the prohibitive computational cost, the approach was revised to individual thermo-mechanical simulations of each part, lumping 10 layers per time-step. In contrast to the preceding chapter on DED, where high-fidelity thermo-mechanical simulations remained computationally tractable, this case underscores the steep computational cost of LPBF modeling. As discussed in chapter 1, the separation of scales in LPBF is much more pronounced, rendering high-fidelity simulation of full builds unfeasible without resorting to extreme simplifications.

This underlines the need for advanced numerical techniques, such as those developed later in this thesis (chapters 7 and 8), to achieve part-scale LPBF simulations without excessive simplifications.

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Article

Recoater-Induced Distortions and Build Failures in Selective Laser Melting of Thin-Walled Ti6Al4V Parts

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Abstract: Additively manufactured thin-walled structures through selective laser melting (SLM) are of great interest in achieving carbon-neutral industrial manufacturing. However, residual stresses and warpages as well as recoater crashes often occur in SLM, leading to the build failure of parts, especially for large-scale and lightweight geometries. The challenge in this work consists of investigating how the recoater affects the warpage and (sometimes) causes the failure of different thin-walled Ti6Al4V parts (wall thickness of 1.0 mm). All these parts are printed on the same platform using a commercial SLM machine. After the loose powder removal and before the cutting operation, a 3D-scanner is used to obtain the actual warpage of each component. Next, an in-house coupled thermo-mechanical finite element model suitable for the numerical simulation of the SLM process is enhanced to consider the recoater effects. This numerical framework is calibrated to predict the thin-walled warpage as measured by the 3D-scanner. The combination of numerical predictions with experimental observations facilitates a comprehensive understanding of the mechanical behavior of different thin-walled components as well as the failure mechanism due to the recoater. The findings show that the use of a higher laser energy input causes larger residual stresses and warpage responsible for the recoater crashes. Finally, potential solutions to mitigate the warpage and the recoater crashes in the SLM of lightweight structures are assessed using the validated model.

Keywords: additive manufacturing; selective laser melting; recoater crashes; lightweight parts; thermo-mechanical finite element simulation



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1. Introduction

Selective Laser Melting (SLM) is one of the most used Additive Manufacturing (AM) technologies allowing for the cost-effective production of metallic components with highly complex geometries [1,2]. SLM is currently being adopted in different industrial sectors, such as bio-medical, aerospace and automotive engineering [3,4]. The SLM uses a laser heat source to selectively melt the metallic powder bed following a layer-by-layer sequence till completing the 3D printing of the components.

Figure 1 shows the steps of the SLM process: (1) the recoater blade spreads a new layer of metallic powder with a thickness of around 30~60 μ m; (2) a high-energy laser beam selectively melts the powder that defines the actual cross-section of the component according to a pre-defined scanning sequence generated by the slicer; (3) the printing platform is lowered to accommodate a new powder layer; (4) steps (1)~(3) are repeated until completing the printing of the whole part; (5) the loose powder is removed and the printed components are cut away from the base plate [5].

In SLM processes, the high-energy laser is very localized and the metallic powder is melted at a very high scan speed (close to 1 m/s). Thus, a very small melting pool is formed so that sharp temperature gradients (up to 10^7 °C/m) and significant cooling rates often exceeding 10^5 °C/s are observed in the heat-affected zone surrounding the

melting pool [6–8]. As a consequence, either large residual stresses (for thick components) or warpages (for thin-walled structures) are generated. Hence, the SLM process often fails because of excessive part distortion, cracking of the supporting structures due to the high residual stresses, and recoater crashes [9–11].

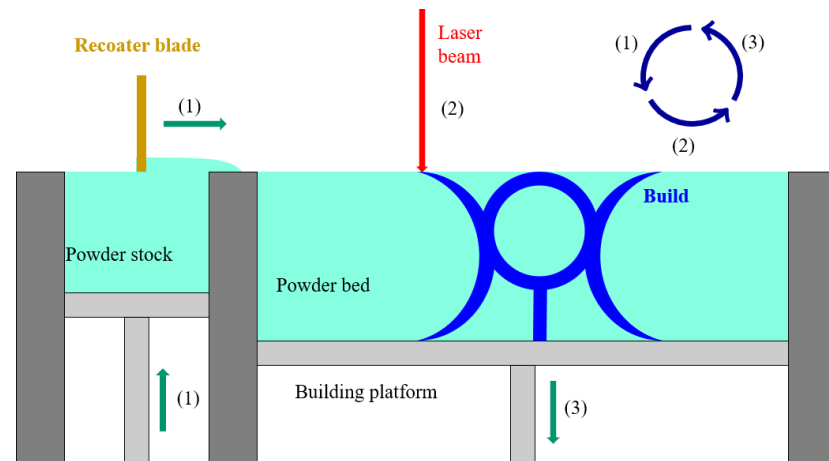


Figure 1. Schematic drawing of the workflow of the typical SLM process where the part shape is not fixed.

To reduce the carbon footprint, the manufacturing of lightweight structures is preferred, e.g., thin-walled titanium components used in the aerospace engineering sector, heat exchangers, and antennas [12–19]. Nonetheless, compared to thick and bulky components, the AM fabrication of lightweight parts is more challenging because they are more prone to warpages; as the building height increases, the mechanical constraint gradually reduces. Moreover, the temperature field increases because of the slow heat dissipation. Consequently, the residual stresses induced by the repeated laser melting and cooling processes generates large deformations, which increase with the printing height further from the building platform. When the vertical displacements at the top surface of the build exceed the pre-set thickness of the powder layer, the structural warpage of the build affects the recoating operation [20]. As a result: (i) the powder spreading is no longer uniform; (ii) the recoater deforms the underlying layers, plastifying the (hot) material; (iii) the warpage precludes the recoater’s movement, causing damages to the AM machine [21]; thus, the build-up fails before completing the whole printing.

Recoater crashes resulting from thermally-induced part deformations could be avoided by optimizing the process parameters, modifying the component design and its orientation in the building chamber, or optimizing the configuration of supporting structures [22–28]. For instance, Promoppatum et al. [25] investigated the influence of energy density (ED) on residual stresses and part deformations. They found that keyholing defects can be generated if the energy input is higher than 2.94 J/mm^2 , and an optimal ED of 2.0 J/mm^2 is recommended. Wang et al. [26,27] studied how to improve the quality of the surface roughness of overhanging structures caused by the melting of the powder bed during SLM fabrication. They found that to avoid any damage to the recoating device, the use of low-energy input and short scanning tracks is recommended. Additionally, Yakout et al. [28] found that adopting excessively high energy power ($>350 \text{ W}$) leads to improper layer melting, which favors the contact between the recoater and the asperities generated on the top surface of the build. Higher ED results in higher peak temperatures and a larger volume of the melting pool. Thus, higher thermal gradients and larger residual stresses are formed, contributing to more pronounced part warpages. Focusing on thin-walled geometries, characterized by poor structural stiffness, these distortions (e.g., vertical displacements) can cause the recoater crashes. Additionally, Le et al. [29] analyzed the quality of the powder bed as a function of the feedstock and different recoating strategies. Their results showed that rubber recoating blades with a larger contact surface area and mid-range recoating

velocities (10–80 mm/s) yield more uniform and compact powder layers, improving the printing quality while reducing the risk of recoater damages. Finally, it was found that the recoating speed directly affects the inter-layer cooling time and, thus, the heat accumulated in the build as well as its mechanical response [30,31]. Hence, using the right recoating speed helps to reduce the risk of the recoater impacting the deformed geometry of the AM build.

Lightweight structures are a critical component of many functional products. Thus, the analysis of build failures related to part deformations and the powder recoating system is of paramount importance for promoting their industrial application. At present, trial-and-error approaches as well as the technician's expertise operating the AM machines can prevent the recoater from crashing. Alternatively, numerical simulation provides a feasible and efficient approach to predict the thermal history and mechanical response during the whole AM process [32–35]. Thus, it is possible to identify the underlying cause of possible problems in the fabrication early and take the necessary measures to solve them. Kobir et al. [33] developed a thermomechanical modeling approach based on graph theory to predict the probability of the occurrence of recoater crashes in the SLM fabrication process and achieved high computational efficiency. Lu et al. [1] employed a coupled thermomechanical model to investigate the influence of the substrate design on the mechanical response in SLM of T-shaped Ti6Al4V parts. Their results showed that crack-free components can be printed by adding grooves within the substrate. Chakraborty et al. [10] numerically analyzed the in-process failure during the SLM process of thin-walled RENE65 and RENE108 parts. The finite element (FE) simulations of the AM process clearly show that the thermal stresses generated in thin-walled structures cause more pronounced warpages and, consequently, these light-weight structures are more prone to printing failures. Vastola et al. [35] simulated the SLM process to investigate the buckling phenomena of thin-walled tubular components, analyzing different structural designs. They found that part distortions can be mitigated by rounding the sharp edges in IN718 parts with a wall thickness of 0.4 mm. Li et al. [36] numerically studied the effect of the scan length on the deformation of thin-walled Ti6Al4V parts and found that the scan length of 4–6 mm is most suitable. Additionally, Chen et al. [37] used a layer-by-layer FE model to study the influence of the part dimension on the warpage of thin Ti6Al4V single-walls fabricated by SLM. They found that increasing the part thickness helps to reduce maximum deformation.

Recent studies suggested that the structure and size of grains formed during AM affect the strength and ductility of the printed material, as well as the residual stresses on a micro-scale [2,4]. However, for macro residual stresses and part deformations, these effects can be negligible when compared to the large thermal gradients induced by the high-energy laser beam in AM. Specifically, this work aims to understand the complicated interactions between the structural features of different thin-walled builds, thermal stresses, part deformation, and recoater effects on a macro-scale.

In this study, three kinds of thin-walled geometries are analyzed: single-wall, open, and closed structures. First, these structures are built using a SLM machine. Next, an in-house coupled thermo-mechanical FE software is enhanced to consider the interaction between the recoating system and the underlying printed layers. The validation and calibration of this model are accomplished by comparing the numerical predictions with the measured displacements obtained by a 3D-scanner. Finally, potential solutions are suggested to mitigate the component warpage induced by the AM process.

2. Experimental Campaign

The 3D printing fabrication is performed using a RENISHAW RenAM 500Q, (Wotton-under-Edge, UK) machine equipped with a 500 W YB-fiber laser system, with a wavelength of 1070 nm and a laser spot diameter of 75 μm . The AM takes place in a high-purity argon atmosphere in order to ensure a lower oxygen content (less than 1000 ppm) during the whole printing process.

In this work, gas-atomized Ti6Al4V powder with a particle size of 15~45 μm is used. The powder is dried in a vacuum oven (vacuum degree < 80 kPa) at 120 $^{\circ}\text{C}$ for 3.0 h. An annealed Ti6Al4V base-plate of $250 \times 250 \times 40 \text{ mm}^3$ is adopted to build different thin-walled structures. The scanning sequence is based on a 67° rotating deposition pattern. Table 1 lists the optimized SLM processing parameters used in this research, guaranteeing the fabrication of fully dense Ti6Al4V parts. A relatively high ED of 6.12 J/mm^2 is adopted to amplify the mechanical effects in lightweight parts.

Table 1. Printing parameters used for the SLM process.

Laser Power (W)	Layer Thickness (μm)	Scan Speed (mm/s)	Hatch Spacing (μm)	Laser Beam Diameter (μm)
300	40	700	70	70

Figure 2 shows the nominal CAD models of different thin-walled structures sent to the slicing tool to generate the scanning sequence for the SLM machine. After build-up; the actual printed parts are measured by the Breuckmann Smart SCAN3D scanner with a measurement accuracy of 0.015 mm. The corresponding displacements causing the part warpage are obtained by the Geomagic Control X software by comparing the scanned images with the nominal CAD geometries. The thin-walled structures are not cut from the substrate when their distortions are measured

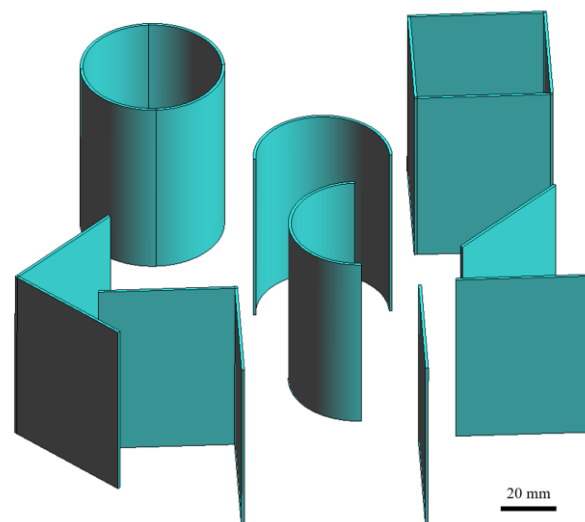


Figure 2. Nominal CAD models of different thin-walled structures sent to the slicing tool to generate the scanning sequence for the SLM machine.

3. Computational Simulation

A coupled thermo-mechanical FE model implemented in the in-house COMET software [38,39] is employed to simulate the SLM process. The fractional step method is used to obtain a staggered solution. Thus, the thermal problem is solved first, followed by the mechanical analysis, at each time-step of the AM process. A detailed description of the thermo-mechanical model used for AM can be found in previous publications [40,41].

3.1. Thermal Problem

The balance equation governing the transient thermal analysis [40] can be written as:

$$\dot{H} = -\nabla \cdot \mathbf{q} + \dot{Q} \quad (1)$$

where $\dot{H}$ is enthalpy rate, $\mathbf{q}$ is heat flux and $\dot{Q}$ is the volumetric heat source (per unit of volume). Here, $\dot{Q}$ is characterized by the total laser input $\dot{P}$ and the actual energy efficiency η_p , applied in the melting-pool volume $V_{mp}^{\Delta t}$:

$$\dot{Q} = \frac{\eta_p \dot{P}}{V_{mp}^{\Delta t}} \quad (2)$$

The heat flux, $\mathbf{q}$, is defined by Fourier's law:

$$\mathbf{q} = -k \nabla T \quad (3)$$

where k is the (temperature-dependent) thermal conductivity, and ∇T is the thermal gradient.

Three different heat dissipation mechanisms are considered: (i) the heat conduction through the substrate (the platform or previously deposited layers) and through the surrounding loose powder, (ii) heat convection, and (iii) radiation at the top surface to the environment before the next layer is deposited.

The heat loss by convection is defined via Newton's law:

$$q_{conv} = h_{conv}(T - T_{room}) \quad (4)$$

where h_{conv} is the Heat Transfer Coefficient (HTC) due to convection, T and T_{room} are the surface temperature of the build and the ambient temperature, respectively.

The heat dissipation by radiation, q_{rad} , is computed by Stefan–Boltzmann's law: where ε_{rad} is the surface emissivity and σ_{rad} is the Stefan–Boltzmann constant.

$$q_{rad} = \varepsilon_{rad} \sigma_{rad} (T^4 - T_{room}^4) \quad (5)$$

3.2. Mechanical Analysis

The mechanical analysis is carried out by solving the balance of momentum and the continuity equations [41]:

$$\nabla \cdot \mathbf{s} + \nabla p + \mathbf{b} = 0 \quad (6)$$

$$\left(\nabla \cdot \mathbf{u} - e^T \right) - \frac{p}{K(T)} = 0 \quad (7)$$

where $\mathbf{b}$ represents the body force (per unit of volume), $K(T)$ is the (temperature-dependent) bulk modulus, and σ stands for the Cauchy stress tensor, which can be split into its spherical p and deviatoric $\mathbf{s}$ parts, respectively:

$$\sigma = p\mathbf{I} + \mathbf{s}(\mathbf{u}) \quad (8)$$

The thermal strains, e^T , are defined as following:

$$e^T(T, f_s) = e^{cool}(T) + e^{pc}(f_s) \quad (9)$$

where $e^{cool}(T)$ and $e^{pc}(f_s)$ are the thermal deformations and the thermal shrinkage during the liquid-to-solid phase change, expressed as:

$$e^{cool}(T) = \alpha(T - T_0) \quad (10)$$

$$e^{pc}(f_s) = \beta f_s \quad (11)$$

where T_0 is the initial temperature, f_s is the solid fraction, α and β are the thermal expansion and thermal shrinkage coefficients, respectively.

Due to the repeated heating and cooling cycles in the SLM process, the cycling thermal loads during the metal depositions vary between room temperature (T_{room}) and the high temperatures above the melting point (T_{melt}) when the laser source is applied. Hence, the

material behavior must be characterized within the entire temperature range, including solid, mushy, and liquid phases. In this work, a J2-thermo-elasto-visco-plastic model [22] is used for the solid phase for temperatures varying between T_{room} and the annealing temperature, T_{anneal} . The von-Mises yield surface is defined as:

$$\Phi(\mathbf{s}, q_h, T) = \|\mathbf{s}\| - \sqrt{\frac{2}{3}} [\sigma_y(T) - q_h] \quad (12)$$

where σ_y is the (temperature-dependent) yield stress and q_h , the stress-like variable controlling the isotropic strain hardening [40], expressed as:

$$q_h(\xi, T) = -[\sigma_\infty(T) - \sigma_y(T)] [1 - e^{-\delta(T)\xi}] - h(T)\xi \quad (13)$$

where ξ is the isotropic strain-hardening variable, σ_∞ is the (temperature-dependent) saturation flow stress, while δ and h are the parameters used to control the exponential and linear hardening laws, respectively.

The deviatoric part of Cauchy's stress tensor $\mathbf{s}$ can be written:

$$\mathbf{s} = 2G(\mathbf{e} - \mathbf{e}^{vp}) \quad (14)$$

where G is the (temperature-dependent) shear modulus, $\mathbf{e}$ are the total (deviatoric) strains obtained from the total strain tensor $\boldsymbol{\varepsilon}(\mathbf{u}) = \nabla^{sym}(\mathbf{u})$, and $\mathbf{e}^{vp}$ are the deviatoric visco-plastic strains. The evolution laws of both the visco-plastic strain tensor and the isotropic strain-hardening variable are obtained from the principle of maximum plastic dissipation as:

$$\dot{\mathbf{e}}^{vp} = \dot{\gamma}^{vp} \frac{\partial \Phi(\mathbf{s}, q_h, T)}{\partial \mathbf{s}} = \dot{\gamma}^{vp} \frac{\mathbf{s}}{\|\mathbf{s}\|} = \dot{\gamma}^{vp} \mathbf{n} \quad (15)$$

$$\dot{\xi} = \dot{\gamma}^{vp} \frac{\partial \Phi(\mathbf{s}, q_h, T)}{\partial q_h} = \sqrt{\frac{2}{3}} \dot{\gamma}^{vp} \quad (16)$$

where $\mathbf{n}$ represents the normal yield surface, and $\dot{\gamma}^{vp}$ stands for the visco-plastic multiplier:

$$\dot{\gamma}^{vp} = \left\langle \frac{\Phi(\mathbf{s}, q_h, T)}{\eta} \right\rangle^{\frac{1}{m}} \quad (17)$$

where $\langle \cdot \rangle$ are the Macaulay brackets, m and η are the sensitivity rate and plastic viscosity, respectively.

Ti6Al4V is characterized by a solid-state phase change (SSPC) which affects the mechanical behavior of the material. Denlinger et al. [42] proposed using an annealing temperature of 690 °C to consider the SSPC-induced stress relaxation in the coupled thermal-stress simulations of AM Ti6Al4V. A good agreement between the simulated and measured results is proven. However, Chen et al. [43] investigated the wire-fed electron-beam AM via variable temperature XRD measurements, and the annealing temperature is finally set to 850 °C in their thermo-mechanical simulations. The difference in the definition of the material constitutive laws used to simulate the mechanical behavior of AM Ti6Al4V is identified as being mainly responsible for the non-unique annealing temperature definition. In our previous numerical study [41], an annealing temperature of 750 °C was selected based on the in situ strain measurements during AM.

When the temperature T increases to T_{anneal} , the yield stress σ_y gradually reduces until vanishing and a mushy/liquid behavior can be observed. When $T > T_{anneal}$, the deviatoric Cauchy stress is characterized by a purely viscous law, which can be deduced from Equation (18) when $\sigma_y \rightarrow 0$ [44]. Thus:

$$\mathbf{s} = \eta_{eff} \dot{\mathbf{e}}^{vp} \quad (18)$$

where $\eta_{eff} = \eta \left(\dot{\gamma}^{vp} \right)^m$ stands for the effective viscosity. Typically, a non-Newtonian behavior with $m > 1$ is adopted for the mushy phase ($T_{anneal} < T < T_{melt}$), while Newtonian behavior ($m = 1$) is used for the liquid phase ($T \geq T_{melt}$) [39].

3.3. Computational Modeling of SLM

In this work, a time-marching scheme is used to simulate the SLM process. The heat source moves step-by-step from the location at time t^n to the next position at time t^{n+1} . During this time step, $\Delta t = t^{n+1} - t^n$, a heat source is applied to the affected elements. The *birth-death-element* technique is adopted to activate the corresponding elements belonging to each layer, according to the actual building sequence defined by the slicing tool (e.g., Cura). Both the SLM machine and the software read the same input file defined in Common Layer Interface (CLI) or g-code formats [45].

Figure 3 shows the FE meshes of five different thin-walled structures characterized by the same wall thickness of 1.0 mm. The numbers of hexahedral elements and nodes used for these geometries are listed in Table 2.

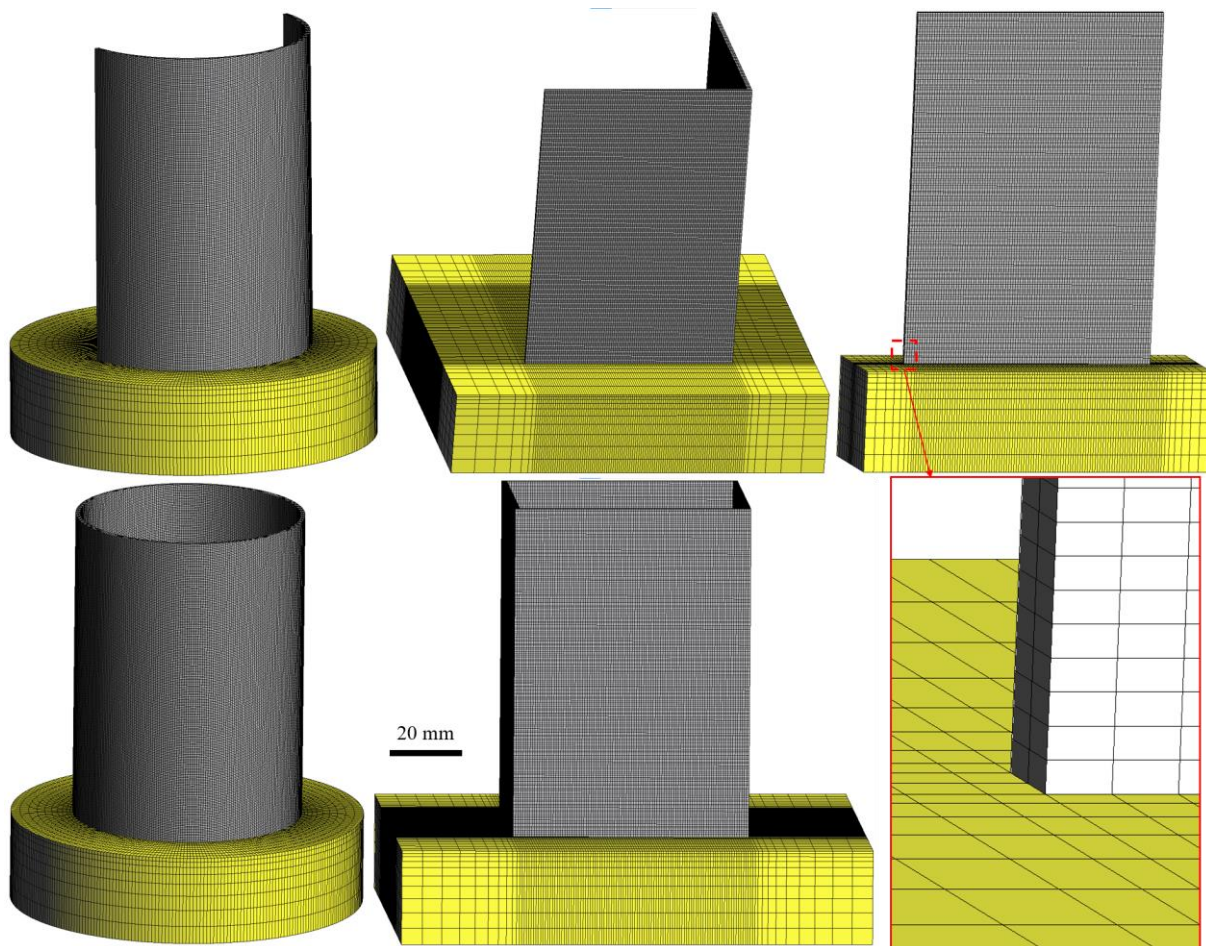


Figure 3. 3D FE mesh models of different thin-walled structures.

In order to reduce the computational cost while preserving the simulation precision, 10 physical layers are lumped into one with an equivalent height of 0.4 mm [46]. The meshes generated have a fixed size of approximately $0.5 \times 0.5 \times 0.2 \text{ mm}^3$ for the built parts, while a coarser mesh is utilized for the base plate [47].

Table 2. Numbers of the FE elements and the nodes for different thin-walled geometries.

Thin-Walled Structures	Number of FE Elements	Number of Nodes
Cylindrical part	244,480	352,320
Semi-cylindrical part	145,280	204,450
Square part	339,840	477,309
L-shape part	219,560	295,959
Single-wall part	65,680	94,395

3.4. Material Properties and Boundary Conditions

Temperature-dependent Ti6Al4V material properties used for both the printed parts and the substrate are shown in Table 3 [38]. The environment temperature is set to 23 °C during the whole SLM process. The loose powder surrounding the SLM parts is not included in the computational domain, and an equivalent boundary condition ($HTC = 5 \text{ W}/(\text{m}^2 \cdot ^\circ\text{C})$) is used to consider its effect [34]. The heat loss at the top surface of the last printed layer is defined by a heat convection coefficient of $12.7 \text{ W}/(^{\circ}\text{C} \cdot \text{m}^2)$ and an emissivity of 0.7 [48]. The laser efficiency during the SLM process of Ti6Al4V is set to $\eta = 0.4$ [1]. An initial temperature of 23 °C is set for the new elements in the building layers. The bottom surface of the substrates is fixed as in the actual SLM machine.

Table 3. Temperature-dependent material properties of Ti6Al4V.

Temperature (°C)	Density (kg/m ³)	Specific Heat (J/(kg·°C))	Thermal Conductivity (W/(m·°C))	Poisson's Ratio	Young's Modulus (GPa)	Thermal Dilatancy (μm/m/°C)	Yield Stress (MPa)
20	4420	546	7.0	0.345	110	8.78	850
205	4395	584	8.75	0.35	100	10.0	630
500	4350	651	12.6	0.37	76	11.2	470
995	4282	753	22.7	0.43	15	12.3	13
1100	4267	641	19.3	0.43	5	12.4	5
1200	4252	660	21.0	0.43	4	12.42	1
1600	4198	732	25.8	0.43	1	12.5	0.5
1650	3886	831	35	0.43	0.1	12.5	0.1
2000	3818	831	35	0.43	0.01	12.5	0.01

3.5. Modeling of the Recoater Action

In the deposition process, contact between the recoater and the component happens when the warpages of the printed thin-walled structure reach the threshold of the used SLM machine ($\approx 40 \text{ μm}$). In this instance, the friction force between the recoater and the part acts on the top surface of the newly deposited layer. The accumulated effect of this lateral force increases as both the height of the part and its warpages increase. Therefore, the effect of the recoater force is similar to that of the vertical gravity load of the deposited material.

In this work, the recoater action is modeled as an external volumetric load in the direction of the recoater blade (Y-axis), gradually applied to the growing structures with continuous layer-by-layer element activation in the mechanical simulations. Specifically, a lateral Y-directional volumetric force of $2.2 \times 10^{-3} \text{ N}/\text{mm}^3$ is applied to the newly activated elements according to the model calibration against the experimental measurements.

4. Results and Discussion

In this section, the warpage and build failures of three types of lightweight geometries with increasing structural stiffness are investigated and discussed: (i) single-wall structures; (ii) open structures; and (iii) closed geometries, as shown in Figure 4. The corresponding geometrical dimensions are shown in Table 4. Note that the actual height of the printed components does not reach the nominal value and a rough top surface for all the thin-walled structures appears. This is due to the contact between the recoater blade and the top surface of the builds during the powder spreading process in the final stage of the AM

process [27]. If the contact occurs when the solidified material is still hot and deformable, proceeding with the building process can lead the recoater blade to crash [10].

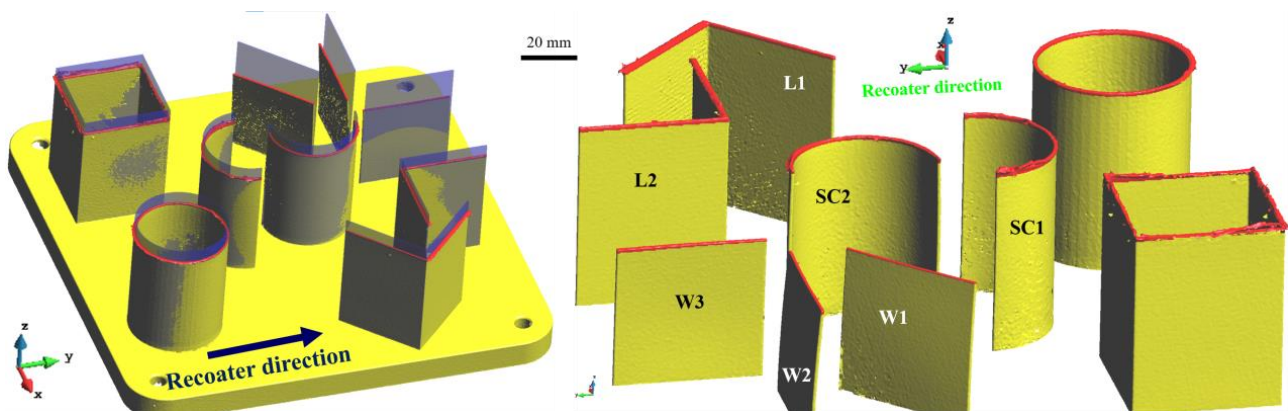


Figure 4. Thin-walled structures: nominal CAD model in blue, while printed parts are depicted in yellow color. The roughness of the top surfaces induced by the recoater is highlighted in red. (W1, W2, etc. are the sample names.)

Table 4. Geometrical dimensions of different thin-walled structures.

Part Shape	Horizontal Size (mm)	Wall Thickness (mm)	Designed Building Heights (mm)	Actual Building Heights (mm)
Cylinder	Ø50.0	1.0	70.0	≈62.0
Semi-cylinder	Ø50.0	1.0	70.0	≈62.0
L-shape	50.0 × 50.0	1.0	70.0	≈62.0
Square	50.0 × 50.0	1.0	70.0	≈62.0
Single-wall	50.0 × 1.0	1.0	70.0	≈50.0

To calibrate the thermo-mechanical FE model for the SLM process, the predicted part warpages are compared to the measured displacements (by 3D-scanner) with respect to the nominal CAD geometries.

4.1. Single-Wall Structures

Figure 5 shows the uncompleted build of 3 single-wall parts and the corresponding nominal CAD geometries. Note that large distortions, up to 3 mm, are measured at the top surface of the builds. The lower section of the walls deforms in the recoating direction while the upper part is opposite to it. This depends on the induced thermal stresses and the interaction with the recoating system. Hereby, the residual longitudinal (σ_{xx}) and vertical (σ_{zz}) stresses are shown in Figure 6. It can be seen that high tensile stresses are generated at the top and the bottom layers as well as at both lateral edges, while the central area of the single-wall presents compressive stresses. This leads to the buckling of the thin-walls when any out-of-plane load such as the recoating process is applied.

Tensile stresses appear when the first layers are printed on the thick and cold substrate which induces a strong mechanical constraint. Similarly, at the top surface as well as at the edges of the wall, high thermal gradients (up to 1×10^7 °C/m) are induced and the faster cooling at these locations results in large tensile stresses [1]. These residual stresses induce the warpage of thin-walled structures because of their poor structural stiffness. A similar phenomenon has been previously reported through numerical studies in references [10,37].

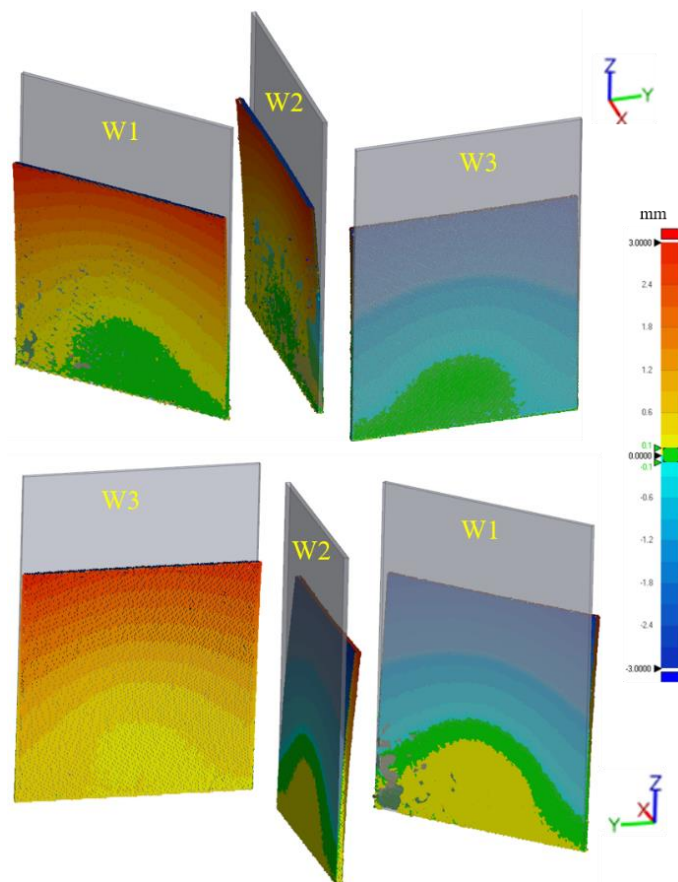


Figure 5. Comparison between the unfinished single-wall parts and the corresponding nominal CAD (grey) geometries.

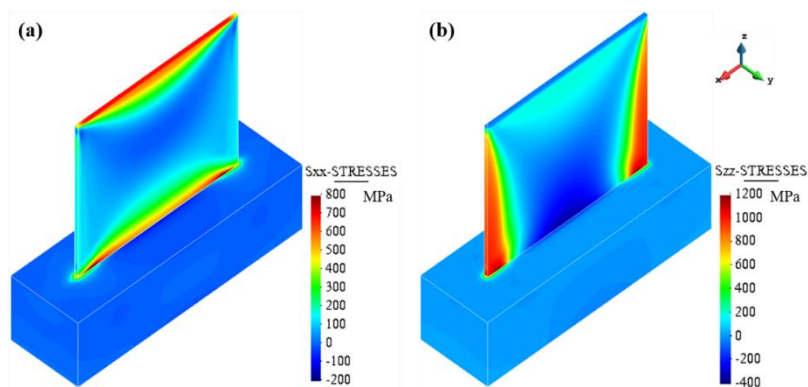


Figure 6. Residual stress distribution of the single-wall part at the end of the printing: (a) longitudinal σ_{xx} stresses; (b) vertical σ_{zz} stresses.

4.2. Open Thin-Walled Structures

The 3D-printing of two different open structures (semi-cylindrical and L-shape parts) is investigated in this section. Figures 7 and 8 show the displacement distributions of two semi-cylindrical parts (SC1 and SC2) with different orientations with respect to the recoating system, as shown in Figure 4. The predicted warpage profiles are in good agreement with the experimental results.

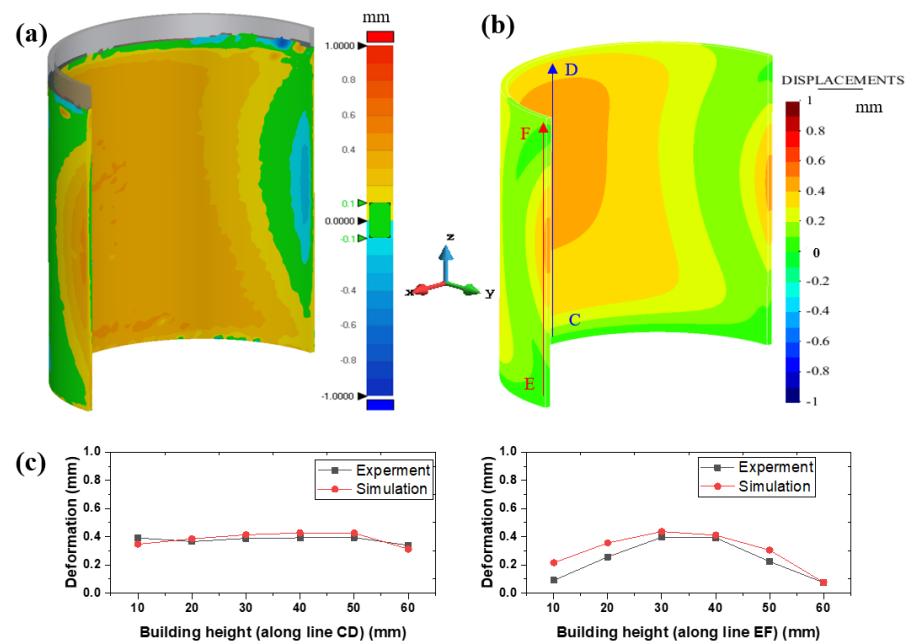


Figure 7. Semi-cylindrical (SC1) part: comparison between the (a) experimental and (b) simulated displacement distribution. (c) The deformation distribution along the lines CD and EF, which are located at the center of the inner surface and at the edge of the outer surface, respectively.

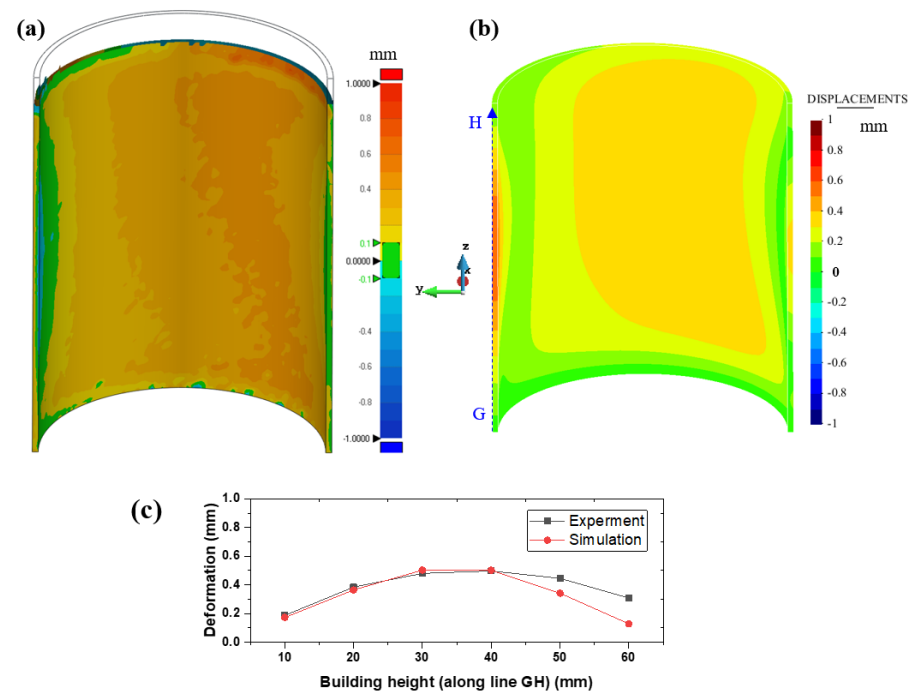


Figure 8. Semi-cylindrical (SC2) part: comparison between the (a) experimental and (b) simulated displacement distributions. (c) The deformation distribution along the line GH, located at the edge of the build.

It can be seen from Figure 7 that large displacements (up to 0.4 mm) are produced in the central region of the SC1 sample. The observed bulging is due to the residual stresses induced by the SLM fabrication process. Similar to the single-wall parts, these open semi-cylindrical geometries suffer of high tensile stresses along the top and bottom circumferential sides as well as at both vertical edges. As shown in Figure 9, the external

surface of the inner region is characterized by tensile stresses, while the inner surface is compressed. This produces the bulging, as also reported in [49,50].

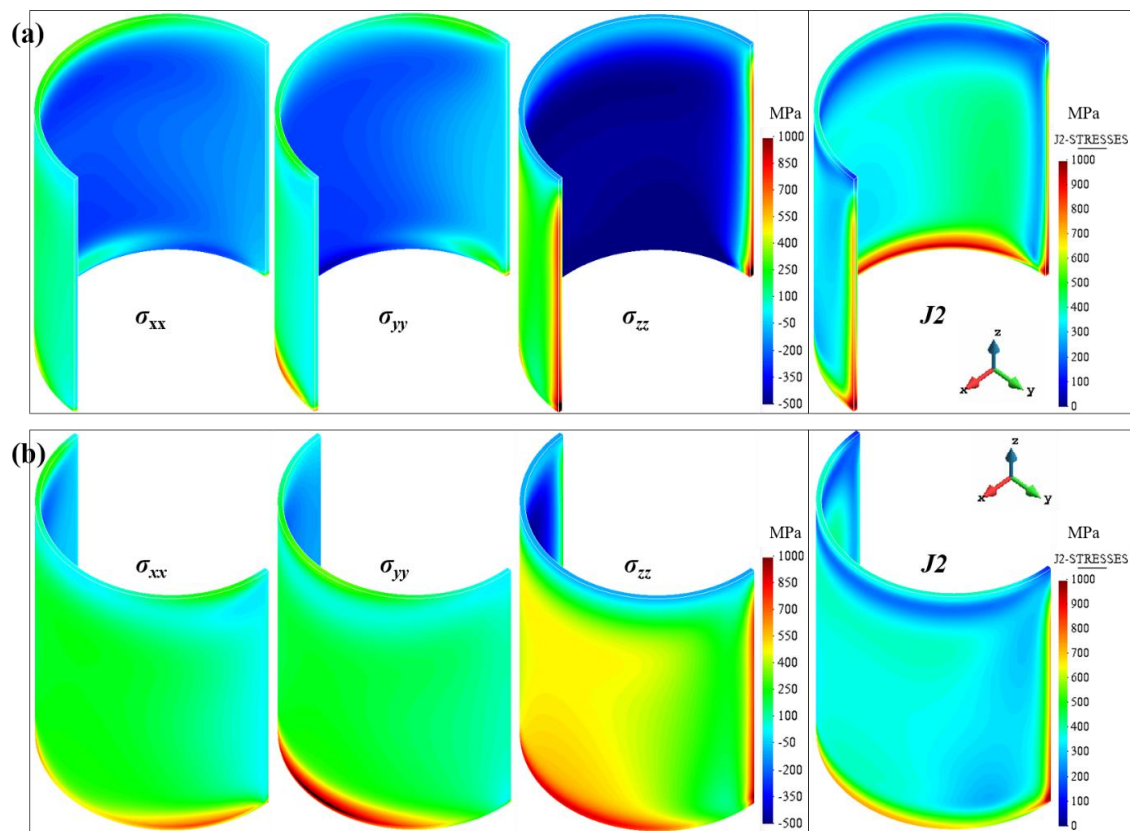


Figure 9. Residual stresses in three orthogonal directions and von Mises stress fields: (a) semi-cylindrical (SC1) part; (b) semi-cylindrical (SC2) part.

The bulging also induces vertical displacements which interfere with the powder spreading by the recoating system. As a consequence, the top surface presents a roughness deteriorating the printing job until, eventually, the recoater crashes. This interference also provokes the appearance of forces typically in the recoater advancing Y-direction, and, consequently, forcing bending in this direction (see Figure 7a).

Similar considerations apply for the semi-cylindrical (SC2) structure, as shown in Figure 8. In this case, the bulging is even more pronounced (approximately 0.5 mm).

The comparison between the predicted and measured out-of-plane displacements of the two L-shape parts, namely the L1 and L2 samples, is shown in Figures 10 and 11, respectively.

The difference in the manufacturing process between these two thin-walled structures is due to their orientations with respect to the recoating movement. In particular, sample L2 has one of the two walls parallel to the movement of the recoater (see Figure 4). Thus, its structural stiffness to the recoater loading is higher than the one of sample L1. This can be easily appreciated when comparing the warpages of L1 and L2 and keeping in mind that the recoater loading is in the Y-direction.

Figure 12 shows the residual stresses for the two L-shaped parts. The stress distributions are similar for both cases, mainly depending on the thermal deformations during the printing process. As for the single-wall builds, the L-shaped structures present high tensile stresses at the external edges as well as at the top and bottom layers. At the sharp corner, a similar vertical stress concentration can also be appreciated. Similar stress results can be found in [51,52]. This stress field is responsible for the pronounced double buckling shown in Figures 10 and 11.

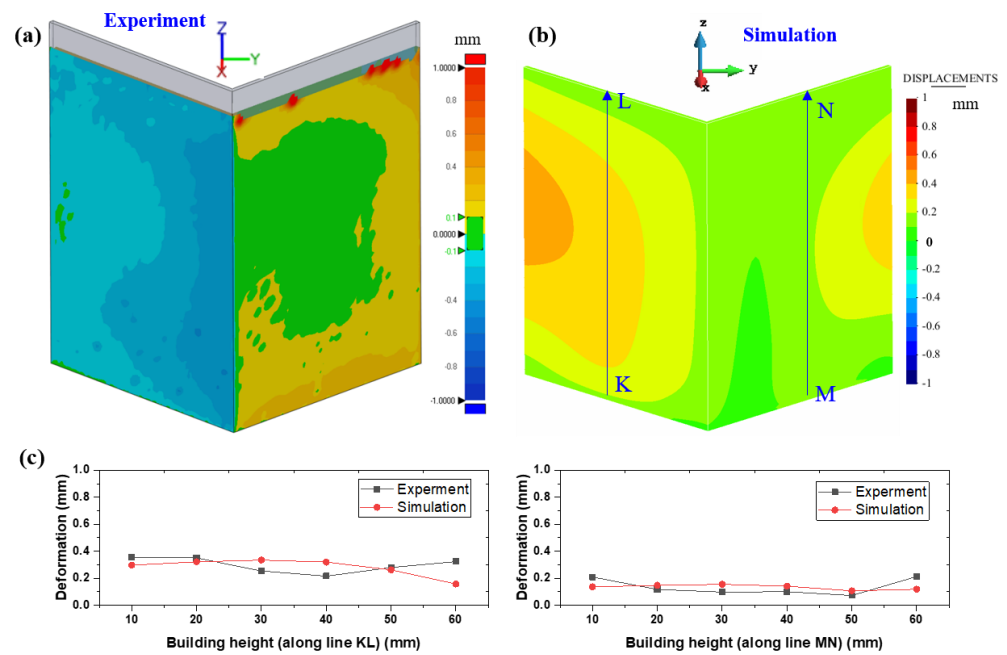


Figure 10. L-shape (L1) part: comparison between the (a) experimental and (b) simulated displacement distributions. (c) The deformation distribution along the lines KL and MN, which are located at the center of the two outer surfaces of the build, respectively. The negative value of the displacements in the experimental results means that the distortion is towards the inside of the CAD geometry.

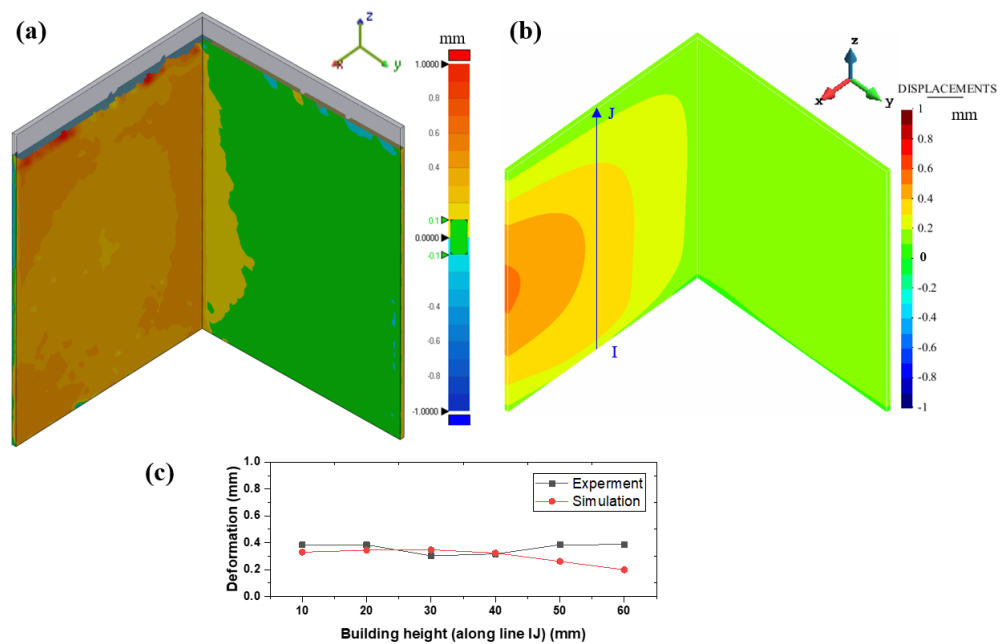


Figure 11. L-shape (L2) part: comparison between the (a) experimental and (b) simulated displacement distributions. (c) The deformation distribution along the line IJ located at the center of the inner surfaces of the build.

4.3. Closed Thin-Walled Structures

In this section, the mechanical behavior of two closed structures, the hollow cylindrical and square geometries, is studied to assess the influence of recoater interference during the SLM process.

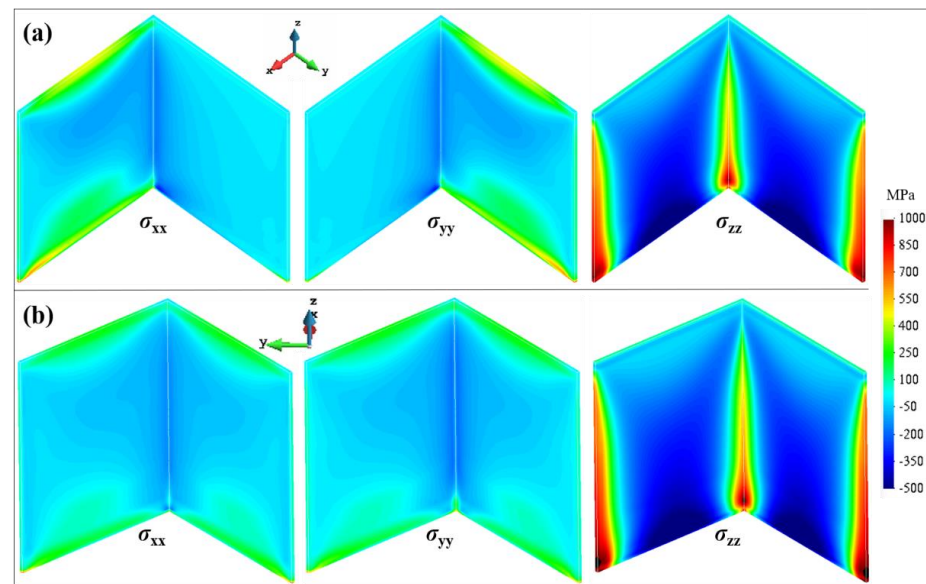


Figure 12. Residual stresses in three orthogonal directions: (a) L1 case; (b) L2 case.

Figure 13 compares the simulated displacement distributions and the experimental 3D-scan measurements for the cylindrical part. Figure 14 shows the corresponding residual stress field. Note that compressive stresses are produced on the inner surface of the cylinder while its external surface suffers tensile stresses. Thus, the cylinder contracts in the radial direction during the cooling process, and relatively small radial displacements are generated due to the higher structural stiffness of closed geometries compared to the open ones [53,54]. However, also in this case, a large Y-displacement, up to 0.5 mm, can be appreciated (Figure 13). Moreover, the build is uncompleted due to the collision between the scraper and the distorted part.

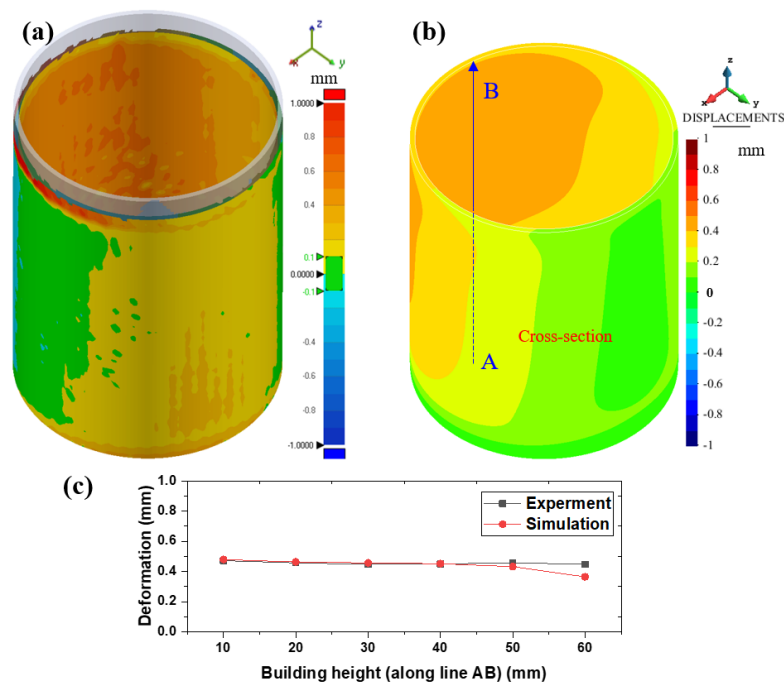


Figure 13. Comparison between the (a) experimental and (b) simulated displacement distributions of the hollow cylindrical part. (c) The deformation distribution along the line AB located at the center of the inner surfaces of the build.

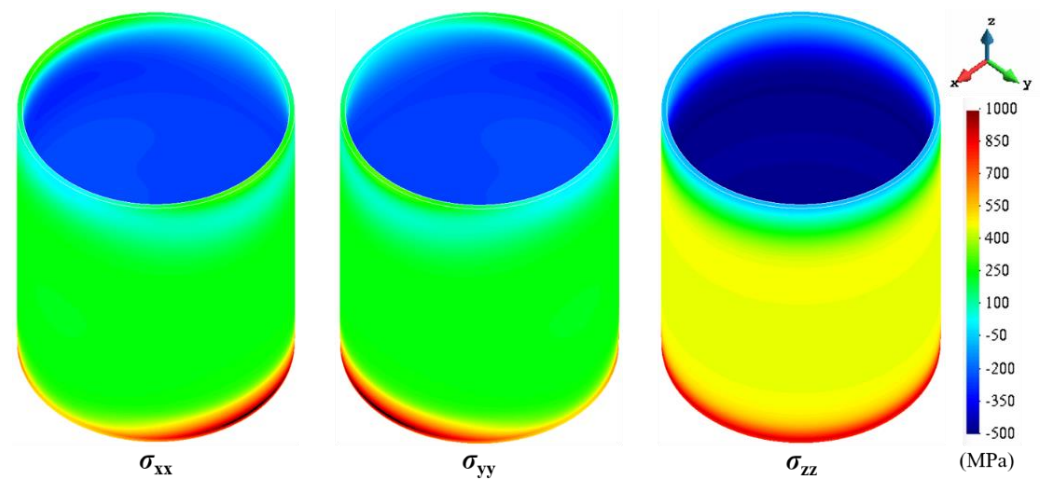


Figure 14. Hollow cylindrical part: residual stresses in three orthogonal directions.

Similar considerations apply for the hollow square part in terms of both warpage (see Figure 15) and stress distributions (see Figure 16). The higher stiffness of this geometry compared to the single-wall or the L-shape structures implies a smaller distortion of the build. However, in Figure 15a, the same bulging phenomenon can be appreciated, being more pronounced in the surfaces orthogonal to the recoating direction.

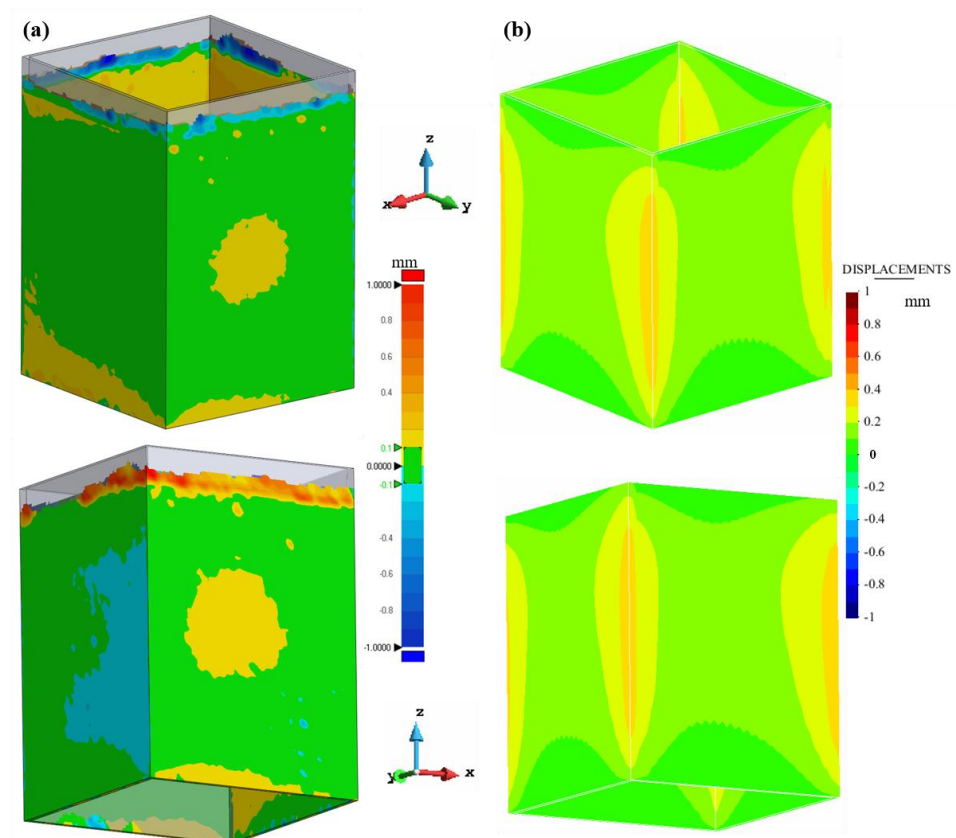


Figure 15. Comparison between the (a) experimental and (b) simulated displacement distributions of the hollow square part.

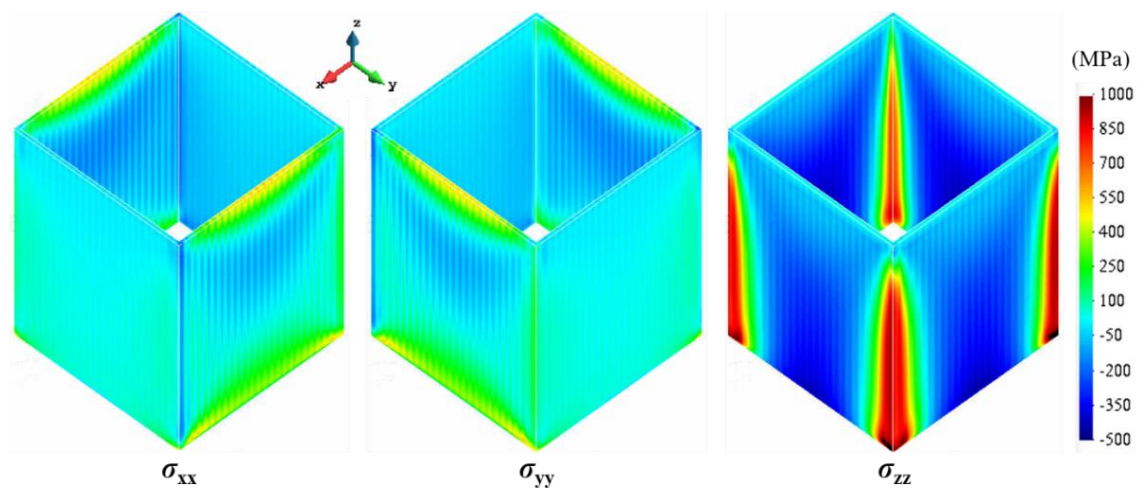


Figure 16. Hollow square part: residual stresses in three orthogonal directions.

5. Proposed Strategies to Reduce the Warpage of Thin-Walled Structures

This numerical study demonstrates that the residual stresses generated by the AM fabrication process can lead to large distortions and buckling phenomena, particularly when thin-walled structures are printed. The structural stiffness of the geometry is one of the key factors to mitigate the final warpage of the builds. A possible strategy to mitigate the distortions during the AM process is the component integration, as shown in Figure 17. This implies that the manufacturing process must include two stages: (i) 3D printing and (ii) separation of parts (e.g., cutting). The effectiveness of this procedure is evident for the geometries investigated in this work. However, more complex geometries can be placed on the base platform, keeping in mind these results; different components to be printed could share some of the surfaces, edges, etc.

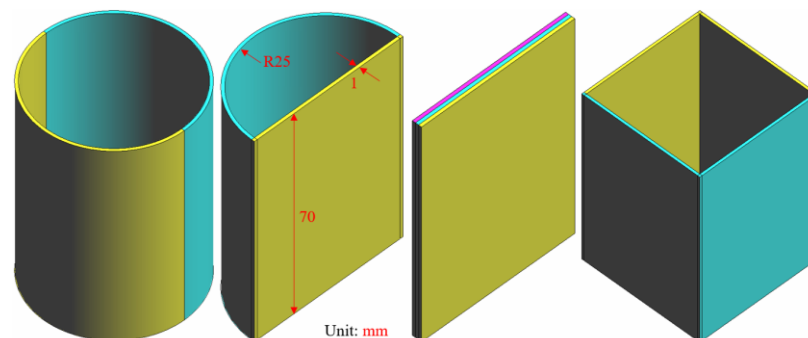


Figure 17. Component integration for improving the SLM process of different open thin-wall geometries. Each color corresponds to one part.

The benefits of component integration not only include increased global stiffness of the thin-walled structures but also an improved temperature field. In fact, the stress concentration at the lateral edges is due to their faster cooling. Thus, agglomerating the parts and integrating them by sharing some of the geometrical features (edges, surfaces, etc.) can produce a more uniform temperature field. Thus, the temperature gradients responsible for the thermal stress concentrations can be effectively mitigated.

Geometry compensation is another possibility to guarantee the geometrical precision of thin-walled lightweight structures fabricated by SLM [55,56]. This is an inverse engineering strategy used to modify the nominal CAD geometry considering the part warpage predicted by the numerical simulation to iteratively compensate the initial CAD model.

Figure 18 demonstrates the effectiveness of using geometric compensation after one iteration. Observe that high residual stresses still persist. However, these can be addressed through post annealing treatment.

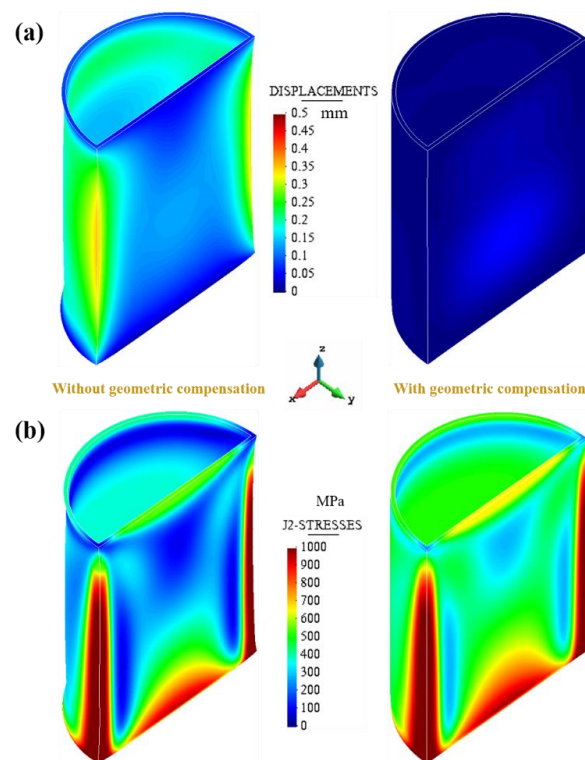


Figure 18. One integrated component from Figure 17 without and with geometric compensation: (a) distortions; (b) residual stresses.

Finally, using a softer scraper in the current SLM machine would also be beneficial for reducing part deformations and damages to the recoating system.

6. Conclusions

In this work, the 3D-printing of different lightweight geometries of Ti6Al4V is investigated. In-house FE thermo-mechanical software has been enhanced to consider the recoating effects. The numerical framework has been calibrated using the experimental results obtained by a 3D scanner. The following validation has demonstrated good agreement between the simulated displacements and the experimental measurements of different thin-walled structures. Finally, the validated model is used to analyze the residual stress evolution during the whole printing process.

The major conclusions of this study are the following:

1. The recoating system affects the residual warpage of the build. Thus, the orientation of the part on the build-plate with respect to the recoating direction makes a difference. This effect is more pronounced when open structures are considered. The higher structural stiffness of the closed-structures mitigates this phenomenon.
2. The vertical displacements at the top surface of the build are amplified by the bulging phenomenon shown by these kinds of structures. The interference between the recoating system and the roughness generated by the non-uniform powder bed spreading generates increased loading in the direction of the recoater's movement. The induced bending is more pronounced when these loads are orthogonal to the thin surfaces. Thus, the orientation of the lightweight structures on the base platform is relevant.

3. Open lightweight structures are more prone to warpage due to their reduced structural stiffness compared to closed ones. However, higher residual stresses appear on the latter and can be relaxed through post-annealing treatment. Therefore, component integration is a possible solution to increase the overall stiffness of the build to better resist the thermal stresses induced by the fabrication process as well as generate a more uniform temperature field, thus lowering temperature gradients and stress concentrations.
4. Geometry compensation is a good inverse engineering strategy to modify the original nominal geometry, accounting for the part warpage due to the AM process and ensuring optimal geometrical accuracy in SLM-parts.

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INTRODUCTION

This chapter introduces a novel method to simulate the thermal field in part-scale LPBF problems. As discussed throughout this thesis, the ratio of time-scales in these problems is extremely large, imposing a prohibitively large number of time-steps.

Concretely, to capture the laser motion without skipping over elements, time-steps must respect the condition

$$\Delta t < T_{hs} = \frac{R}{V} \quad (47)$$

where R is the laser radius and V is the laser speed; exceeding this limit would cause the heat source to skip over elements. In contrast, the net print time is on the order of $T_{print} = \mathcal{O}\left(\frac{L^3}{R^2 V}\right)$ and the resulting ratio of time-scales is proportional to $(L/R)^3$ (see chapter 1).

Uniform time-stepping therefore requires an exorbitant number of time-steps, e.g. on the order of hundreds of millions or even billions to simulate a centimeter-scale LPBF part, resulting in days or weeks of computation for builds that take only minutes or hours in practice.

Since constraint (47) is too expensive to satisfy for part-scale problems, this chapter proposes a method to bypass it by reformulating the model so that the time-scale of the moving heat source is effectively increased. During preliminary discussions, the authors agreed that in a long enough track, the thermal field in the vicinity of the heat source remains nearly unchanged, simply advecting with the moving laser. Several strategies were considered to exploit this behavior, ranging from alternative integration schemes to data-driven surrogates. However, the key insight is that if it barely changes, it must be steady in the moving frame of the heat source. This observation, while not new [Mundra et al., 1996, Van Elsen et al., 2007, Storti et al., 2022, Jia et al., 2024], had not yet been leveraged as a means to increase the admissible time-step size in high-fidelity simulations.

The model proposed in this chapter introduces a moving subdomain attached to the heat source. Inside this subdomain, the problem is posed in the reference frame of the moving heat source, while the unmodified problem is solved elsewhere.

For long enough tracks, the solution in the moving subdomain is quasi-steady, allowing for significantly larger time-steps. The proposed workflow measures the steadiness of the solution at the end of each time-step to increase the time-step once the solution is steady enough.

SUMMARY & CONCLUSIONS

The method was implemented in a custom FEM code [Slimani, 2024]¹ for linear thermal problems with moving Gaussian sources and a simplified, collision-based, phase change model. The work included simplified benchmarks and a single-track thin wall.

Unexpectedly, the method considerably improved accuracy in the HAZ. In particular, the resulting heat-front is steeper and the heat-tail is longer in comparison to the standard FEM solution. These features are consistent with experimental observations of melt pool asymmetry and with the correction originally introduced by Goldak et al. [1984] via the double-ellipsoid heat source. This alignment with established modeling

In this publication, the authors chose to highlight the “Chimera” nature of the method in the title, as the implementation relies on multiple meshes. However, the method was renamed to “advected subdomain” in later works, to better reflect its essence. The Chimera aspect is a means to an end, while the introduction of advection is the defining feature of the method.

¹ Openly available at <https://github.com/ordinary-slim/moving-heat-source>.

practice highlights that the advected subdomain enhances the fidelity of the simulation in the melt pool vicinity.

The method is not without limitations. It struggles with multi-track geometries, where accuracy deteriorates after direction changes; the scheme must be switched off during turns and reactivated afterwards. Implementation is more complex due to the motion of the subdomain, which requires additional boolean operations and interpolations at each time-step.

Individual time-steps are more expensive due to loss of symmetry in the stiffness matrix and the introduction of advection ($\approx 2\times$). This extra cost is amortized by the larger time-steps for long enough tracks: in the single-track thin wall, time-steps up to $8T_{hs}$ were achieved, reducing the total number of time-steps by a factor of 6 and the run time by a factor of 3 in the considered example.

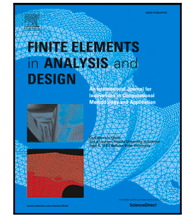
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A Chimera method for thermal part-scale metal additive manufacturing simulation[☆]

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ABSTRACT

This paper presents a Chimera approach for the thermal problems in welding and metallic Additive Manufacturing (AM). In particular, a moving mesh is attached to the moving heat source while a fixed background mesh covers the rest of the computational domain. The thermal field of the moving mesh is solved in the heat source reference frame. The chosen framework to couple the solutions on both meshes is a non-overlapping Domain Decomposition (DD) with Neumann–Dirichlet transmission conditions.

Increased steadiness and accuracy within the vicinity of the Heat Affected Zone (HAZ) are the main advantages of this approach. The steadiness gain allows for the use of larger time steps, which is vital in AM applications and, in particular, Laser Powder Bed Fusion (LPBF), where the disparity of time scales represents a major hurdle. Moreover, enhanced accuracy can be observed in the resulting morphology of the melt pool. It will be shown that the method addresses classical shortcomings pointed out by Goldak without requiring the use of an asymmetrical heat source profile.

1. Introduction

Thermal part-scale simulation of metallic AM is necessary to analyse microstructure characteristics and detect regions with high thermal gradients [1,2]. However, this is a daunting task, often implying long execution times and high computational costs. Modelling these problems is challenging due to their “extremely multiscale” nature [3]. In these applications, builds of characteristic size L_{print} are driven by a laser of characteristic size L_{hs} , where the ratio L_{print}/L_{hs} is about 100 – 1000.

The discrepancy of temporal scales is even more marked. The timescale of the heat source, T_{hs} , can be estimated as the time required by the laser to travel one radius R , $T_{hs} = R/V$, with V the speed of the heat source. T_{hs} will be used as a unit of time in the remainder of this work. In LPBF, it is in the order of 10^{-4} seconds. This is prohibitively small compared to the *net printing time*, the total time the laser is turned on. The ratio T_{print}/T_{hs} can be orders of magnitude bigger than 10^5 .

In practice, the timescale T_{hs} dictates the following constraint on the time-step Δt :

$$\Delta t \leq T_{hs} \quad (1)$$

If inequality (1) is not respected, the numerical solution will display a spotty pattern: elements are skipped over resulting in numerous erroneous temperature peaks as can be observed on Fig. 1(b). Many authors opt for $\Delta t = 0.5 T_{hs}$ [4–7] and commercial software packages like Netfabb warn against time-steps bigger than a T_{hs} .¹ For sizeable builds, this constraint is too restrictive and renders “naive modelling”² infeasible: Hodge [3] estimates that the simulation of a 19.2 mm cube printed using typical LPBF

[☆] Supplementary video related to this article is available at “https://github.com/ordinary-slim/media_moving_heat_source/blob/master/animation.gif”.

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¹ <https://help.autodesk.com/view/NETF/2021/ENU/?guid=GUID-67A6D8F0-AA04-436B-9FAF-A912BE00B497>.

² As in comprehensive first-principles modelling. Wording from [3,8].

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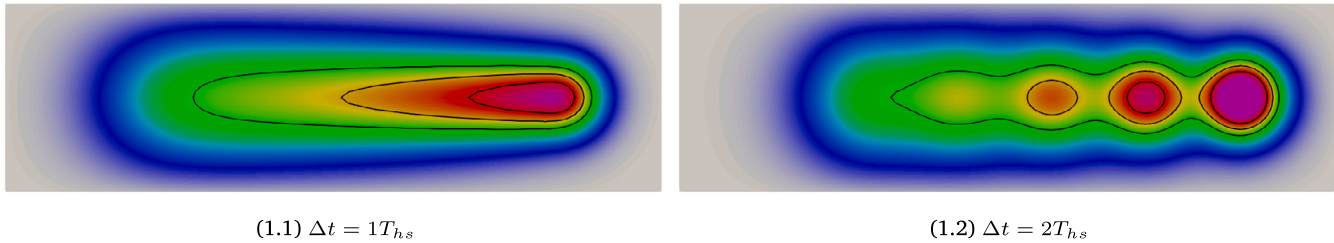


Fig. 1. 2D heating track example with admissible and inadmissible time-step sizes according to inequality (1).

parameters would take $\mathcal{O}(10^8)$ time-steps. In the quest to obtain results within a reasonable time interval (in the order of days) for builds of practical interest, a time-step should span tens of microseconds at most [7].

On the one hand, the contrast of spatial scales has been amply studied and is typically addressed through Adaptive Mesh Refinement (AMR) [9–11]. On the other hand, the disparity of time scales has only recently picked up the interest of researchers and there does not exist a standard solution yet. There are 2 classes of solutions in the literature to reduce the number of time-steps of the whole structure: *lumped heat sources* and *substepping*, the former being the most popular of the two.

Replacing the accurate heat source profile by an averaged source term like in [11–13] allows bypassing the restriction of the heat source timescale to advance hatch-by-hatch or even layer-by-layer at the cost of accuracy. Van Elsen et al. [14] shows that although the temperature field far from the HAZ is matched, the size of the melt pool as well as the peak temperature are underestimated. One can compensate by numerically calibrating other problem parameters as is done in *flash heating* [4]: the deposition speed is artificially increased in order to obtain more faithful peak temperatures.

As an alternative, *substepping* does not necessarily compromise the accuracy of the results. Rather than taking uniform time-steps for the whole structure, finer time-steps are taken close to the heat source and coarser time-steps far from it. Pusio and Hodge [15] showcases speedup of factors 20–90 as their numerical example is scaled up. This is achieved through a “multirate integration scheme” [3] so that the degrees of freedom (DOFs) are spatially partitioned into fast and slow. A time-step is then subdivided into (1) a global predictor step using a large Δt , (2) corrector steps using a small Δt for the fast DOFs and (3) a final corrector step for all DOFs. Viguerie et al. [16] uses a similar predictor–corrector scheme together with the overlapping DD framework approach described in [17]. They obtain a computational speedup of 2.44 in a 3D welding example.³ The work of Soldner and Mergheim [11] showcases a DD framework with heterogeneous time-steps combined with a lumped heat source. Kopp et al. [18] is able to naturally address both the spatial and temporal multiscale natures of their welding examples through space–time FEM: the time interval is meshed and its (de)refinement is handled with AMR.

There also exist techniques to reduce the computational cost of a single time-step. In recent years, GPU based software has been performing very well [19,20]. Proell et al. [7] also attains good performance using CPU vectorization, although they declare in their conclusion that they will make their software GPU compliant in the future. Explicit time-stepping can also be used as a speedup technique: although it brings up stability concerns, the critical time-step is less restrictive than constraint (1) by a factor of 5–10 in the examples of Essongue et al. [21].

The model proposed in this work is intended to bypass constraint (1) without artificially altering the power distribution profile. The driving hypothesis is that for a long enough heating track, the thermal field will reach a steady state in the reference frame of the heat source. Once steady, larger time-steps are allowed. In the welding literature, multiple authors have observed that steady state is reached rather quickly [14,22,23]. Computing the whole problem in the reference frame of the heat source is unwise since it introduces transitoriness in far away regions and at the boundaries of the build. Hence, a Chimera approach [24] is applied: a patch mesh is attached to the laser and the rest of the domain is covered by a background mesh. The thermal field in the patch mesh is computed in the heat source reference frame while the background mesh does it in the laboratory reference frame. The two meshes are coupled at their interface through Neumann–Dirichlet transmission conditions. This framework is similar to the one presented by Storti et al. [25], the main difference being the coupling of subdomains.

Furthermore, it will be observed that this approach offers accuracy gains in the HAZ. Goldak et al. [26] noted that the temperature gradient obtained with an ellipsoidal heat source is inaccurate in the proximity of the meltpool. In its back, the gradients are too steep, while in its front, they are too flat. To remediate this issue, the double ellipsoidal heat source profile was proposed, which to this day is still widely used to conform to the final asymmetric shape of the meltpool: note on Fig. 2 that a shorter ellipsoid will be placed in the front of the welding path and a longer one at the rear. Thus, the symmetrical Gaussian profile is artificially modified to account for the missing heat advection induced by the fast motion of the heat source. Moreover, the determination of the parameters characterizing the double ellipsoid is not straightforward [8]. This work will show that using the heat source reference frame will naturally remediate the advection effect described by Goldak without requiring the use of an asymmetrical profile.

It is remarked that Chimera methods also allow for the use of a finer patch mesh compared to the background mesh (cf. Fig. 3), avoiding the use of AMR in the HAZ and the associated time due to the recomputation of connectivities at every time-step [17,25]. In the work of Leonor and Wagner [20], 3 different subdomains are used to resolve fine, meso- and macroscales.

³ Note that the potentially obtainable speedup factor for a given method is problem dependent.

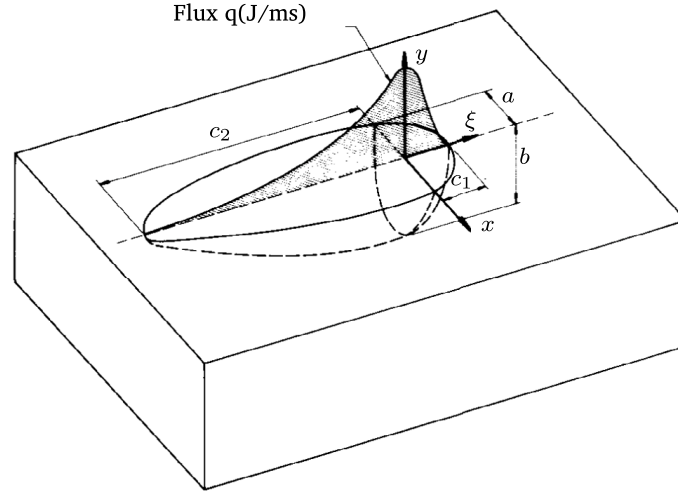


Fig. 2. Double ellipsoidal profile [26]. ξ is the welding direction.

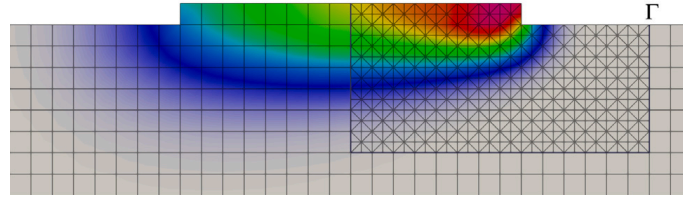


Fig. 3. The subdomain of the HAZ can be meshed with a different element type, size or degree.

2. Methodology

This section is structured as follows: first, the standard approach in the laboratory reference frame is presented. For the remainder of this work, it will be referred to as *reference model*. Then the Chimera method is described.

2.1. Reference model

The reference model in this work consists of the balance of energy equation for AM. For the sake of simplicity neither the thermal dependency of the material parameters nor the latent heat are accounted for. The problem statement is as follows: solve for the temperature field $T = f(\mathbf{x}, t) : \Omega(t) \mapsto \mathbb{R}$ such that

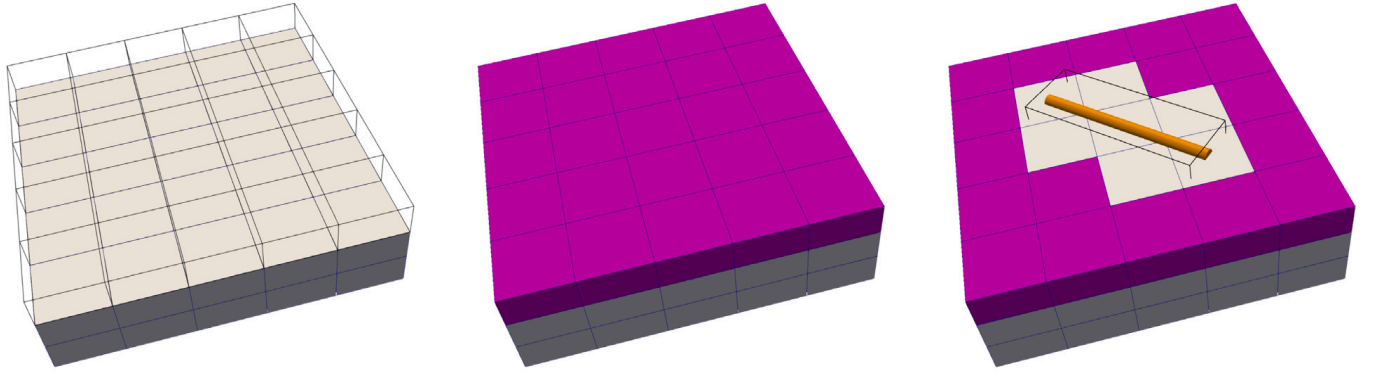
$$\begin{aligned} \rho c_p \partial_t T(\mathbf{x}, t) - \nabla \cdot (k \nabla T(\mathbf{x}, t)) &= r(\mathbf{x}, t) & \forall \mathbf{x} \in \Omega(t) \\ q_{conv} &= h_{conv}(T(\mathbf{x}, t) - T_{env}) & \forall \mathbf{x} \in \partial\Omega_{conv}(t) \\ T(\mathbf{x}, 0) &= T_0(\mathbf{x}, 0) & \forall \mathbf{x} \in \overline{\Omega}(0) \\ T(\mathbf{x}, t) &= T_{dep} & \forall \mathbf{x} \in \overline{\Omega}(t) \mid \forall t' < t, \mathbf{x} \notin \overline{\Omega}(t') \end{aligned} \quad (2)$$

where ρ , c_p , k , r , q_{conv} , h_{conv} and T_{dep} denote the density, the specific heat, the conductivity, the volumetric heat source, the convection heat flux, the convection coefficient and the deposition temperature, respectively. The heat source adopted in this work is the standard Gaussian distribution.

$$r_{2D}(\mathbf{x}, t) = \frac{2P(t)}{\pi R^2} \exp\left(\frac{-2\|\mathbf{x} - \mathbf{x}_{hs}(t)\|_2^2}{R^2}\right) \quad r_{3D}(\mathbf{x}, t) = \frac{6\sqrt{3}P(t)}{\pi^{3/2}R^3} \exp\left(\frac{-3\|\mathbf{x} - \mathbf{x}_{hs}(t)\|_2^2}{R^2}\right) \quad (4)$$

where P , R and $\mathbf{x}_{hs}$ denote respectively the net power supply, the radius and the current position of the heat source. Note the time dependency of $\mathbf{x}_{hs}$ in the laboratory reference frame.

In this work, the powder bed is included in the simulation domain when considering LPBF applications. However, a surrogate model is used for the transformation of loose powder into bulk material. Elements affected by the HAZ are automatically set to bulk elements by increasing their conductivity by a factor of 100 as done in [27]. Said elements are detected through a collision test as depicted in Fig. 4(c).



(4.1) Bare substrate below an inactive layer.

(4.2) A powder layer is activated.

(4.3) The material of the elements which collide with the deposited hatch is set to bulk.

Fig. 4. Illustration of simplified melting. () Powder () Bulk

The time dependency of the computational domain $\Omega(t)$ in Eq. (2) is due to the deposition process. Numerically, it is modelled using the born-dead element technique [28]. Elements of a layer that are yet to be deposited are *inactive* and are not included in the computational domain (cf. Fig. 4(a)). During the recoating step, a new layer of powder elements is activated as shown in Fig. 4(b).

2.2. Chimera model

This section presents the Neumann–Dirichlet scheme employed in this work. In the context of this problem, it can be used for both overlapping and non-overlapping decomposition: the classic version is non-overlapping, and Houzeaux and Codina [29] shows its validity in overlapping settings. For the sake of simplicity, the non-overlapping version is the one featured in the body of the work while the overlapping one is discussed shortly in the Appendix.

In the vicinity of the HAZ, the problem is modelled in the reference frame of the moving heat source. To this end, a moving subdomain $\Omega_m(t) \subset \Omega$ is attached to the source, such that the latter appears fixed in space when observed from Ω_m . Let ξ denote the spatial coordinate in this frame and $\mathbf{v} = \frac{d\mathbf{x}_{hs}}{dt}$ the speed of the laser. The change of coordinate system can be expressed as

$$\xi = \mathbf{x} - \int_0^t \mathbf{v}(t) dt$$

In this framework, the balance of energy (2) can be rewritten for $T^m : \Omega_m \rightarrow \mathbb{R}$

$$\rho c_p \left(\partial_t T^m(\xi, t) - \mathbf{v}(t) \cdot \nabla T^m(\xi, t) \right) - \nabla \cdot (k \nabla T^m(\xi, t)) = r(\xi, t) \quad \xi \in \Omega_m(t) \quad (5)$$

Note the introduction of an advection term to account for the motion of the mesh. Moreover, the power source only depends on time through the power P : $\mathbf{x}_{hs}$ is now fixed.

The speed $\mathbf{v}$ is translational; in the case of an angular speed ω , $\mathbf{v}$ should be replaced by $\omega \times (\xi - \xi_0)$ in Eq. (5), where ξ_0 is the centre of rotation of the heat source. Only cases with translational speeds are considered in this work.

The rest of the computational domain is *fixed* and denoted by $\Omega_f(t) = \text{int}(\Omega \setminus \Omega_m(t)) \subset \Omega$. The fixed subproblem is posed in the usual laboratory reference frame. If Ω_m is big enough to contain the whole support of the source, the balance equation for Ω_f can be written as follows for $T^f : \Omega_f \rightarrow \mathbb{R}$

$$\rho c_p \partial_t T^f(\mathbf{x}, t) - \nabla \cdot (k \nabla T^f(\mathbf{x}, t)) = 0 \quad \mathbf{x} \in \Omega_f(t) \quad (6)$$

Both subdomains form a decomposition of Ω at t^{n+1} and are coupled through Neumann–Dirichlet transmission conditions at their interface, $\Gamma(t) = \partial\Omega_m \cap \partial\Omega_f$, as shown on Fig. 5.

$$k \partial_n T^m(\xi, t) = k \partial_n T^f \quad \xi \in \Gamma(t) \quad (7)$$

$$T^f(\mathbf{x}, t) = T^m \quad \mathbf{x} \in \Gamma(t) \quad (8)$$

The remaining heat transfer and initial conditions write

$$\begin{aligned} q_{\text{conv}} &= h_{\text{conv}}(T^m(\xi, t) - T_{\text{env}}) & \xi \in \partial\Omega_{m, \text{conv}}(t) \\ T^m(\xi, 0) &= T_0(\xi, 0) & \xi \in \bar{\Omega}_m(0) \\ T^m(\xi, t) &= T_{\text{dep}} & \mathbf{x}(\xi) \in \bar{\Omega}(t) \mid \forall t' < t, \mathbf{x}(\xi) \notin \bar{\Omega}(t') \end{aligned} \quad (9)$$

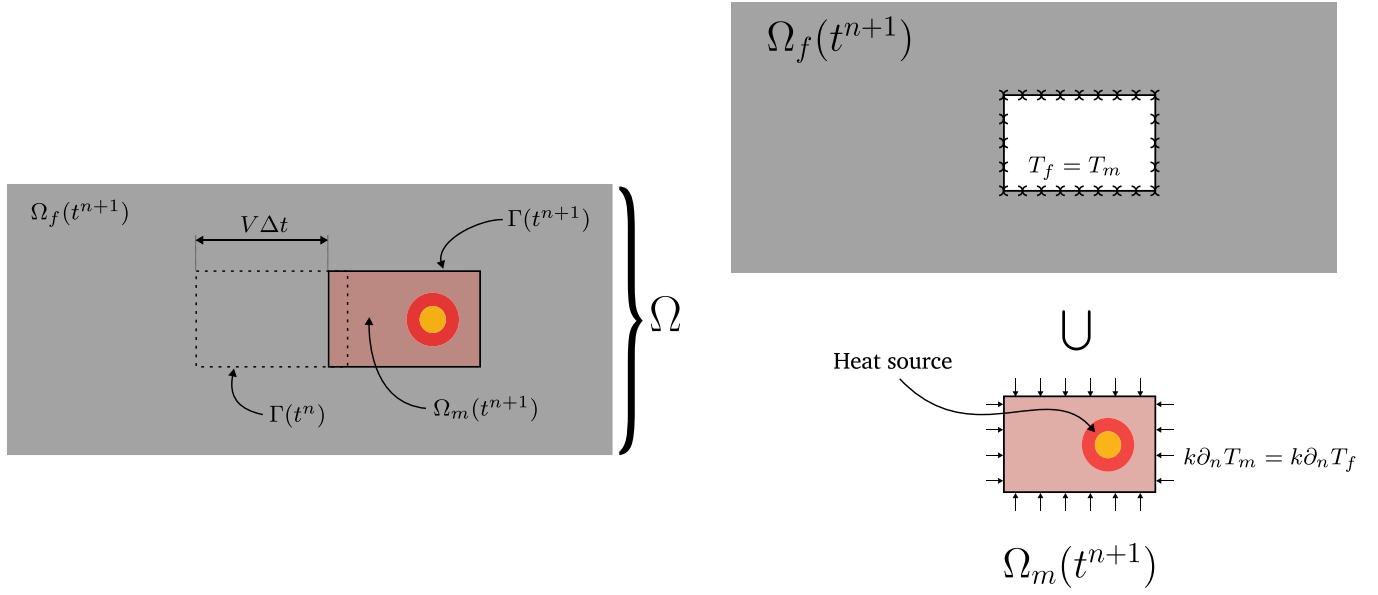


Fig. 5. Schematic of Chimera model with non-overlapping decomposition.

$$\begin{aligned}
 q_{\text{conv}} &= h_{\text{conv}}(T^f(\mathbf{x}, t) - T_{\text{env}}) & \mathbf{x} &\in \partial\Omega_{f,\text{conv}}(t) \\
 T^f(\mathbf{x}, 0) &= T_0(\mathbf{x}, 0) & \mathbf{x} &\in \bar{\Omega}_f(0) \\
 T^f(\mathbf{x}, t) &= T_{\text{dep}} & \mathbf{x} &\in \bar{\Omega}(t) \mid \forall t' < t, \mathbf{x} \notin \bar{\Omega}(t')
 \end{aligned}$$

Note that Eq. (9) is not applied to new nodes in ξ but to new nodes in the corresponding $\mathbf{x}$. This is because in the heat source reference frame there are no newly deposited nodes since the deposition front is stationary. A more accurate wording would be *replaced* nodes, since nodes with hot material are replaced with ones with cold material.

At time t^{n+1} , Ω_m and Ω_f are discretized in space by the FE meshes $\mathcal{T}^m(t)$ and $\mathcal{T}^f(t)$. *Streamline Upwind Petrov–Galerkin* (SUPG) is chosen to stabilize the advection term in Eq. (5). The resulting coupled integral equations in $T_h^m \in V_h^m$ and $T_h^f \in V_h^f$ write as follows

$$\begin{aligned}
 & \int_{\Omega_m} \phi_m \rho c_p \partial_t T_h^m - \int_{\Omega_m} \phi_m \rho c_p \mathbf{v} \cdot \nabla T_h^m \\
 & + \int_{\Omega_m} k \nabla \phi_m \cdot \nabla T_h^m - \int_{\partial\Omega_{m,\text{conv}}} \phi_m h_{\text{conv}} T_h^m \\
 & - \int_{\Gamma} k \phi_m \nabla T_h^f \cdot \hat{n} + \int_{\Omega_m} \tau R_h \Big|_{T_h^m} \rho c_p \mathbf{v} \cdot \nabla \phi_m = \int_{\Omega_m} \phi_m r + \int_{\partial\Omega_{m,\text{conv}}} \phi_m h_{\text{conv}} T_{\text{env}} \quad \forall \phi_m \in V_h^m \\
 & \int_{\Omega_f} \phi_f \rho c_p \partial_t T_h^f + \int_{\Omega_f} k \nabla \phi_f \cdot \nabla T_h^f - \int_{\partial\Omega_{f,\text{conv}}} \phi_f h_{\text{conv}} T_h^f = \int_{\Omega_f} \phi_f r + \int_{\partial\Omega_{f,\text{conv}}} \phi_f h_{\text{conv}} T_{\text{env}} \quad \forall \phi_f \in V_h^f
 \end{aligned} \tag{10}$$

$$V_h^m \subset H^1(\Omega_m) \quad V_h^f \subset H^1(\Omega_f) : \forall \phi_f \in V_h^f, \phi_f|_{\Gamma} = 0$$

where $R_h \Big|_{T_h^m}$ denotes the pointwise residual of T_h^m in equation Eq. (5) and τ is an element-wise scalar stabilization coefficient chosen according to Codina [30]. Backward Euler is adopted for the time integration. Note that higher order time integrations such as Crank–Nicholson can introduce oscillations (see [15]). After time discretization, the algebraic form of the problem is

$$\begin{pmatrix} \frac{\tilde{M}_m}{\Delta t} + K_{m,m} & K_{m,m_\Gamma} & 0 & 0 \\ K_{m_\Gamma,m} & \frac{\tilde{M}_{m_\Gamma}}{\Delta t} + K_{m_\Gamma,m_\Gamma} & 0 & N \\ 0 & 0 & \frac{\tilde{M}_f}{\Delta t} + K_{f,f} & K_{f,f_\Gamma} \\ 0 & D & 0 & -I \end{pmatrix} \begin{pmatrix} T^{m,n+1} \\ T^{m_\Gamma,n+1} \\ T^{f,n+1} \\ T^{f_\Gamma,n+1} \end{pmatrix} = \begin{pmatrix} F_m + \frac{\tilde{M}_m}{\Delta t} T^{m,n} \\ F_{m_\Gamma} + \frac{\tilde{M}_{m_\Gamma}}{\Delta t} T^{m_\Gamma,n} \\ F_f + \frac{\tilde{M}_f}{\Delta t} T^{f,n} \\ 0 \end{pmatrix} \tag{12}$$

On the left-hand side, the $T^{\cdot,k}$ -vectors contain the nodal values of the solutions at time t^k , the $\tilde{M}$ -matrices denote the modified mass matrices with an extra SUPG term associated to the time derivative, the $K_{\cdot,\cdot}$ matrices contain diffusion, advection and convection contributions from the nodes of the second subscript to the nodes of the first subscript, matrix N contains the Neumann contribution from the Γ -nodes of $\mathcal{T}^f$ to the Γ -nodes of $\mathcal{T}^m$, and the last row corresponds to the Dirichlet condition (8). D is such that, at time t^k ,

$$\text{row}_i D \cdot T^{m,k} = T_h^m(\xi_i, t^k) = T_h^m(\mathbf{x}_i - \int_0^{t^k} \mathbf{v} dt, t^k) \quad \forall \mathbf{x}_i \mid \mathbf{x}_i \text{ is a } \Gamma\text{-node of } \mathcal{T}^f$$

and I is an identity matrix of the appropriate size. Slightly abusing notation, the 0s denote null matrices of varying sizes. On the right-hand side, the F -vectors contain power density and convection contributions. Notice that, for a monolithic solve, the Dirichlet and Neumann conditions need to be assembled to the left-hand side of Eq. (12) since they depend on the solution at t^{n+1} .

Matrix (12) is non-symmetric: $K_{m,m}$, K_{m,m_f} and $K_{m_f,m}$ contain advection contributions and matrices N and D are unrelated.

In the numerical examples, the linear system (12) will be solved monolithically at each time-step. In contrast, the reference model only requires the solution of a Symmetric Positive Definite (SPD) matrix. The performance of the method could be enhanced by solving for Ω_f and Ω_m in a staggered fashion. Although the matrix of the moving subproblem would remain non-symmetric, the matrix of the fixed subproblem will be SPD.

As the moving subproblem grows steadier, larger Δt and Ω_m are chosen according to the following workflow

$$\text{steadiness_metric}(T_h^m) < \alpha \longrightarrow \text{Increase } \Delta t \longrightarrow \text{Resize } \Omega_m \quad (13)$$

where $\alpha > 0$ is an given threshold. This is checked at the end of each time-step, and Δt is generally increased by a constant value $0.5 T_{hs} - 1 T_{hs}$. The following ratio of L_2 norms is utilized:

$$\text{steadiness_metric}(f) := \frac{\|f|_{t^{n+1}} - f|_{t^n}\|_2}{\|f|_{t^{n+1}}\|_2} \quad (14)$$

That is, the solution at t^n and t^{n+1} is used to determine whether Δt in $t^{n+2} = t^{n+1} + \Delta t$ can be increased. This metric does not take into account changes in the motion of the heat source, the material composition, nor the geometry. In this work, the former is taken care of by resetting Δt upon starting a new heating track, but the other factors mentioned are currently left unaddressed. If one wanted to address e.g. geometry changes, it would be necessary to keep track of whether the active elements array of $\mathcal{T}^m$ changed. The closer the change is to the heat source, the more weight it should be given.

Regarding the shaping and sizing of Ω_m , the following considerations must be taken into account:

1. $\Omega_m \subset \Omega$. Since $\mathcal{T}^m$ is moving, it is necessary to check whether any elements went out of bounds. In particular, assuming a first order time integration, one needs to ensure that

$$\Omega_m(t^n) \subset \Omega(t^n) \quad (15)$$

$$\Omega_m(t^{n+1}) \subset \Omega(t^{n+1}) \quad (16)$$

The first condition ensures that the previous solution is available, and the second condition is trivially necessary.

2. Ω_m should be big enough to contain the heat source so that it can be omitted in Eq. (6). If a portion of its support is left out of Ω_m , the right-hand side of Eq. (6) is non-zero and the spotty pattern of Fig. 1(b) might reappear. For the 3D heat source of Eq. (4), the minimum size of Ω_m should be about 1.5–2 radii, since, at that distance, the relative power density is negligible.

Note that it is not always possible to guarantee this minimum size since condition (15) might interfere: consider the situation described in Fig. 6 where the heat source at t^{n+1} is at a boundary of the domain and its speed is perpendicular to the normal i.e. $\mathcal{T}^m$ is coming onto the domain. Although subset B belongs to Ω , it cannot be included in Ω_m since, at t^n , it was outside Ω and breaks (15). In this case, since B contains an important portion of the support of the heat source, the scheme is restricted to small time-steps, or it can revert to the reference model by engulfing all of Ω in Ω_f .

3. Ω_m should be long enough not to skip over a portion of Ω_f i.e. its back length must be bigger than $V\Delta t$. This is analogous to constraint Eq. (1), with the advantage here that Ω_m can be sized at each time-step.
4. Ω_m should not include regions of the solution which are steadier in the laboratory reference frame e.g. boundaries that are not the deposition front.

At the implementation level, Ω_m is sized according to the following parameters: front, back, side, top and bottom lengths with respect to the position of the heat source. The front, side, top and bottom lengths are usually set according to item 2. To set the back length, a function of Δt is provided to the software keeping in mind item 3. Item 1 is enforced at the level of the driver using boolean operations before and after the motion of Ω_m as will be explained shortly.

The necessary degree of flexibility in adapting Ω_m at each time-step is achieved by employing a mesh larger than necessary and deactivating elements until the desired shape and size are attained. This process is illustrated in Fig. 7. Let $\mathcal{T}_{bg}^m$ denote this background mesh, such that $\mathcal{T}^m$ now refers to the active mesh of Ω_m . A time-step starts by resetting $\mathcal{T}^m$ and $\mathcal{T}_{bg}^f$ to $\mathcal{T}_{bg}^m$ and a mesh of $\Omega(t^n)$, respectively. When a new heating track starts, $\mathcal{T}_{bg}^m$ is aligned with the new heat source direction through a rotation. Then, $\mathcal{T}_{bg}^m$ is progressively reduced to $\mathcal{T}^m$ through multiple intersections. First, the routine `shapeSubdomain` sets the desired lengths by intersecting $\mathcal{T}_{bg}^m$ with oriented boxes or/and spheres of the corresponding sizes. Then, $\mathcal{T}^m \leftarrow \text{intersect}(\mathcal{T}_{bg}^m, \mathcal{T}^f)$ is performed to enforce Eq. (15). After the motion of $\mathcal{T}^m$ from t^n to t^{n+1} , $\mathcal{T}^m \leftarrow \text{intersect}(\mathcal{T}^m, \mathcal{T}^f)$ is carried out again so that Eq. (16) is respected. Finally, the *hole cutting* operation is performed: the resulting mesh for $\mathcal{T}^m$ is subtracted from the mesh of $\mathcal{T}^f$, i.e. $\mathcal{T}^f \leftarrow \text{subtract}(\mathcal{T}^f, \mathcal{T}^m)$.

Activation is kept track of through the `activeElements` and `activeNodes` arrays. The aforementioned boolean operations are implemented by interpolating the `activeNodes` array as a finite element function from a mesh to another. At the receiving

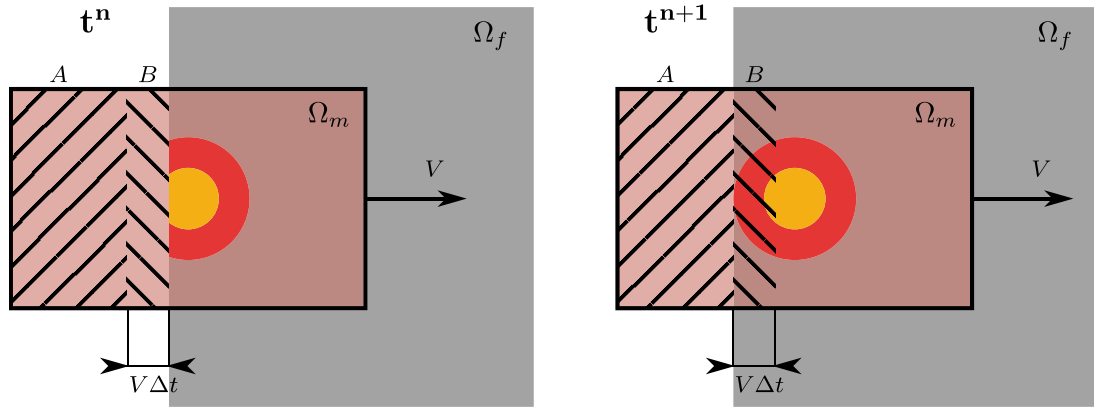


Fig. 6. Schematic with Ω_m coming onto the domain. A and B violate conditions (16) and (15), respectively: at time t^n , B was out of bounds, hence the time derivative cannot be computed on $B \subset \Omega_m$. Consequently, it has to be included in Ω_f .

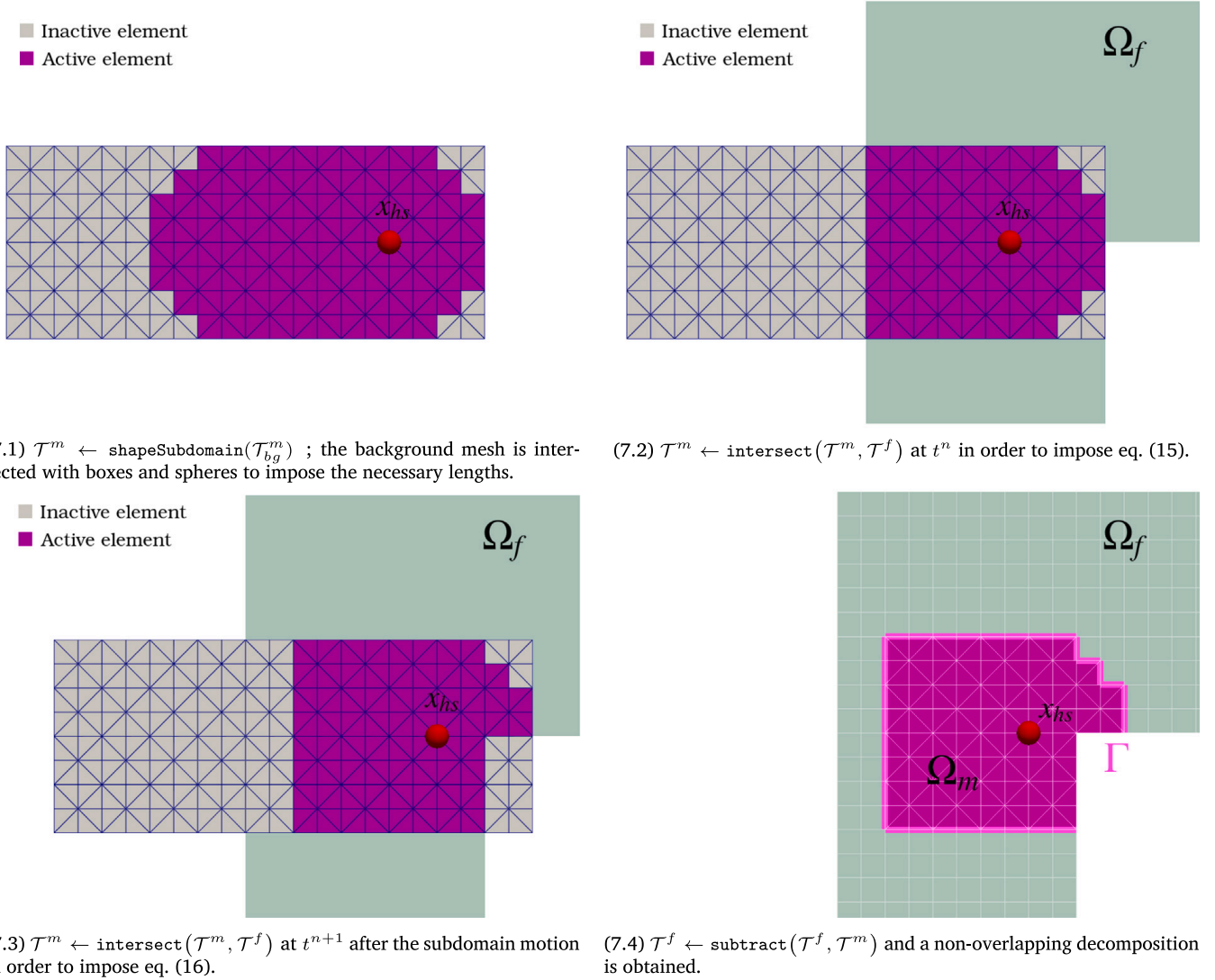


Fig. 7. Illustration of the meshing process for Ω_m and the boolean operations carried out during an iteration.

end of the projection, elements whose nodes are all 1-valued are marked as active in the other mesh. The values of the `activeElements` array are modified accordingly: for `intersect`, an element is kept active only if active in both meshes, and for `subtract`, an element is deactivated only if active in the other mesh. The latter can result in overlaps if the boundary of $\mathcal{T}_m$ lies in the middle of elements of $\mathcal{T}_f$. This case will be discussed in the [Appendix](#). In the numerical examples, only small overlaps will occur, since, after the hole cutting, no distance computations are performed to enlarge the overlap.

Algorithm 1 describes the driver routine of the Chimera method. Note that although the Chimera method adds a considerable amount of operations, most of these are projections and spatial searches whose cost is negligible compared to the assembly and the solution of the linear system.⁴ This driver routine would need to be modified for another choice of integration scheme to check a condition analogous to (15) for e.g. t^{n-1} , requiring an extra intersection.

Algorithm 1 Driver routine for LPBF time-step of Chimera method

Additional operations with respect to reference method are highlighted.

- 1: $\mathcal{T}^m \leftarrow \mathcal{T}_{bg}^m$ $\triangleright$ Reset activation of $\mathcal{T}^m$
 - 2: $\mathcal{T}^f \leftarrow \text{Mesh of } \Omega(t^n)$ $\triangleright$ Set Ω_f to physical domain
 - 3: **if** on new layer **then**
 - 4: Activate powder layer
 - 5: **if** on new track **then**
 - 6: Set heat source power and speed $\triangleright$ In Ω_f
 - 7: Realign $\mathcal{T}^m$, set advection and domain speeds
 - 8: $\mathcal{T}^m \leftarrow \text{shapeSubdomain}(\mathcal{T}_{bg}^m)$ $\triangleright$ Shape $\mathcal{T}^m$ by intersecting its background mesh with boxes or/and spheres
 - 9: $\mathcal{T}^m \leftarrow \text{intersect}(\mathcal{T}^m, \mathcal{T}^f)$, ensuring $\Omega_m \subset \Omega(t^n)$
 - 10: Advance time to t^{n+1} $\triangleright$ Update heat source position, mesh motion, etc.
 - 11: $\mathcal{T}^m \leftarrow \text{intersect}(\mathcal{T}^m, \mathcal{T}^f)$, ensuring $\Omega_m \subset \Omega(t^{n+1})$
 - 12: **for all** elements which collide with deposition **do**
 - 13: Set material to bulk $\triangleright$ Simplified melting
 - 14: $\mathcal{T}^f \leftarrow \text{subtract}(\mathcal{T}^f, \mathcal{T}^m)$
 - 15: Locate Γ_m and Γ_m $\triangleright$ Locate the interface facets of both domains
 - 16: Set Γ_f to Dirichlet and Γ_m to Neumann boundary conditions
 - 17: Set convection boundary conditions on external boundary $\triangleright \partial\Omega \setminus \Gamma$, necessary to update since the meshes are changing
 - 18: Assemble and solve the finite element problem
 - 19: Communicate solution across meshes
 - 20: Compute steadiness of moving problem and new Δt
-

3. Numerical examples

Both the reference and the Chimera methods were implemented in a C++ library. All the code for both the algorithm and the cases run is made available online at the following link: https://github.com/ordinary-slim/moving_heat_source. The main routines are exposed to Python through Pybind [31] in order to write the driver code in a high level language. Third party pre and post-processing libraries are invoked through their Python APIs (Application Programming Interface). Namely, the libraries gmsh and meshio are extensively used [32,33].

For the processing, both the Eigen library [34] and MATLAB [35] are used for linear algebra, the later being invoked through its C++ API. Geometrical operations (convex polyhedra collision, fast spatial search) are implemented using CGAL [36,37].

For each numerical example, both the reference and the proposed models described in Section 2 are exposed. All the domains are meshed using first order quadrilateral and hexahedral elements.

The first example will showcase the accuracy of the proposed model in the vicinity of the heat source and illustrate a problem encountered by the Chimera model with large time-steps when Γ is ill-placed. The second example features a slightly more complex heating track with the issues that come along it. Finally, the third example treats a 3D printing case, a thin wall printed using LPBF.⁵

⁴ Section 3.3 contains a short discussion on the main costs of an iteration.

⁵ It is worth mentioning that the authors tried applying the presented methodology to DED (Directed Energy Deposition) without success in reducing the total number of time-steps. The key difference with an LPBF simulation is that DED involves simultaneous heating and deposition at every printing step. Hence, at every time-step, the newly deposited nodes have a high time derivative of the solution and the moving subproblem is never steady. In discrete terms, upon activation of a node, T^n is set at the deposition temperature T_{dep} , resulting in $\Delta_h^t T^{n+1} = \frac{T^{n+1} - T_{\text{dep}}}{\Delta t} \gg 0$ in general.

Table 1
Material properties and process parameters for Sections 3.1 and 3.3.

Symbol	Parameter	Value	Unit
ρ	Density	4300	kg/m ³
c_p	Specific heat	700	J/kg K
k	Conductivity	10	W/m K
V	Speed V	1000	mm/s
R	Radius R	0.1	mm
P	Power	50	W
$T_{0/env/dep}$	Initial/environment/deposition temperature	25	°C

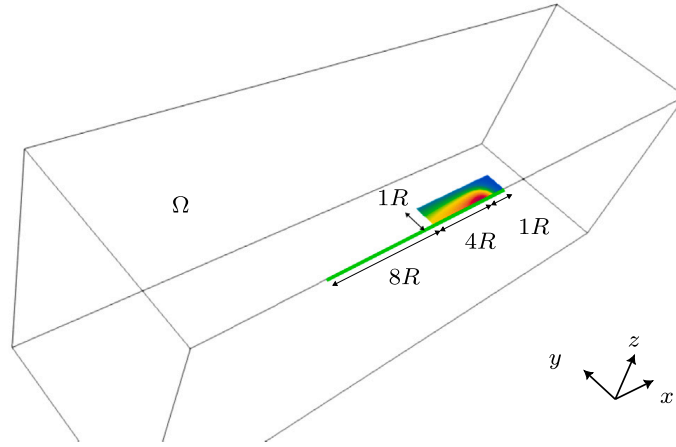


Fig. 8. Computational domain Ω , subdomain of Fig. 9 and line for profile of Fig. 10(b).

3.1. 3D track in infinite body

The performance of the Chimera model is studied in the context of a single track in an infinite medium. Analytical solutions of several 3D heat source profiles ranging from ellipsoidal to uniform distributions are available [14,38]. Throughout this work, Ti64 material is utilized alongside LPBF-like parameters. The data is reported in Table 1.

The accuracy of the steady state solution in the proximity of the heat source as well as the effect of the interface Γ will be examined. The simulation domain Ω , although finite, is chosen big enough to neglect boundary effects in the subdomain of interest, cf. Fig. 8. All the boundaries are insulated (null Neumann): the top and right surfaces are planes of odd symmetry of the solution and the remaining boundaries are assumed to be far enough so that the solution does not vary anymore.

For the proposed model, a relatively large time-step of $\Delta t = 2 T_{hs}$ is adopted in order to quickly reach steady state. In contrast, since the system is ever-transient in the reference model, it is necessary to use increasingly smaller time-steps in order to obtain convergence.

Fig. 9 compares isothermal lines and peak temperatures of the analytical, the proposed and the reference models upon reaching quasi steady state. The reference model uses $\Delta t = 0.25 T_{hs}$ while the proposed model employs the aforementioned $\Delta t = 2 T_{hs}$. Both solutions are computed with a mesh density of 8 elements per radius. Note that the region shown is fully contained in Ω_m i.e. the temperature field of the proposed model is computed from the heat source reference frame. As expected, by virtue of being a better choice of reference frame, results are more accurate both in terms of peak temperature and isotherms. This is confirmed by Table 2; at the finest spatial resolution, the solution in the heat source reference frame with $\Delta t = 2 T_{hs}$ is still better than the solution in the laboratory reference frame with $\Delta t = \frac{1}{16} T_{hs}$. The latter is comparable to the 4 elements per radius solution in the heat source reference frame. Note from Table 2b that, at a constant Δt , the error does not diminish with spatial refinement; indicating that it is solely affected by temporal refinement. Nonetheless, spatial refinement is still necessary in order to obtain convergence since the motion of the heat source must be resolved to avoid steps smaller than the size of an element: if the mesh has N elements per radius, $\Delta t \geq \frac{1}{N} T_{hs}$. Hence, convergence in the reference model needs both spatial and temporal refinement while it only involves spatial refinement in the proposed model due to it reaching steady state in Ω_m .

The error is concentrated at the thermal front since the steepest gradients are located there. The pointwise error there is particularly high in Fig. 9(f) because the predicted isotherms are too spread as illustrated on Fig. 9(d), resulting in an underprediction of the gradients along the heating track. Conversely, in the thermal tail, the isotherms are too close, and the gradients are overpredicted. This issue is well known in the literature; Goldak et al. [26] proposed an asymmetrical double ellipsoidal heat source with a smaller ellipsoid at the front and a longer ellipsoid at the back in order to compensate for these over- and underpredictions. Goldak suggests that the dimensions of these ellipsoids should correspond to the melt pool. Van Elsen et al. [14] argues that such a heat source is artificial since physical heat sources are symmetrical. Note that this issue is absent in the Chimera method due

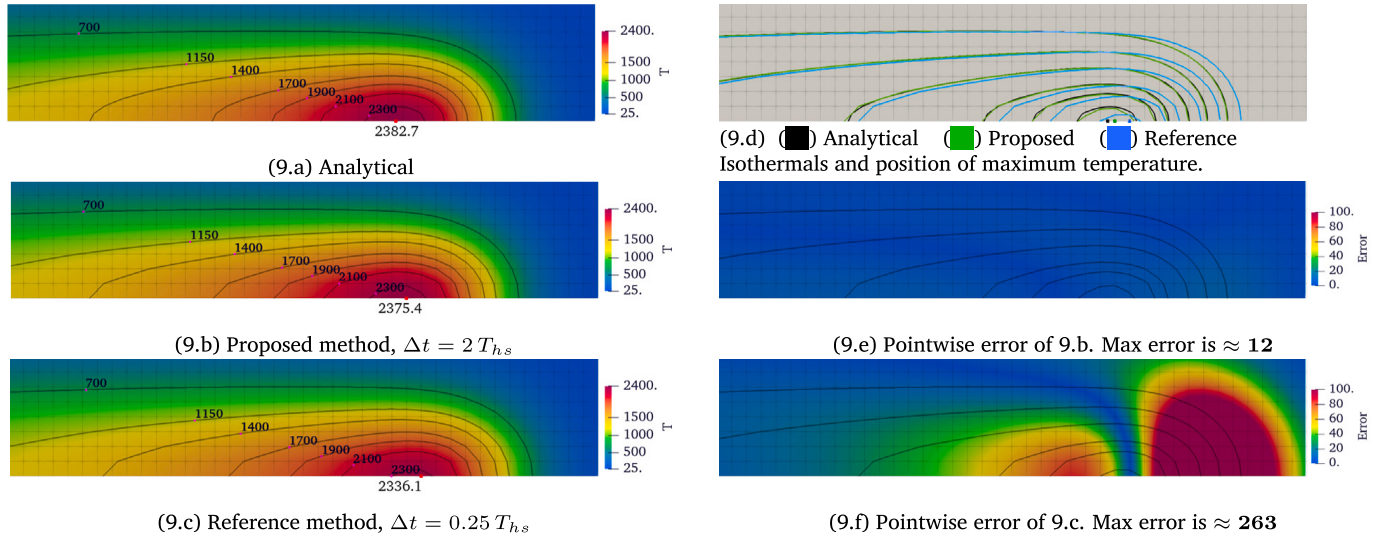


Fig. 9. Solution (left) and error (right) contour fields. Spatial resolution is 8 elements per radius.

Table 2

Relative L2 error $\frac{\|T_h - T_{\text{anal}}\|_2}{\|T_{\text{anal}}\|_2}$ for 3D welding case.

(a) Proposed method		(b) Reference method				
	$\Delta t = 2T_{hs}$		$\Delta t = 0.5T_{hs}$	$\Delta t = 0.25T_{hs}$	$\Delta t = 0.125T_{hs}$	$\Delta t = 0.0625T_{hs}$
2 els./radius	181.23%	2 els./radius	403.41%	–	–	–
4 els./radius	44.73%	4 els./radius	414.16%	208.76%	–	–
8 els./radius	14.32%	8 els./radius	427.43%	216.71%	108.57%	–
16 els./radius	5.46%	16 els./radius	431.37%	219.83%	110.99%	55.44%

to the advection, which, in the first place, was the one introducing the asymmetry: it brings closer the isotherms at the front and further apart the isotherms at the back by adding a thermal flux in the direction opposite to the laser speed. Concerning the peak temperature, the reference model predicts its position too far to the front. The Chimera model is again more accurate thanks to the presence of advection which pushes it further back.

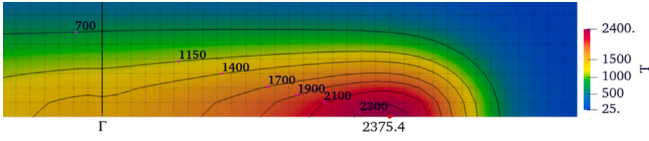
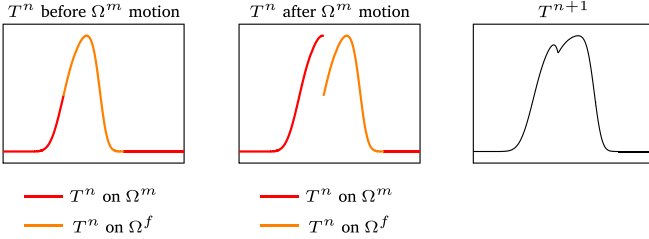
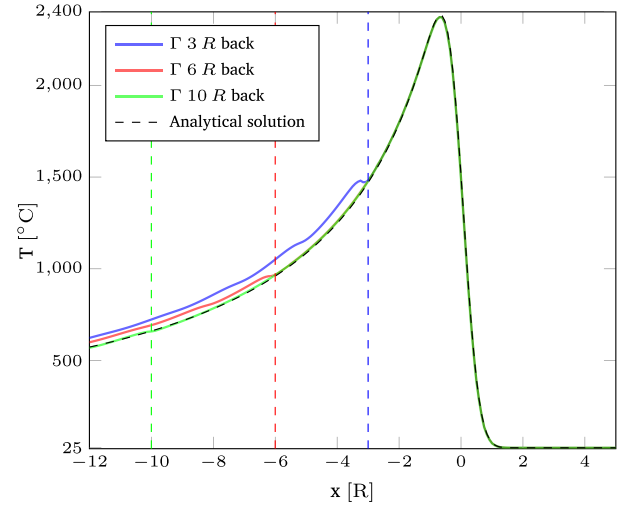
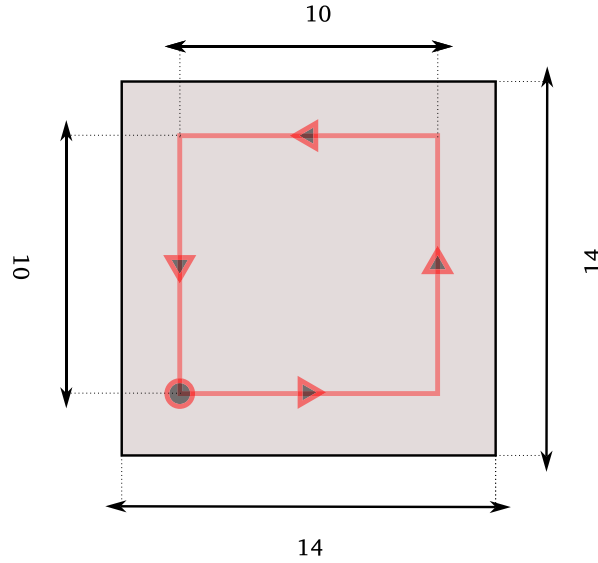
In order to study the effect of the interface Γ , its position is brought much closer to the heat source as shown on Fig. 10(a). Here, Γ is situated $3R$ behind the heat source, while keeping the same time-step $\Delta t = 2T_{hs}$. This change introduces oscillations as can be observed on the figure when the isotherm crosses Γ . This is a discretization effect due to the interface being located in a region with high gradients and the time-step being relatively too large.⁶ The issue is expanded upon by Fig. 10(b) which shows profile plots along the heating track over the line shown on Fig. 8 for interface positions of $3R$, $6R$ and $10R$ behind the heat source. The $3R$ profile shows the highest oscillation, and, the further back the interface is positioned, the smaller the oscillation. The cause is depicted on Fig. 10(c): T_h^n exhibits a spatial discontinuity at Γ after the motion of Ω_m . The moving subproblem carries over $T_h^{m,n}$ of its previous position to its new position, discarding $T_h^{f,n}$ there. The resulting T_h^n has a discontinuity across Γ which in turn causes a discontinuity in the discrete time derivative $\Delta_t T_h^{n+1} = \frac{T_h^{n+1} - T_h^n}{\Delta t}$, and an oscillation of T_h^{n+1} . In 1D, the magnitude of the discontinuity is

$$\|T_h^n\|_{\Gamma^{n+1}} = \int_{x|_{\Gamma^n}}^{x|_{\Gamma^{n+1}}} \partial_x T_h^{f,n} dx = \int_{x|_{\Gamma^n}}^{x|_{\Gamma^n} + V\Delta t} \partial_x T_h^{f,n} dx \quad (17)$$

It is proportional to Δt and to the norm of the gradients in the region. If small enough, the discontinuity will be absorbed by diffusion as shown on Fig. 10(b). The oscillation is proportional to the speed of the heat source seeing as, for higher speeds, lower time-steps are required to advance the same distance, limiting the time over which the discontinuity can dissipate. Hence, the oscillation is proportional to the Péclet number. In the context of our problem, once the thermal tail is formed, it is advantageous to place the interface far behind as shown in Fig. 10(b) so as to position Γ where gradients are low.

This oscillation could also be interpreted as a violation of the flux continuity condition in Eq. (7), which is only weakly enforced. The issue could potentially be addressed by using a Lagrange multiplier approach which would allow giving bigger weight to Eq. (7).

⁶ To the knowledge of the authors, this effect has not been studied previously.

10.1: Proposed model, interface Γ 3R behind the heat source.10.3: Illustration of T^n discontinuity at t^{n+1} resulting in oscillation in T^{n+1} .10.2: Temperature profiles along line shown on Fig. 8 for Chimera model. Distance is measured in radii and heat source is located at 0. The closer the interface Γ is brought, the larger the oscillation.**Fig. 10.** Contour, profiles and schematic analysing oscillation in the solution due to large time step relative to the interface position.**Fig. 11.** Domain and heating track for Section 3.2.

3.2. 2D square track

A 2D square welding track is featured here to show an example with sharp direction changes. The domain and the heating track are depicted on Fig. 11. The material parameters are the same as in Table 1. The speed is set to 100 mm/s, the radius to 0.2 mm and the power to 100 W. A convection boundary condition is chosen with a coefficient of 20 W/m and $T_{env} = 25$.

The spatial resolution of both models is 4 elements per radius. The reference model uses $\Delta t = 0.5 T_{hs}$ while the Chimera model progressively increases from $0.5 T_{hs}$ to $5.5 T_{hs}$.

Snapshots of the thermal fields towards the end of the simulation are shown on Fig. 12. The reference method needs 400 time-steps, while the Chimera method achieves qualitatively similar results in 129 time-steps. The shape of Ω_m in Fig. 12 is obtained by intersecting the rectangular background mesh with 2 circles and a rectangle following the procedure described in Section 2. Note that the elongated rectangle has to be realigned through a rotation at the beginning of each track.

Fig. 13 zooms into the bottom right turn. The issue with sharp direction changes is depicted in Fig. 13(b): the advection of the current heating track shears the previous thermal tail. Note that as the time-step is decreased, so does the shearing, as illustrated

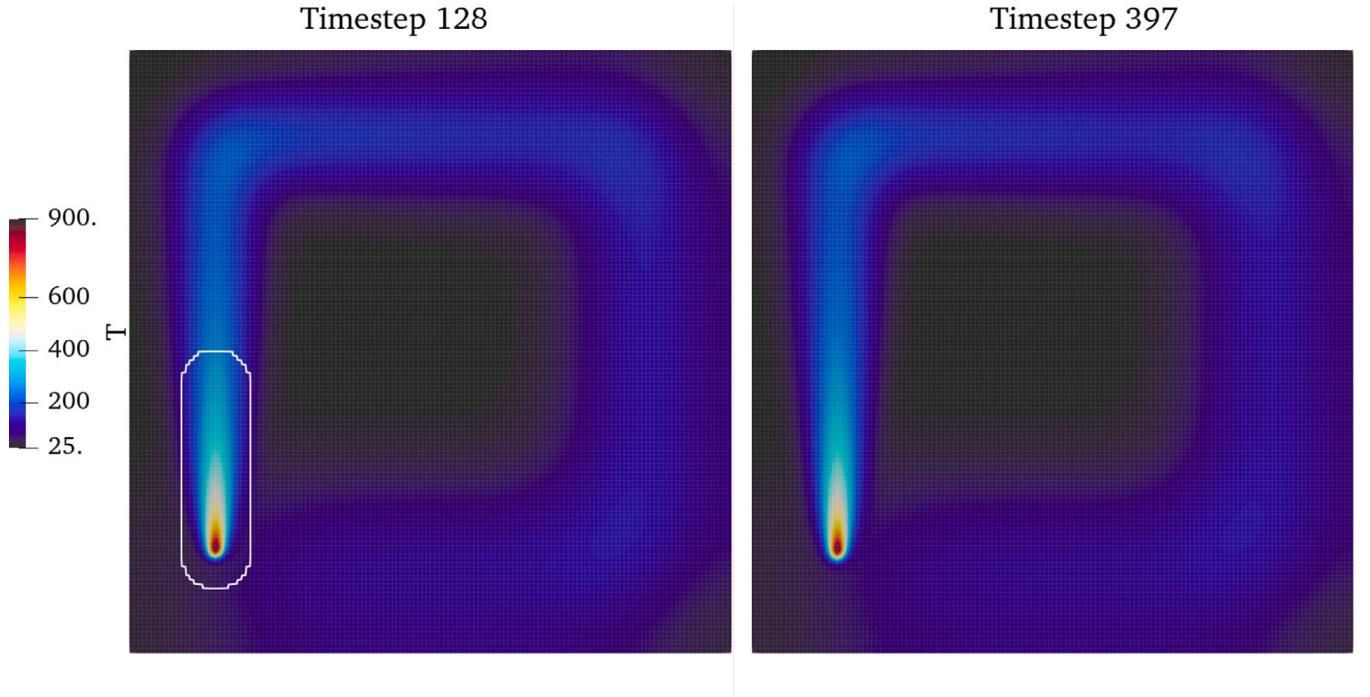
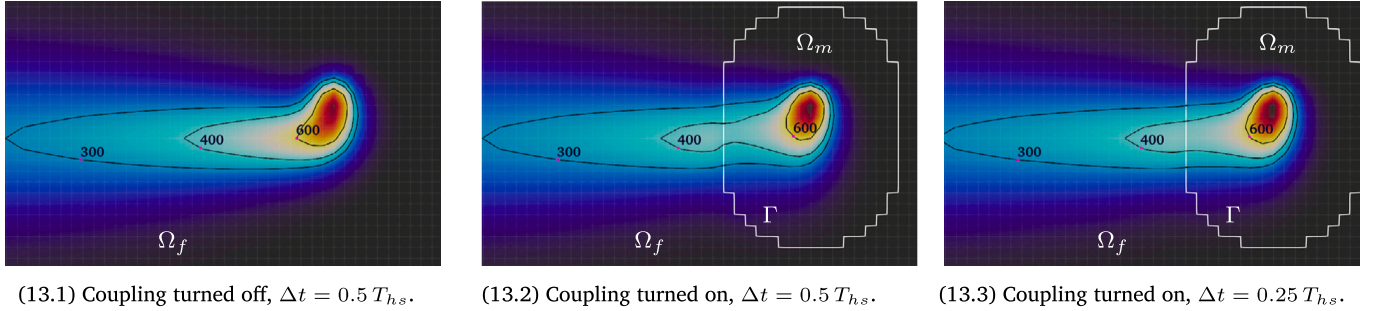


Fig. 12. Proposed and reference method towards the end of the square track. The outline of Ω_m is shown in white after a time-step of $\Delta t = 5 T_{hs}$.



(13.1) Coupling turned off, $\Delta t = 0.5 T_{hs}$.

(13.2) Coupling turned on, $\Delta t = 0.5 T_{hs}$.

(13.3) Coupling turned on, $\Delta t = 0.25 T_{hs}$.

Fig. 13. Bottom right 90° turn. Γ is outlined in white. If coupling is on during sharp turns, shearing of the previous thermal tail is observed on the right.

by Fig. 13(c). The approach adopted to overcome this issue in the rest of this work is to turn off the scheme at the beginning of a heating track i.e. revert to the reference model. In Fig. 13(a), right after a turn, Ω_f covers the whole domain. In the next time-steps, the solution will be projected on Ω_m , and whenever Eq. (13) is satisfied for the first time along a track, the coupling will be turned back on. It is worth mentioning that upon turning the coupling back on, the temperature peak overshoots by around 5 – 10% and goes back down after a couple of time-steps.

The homepage of the code repository showcases a video of this example.

3.3. LPBF thin wall

The build of a LPBF thin wall is modelled with both the reference and the Chimera methods. The material and process parameters of Table 1 are reused in this section. The wall is 10 mm in length, 0.1 mm in width and 0.25 mm in height and the layer thickness is 25 μm i.e. the simulation spans 10 layers. Each layer consists of a single track, whose direction alternates from one layer to the next. It is built on top of a 12 mm $\times$ 2 mm $\times$ 1 mm substrate. Heat is convected across the boundary of the domain with $h_{conv} = 20 \text{ W/m}^2$ and $T_{env} = 25$. Interlayer cooling time is set to two seconds, after which the build is recoated by activating a new powder layer, as depicted on Fig. 4(b).

Three solutions are compared: a solution with the Chimera model with increasing time-steps, a reference model solution with a standard $\Delta t = 0.5 T_{hs}$ and a fine reference model solution with $\Delta t = 0.125 T_{hs}$. The first two have a spatial resolution of 4 elements per radius in-plane and 1 element through the layer thickness. The fine solution has double the aforementioned resolution. The total number of DOFs is approximately the same for the first two solutions; it is slightly larger for the Chimera method since the interface

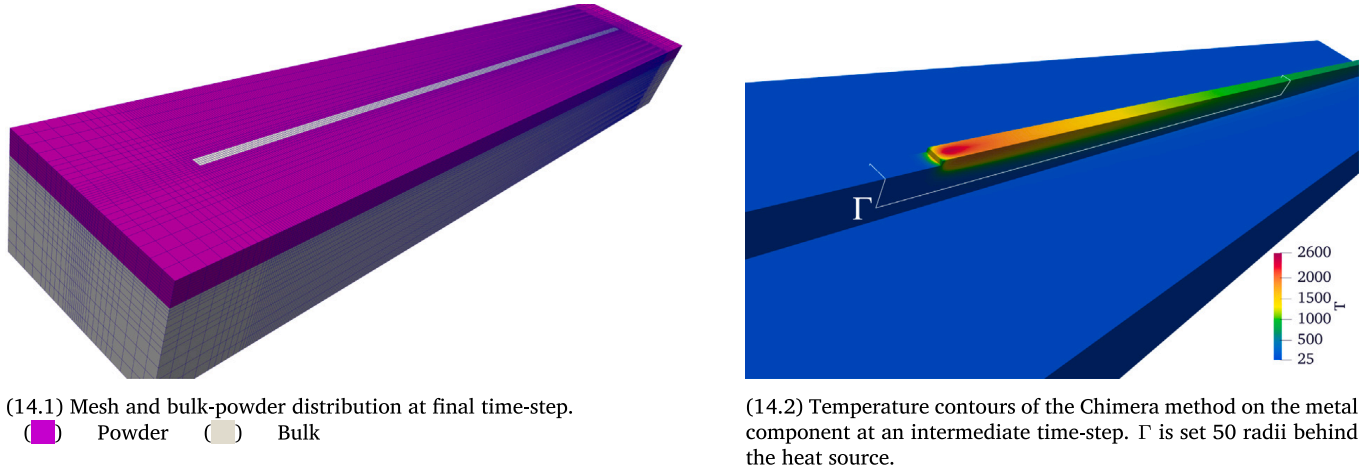
Fig. 14. Mesh and Ω_m used in Section 3.3.

Table 3

Cost of simulation in terms of number of time-steps and elapsed time for reference and Chimera methods. The solution of matrix equations is performed by MATLAB.

	Reference method, $\Delta t = 0.5 T_{hs}$	Proposed method, adaptive Δt
Total printing time-steps	2000	331
Total duration printing time-steps [s]	22 733	6832
Total Chimera time-steps	–	251
Average number of DOFs	258 122	264 168
Average duration printing time-step [s]	11.37	20.64
Average duration Chimera time-step [s]	–	23.32

nodes are duplicated. Fig. 14(a) shows their mesh and bulk-powder distribution at the final time-step. The mesh shown has 293 K elements while the mesh of the fine solution has 1.891 M elements.

The time-step of the Chimera starts off at $0.5 T_{hs}$ and increases in increments of $0.5 T_{hs}$ until reaching $8 T_{hs}$ towards the end of the track. As in the previous section, the coupling is turned off as appropriate: cooling time-steps and starts of tracks are modelled entirely from the laboratory reference frame i.e. the first heating time-steps of a track are solved in Ω_f and the solution is projected at each time-step to Ω_m . Similarly to Section 3.2, the coupling is turned back on the first time that the solution in Ω_m satisfies Eq. (14), meaning here the first time-step with $\Delta t = 1 T_{hs}$.

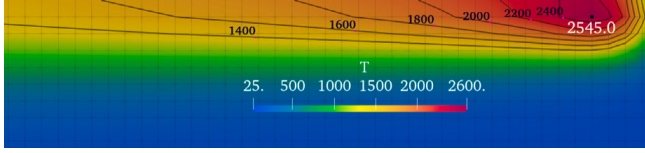
The back length of Ω_m is chosen rather large so that the subdomain extends well into the thermal tail. This is done in order to mitigate oscillations as explained in Section 3.1. For $\Delta t = 3 T_{hs}$ and $8 T_{hs}$, the back length is set to $10.25R$ and $50R$, respectively. Fig. 14(b) shows the outline of Ω_m after a time-step with $\Delta t = 8 T_{hs}$.

Fig. 15 compares contours and profiles of the solutions. Figs. 15(a), 15(d) and 15(e) display snapshots towards the end of the fifth layer while Figs. 15(b), 15(c) and 15(f) show the end of the last track. For the proposed model, the size of the last time-step taken was $8 T_{hs}$ and $1 T_{hs}$ in Figs. 15(e) and 15(f), respectively. Note that the back of Ω_m is out of frame in the former while it is in frame in the latter. Oscillations are absent from Figs. 15(e) and 15(f) due to the appropriate choice of time-step & back length combination. The trend observed in Section 3.1 repeats here: isotherms obtained with the Chimera model are denser at the thermal front and looser at the tail, generally closer to the fine solution than the $0.5 T_{hs}$ -solution. In terms of peak temperature, both the Chimera and $0.5 T_{hs}$ solutions are off by 30–80 °C.

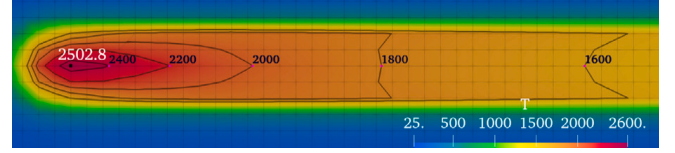
Figs. 15(g) and 15(h) show temperature profiles along the centreline at the top of the build. Similarly to the previous figures, they are timed towards the end of the fifth and tenth layers, respectively. Note that at $x = -5$ and $x = 5$, the material transitions from bulk to powder at the beginning/end of each hatch. In comparison to the $0.5 T_{hs}$ -solution, the Chimera one is slightly closer to the fine solution in the proximity of the HAZ but it is off by 30 °C in the back of the thermal tail. Slight oscillations are observable at the previous positions of Γ , especially on Fig. 15(g) due to the issue explained in Section 3.1. Note that only the fine solution is able to resolve the temperature spike at the bulk-powder interface.

Table 3 reports simulation costs in terms of time-steps and elapsed time for the Chimera and the $0.5 T_{hs}$ solutions. Both methods are using MATLAB's linear system solver. The Chimera method takes around 6 times less time steps and about 3.3 times less execution time. Note that the average Chimera iteration is around 2 times more expensive than the average iteration from the reference model despite the similar number of DOFs. This stems from the SPD-ness of the matrix of the reference model, which is a big advantage compared to the asymmetric monolithic matrix in (12).

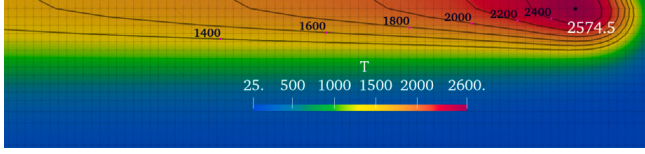
The main costs of an iteration were studied using profiling results for the problem of Section 3.1. In the 8 elements per radius case, $\mathcal{T}^f$ has 282.9K nodes. This results in a system of 282.9K DOFs for the reference model and 286.6K DOFs for the Chimera one



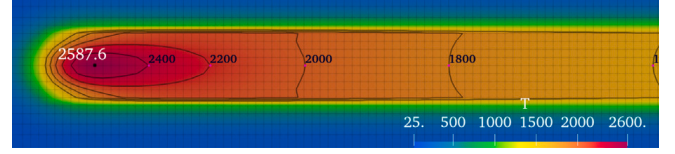
15.1: Side view of reference model solution towards the end of the fifth layer, $\Delta t = 0.5 T_{hs}$



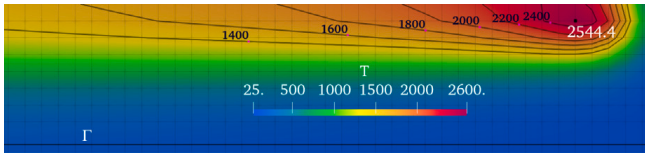
15.2: Bird view of reference model solution towards the end of the last layer, $\Delta t = 0.5 T_{hs}$



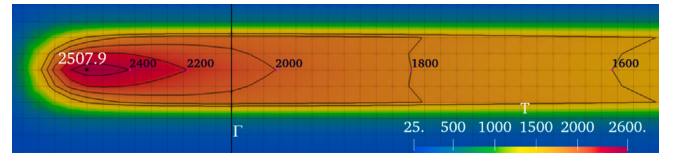
15.3: Side view of fine solution towards the end of the fifth layer, $\Delta t = 0.125 T_{hs}$



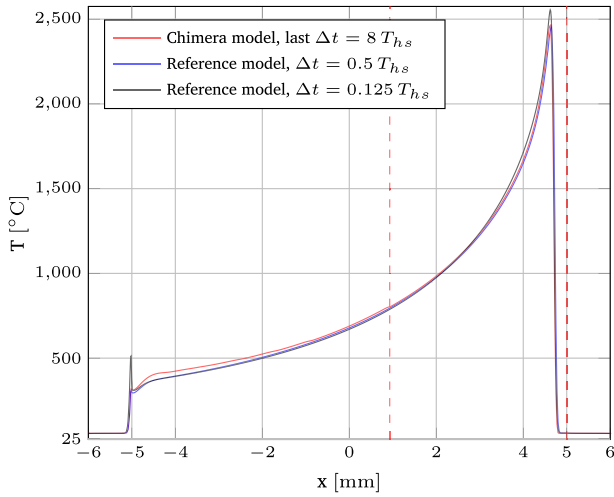
15.4: Bird view of fine solution towards the end of the last layer, $\Delta t = 0.125 T_{hs}$



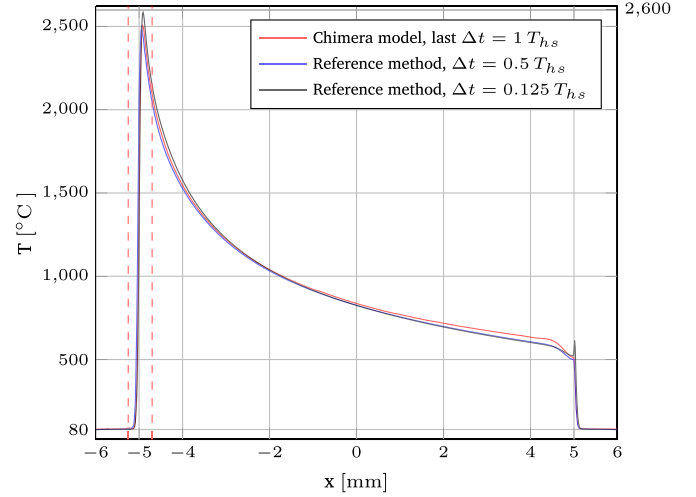
15.5: Side view of Chimera model solution towards the end of the fifth layer, last $\Delta t = 8 T_{hs}$



15.6: Bird view of Chimera model solution towards the end of the last layer, last $\Delta t = 1 T_{hs}$



15.7: Plot along top centerline of build towards end of fifth layer.



15.8: Plot along top centerline of build towards end of tenth layer.

Fig. 15. Contours, peak temperatures and profiles along printing direction for intermediate (left, side view) and final times (right, bird view).

Table 4
Costs of iteration using model problem from Section 3.1.

	Reference method	Chimera method	Reference method with Ω_m in background
Total time [s]	8.5	12.0	9.5
Assembly [%]	93.8	70.3	84.4
Linear system solution	5.8	16.7	5.2
Boolean operations [%]	0.0	6.6	5.7
Interface location [%]	0.0	4.0	0.0
Interpolations [%]	0.0	2.0	2.9

since the interface DOFs are duplicated. The size of Ω_m is chosen so that it has 29K DOFs i.e. approximately 10% of total DOFs. The linear systems of the reference and Chimera models are solved using conjugate gradient and biconjugate gradient stabilized method, respectively.

Table 4 presents the aforescribed profiling results. The time spent for an iteration as well as the fraction of time spent on the main tasks of Algorithm 1 are reported. In this case, a single time-step of the Chimera model is about 40% more expensive than

that of the reference model, hence a reduction of 30% in the total number of time-steps is necessary in order to offset this cost. Assembly takes about the same time, but the linear system solve is 4 times more expensive, although the latter is far outweighed by the former. Extra-operations only present in the Chimera model account for about 12% of its iteration cost. This could be further reduced by implementing the boolean operations (shaping of $\mathcal{T}^m$ and hole cutting) and the location of the interface using tree based algorithms [39]. In this work, they are implemented suboptimally using projections.

In the case of a reference model iteration with a moving subdomain in the background i.e. an iteration with the coupling turned off, its cost is about 12% higher than if Ω_m was absent. As mentioned previously, the 5.7% from the boolean operations could be lowered. Compared to the Chimera iteration, there is one less boolean operation ($\mathcal{T}^f \leftarrow \text{subtract}(\mathcal{T}^f, \mathcal{T}^m)$) and one less interpolation (from $\mathcal{T}^m$ to $\mathcal{T}^f$).

4. Conclusions

This work presents a novel FEM Chimera approach for the thermal modelling of moving heat sources. The problem in the HAZ is posed in the reference frame of the heat source while the rest of the domain is solved in the laboratory reference frame.

The main pros of the approach are an accuracy improvement in the HAZ and an increase in steadiness which can be exploited to take bigger time-steps since the formulation is not constrained by Eq. (1). Both are due to the better choice of reference frame. In particular, the advection in the moving frame recovers a shorter front and a longer tail without requiring the use of an asymmetrical profile [26].

Its main cons are a higher algebraic complexity compared to the standard approach and the potential presence of oscillations in the solution depending on the choice of parameters and time-step. Concerning the former, advection loses the SPD-ness of the original problem and leads to a higher computational cost as described in Section 3.3. Regarding the latter, formulations with moving subdomains present a discontinuity in the solution at the previous time-step. If this discontinuity is big enough, it can result in an oscillation as described in Section 3.1. In the context of the problem at hand, this discontinuity can be minimized by optimizing the position of Γ at the thermal tail. A possibility is a spatial search in order to minimize a multidimensional version of Eq. (17).

Since the presented algorithm relies on the subproblem reaching steady state to speed up the simulation, it will perform worse the more the part is subdivided in different scanning tracks, such as in the case of island scan strategies. Although how fast the subproblem reaches steady state in a given track depends also on the Péclet number, the authors estimate that a track should be at least $5R$ to profit from the algorithm. For problems with short tracks, the simulation will certainly not be sped up, although they may still obtain accuracy improvements in the HAZ using the presented model.

The authors believe that this approach can be combined with a substepping algorithm [15,16] in order to further reduce simulation cost while retaining the aforementioned pros. Future works could also explore other choices of domain decomposition frameworks [17,25].

CRedit authorship contribution statement

Mehdi Slimani: Writing – original draft, Validation, Software, Methodology, Investigation, Formal analysis, Conceptualization. **Miguel Cervera:** Writing – review & editing, Supervision, Project administration, Funding acquisition. **Michele Chiumenti:** Writing – review & editing, Supervision, Project administration.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

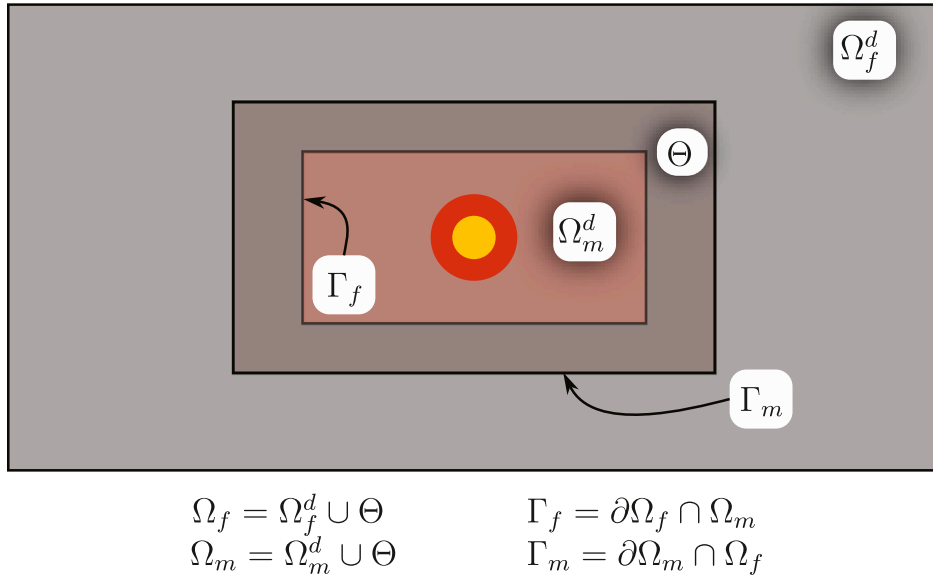
Data availability

No data was used for the research described in the article.

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Fig. A.16. Overlapping decomposition of Ω .

Appendix. Overlapping decomposition

Section 2 describes a non-overlapping Neumann–Dirichlet domain decomposition scheme. For the problem at hand, the same scheme is also valid in an overlapping setting [29,40]. Let Ω_m^d , Ω_f^d and Θ denote the disjoint parts of the moving and fixed domains and the overlap, respectively. The decomposition is

$$\begin{aligned}\Omega &= \text{int}(\overline{\Omega_m^d \cup \Omega_f^d \cup \Theta}) \\ \Omega_m &= \Omega_m^d \cup \Theta \\ \Omega_f &= \Omega_f^d \cup \Theta\end{aligned}$$

with interfaces Γ_m and Γ_f as depicted on Fig. A.16. For this decomposition, the system of differential equations becomes

$$\begin{aligned}\rho c_p \left(\partial_t T^m(\xi, t) - \mathbf{v}(t) \cdot \nabla T^m(\xi, t) \right) - \nabla \cdot (k \nabla T^m(\xi, t)) &= r(\xi) & \xi \in \Omega_m \\ \rho c_p \partial_t T^f(\mathbf{x}, t) - \nabla \cdot (k \nabla T^f(\mathbf{x}, t)) &= 0 & \mathbf{x} \in \Omega_f \\ k \partial_n T^m(\xi, t) &= k \partial_n T^f & \xi \in \Gamma_m \\ T^f(\mathbf{x}, t) &= T^m & \mathbf{x} \in \Gamma_f \\ q_{\text{conv}} &= h_{\text{conv}}(T^m(\xi, t) - T_{\text{env}}) & \xi \in \partial\Omega_{m, \text{conv}} \\ T(\xi, 0) &= T_0(\xi, 0) & \xi \in \Omega_m \Big|_{t=0} \\ q_{\text{conv}} &= h_{\text{conv}}(T^f(\mathbf{x}, t) - T_{\text{env}}) & \mathbf{x} \in \partial\Omega_{f, \text{conv}} \\ T(\mathbf{x}, 0) &= T_0(\mathbf{x}, 0) & \mathbf{x} \in \Omega_f \Big|_{t=0}\end{aligned} \tag{A.1}$$

where the only difference lies in the transmission conditions being imposed at Γ_m and Γ_f instead of Γ . In its weak form, this domain decomposition scheme is the same as the one in proposition 4.1 of Houzeaux [40]. Although at a first glance they might appear different since the aforementioned is homogeneous, the heterogeneity is taken care of by expressing both PDEs in the same reference frame.

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SUBSTEPPING METHODS

This chapter presents the author’s most recent work, currently under peer review, and constitutes the principal contribution of this thesis.

INTRODUCTION

Building on the advected subdomain method described in the previous chapter, this work turns its attention to substepping techniques. These approaches have recently gained attention in the literature, notably with the works of [Hodge \[2021\]](#), [Viguerie et al. \[2022\]](#), with [Hodge \[2021\]](#) reporting significant speed-ups. Substepping directly addresses the fundamental bottleneck of [LPBF](#) simulation —the severe disparity of time-scales— making it a natural candidate for part-scale modeling.

These methods are known under various names, such as subcycling, multirate and multi-step methods. They partition the computational domain into subdomains that can be advanced in time with different time-step sizes and/or integration schemes. They naturally fit problems with strong time-scale disparities, where the smallest one only affects a small region of the domain, such as [LPBF](#).

So far in the [LPBF](#) literature, these methods have only been employed to vary the time-step size. The computational domain Ω is typically divided into two regions, Ω_f and Ω_s , with time-steps Δt_f and $\Delta t_s = m \Delta t_f$, respectively, for some integer $m > 1$. Ω_f is a small region around the moving heat source and Ω_s covers the rest of the domain. The constraint on the time-step size (47) only applies to Ω_f , while Ω_s can be advanced with a larger time-step.

A review of the literature revealed that a variety of [DD](#) methods are employed to couple Ω_f and Ω_s , but common patterns could be identified in their overall structure.

In particular, these schemes generally start with a predictor step, estimating the solution at t^{n+1} and feeding it to Ω_f . After advancing both subdomains to t^{n+1} , one could take the new solution at t^{n+1} and feed it back to Ω_f , repeating this process until convergence. In practice, however, this is not done, as cost reduction is the main objective of these methods. Hence, these schemes can be regarded as staggered [DD](#) methods truncated after a single iteration. Two main approaches were identified in the literature: *fully staggered* [[Cheng and Wagner, 2021](#), [Elahi et al., 2025](#)] and *semi-monolithic* [[Viguerie et al., 2022](#), [Hodge, 2021](#)].

This chapter presents a novel fully staggered Robin-Robin scheme with custom Robin coefficients [[Chen et al., 2014](#)] and compares it to the semi-monolithic scheme of [Hodge \[2021\]](#).

Additionally, the advected subdomain method is embedded into the fast partition in an attempt to compound its speed-up with that of substepping. From a computational standpoint, both methods mesh well together, as substepping restricts the presence of advection to Ω_f only.

SUMMARY & CONCLUSIONS

The methods were implemented in Python / C++ as a FEniCSx extension [[Baratta et al., 2023](#)], which was extended to support growing domains using `multiPhenicsx` [[Ballarin, 2020](#)], and `multimesh` staggered and monolithic [DD](#) schemes using custom assembly routines.

The implemented thermal model includes latent heat effects and temperature-dependent material properties. The cases considered include a 2D benchmark, 3D experimental melt pool measurements and 3D [LPBF](#) cubic parts of increasing size.

The authors first considered a fully staggered Dirichlet-Neumann approach. It was found to perform poorly, requiring both relaxation and more iterations to converge than Robin-Robin. This result is in line with the findings of [Canuto and Lo Giudice \[2019\]](#).

The Robin-Robin scheme is found to perform better, obtaining similar or marginally better accuracy than the semi-monolithic Dirichlet approach of [Hodge \[2021\]](#), but at a lower computational cost, since the latter requires an additional global assembly / solve.

Observed speed-ups depend mainly on the fraction of total DOFs contained in Ω_f , which decreases the relative cost of the “fast” solve. Increasing the ratio $m = \Delta t_s / \Delta t_f$ decreases the frequency of “slow” solves, but can increase the ratio of DOFs in Ω_f : beyond a certain m , a *slow down* is observed due to the larger Ω_f . For $\Delta t_f = 0.5T_{hs}$, $\Delta t_s \in [5, 10]T_{hs}$, one can expect speed-ups in the range 2-5 for DOFs ratios in the range 5-20%.

These speed-up numbers are modest in comparison to the ones advertised in [Hodge \[2021\]](#), [Puso and Hodge \[2023\]](#), [Cheng and Wagner \[2021\]](#) and more in line with the findings of [Viguerie et al. \[2022\]](#). After closer inspection, the author realized that [Hodge \[2021\]](#) operated in a different regime, with extremely fine time-steps $\Delta t_f \approx 0.03T_{hs}$. The current work employs $\Delta t_f = 0.5T_{hs}$, and Viguerie was closer to $\Delta t_f = 1T_{hs}$. It was concluded that Hodge required such fine time-steps (subelement scale) due to the chosen latent heat model (apparent heat capacity and heat integration scheme). In the appendix of this chapter, the apparent heat capacity model is compared to the enthalpy-based model used in this work and [Viguerie et al. \[2022\]](#). The latter is found to be much more robust, allowing for coarser time-steps.

The advected subdomain was found to accelerate simulations for sufficiently long tracks. This chapter reiterates the finding of the previous chapter, proving that the method improves accuracy in the [HAZ](#). However, it performed poorly for the cube prints: neighboring tracks were too close relative to the subdomain size, so the advection sheared away the thermal tails of the previous track, negatively impacting accuracy. The work concludes that this method is best suited to simple scan patterns with long straight tracks, and its use should be avoided for general speed-up purposes.

Additional findings include:

- The truncation of the substepping schemes to a single iteration has a negligible impact on accuracy in the considered 2D benchmark.
- The Dirichlet scheme of [Hodge \[2021\]](#) does not let the solution deviate from the predictor. A predictor step without the heat source is found to improve the accuracy of this scheme.
- The thermal model considered (heat equation with melting phase change) is able to reproduce experimental melt pool measurements without prior calibration if coupled with a thermally dependent absorptivity. The absorptivity curve was calibrated on *training* measurements and then used as-is to successfully predict a *test* measurement. However, the calibrated curve shows a drop in absorptivity after melting, which is not physically expected. It most likely compensates for an absent heat sink due to fluid flow effects.

Overall, this chapter provides a comprehensive evaluation of substepping strategies for LPBF thermal modeling, clarifying their components, performance and limitations.

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Substepped and advected subdomain methods for part-scale LPBF modeling

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Abstract

This work presents substepping schemes for part-scale Laser Powder Bed Fusion (LPBF) modeling where the computational domain is divided into a fast partition with a small time-step and a slow one using a large time-step. These schemes are of special interest due to the disparity of time scales present in LPBF applications, which renders simulation prohibitively expensive unless simplifications are made. A Robin-Robin substepper is proposed and compared to the scheme proposed by Hodge (2021).

Additionally, the introduction of an advected subdomain in the fast partition is proposed. This approach was first presented in Slimani et al. (2024) and allows for larger time-steps, as the problem in the Heat Affected Zone (HAZ) is posed in the moving reference frame of the laser, where the thermal field is significantly steadier than in the fixed frame.

These methods are used in combination to obtain a computationally efficient scheme for LPBF thermal simulations. The proposed methods are implemented in **FEniCSx**. Their strengths and weaknesses are evaluated through 2D benchmarks, comparison with experimental melt pool data, and 3D LPBF simulations.

1. Introduction

Thermal modelling of LPBF processes is necessary in order to optimize the microstructure and the scan path to reduce warpage and residual stresses. However, part-scale simulation is especially costly due to the “extremely multiscale” nature of the process (Hodge, 2021).

As an example, consider the bridge structures proposed in the AM Bench 2022 challenge (Yeung et al., 2022): the smallest and largest lengths are 40 μm (laser radius) and 75 mm (part length), resulting in a ratio of spatial scales in the order of 10^3 . The disparity is even greater for temporal scales: the cumulative laser-on time is about 15 minutes, while the time it takes for the laser to move by one radius, T_{hs} , is about 40 μs . The resulting ratio of scales is in the order of 10^7 , imposing a prohibitively high number of time-steps to accurately resolve the HAZ. This issue is hard to circumvent, since, when modelling in the laboratory reference frame, if the time-step Δt does not satisfy the constraint

$$\Delta t \leq T_{hs} \quad (1)$$

the resulting temperature field exhibits spurious oscillations, rendering the solution qualitatively and quantitatively unacceptable. To achieve accurate results, typical values of the employed time-step are around 0.2–0.5 T_{hs} (Viguerie et al., 2022; Patil et al., 2021; Proell et al., 2024).

Since employing an accurate power density profile comes at a high cost, the most common approach is to utilize *lumped heat sources*, encompassing techniques such as *hatch lumping*, *layer lumping* and *flash heating* (Chiumenti et al., 2017; Malmelöv et al., 2019; Soldner and Mergheim, 2019). A time-step is decided without regard for constraint (1) and the laser’s energy input is evenly distributed along its path. Although this approach allows for feasible simulations, it comes at the cost of accuracy. Van Elsen et al. (2007) shows that while temperature contours far from the HAZ might coincide, peak temperature is grossly underestimated,

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possibly resulting in the absence of a melt pool. *Flash heating* addresses this issue by artificially increasing the deposition speed in order to recover a more faithful melt volume (Patil et al., 2021), hence requiring numerical calibration.

Recent literature has pursued two avenues to render part-scale simulations feasible without lumped heat sources: optimizing the computation of a single time-step and using small time-steps only where necessary.

Many approaches exist to reduce the cost of a given time-step, such as matrix-free FEM (Dugast et al., 2021), the use of GPUs (Leonor and Wagner, 2024; Dugast et al., 2021) and CPU vectorization (Proell et al., 2024). Essongue et al. (2022) advocates for explicit time integration schemes, as in LPBF applications, constraint (1) is more restrictive than the stability threshold. In their follow-up work, Essongue et al. (2024) demonstrate that the speed-up is significantly lower in Directed Energy Deposition modelling due to the reduced contrast in time scales.

Note that although Proell et al. (2024) achieves a considerable speed-up by combining many of these methods together with additional compiler level optimizations, they still consider the simulation of decimeter-scale parts unrealistic.

Since constraint (1) must only be enforced near the HAZ, multiple authors have proposed methods that allow different time-steps in different subdomains. Kopp et al. (2022) shows welding examples with space-time FEM: because the time axis is included in the mesh, adaptive mesh refinement is applied in order to use smaller time-steps in the HAZ. Few references have adopted this technique, since the dominant trend in the field are implementations based on finite difference discretizations in time.

Conversely, substepping has seen broader adoption due to its easier integration into existing software. The first substepping work in AM was introduced by Soldner and Mergheim (2019), who combined it with a lumped heat source model. Following the approach of Nakshatrala et al. (2009), they evaluated the interface terms explicitly at t^n , introducing a stability constraint on the macro time-step Δt_s .

Viguerie et al. (2022) presents a substepping approach based on a custom domain decomposition (DD) scheme. In their welding examples with IN625, they employ micro-steps of $1T_{hs}$ and macro-steps of $4T_{hs}$, obtaining a speed-up of 2.5. In comparison, Hodge (2021) claims much larger speed-ups in the order of 100, albeit with much smaller micro-steps of approximately $0.02T_{hs}$, and similarly sized macro-steps of $3T_{hs}$. Although the two substepping schemes are structurally similar, the treatment of the phase change in the latter necessitated very fine time discretization (apparent heat capacity and heat integration methods). In their follow-work, Puso and Hodge (2023) showcase the substepping scheme in a practical example using micro-steps of about $0.04T_{hs}$ and macro-steps of $7.7T_{hs}$.

Cheng and Wagner (2021) derive an efficient substepping scheme based on Dirichlet-Robin interface conditions. The Robin coefficient is analytically derived from a linear 1D problem, resulting in high accuracy at the interface. They showcase their scheme with micro-steps of $0.07T_{hs}$ and macro-steps of $7T_{hs}$, yielding a reported speed-up of 100.

In their recent work, Elahi et al. (2025) extend the three level scheme DD of Leonor and Wagner (2024) to employ different time-steps in each level. They present an extremely efficient GPU-based scheme, using micro-steps of $0.086T_{hs}$ at the finest level, and macro-steps of $5.5T_{hs}$ at the coarsest level. It is apparent from this quick overview of the literature that most substepping references adopt macro-steps of a few T_{hs} .

In previous work, the authors pursued a different strategy to speed-up LPBF simulations by attaching a moving subdomain to the heat source and performing computations in its reference frame (Slimani et al., 2024). In this frame, where the laser remains stationary, the thermal field is steadier, allowing for significantly larger time-steps for long scan tracks. However, the work only addressed the linear heat equation and the overall speed-up was limited by the increased computational cost introduced by the advection terms.

Although originally referred to as *Chimera* due to the use of two meshes, the core feature of the method is the subdomain attached to the heat source. The heat equation is posed in the moving reference frame, which introduces advection terms that are central to the model’s behavior and performance. Hence, the name *advected subdomain* is used in this work to better reflect the method’s defining characteristics.

In this work, the authors implement the substepping scheme described by Hodge (2021) as well as an additional Robin-Robin scheme and add their advected subdomain method in the fast subdomain. Thermally dependent material properties as well as phase change are considered in order to present a realistic thermal model of LPBF. The numerical examples will examine both the accuracy and efficiency of the various models proposed.

2. Methodology

This section describes the modeling frameworks adopted in this work. First, the balance of energy equation is presented, along with the phase change and growing domain treatments. Next, a Robin-Robin variant of the advected subdomain method presented in Slimani et al. (2024) is described. The section concludes with a short overview of multi-timestep methods and details the substepping approaches used in this work. Specifically, the substepper presented in Hodge (2021) is used throughout the work as a baseline, and a novel Robin-Robin substepper with Robin coefficients based on Chen et al. (2014) is proposed.

2.1. Problem statement

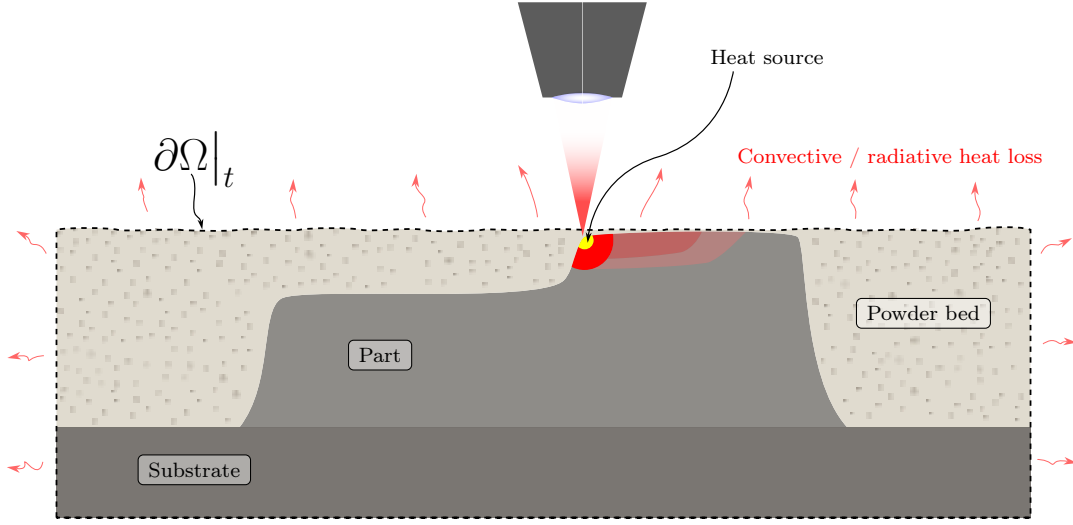


Figure 1: Schematic of the LPBF computational domain $\Omega(t)$, encompassing the bulk (part and substrate) and powder bed regions, together with the applied heat source and convective/radiative heat losses.

The governing PDE is the energy balance including diffusion, heating and latent heat effects; a temperature field $T = f(\mathbf{x}, t) : \Omega \rightarrow \mathbb{R}$ is sought such that

$$\begin{aligned} \rho c_p \partial_t T(\mathbf{x}, t) + \rho L \partial_t f_l - k \Delta T(\mathbf{x}, t) &= r(\mathbf{x}, t) & \forall \mathbf{x} \in \Omega(t) \\ \partial_n T &= h(T - T_{\text{env}}) & \forall \mathbf{x} \in \partial\Omega_{\text{conv}}(t) \\ \partial_n T &= \varepsilon \sigma (T^4 - T_{\text{env}}^4) & \forall \mathbf{x} \in \partial\Omega_{\text{rad}}(t) \end{aligned} \quad (2)$$

where ρ, c_p, L, f_l and r denote respectively the density, specific and latent heats, liquid fraction and power density. $h_{\text{conv}}, \varepsilon$ and σ are the convection heat transfer coefficient, the emissivity and the Stefan-Boltzmann constant, and T_{env} is the environment temperature. Figure 1 presents the computational domain for the case of LPBF.

This work adopts the latent heat treatment proposed in Kollmannsberger et al. (2018), which uses a variant of the source-based approach presented in Celentano et al. (1994). Rather than using the chain rule to express $\partial_t f_l$ as a function of $\partial_t T$, as done in the apparent heat capacity method, the time derivative is kept as-is (Celentano et al., 1994) and f_l is regularized using a hyperbolic tangent (Kollmannsberger et al., 2018):

$$f_l(T) = \frac{1}{2} \left[\tanh \left(S \frac{2}{T_l - T_s} \left(T - \frac{T_s + T_l}{2} \right) \right) + 1 \right] \quad (3)$$

where T_l, T_s and S correspond to the liquidus and solidus temperatures and a smoothing parameter. f_l and its derivative are plotted in fig. B.26 for several values of S : as S increases, f_l approaches the step function and the phase change becomes isothermal.

$\partial_t f_l$ is computed as part of the time integration scheme and can be regarded as an additional heat sink term depending on the temperature history. The authors find that this approach is much more robust than the apparent heat capacity method, see appendix Appendix B for a comparison.

The time dependency of the computational domain in eq. (2) arises from the domain growth associated with the LPBF recoating process. It is numerically modelled using the born-dead element technique (Chiu-mentti et al., 2010). The deposition and melting processes are illustrated in fig. 2. Figure 2a shows a bare substrate below an *inactive* powder layer, which does not take part in the thermal problem. Figure 2b shows the activation of the powder layer, which will be subsequently heated by the moving heat source. Then, at the end of a given time-step, powder elements whose average temperature surpasses the melting point $T_m = \frac{T_s + T_l}{2}$ are set to bulk, as shown in fig. 2c. Following Kollmannsberger et al. (2018), the material properties of both powder and bulk are temperature-dependent and become identical above the melting point, so that powder elements are indistinguishable from bulk elements once melted.

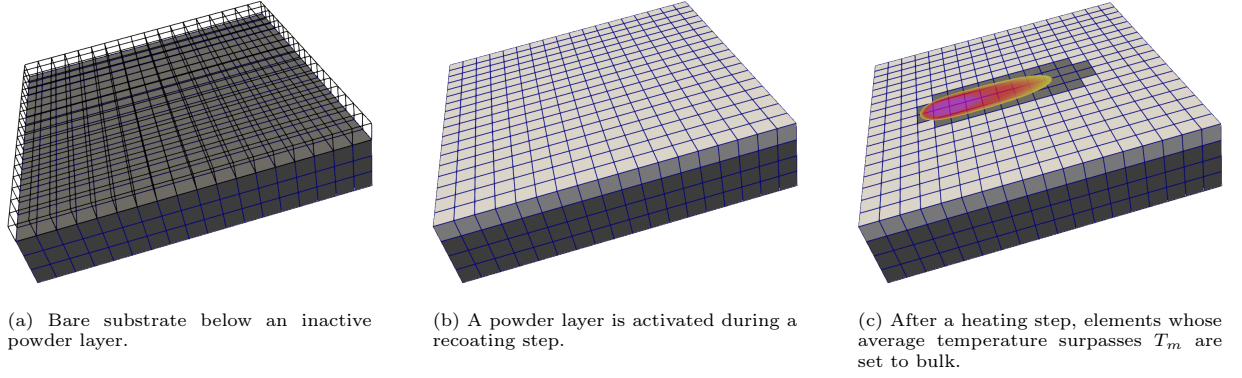


Figure 2: Illustration of deposition and melting processes. Powder Bulk

In the remainder of this work, the solution of eq. (2) using FEM and uniform Backward-Euler time integration is referred to as the *standard model*, and serves as a reference for the proposed substepping schemes.

2.2. Advected subdomain model

The motivation for the advected subdomain method lies in the observation that the strong transience of the HAZ is primarily due to the motion of the heat source. By reformulating the problem in the frame of the moving heat source, the thermal field becomes significantly steadier, allowing for much larger time-steps.

However, this approach is only meaningful in the vicinity of the heat source, as it would introduce unnecessary complexity elsewhere. Hence, in their previous work (Slimani et al., 2024), the authors subdivided the computational domain in two zones: a moving subdomain $\Omega_m(t)$ attached to the heat source, where the governing equations are posed in the moving reference frame, and a fixed subdomain $\Omega_f(t) = \text{int}(\Omega \setminus \Omega_m(t))$, where the equations remain unaltered. Let $\mathbf{v} = \frac{d\mathbf{x}_{hs}}{dt}$ denote the laser velocity; the change of coordinate system can be expressed as

$$(\mathbf{x}, t) \longrightarrow (\boldsymbol{\xi}, \eta), \begin{cases} \boldsymbol{\xi} = \mathbf{x} - \int_0^t \mathbf{v}(t) dt \\ \eta = t \end{cases} \implies \begin{cases} \partial_{x_i} = \partial_{\xi_i} \Rightarrow \nabla_{\mathbf{x}} = \nabla_{\boldsymbol{\xi}} \\ \partial_t = \partial_{\eta} - v_i \partial_{\xi_i} = \partial_{\eta} - \mathbf{v}(t) \cdot \nabla_{\boldsymbol{\xi}} \end{cases}$$

Denoting η by t for clarity, eq. (2) rewrites as follows for $T_m : \Omega_m \rightarrow \mathbb{R}$:

$$\rho c_p \partial_t T_m(\boldsymbol{\xi}, t) + \rho L \partial_t f_l - \rho(c_p + L f_l') \mathbf{v} \cdot \nabla_{\boldsymbol{\xi}} T_m(\boldsymbol{\xi}, t) - k \Delta_{\boldsymbol{\xi}} T_m(\boldsymbol{\xi}, t) = r(\boldsymbol{\xi}) \quad \forall \boldsymbol{\xi} \in \Omega_m(t) \quad (4)$$

where the source term only depends on space since it is stationary in the moving frame.

As mentioned earlier, the PDE on Ω_f remains unchanged with respect to eq. (2). If the support of the source term is fully contained in Ω_m , the right-hand side is null:

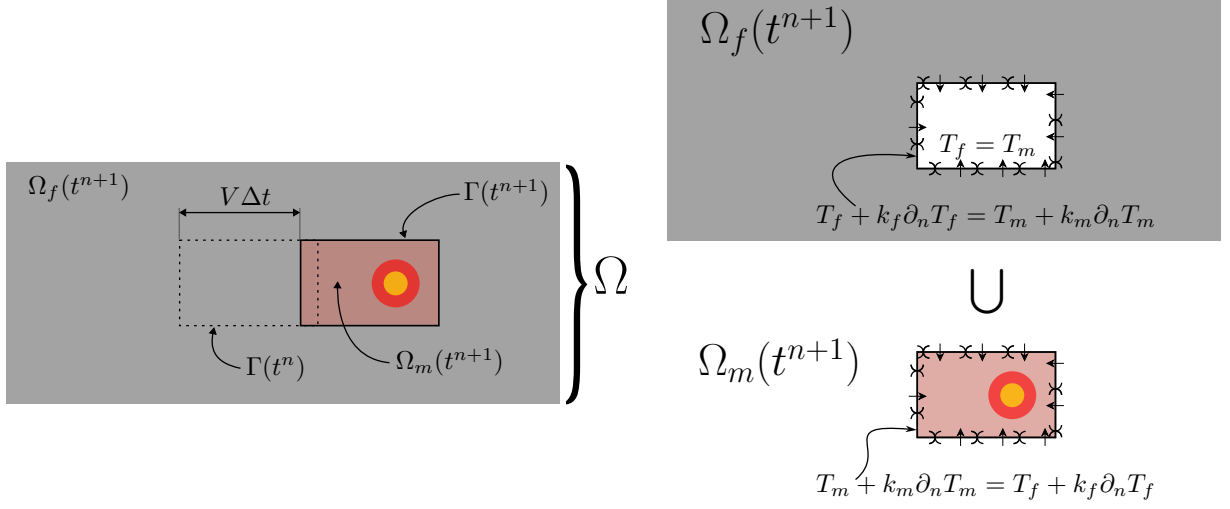


Figure 3: Schematic of non-overlapping advected subdomain with Robin-Robin coupling. The arrows represent fluxes, and the links embody coupling of the solutions on either side. The combination of arrows and links represents the Robin conditions.

$$\rho c_p \partial_t T_f(\mathbf{x}, t) + \rho L \partial_t f_l - k \Delta T_f(\mathbf{x}, t) = 0 \quad \forall \mathbf{x} \in \Omega_f(t) \quad (5)$$

In Slimani et al. (2024), the authors considered Dirichlet-Neumann coupling between the two subdomains. In this work, Robin-Robin coupling is adopted instead, as it is arguably easier to implement (same type of condition on both sides of the interface) and exhibits better staggered convergence properties than Dirichlet-Neumann (Canuto and Lo Giudice, 2019). Figure 3 illustrates a non-overlapping decomposition of Ω into Ω_m and Ω_f and the Robin-Robin coupling conditions applied on the interface $\Gamma(t) = \partial\Omega_m \cap \partial\Omega_f$:

$$T_m + k|_{T_m^{n+1}} \partial_n T_m = T_f + k|_{T_m^{n+1}} \partial_n T_f \quad \xi \in \Gamma(t) \quad (6)$$

$$T_f + k|_{T_f^{n+1}} \partial_n T_f = T_m + k|_{T_m^{n+1}} \partial_n T_m \quad x \in \Gamma(t) \quad (7)$$

The remaining heat transfer and initial conditions take the form

$$\begin{aligned} q_{\text{conv}} &= h_{\text{conv}}(T_m(\xi, t) - T_{\text{env}}) & \xi \in \partial\Omega_{m, \text{conv}}(t) \\ q_{\text{rad}} &= \varepsilon \sigma (T_m(\xi, t)^4 - T_{\text{env}}^4) & \xi \in \partial\Omega_{m, \text{rad}}(t) \\ T_m(\xi, 0) &= T_0(\xi, 0) & \xi \in \bar{\Omega}_m(0) \\ T_m(\xi, t) &= T_{\text{dep}} & x(\xi) \in \bar{\Omega}(t) \mid \forall t' < t, \ x(\xi) \notin \bar{\Omega}(t') \\ q_{\text{conv}} &= h_{\text{conv}}(T_f(x, t) - T_{\text{env}}) & x \in \partial\Omega_{f, \text{conv}}(t) \\ q_{\text{rad}} &= \varepsilon \sigma (T_f(x, t)^4 - T_{\text{env}}^4) & x \in \partial\Omega_{f, \text{rad}}(t) \\ T_f(x, 0) &= T_0(x, 0) & x \in \bar{\Omega}_f(0) \\ T_f(x, t) &= T_{\text{dep}} & x \in \bar{\Omega}(t) \mid \forall t' < t, \ x \notin \bar{\Omega}(t') \end{aligned} \quad (8)$$

Let $\mathcal{T}_m(t)$ and $\mathcal{T}_f(t)$ denote the active finite element meshes of Ω_m and Ω_f . Let V_m and V_f be the finite element spaces associated with $\mathcal{T}_m$ and $\mathcal{T}_f$. The residual weak forms $\mathcal{R}_m$ and $\mathcal{R}_f$ of the moving and fixed subproblems are included in Appendix A. Together, they define a coupled system of nonlinear integral equations for $T_m^{n+1} \in V_m$ and $T_f^{n+1} \in V_f$:

$$\begin{aligned}
\mathcal{R}_m(T_m^{n+1}, T_f^{n+1}) &= 0 & \forall \phi_m \in V_m \\
\mathcal{R}_f(T_m^{n+1}, T_f^{n+1}) &= 0 & \forall \phi_f \in V_f
\end{aligned}$$

These equations are solved using Newton-Raphson iterations: given current guesses $T_m^{n+1,i}$ and $T_f^{n+1,i}$, find δT_m and δT_f such that

$$\frac{\partial \mathcal{R}_m}{\partial T_m} \delta T_m + \frac{\partial \mathcal{R}_m}{\partial T_f} \delta T_f = -\mathcal{R}_m \quad \forall \phi_m \in V_m \quad (9)$$

$$\frac{\partial \mathcal{R}_f}{\partial T_m} \delta T_m + \frac{\partial \mathcal{R}_f}{\partial T_f} \delta T_f = -\mathcal{R}_f \quad \forall \phi_f \in V_f \quad (10)$$

and update the solutions $T_m^{n+1,i+1} \leftarrow T_m^{n+1,i} + \delta T_m$ and $T_f^{n+1,i+1} \leftarrow T_f^{n+1,i} + \delta T_f$ until the increments δT_m and δT_f are sufficiently small.

If material properties are averaged over each element, the matrix forms of $\frac{\partial \mathcal{R}_f}{\partial T_f}$, $\frac{\partial \mathcal{R}_f}{\partial T_m}$ and $\frac{\partial \mathcal{R}_m}{\partial T_f}$ are symmetric. In contrast, the Jacobian block $\frac{\partial \mathcal{R}_m}{\partial T_m}$ is non-symmetric due to advection. When both subproblems are solved together i.e. monolithically, the overall system matrix is therefore non-symmetric. Alternatively, a staggered approach can be employed in which the moving and fixed subproblems are solved sequentially, feeding the solution of one into the other until convergence. This confines the asymmetry to the moving subproblem, but requires an additional loop on top of the Newton-Raphson iterations to enforce coupling consistency.

Both monolithic and staggered approaches are implemented in this work, and their performance is compared in section 4.3.

As mentioned earlier, the goal of the advected subdomain method is to enable larger time-steps as the thermal field in Ω_m becomes steadier. In Slimani et al. (2024), the authors measured the steadiness of the solution by computing the relative L2 norm of the increment between two consecutive time-steps. In this work, the maximum value of the time derivative of T_m is adopted instead. When this value falls below a threshold ϵ , the time-step size Δt is increased for the next step:

$$\text{steadiness_metric}(T_m) := \max_{\Omega_m} \left| \frac{T_m^{n+1} - T_m^n}{\Delta t} \right| < \epsilon \implies \text{Increase } \Delta t \text{ for } t^{n+2} = t^{n+1} + \Delta t \quad (11)$$

The maximum is more robust than the relative L2 norm, as the latter is sensitive to the size of Ω_m .

The motion of Ω_m requires a special workflow of boolean operations to ensure that $\Omega_m(t^n)$ and $\Omega_m(t^{n+1})$ remain subsets of Ω at all times. Mesh intersection and subtraction are implemented efficiently using bounding box trees, making their computational cost negligible compared to assembly and solve. Additional details on the workflow itself can be found in Slimani et al. (2024), or in the open-source code repository (Slimani, 2025).

2.3. Substepping

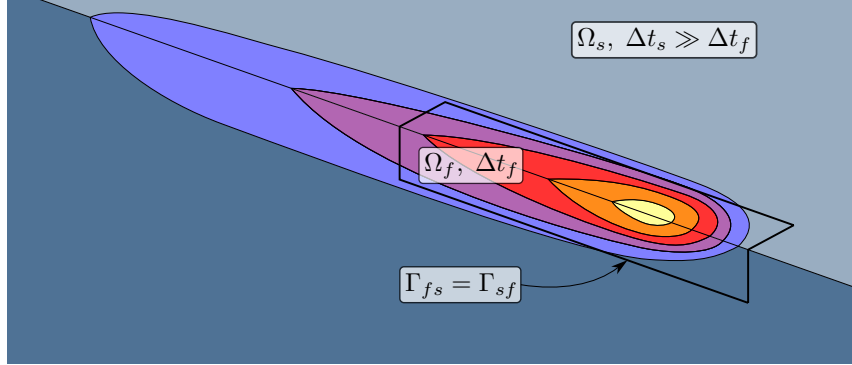


Figure 4: Non-overlapping substepping decomposition. The HAZ is included in the fast partition Ω_f . The remainder of the domain belongs to the slow partition Ω_s .

Substepping methods are known under various names in the literature, including multirate, subcycling, local time-stepping, multistep, etc. They consist in partitioning the domain into subdomains and marching them in time with their own time-steps and/or integration schemes.

Figure 4 illustrates a disjoint partition $\Omega = \Omega_f \sqcup \Omega_s$, where the subscripts f and s denote the *fast* and *slow* subdomains, respectively. Throughout this work, the previously defined fixed subproblem is always contained within the fast partition, so the notation is unambiguous. Let $\Gamma_{fs} = \Gamma_{sf}$ denote the interface between the two partitions. The slow partition Ω_s advances from t^n to $t^{n+1} = t^n + \Delta t_s$ in a single *macro-step*, while the fast partition Ω_f subdivides the same interval in M *micro-steps* of size $\Delta t_f = \frac{\Delta t_s}{M}$.

Let $T_s : \Omega_s \rightarrow \mathbb{R}$ and $T_f : \Omega_f \rightarrow \mathbb{R}$ denote the solutions in the slow and fast partitions. Following domain decomposition principles, they must be coupled across the interface to ensure that *transmission conditions* are satisfied. Let the superscript $\frac{n}{M}$ denote the time index at the n -th micro-step, $t^n + m\Delta t_f$, $m \in [1, M]$. The transmission conditions read

$$T_f^{n+\frac{m}{M}} = T_s^{n+\frac{m}{M}} \quad k\partial_n T_f^{n+\frac{m}{M}} = k\partial_n T_s^{n+\frac{m}{M}} \quad (12)$$

$$T_s^{n+\frac{m}{M}} \approx \left(1 - \frac{m}{M}\right)T_s^n + \frac{m}{M}T_s^{n+1} \quad (13)$$

$$m \in [1 \dots M]$$

That is, both the solution and its flux must remain continuous across the interface throughout the substepping cycle. In a FEM setting, flux continuity is satisfied only in the weak sense via the variational formulation. Since the slow solution is only available at macro-step endpoints, it is approximated at the micro-steps using linear interpolation (13), which introduces a consistency error of order $\mathcal{O}(\Delta t_s)$. The impact of this approximation on the overall accuracy of the substepping scheme is revisited in section 4.1.2.

A review of the literature reveals several substepping schemes proposed for AM (Hodge, 2021; Viguerie et al., 2022; Cheng and Wagner, 2021; Soldner and Mergheim, 2019; Elahi et al., 2025), and broader fields (Canuto and Lo Giudice, 2019; Zhao et al., 2016). While these approaches differ primarily in the way the subdomains are coupled, reflecting the wide variety of domain decomposition methods available, a recurring distinction emerges: some schemes fully separate the fast and slow solves, while others perform combined solves, generally at the end of the substepping cycle. In this work, the former is referred to as *fully staggered*, while the latter is termed *semi-monolithic*.

These should be viewed from a domain decomposition perspective. In classical DD methods with two subdomains, there exists only two options to solve the coupled problem: either a staggered approach or a monolithic one. However, with three or more subdomains, intermediate strategies can be devised. Similarly, regarding the intermediate states of the fast partition as separate subdomains, the same classification applies to substepping schemes.

From this viewpoint, the *fully monolithic* approach solves all micro-steps and the macro-step simultaneously within a single global system, as done for instance in Zhao et al. (2016). For a linear problem with Backward-Euler time integration and weak enforcement of the transmission conditions (12), the corresponding linear system can be written as:

$$\begin{pmatrix} +\frac{\mathbf{M}_f}{\Delta t_f} + \mathbf{A}_f & 0 & \dots & 0 & 0 & \frac{1}{M} \mathbf{C}_{fs} \\ -\frac{\mathbf{M}_f}{\Delta t_f} & +\frac{\mathbf{M}_f}{\Delta t_f} + \mathbf{A}_f & \dots & 0 & 0 & \frac{2}{M} \mathbf{C}_{fs} \\ & & \ddots & & & \\ 0 & 0 & \dots & +\frac{\mathbf{M}_f}{\Delta t_f} + \mathbf{A}_f & 0 & \frac{M-1}{M} \mathbf{C}_{fs} \\ 0 & 0 & \dots & -\frac{\mathbf{M}_f}{\Delta t_f} & +\frac{\mathbf{M}_f}{\Delta t_f} + \mathbf{A}_f & \mathbf{C}_{fs} \\ 0 & 0 & \dots & 0 & \mathbf{C}_{sf} & \frac{\mathbf{M}_s}{\Delta t_s} + \mathbf{A}_s \end{pmatrix} \begin{pmatrix} \mathbf{T}_f^{n+\frac{1}{M}} \\ \mathbf{T}_f^{n+\frac{2}{M}} \\ \vdots \\ \mathbf{T}_f^{n+\frac{M-1}{M}} \\ \mathbf{T}_f^{n+1} \\ \mathbf{T}_s^{n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{b}_f^{n+\frac{1}{M}} + \frac{\mathbf{M}_f}{\Delta t_f} \mathbf{T}_f^n + \frac{M-1}{M} \mathbf{C}_{fs} \mathbf{T}_s^n \\ \mathbf{b}_f^{n+\frac{2}{M}} + \frac{M-2}{M} \mathbf{C}_{fs} \mathbf{T}_s^n \\ \vdots \\ \mathbf{b}_f^{n+\frac{M-1}{M}} + \frac{1}{M} \mathbf{C}_{fs} \mathbf{T}_s^n \\ \mathbf{b}_f^{n+1} \\ \mathbf{b}_s^{n+1} + \frac{\mathbf{M}_s}{\Delta t_s} \mathbf{T}_s^n \end{pmatrix} \quad (14)$$

where $\mathbf{M}$ and $\mathbf{A}$ denote the mass and stiffness matrices, $\mathbf{C}$ represents the coupling matrices, and $\mathbf{b}$ corresponds to the source term. A similar approach is adopted in space-time FEM methods, since all “time slabs” are solved simultaneously (Kopp et al., 2022).

Algorithm 1 Substepping workflows

▷ The first superscript indicates the substepping staggered iteration count.

- 1: **if** do_predictor **then**
- 2: | $T_s^{0,n+1} \leftarrow \tilde{T}_s^{n+1}$ from predictor step over Ω at Δt_s
- 3: **else**
- 4: | $T_s^{0,n+1} \leftarrow T_s^n$
- 5: $i \leftarrow 0$
- 6: **while** not converged at Γ_{fs} and $i < i_{\max}$ **do**
- 7: | $i \leftarrow i + 1$
- 8: | Set solution and material composition to values at t^n

- Fully staggered (Cheng and Wagner, 2021; Elahi et al., 2025; Canuto and Lo Giudice, 2019)
- 9: **for** $m = 1, \dots, M$ **do**
 - 10: | Solve for $T_f^{i,n+\frac{m}{M}}$ on Ω_f at Δt_f with boundary condition from

$$T_s^{i-1,n+\frac{m}{M}} = \left(1 - \frac{m}{M}\right) T_s^n + \frac{m}{M} T_s^{i-1,n+1} \quad (15)$$
 - 11: | Solve for $T_s^{i,n+1}$ on Ω_s with boundary condition from $T_f^{i-1,n+\frac{m}{M}}$
 - 12: **end while**
 - 13: $T_s^{n+1} \leftarrow T_s^{i,n+1}, \quad T_f^{n+1} \leftarrow T_f^{i,n+1}$
-

- Semi-monolithic (Hodge, 2021; Viguerie et al., 2022)
- 9: **for** $m = 1, \dots, M-1$ **do** ▷ All substeps but one
 - 10: | Solve for $T_f^{i,n+\frac{m}{M}}$ on Ω_f at Δt_f with boundary condition from eq. (15).
 - 11: | Monolithic solve for $T_s^{i,n+1}$ and $T_f^{i,n+1}$. For a linear problem with weak coupling, the system reads

$$\begin{pmatrix} \frac{\mathbf{M}_f}{\Delta t_f} + \mathbf{A}_f & \mathbf{C}_{fs} \\ \mathbf{C}_{sf} & \frac{\mathbf{M}_s}{\Delta t_s} + \mathbf{A}_s \end{pmatrix} \begin{pmatrix} \mathbf{T}_f^{n+1} \\ \mathbf{T}_s^{n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{b}_f^{n+1} + \frac{\mathbf{M}_f}{\Delta t_f} \mathbf{T}_f^n + \frac{M-1}{M} \mathbf{C}_{fs} \mathbf{T}_s^n \\ \mathbf{b}_s^{n+1} + \frac{\mathbf{M}_s}{\Delta t_s} \mathbf{T}_s^n \end{pmatrix} \quad (16)$$

In practice, most references in the AM literature adopt either fully staggered or semi-monolithic schemes. Algorithm 1 summarizes their respective workflows. Both algorithms start with an optional predictor step to obtain an initial estimate of the slow solution at t^{n+1} . Then, the substepping cycle begins: the fast partition is advanced in time, receiving a boundary condition from the slow partition.

In the fully staggered schemes of Cheng and Wagner (2021); Canuto and Lo Giudice (2019), the fast partition is marched M times until t^{n+1} , and only then the slow partition is advanced separately, receiving a boundary condition from the last micro-step. The authors also classify Elahi et al. (2025) as a fully staggered scheme; although it employs 3 subdomains, all are marched separately i.e. without any combined solve.

In the semi-monolithic schemes of Hodge (2021); Viguerie et al. (2022), the fast partition is marched $M - 1$ times, and then a joint monolithic solve is performed for both partitions at t^{n+1} : the corresponding linear system is given by eq. (16) (see algorithm 1), under the same assumptions as eq. (14).

The advantage of the semi-monolithic approach is that the joint solve at the end of the substepping cycle ensures that transmission conditions (12) are satisfied at t^{n+1} , which is not the case for fully staggered schemes. However, the latter is computationally cheaper and more modular.

Once both partitions have been advanced to t^{n+1} , one could update the interface conditions at the micro-steps and repeat the substepping cycle, until no significant change is observed in the solutions. In practice, no scheme in the LPBF literature performs more than one substepping iteration, since reducing computational cost is the primary motivation. Hence the corresponding superscript in algorithm 1 is omitted in the rest of this document. As it will be shown in section 4.1.3, this truncation has a negligible impact on the accuracy of the solution.

In this work, two substepping schemes are implemented and compared: the semi-monolithic Dirichlet substepper presented in Hodge (2021), and a modified version of the fully staggered Robin-Robin substepper presented in Canuto and Lo Giudice (2019). In the remainder of this document, they will be referred to as the *Dirichlet* and *Robin* substeppers, for brevity.

2.3.1. Dirichlet substepper

Figure 5 illustrates an example step of the Dirichlet substepper. First, the predictor step (fig. 5b) obtains an initial estimate of the slow solution at t^{n+1} , $\tilde{T}_s^{n+1}$. Then, $M - 1$ substeps are performed on Ω_f : fig. 5c shows the solution $T_f^{n+\frac{m}{M}}$, $1 \leq m < M$ after a generic substep. The Dirichlet condition imposed on Γ_{fs} is obtained from the linear interpolation (13) using the previous slow solution T_s^n and the predicted one $\tilde{T}_s^{n+1}$:

$$T_f^{n+\frac{m}{M}} = T_s^{n+\frac{m}{M}} = \left(1 - \frac{m}{M}\right) T_s^n + \frac{m}{M} \tilde{T}_s^{n+1} \quad \forall \mathbf{x} \in \Gamma_{fs} \quad (17)$$

From a transmission conditions standpoint, only the continuity of the solution is enforced at the substeps.

Finally, the monolithic solve (or *corrector step*) solves for both T_f^{n+1} and T_s^{n+1} . Since same mesh DD is employed, the interface DOFs are shared between the two partitions. In this work, they are assigned to the fast partition.

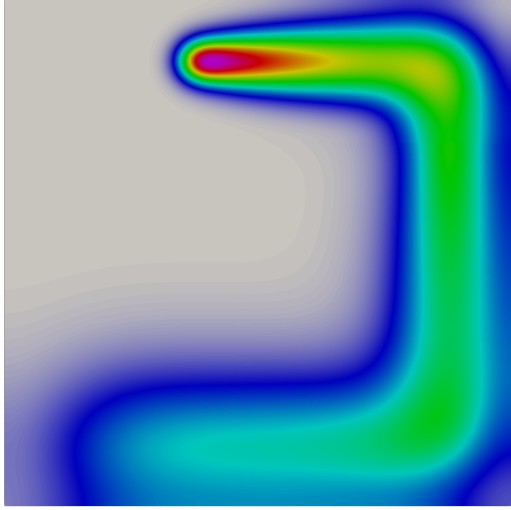
2.3.2. Robin substepper

An example step of the Robin substepper is also shown in fig. 5. The predictor step is identical to the Dirichlet case. Then, M substeps are performed on Ω_f : fig. 5e shows the solution at the m -th substep, $T_f^{n+\frac{m}{M}}$, $1 \leq m < M$. The Robin condition imposed on Γ_{fs} reads

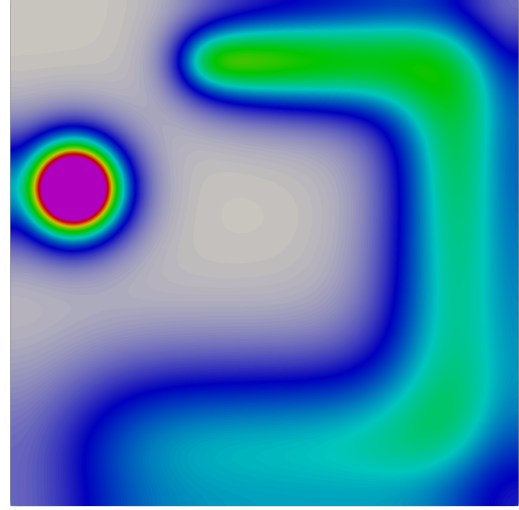
$$\begin{aligned} \gamma_f T_f^{n+\frac{m}{M}} + k_f \partial_n T_f^{n+\frac{m}{M}} &= \gamma_f T_s^{n+\frac{m}{M}} + k_s \partial_n T_s^{n+\frac{m}{M}} & \forall \mathbf{x} \in \Gamma_{fs} \\ \gamma_s T_s^{n+1} + k_s \partial_n T_s^{n+1} &= \gamma_f T_f^{n+1} + k_f \partial_n T_f^{n+1} & \forall \mathbf{x} \in \Gamma_{sf} \end{aligned} \quad (18)$$

where k_f and k_s are the thermal conductivities on the fast and slow partitions, respectively. The coefficients γ_f and γ_s are generally set to 1, see Canuto and Lo Giudice (2019); however, one can attempt to optimize this choice in order to improve the convergence of the staggered scheme, as done analytically in Cheng and Wagner (2021) for Dirichlet-Robin coupling. Following Chen et al. (2014), in this work they are set to $\mathcal{O}(1)$ and $\mathcal{O}(k/h)$, respectively. This choice is “optimal” in the sense that it should result in mesh independent convergence rate of the staggered scheme.

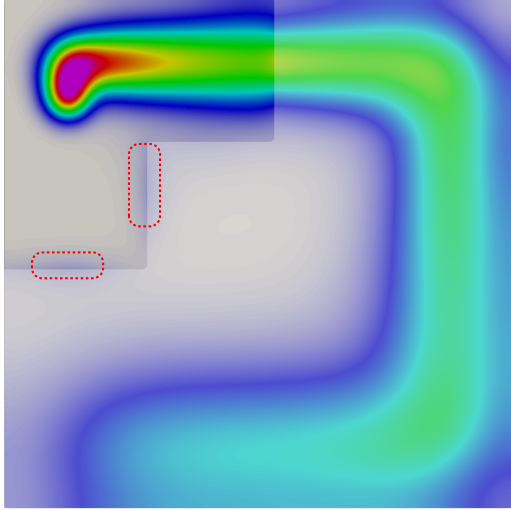
Finally, the *corrector step* solves for T_s^{n+1} on Ω_s , receiving a Robin condition from the last micro-step on Ω_f . Figure 5f shows the solution T_s^{n+1} after the corrector step. Note that the discontinuities at the interface are a natural consequence of the truncated staggered scheme and the weak enforcement of solution continuity.



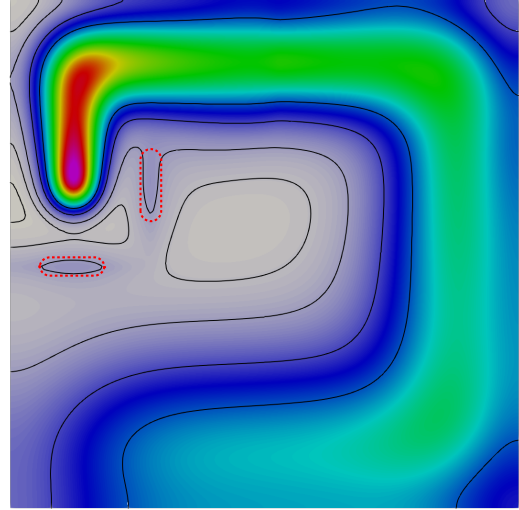
(a) Previous solution T^n



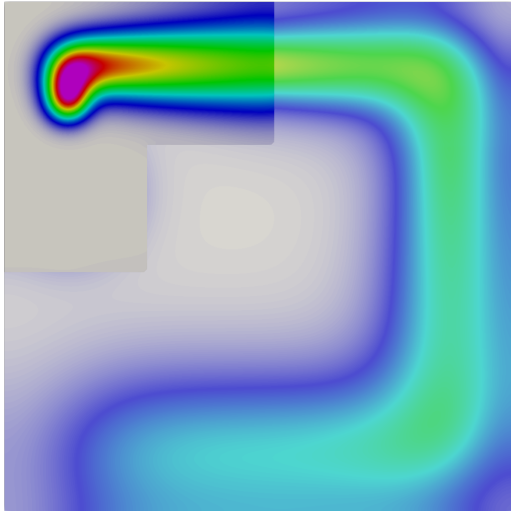
(b) $\tilde{T}^{n+1}$ after predictor step



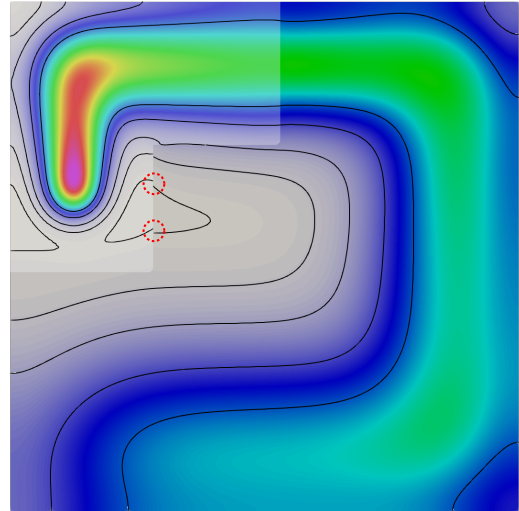
(c) Intermediate **Dirichlet** substep. The Dirichlet condition does not let the solution deviate from the predictor.



(d) **Dirichlet** corrector step. Note the leftover temperature peaks from the predictor.



(e) Intermediate **Robin** substep. Compared to the Dirichlet substep, the solution is free to diffuse away from the predictor.



(f) **Robin** corrector step. Note the discontinuities in the solution.

Figure 5: Examples of Dirichlet and Robin substepping cycles.

It is worth mentioning that the authors initially pursued a Dirichlet-Neumann variant of the substepper; however, as per Canuto and Lo Giudice (2019), the authors found that it lacked both accuracy and robustness, requiring a relaxation parameter to converge (see section 4.1.3).

2.4. Substepped advected subdomain methods

The main purpose of this work is to combine the advantages of the advected subdomain method and the substepping schemes. The moving domain Ω_m is embedded within the fast partition Ω_f , such that the substeps are carried out using the advected subdomain method. This is advantageous compared to the original advected subdomain method since it considerably reduces the size of the asymmetric system by excluding the slow partition.

As a consequence of using of the steadiness workflow of the advected subdomain model, a macro-step is no longer divided into a fixed number of substeps, since Δt_f is increased adaptively. The advected subdomain will be inserted within both the Robin and Dirichlet substeppers described in section 2.3. The resulting schemes can be regarded as three level methods, similar to Leonor and Wagner (2024); Elahi et al. (2025).

3. Implementation

The schemes presented in section 2 were implemented on top of the **FEniCSx** software library (Baratta et al., 2023). For the solution of linear systems, the **PETSc** library was employed. Following the **FEniCSx** design philosophy, high-level functionality was written in **Python**, while performance-critical components were implemented using **C++** and exposed to **Python** via **nanobind** (Jakob, 2022). The code heavily relies on the **multiphenicsx** extension (Ballarin, 2020) of **FEniCSx**, which provides DOF-deactivation functionality used to implement the growth of the domain and the DD routines.

The implementation of the presented substepping strategies was relatively simple in comparison to the implementation of the advected subdomain scheme. In this work, the former are based on same-mesh DD, which is natively supported by **FEniCSx**. However, the latter relies on multi-mesh DD strategies, which required the development of custom interface detection algorithms and assembly routines for both the residual and Jacobian contributions of eqs. (6) and (7), a task further complicated by the distributed-memory setting of MPI, where coupled DOFs often reside on different processes.

Interface detection was implemented as follows: a quadrature rule is generated on all the boundary facets of $\mathcal{T}_i$, where $i = m, f$. For each Gauss point of each facet, a spatial search is performed on the cells of $\mathcal{T}_j$, $j \neq i$. The search returns ownership information in the form of the rank and local element index of the cell of $\mathcal{T}_j$ that contains the point, if any. A boundary facet of $\mathcal{T}_i$ is marked as an interface facet only if all its quadrature points are located in $\mathcal{T}_j$; otherwise it is discarded.

This procedure may produce false positives in corner cases, such as closed quadrature rules and single element protrusions of one mesh into another. Nevertheless, it is robust and efficient, as ownership information is later reused during the assembly of the coupling contributions to associate each Gauss point with the DOFs of the neighboring mesh it must couple to, and the geometry of the cell that contains it. This is necessary in a distributed memory setting, since each process stores only a subset of the global mesh and coupled DOFs of the two meshes will be owned by different processes and continuously change as $\mathcal{T}_m$ moves.

Before assembly starts, basis functions and their gradients are tabulated at each quadrature point of each interface facet, and these values are reused in each subsequent assembly. Figure 6 shows an example of a monolithic step and the corresponding meshes and partitions.

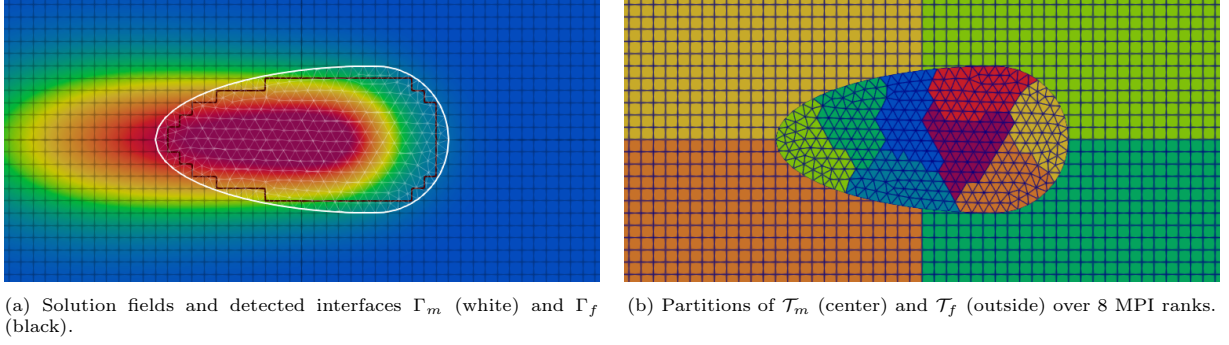


Figure 6: Parallel implementation of the advected subdomain scheme based on multi-mesh DD.

The full implementation is publicly available in the repository associated with this work (Slimani, 2025). A pre-built `Docker` image is also provided to facilitate reproducibility of the results presented in section 4; see the repository’s `README` for detailed instructions.

4. Numerical examples

Throughout the numerical examples, P1 and Q1 elements are used. First, the performance of the proposed substepping schemes is examined in a 2D welding case. Then, the predictive accuracy of the model is demonstrated by reproducing experimental melt pool shape results from the AMB2018-02 benchmark (Lane et al., 2020). Finally, the methodology is applied to 3D LPBF cubes of increasing size to assess the computational speed of the various substeppers.

4.1. 2D square track

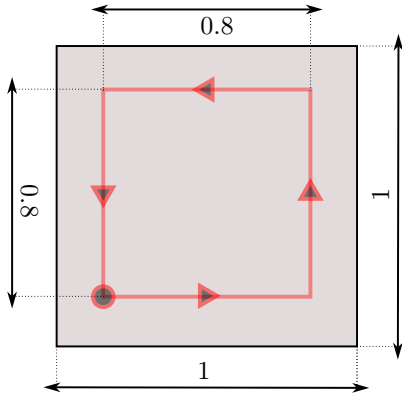


Figure 7: Domain and heating track

Property	Value	Unit
Density ρ	4.3×10^{-6}	kg mm^{-3}
Specific heat c_p	700.0	$\text{J kg}^{-1} \text{ }^\circ\text{C}^{-1}$
Conductivity k	1.0×10^{-2}	$\text{W mm}^{-1} \text{ }^\circ\text{C}^{-1}$
Radius R	0.1	mm
Power P	500.0	W
Speed $\ \dot{\mathbf{x}}_{\text{hs}}\ $	1000.0	mm s^{-1}
Convection coeff. h_{conv}	10	$\text{W mm}^{-1} \text{ }^\circ\text{C}^{-1}$
Solidus temperature T_s	1600.0	$^\circ\text{C}$
Liquidus temperature T_l	1650.0	$^\circ\text{C}$
Latent heat L	350.0	kJ kg^{-1}
Smoothing constant S	0.5	

Table 1: Ti64-like material parameters for 2D square track. Phase change parameters are only used in the non-linear case.

The different substeppers, their accuracy and their respective strengths and weaknesses are studied in the context of a 2D heating path problem. The problem consists of a Gaussian heat source

$$r(\mathbf{x}, t) = \frac{2P}{\pi R^2} \exp\left(\frac{-2\|\mathbf{x} - \mathbf{x}_{\text{hs}}(t)\|_2^2}{R^2}\right)$$

moving along the square path shown in fig. 7. Both linear and non-linear cases are considered, with the latter accounting for phase change effects. Material parameters are listed in table 1.

The first object of study is the temporal convergence behavior of the different substeppers. Each track is $16R$ long, so the coarsest time-steps are chosen as $\Delta t_s = 16T_{hs}$ and $\Delta t_f = 1T_{hs}$, corresponding to one track per macro-step and Δt_f right on the bound of constraint (1). The time-steps are then successively refined in factors of 2 while maintaining the ratio $\Delta t_s/\Delta t_f = 16$, down to $\Delta t_s = 1T_{hs}$ and $\Delta t_f = \frac{1}{16}T_{hs}$. To

isolate temporal from spatial discretization errors, a fine uniform mesh with element size $h = \frac{R}{16}$ is used. The reference solution is computed with a finer discretization of $h = \frac{R}{64}$ and $\Delta t = \frac{1}{64}T_{hs}$, and does not employ substepping.

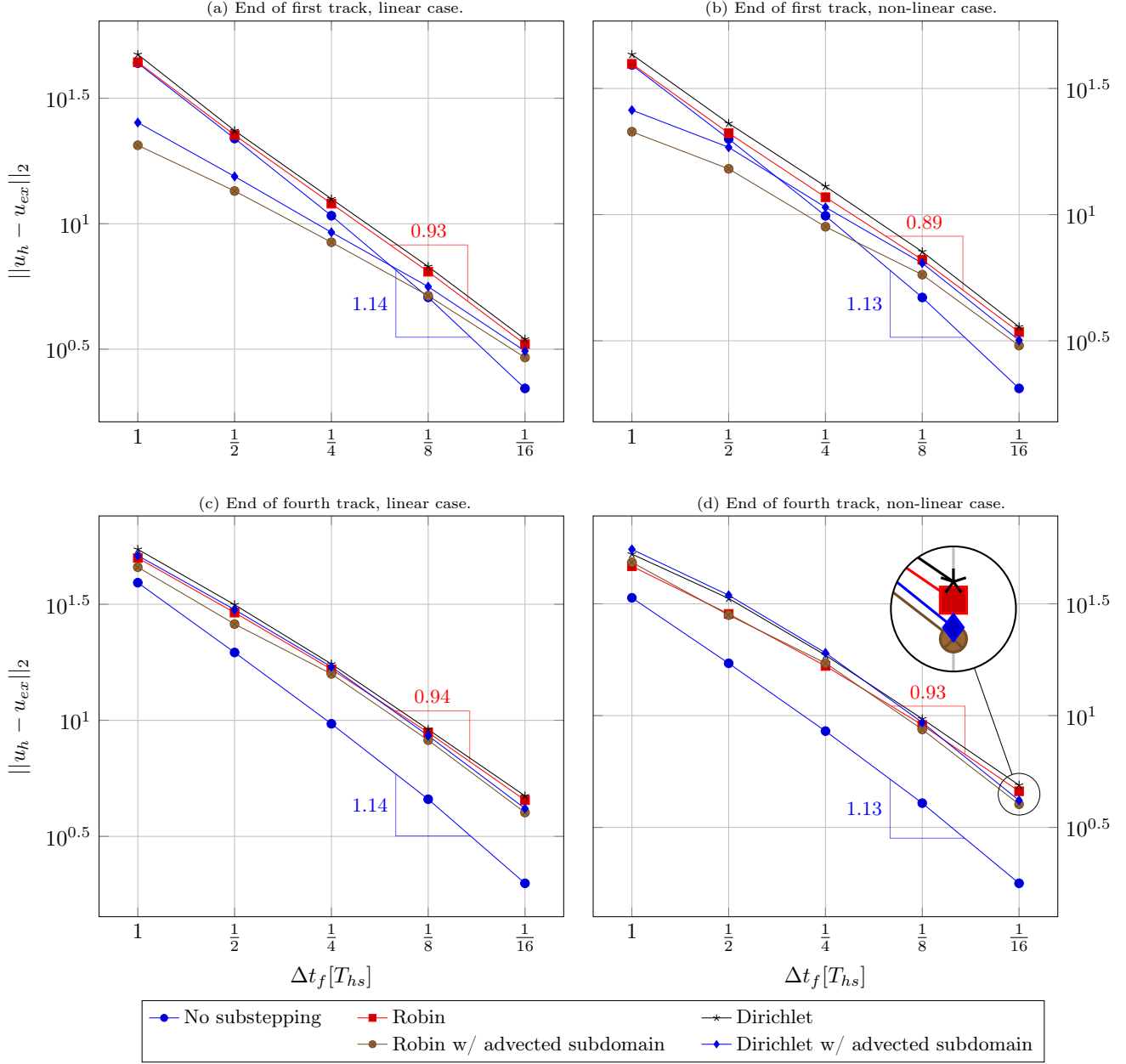


Figure 8: Convergence of the L^2 error at the end of the first (top) and fourth tracks (bottom) for both the linear (left) and non-linear (right) cases. The horizontal axis shows Δt_f , with $\Delta t_s/\Delta t_f = 16$ kept fixed. Results are shown for all substepping strategies (Robin and Dirichlet, with and without advected subdomain), together with the unsubstepped solution for reference.

Figure 8 reports the L^2 error of the solution over the entire domain at the end of the first and fourth tracks in the top and bottom rows, respectively. The substeppers considered are the Robin and Dirichlet substeppers with and without advected subdomains. The solution without substepping and $\Delta t = \Delta t_f$ is included for comparison.

All the substeppers achieve a convergence rate slightly below 1, while the unsubstepped solution achieves

a rate above 1. In all cases, the Robin models perform slightly better than their Dirichlet counterparts in terms of error at a given time-step.

Big differences in performance are only observed at the end of the first track, where the models with advected subdomains vastly outperform the other models, especially for coarse discretizations. This is due to their higher accuracy in the HAZ.

Nevertheless, their performance degrades over time due to their poor handling of sharp turns, as illustrated in fig. 9 which compares solution and error contours for the Robin substepper with and without an advected subdomain. In particular, fig. 9f shows a larger error near the rear of Ω_f compared with fig. 9e.

Leaving the advected subdomain on all the time would shear the solution and introduce large errors (Slimani et al., 2024). Hence, the advected subdomain is turned off at each turn and re-incorporated once the solution has stabilized, typically after a few substeps. However, these switches back and forth lead to an accuracy loss right after each turn, which progressively accumulates over time. By the fourth track, the advantage of the advected subdomain has nearly vanished, as shown in figs. 8c and 8d. Although the models with advected subdomains initially outperform the other models after the first track, their performance becomes comparable by the end of the fourth track.

Nonetheless, the bottom row of fig. 9 clearly demonstrates the benefit of the advected subdomain: the error in the HAZ is much lower than in the unsubstepped solution. This error manifests as a slight forward shift of the melt pool in the latter compared to the former, an effect that could be compensated through calibration of a double-ellipsoidal heat source model (Goldak et al., 1984).

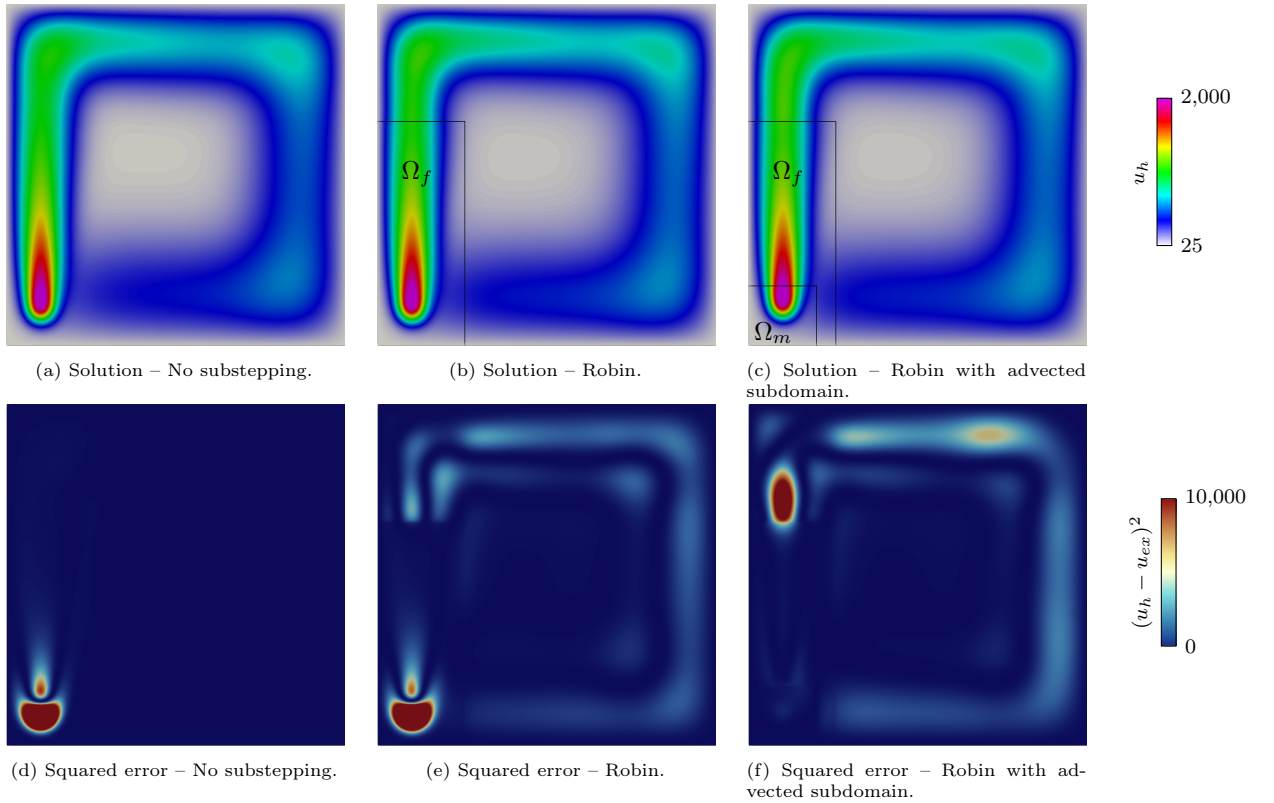


Figure 9: Solutions (top row) and pointwise squared errors (bottom row) in the linear case for the Robin substepper with and without an advected subdomain, with $\Delta t_s = 8T_{hs}$ and $\Delta t_f = 0.5T_{hs}$. The unsubstepped solution with $\Delta t = 0.5T_{hs}$ is shown for reference. The substeppers introduce some error throughout the domain. The advected subdomain reduces the error in the HAZ but increases the error near the track turns.

4.1.1. Comparing predictors

Comparing fig. 5c and fig. 5e, one remarks that the Dirichlet substepper is much more sensitive to the predictor than the Robin substepper. In particular, observe on fig. 5d the spurious temperature peaks at

the interface between the fast and slow regions. These arise because the heat source reaches Γ_{fs} during the predictor step in fig. 5b; the Dirichlet condition preserves this excess heat in subsequent substeps, whereas in the Robin substepper it is allowed to diffuse away.

Since the diameter of the heat spot produced by the predictor is proportional to Δt_s , one can either decrease Δt_s or enlarge Ω_f to mitigate the issue, although both approaches can increase the computational cost.

Since the macro-step size Δt_s is typically much larger than $1T_{hs}$, the predictor step cannot possibly resolve the heat source, making its heating profile unreliable. Nevertheless, a predictor step remains essential as indicated by fig. 10, which illustrates a Dirichlet substepping cycle without a predictor step. The resulting solution is unsatisfactory, as the diffusion at the intersection of Γ_{fs} and the heating track is severely underestimated. Skipping the predictor step is equivalent to using the previous solution as the predictor, which amounts to evaluating the interface terms at t^n , effectively introducing an explicit component in their time integration (Soldner and Mergheim, 2019). Furthermore, in the case of the Dirichlet substepper, the substeps remain constrained to the solution at t^n along the interface, leading to the observed stagnation.

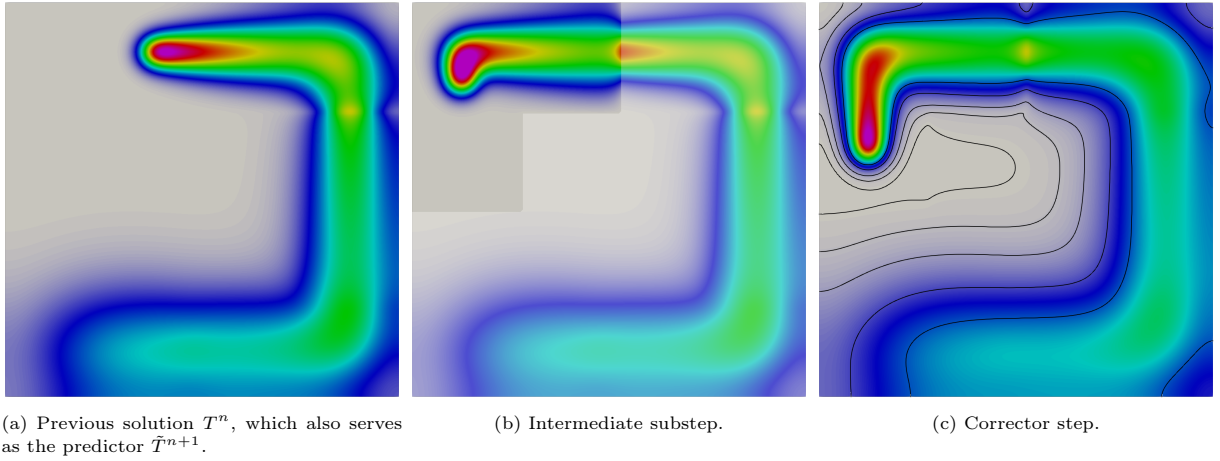


Figure 10: Example of Dirichlet substepper step without a predictor step.

These observations suggest that the predictor should focus on capturing diffusive effects, whose characteristic time scale should be on the order of Δt_s . To explore this, two alternative predictor strategies are considered: 1) **turning off the source term** (fig. 11) and 2) using a **lumped heat source** profile (fig. 12). The former completely foregoes heating, while the latter attempts to approximate heating effects while still employing a large time step, as is common in AM simulations (Moreira et al., 2024; Chiumenti et al., 2010; Soldner and Mergheim, 2019). Standard collision detection algorithms are used to identify the elements affected by the lumped heat source, with a collision box extending $1R$ in the directions transverse to the heat source motion, and delimited by the positions of the heat source at t^n and t^{n+1} along the track direction.

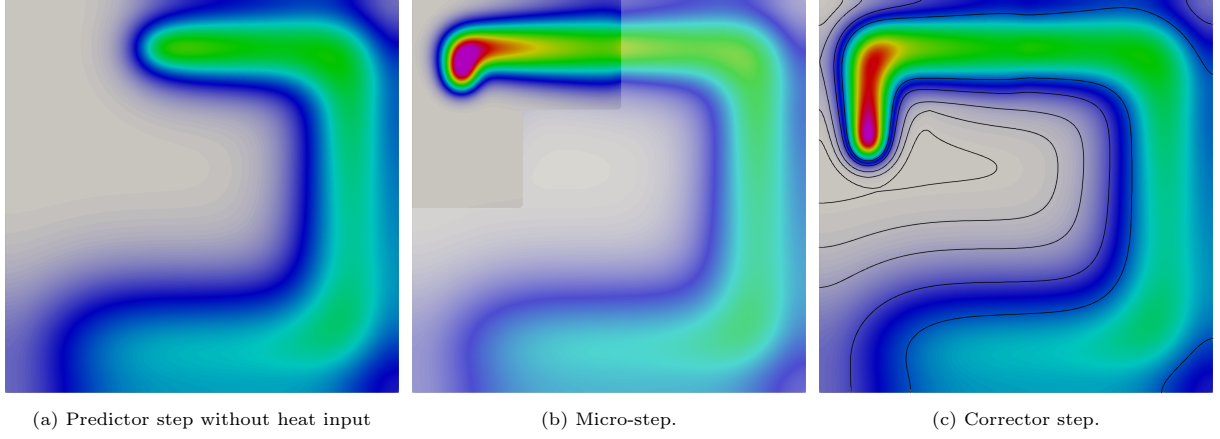


Figure 11: Example of Dirichlet substepper step using a predictor step without including the source term.

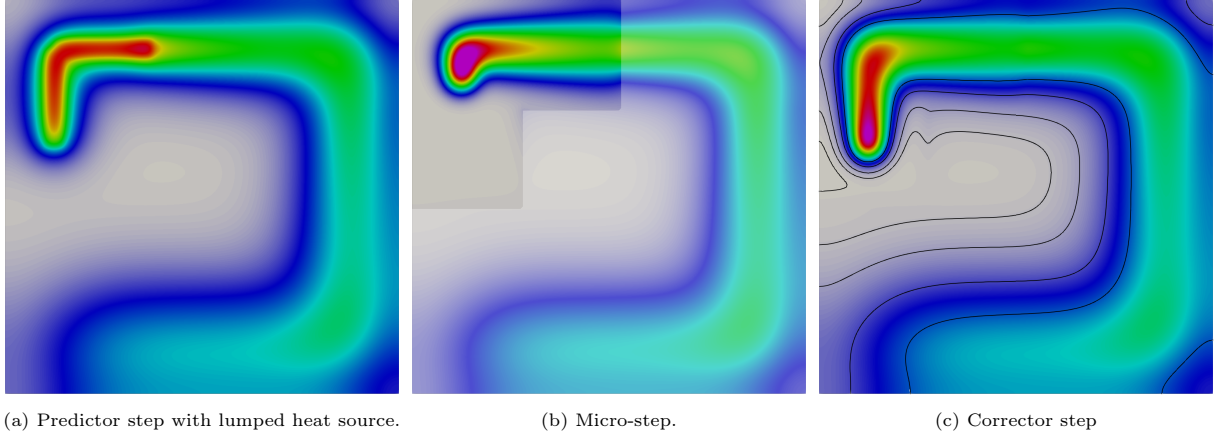


Figure 12: Example of Dirichlet substepper step using a lumped heat source predictor.

Figure 13 compares the three predictor strategies: standard, heat source (HS) turned off and lumped HS. The left panel shows the convergence rates of the three predictors in the linear case for both the Robin and Dirichlet substeppers. The results are reported without the advected subdomain at the end of the fourth track. As expected, the predictor has negligible effect on the Robin substepper. In contrast, the Dirichlet substepper is significantly more sensitive to the predictor choice, especially for coarser time steps Δt_s . This sensitivity decreases as Δt_s is decreased, since the predicted heat output is more localized and no longer reaches Γ_{fs} .

The lumped HS predictor improves the results compared with the standard predictor, but turning off the HS completely is clearly the better option. The right panel of fig. 13 compares solution and error contours for the standard and no-HS predictors. Similarly to fig. 5d, fig. 13c shows residual heating at Γ_{fs} due to the predictor, which translates to elevated error in the same region. These features are absent from figs. 13b and 13d, which achieve a lower error altogether.

An advantage of the no-HS and lumped HS predictors over the standard predictor is that they yield lower temperatures, which fare better with non-linear iterations: as noted in Puso and Hodge (2023), the high temperatures imposed by the standard predictor can cause convergence issues in the non-linear iterations.

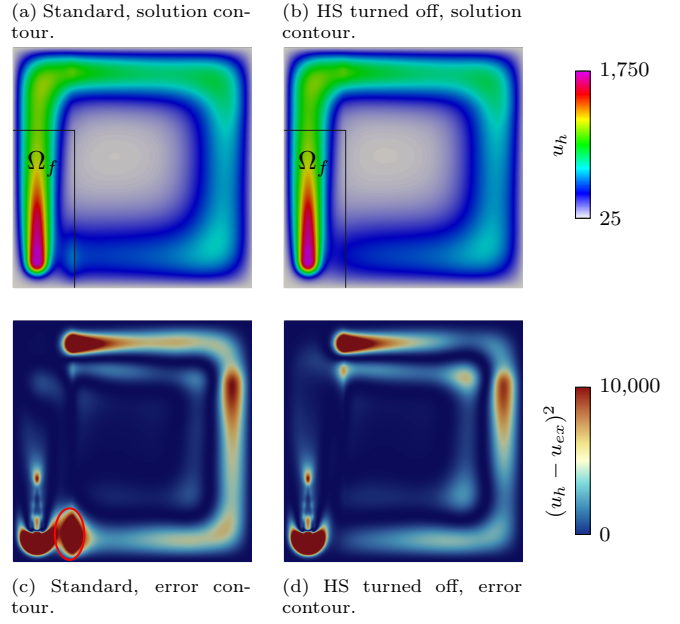
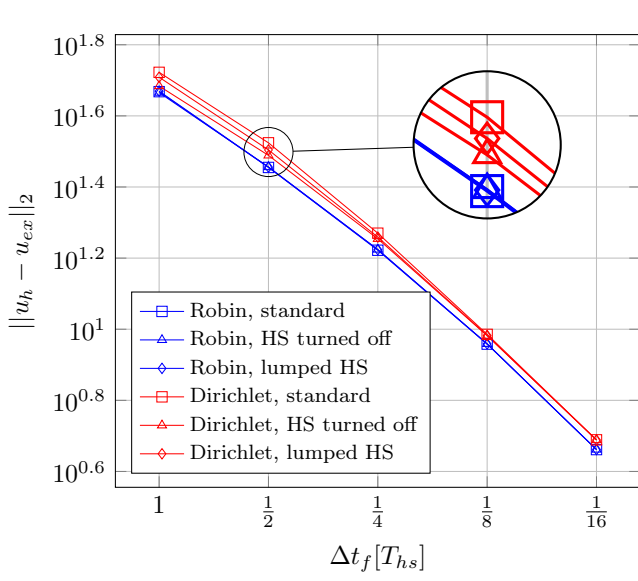


Figure 13: Comparison of predictor strategies. Left, convergence rates in the linear case for the standard, the heat source (HS) turned off and the lumped HS predictors. Right, solutions and errors of the Dirichlet substepper at the end of the fourth track in the non-linear case, using both the standard and the HS turned off predictors, with $\Delta t_s = 16T_{hs}$ and $\Delta t_f = 1T_{hs}$. The boundary of Ω_f is indicated in black.

4.1.2. On the effect of Δt_s

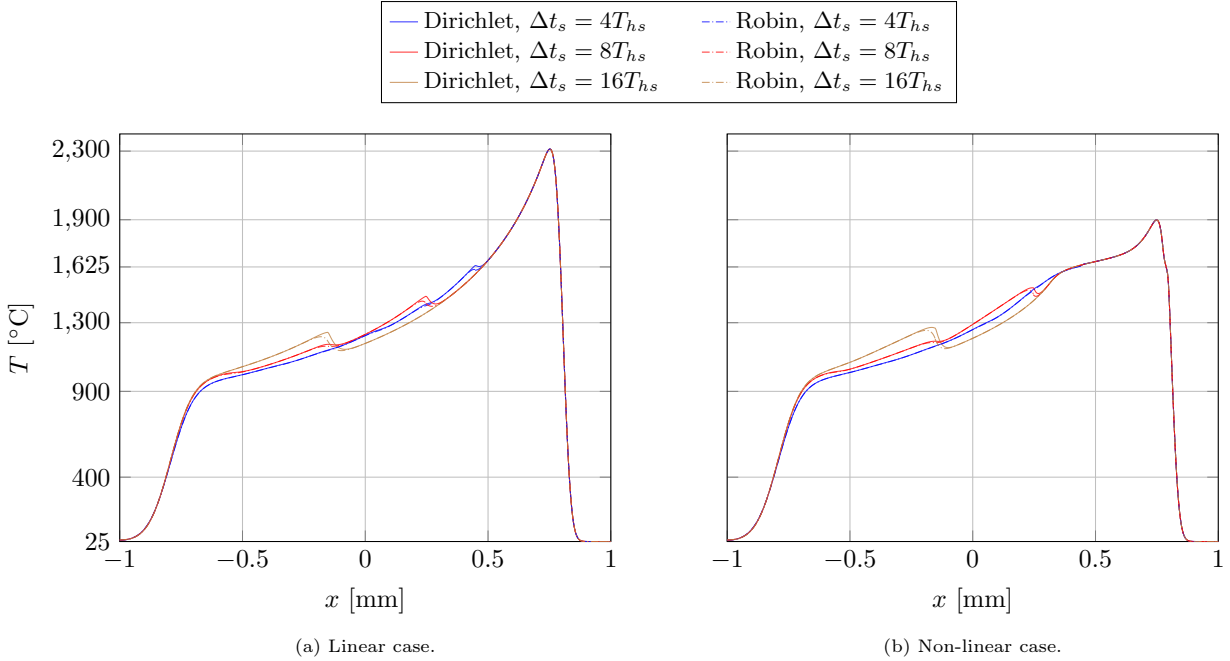
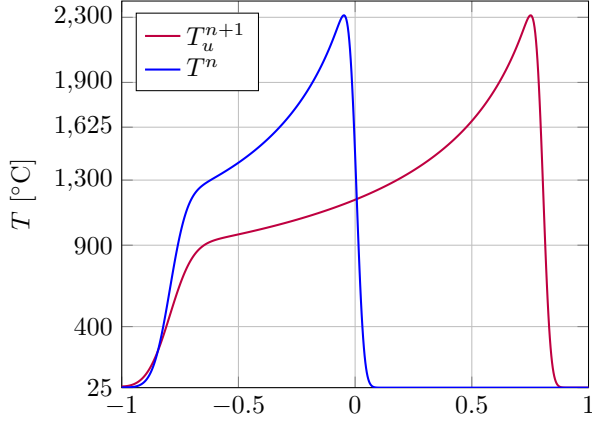
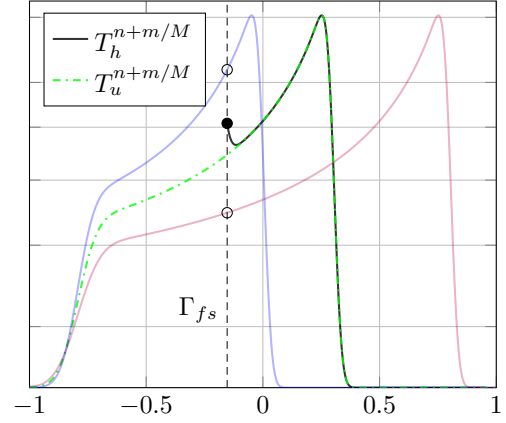


Figure 14: Solution profiles along the first heating track for increasing values of Δt_s and constant $\Delta t_f = \frac{1}{8}T_{hs}$, for both the Dirichlet and Robin substeppers without the advected subdomain. The no-HS predictor is employed.

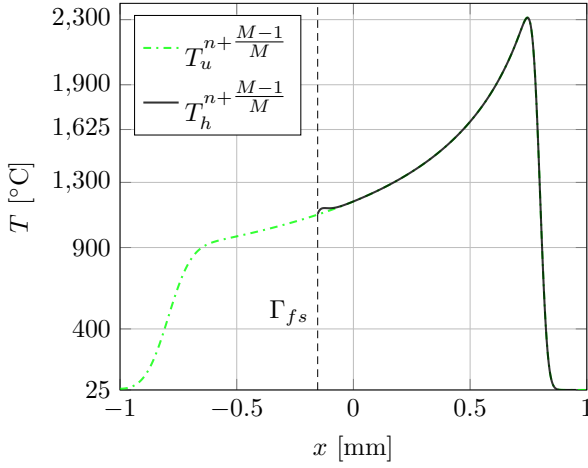
It is important to understand the cost-accuracy trade-off associated with increasing Δt_s . In the authors' experience, it often leads to a jump at the fast-slow interface. To accentuate this effect, the conductivity is



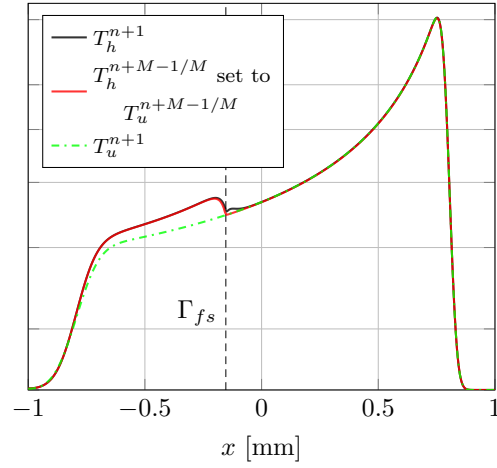
(a) Unsubstepped solution T_u serves as a predictor.



(b) Early in the substepping process, diffusion at the fast-slow interface is severely underestimated by the linear interpolation (13).



(c) At the last substep, the linear interpolation has caught up, with only a small residual wave remaining on the fast side.



(d) The unsubstepped predictor still produces a jump at the interface. Forcing the last substep to match the unsubstepped solution removes the residual wave on the fast side but does not eliminate the jump.

Figure 15: Step-by-step illustration of a linear problem where the Dirichlet substepper uses the unsubstepped solution as a predictor, with $\Delta t_s = 16T_{hs}$ and $\Delta t_f = \frac{1}{8}T_{hs}$.

halved in the following examples to reduce the diffusion of this jump. The advected subdomain is omitted, as it is not relevant to the discussion.

Figure 14 shows the solution profiles along the first heating track for $\Delta t_s = 4, 8, 16T_{hs}$, for both the Dirichlet and Robin substeppers. A fine Δt_f of $\frac{1}{8}T_{hs}$ is kept constant to isolate the effect of Δt_s . For both the linear and non-linear cases, increasing Δt_s leads to progressively larger jumps at the fast-slow interface, with the slow side lagging behind the fast side and overpredicting the temperature in the thermal tail.

To further isolate the effect of Δt_s , the unsubstepped solution is fed as a predictor to the Dirichlet substepper in fig. 15. Figure 15b shows that the linear interpolation of the Dirichlet condition (13) severely underestimates the diffusion at the interface. This occurs because diffusion is strongest when the region is hotter than its surroundings, and gradually slows down as thermal equilibrium is approached, a deceleration that the linear interpolation cannot capture. By the last substep, the linear interpolation (13) catches up, and only a small residual wave remains on the fast side, as shown in fig. 15c.

Still, the jump at the interface persists despite the good predictor, as shown in fig. 15d. Forcing the last substep to the unsubstepped solution does not remove the jump, although it does remove the residual wave on the fast side caused by the linear interpolation. By exclusion, the jump must be due to the poor time

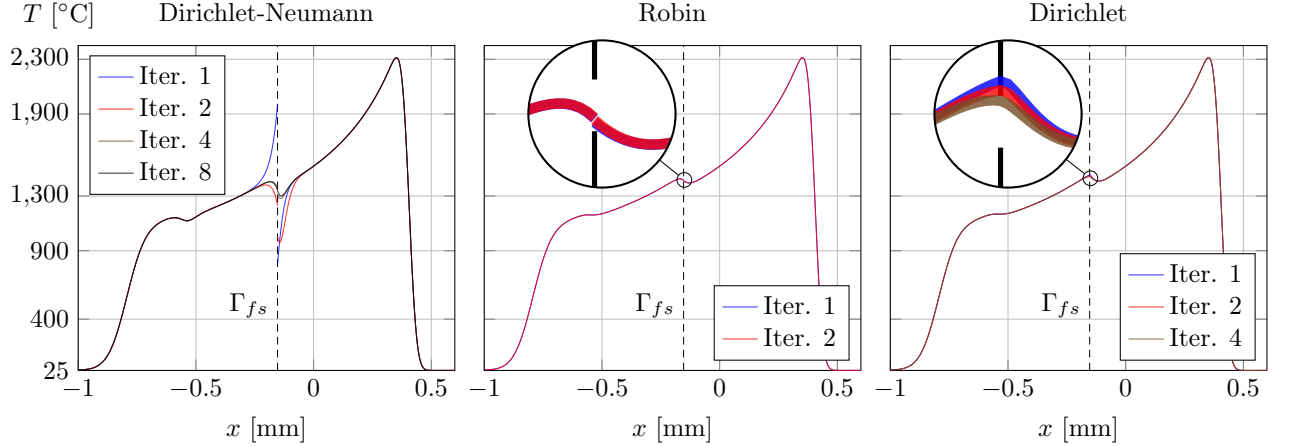


Figure 16: Solution profiles along the heating track after multiple staggered iterations for a linear problem with $\Delta t_s = 8T_{hs}$ and $\Delta t_f = 0.125T_{hs}$. Substeppers from left to right: Dirichlet–Neumann with Aitken relaxation, Robin, and Dirichlet.

integration on the slow side, which underestimates the diffusion in Ω_s .

Note that the issue is encountered at around $\Delta t_s = 5T_{hs}$. As discussed in section 1, no reference in the literature goes over $\Delta t_s = 10T_{hs}$, with most studies operating near $\Delta t_s = 5T_{hs}$. Since these works, like the present one, employ first-order time integration on the slow side, the authors conclude that the current bottleneck on employing larger Δt_s is the time integration on the slow side. Employing higher-order time integration schemes may offer a way forward: although an increase in computational cost is expected, each macro-step advances the solution over a large time interval, maximizing the impact of improved accuracy.

4.1.3. On the effect of truncated staggered iterations

As explained in section 2.3, the presented substepping schemes can be seen as staggered DD schemes truncated at the first iteration. It is therefore natural to investigate whether this early truncation significantly impacts solution accuracy.

Figure 16 shows solution profiles along the heating track for multiple substeppers. The left-most plot corresponds to a fully staggered Dirichlet–Neumann scheme. Without relaxation the scheme diverges, so Aitken relaxation (Yu et al., 2020) is applied. Even with relaxation, convergence is slow, requiring more than 10 iterations.

The central plot shows the Robin substepper, which practically shows no change between the first and second iterations. The coefficient choice proposed by Chen et al. (2014) appears to perform well in this case. The magnified interface region reveals only a very small jump in the solution across Γ_{fs} , which is consistent with the weakly imposed Robin condition. These results corroborate the findings of Canuto and Lo Giudice (2019); Cheng and Wagner (2021), which report that the Robin substepper vastly outperforms the Dirichlet–Neumann one.

The right-most plot shows the Dirichlet substepper, which converges within a few iterations. The solution initially exhibits a peak at the interface which progressively smooths out as the iterations proceed. Nevertheless, the difference between the first and last iterations is relatively small.

Overall, the results suggest that truncating the staggered iterations at the first iteration does not significantly impact accuracy, provided that a suitable substepper is chosen.

4.2. AMB2018-02

As part of the 2018 Additive Manufacturing Benchmark test series (AM-Bench 2018), Lane et al. (2020) conducted a series of single-track experiments on bare IN625 substrates, varying the laser power and the scanning speed and recording the resulting melt pool dimensions. In this section, the model presented in section 2.1 is validated against 3 of those experiments, namely, the ones conducted on the AMMT machine and thermally imaged every 20 μs . These correspond to the last three rows of Table 3 of Lane et al.

(2020) and are denoted tracks A2 ($V = 0.4\text{m s}^{-1}$, $P = 137.9\text{W}$), B3 ($V = 0.8\text{m s}^{-1}$, $P = 179.2\text{W}$) and C1 ($V = 1.2\text{m s}^{-1}$, $P = 179.2\text{W}$).

Kopp et al. (2022) performed a similar experimental validation, focusing on track B3. The material parameters reported in Kopp et al. (2022) are also adopted in this work (see table 2), along with the same heat-source model:

$$r(\xi) = \frac{\nu P}{2\pi R^2} \exp\left(-\frac{\xi_x^2 + \xi_y^2}{2R^2}\right) \frac{2}{\sqrt{2\pi}R_z} \exp\left(-\frac{\xi_z^2}{2R_z^2}\right) \quad (19)$$

which corresponds to a two-dimensional Gaussian of radius R extended along the depth direction by another Gaussian of radius R_z that governs the exponential decay of the heat source with depth.

Kopp observes that “the melt pool reaches steady-state after at most 2 mm”. The authors can corroborate this observation and therefore reduce the problem size to track lengths of 2 mm over substrates of dimensions $4.25 \times 2.05 \times 1.755\text{ mm}^3$. Furthermore, the effects of radiation and convection are neglected since they operate on much larger time scales than those of heating and diffusion (s versus μs) and therefore have a negligible influence on the melt pool shape during the laser scan.

Properties	Value	Unit
Solidus temperature T_s	1290	$^{\circ}\text{C}$
Liquidus temperature T_l	1350	$^{\circ}\text{C}$
Latent heat L	2.8×10^5	J kg^{-1}
Density ρ	8440.0	kg m^{-3}
Specific heat c_p	$\{(0.0, 405), (1320, 723.6), (2000, 723.6)\}$	$(^{\circ}\text{C}, \text{J kg}^{-1} ^{\circ}\text{C}^{-1})$
Conductivity k	$\{(0.0, 9.5), (1320, 28.85), (2000, 28.85)\}$	$(^{\circ}\text{C}, \text{W m}^{-1} ^{\circ}\text{C}^{-1})$

Table 2: Material properties for IN625 used for FEM. From Kopp et al. (2022); Lane et al. (2020).

Results are reported using a fine element size of $h = \frac{1}{8}R$ in the vicinity of the melt pool, and coarser elements elsewhere (fig. 18a). Coarser meshes with $h = \frac{1}{4}R$ are considered for calibration: the melt pool width and depth are practically unaffected, and the melt pool length differs by less than 2%. The slow time-step is fixed to $\Delta t_s = 6T_{hs}$, while Δt_f is set to $2T_{hs}$ and $0.25T_{hs}$ in the cases with and without an advected subdomain, respectively. The advected subdomain is well suited to the task, since the object of study is the steady state melt pool shape. From the conclusions of the previous section, it should provide more accurate results in the HAZ.

First, the results of Kopp et al. (2022) are reproduced for experiment B3. Since the model of Kopp et al. employs the same phase change regularization function as in the present work, the same parameters must to be calibrated: ν , R_z and S . Kopp et al. report $\nu = 0.32$ and $R_z = 0.28R$ based on calibration against the melt pool width and depth, while S is chosen to fit the melt pool length.

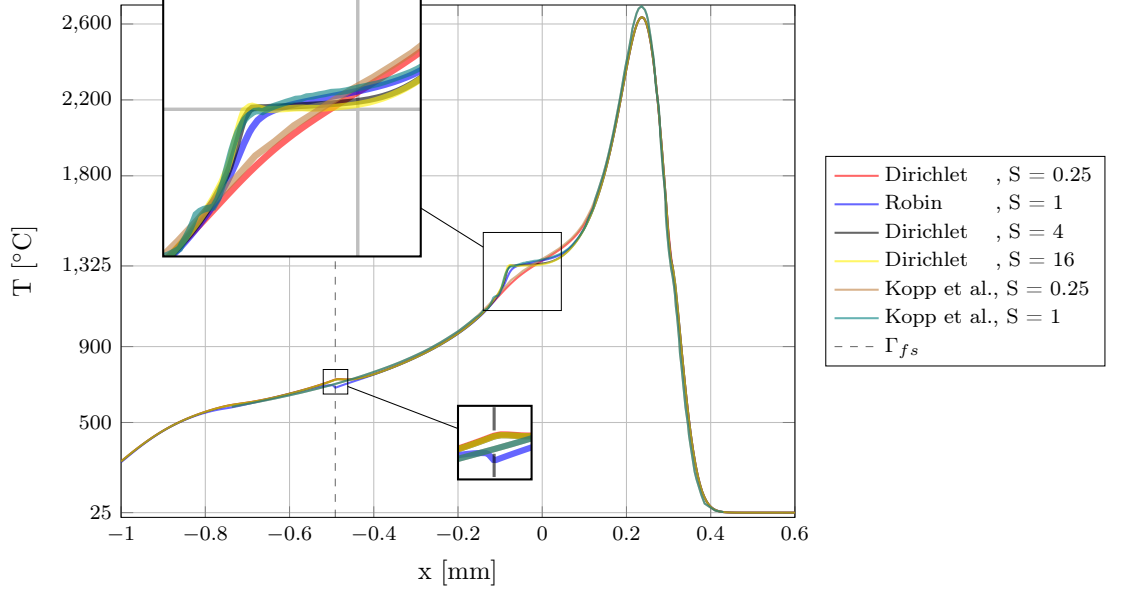


Figure 17: Temperature along the heating track for varying S using both the Robin and Dirichlet substeppers without an advected subdomain. The dashed line indicates the location of the fast-slow interface Γ_{fs} . Results from Kopp et al. (2022) are included for reference.

Figure 17 shows the temperature along the heating track on the top surface of the substrate, using $\nu = 0.32$ and $R_z = 0.28R$ and $S \in \{0.25, 1, 4, 16\}$. Both the Dirichlet and Robin substeppers without an advected subdomain are considered, and the results are compared with those of Kopp et al. for $S = 0.25$ and $S = 1$.

Increasing S produces a flatter temperature profile around the melting point, as expected of a more isothermal melting. This, in turn, leads to a longer melt pool (table 3), while the width and depth remain nearly unchanged. Away from the heat source, the results are otherwise very similar, except for their oscillations at the melting front observed for $S = 1$ in Kopp et al.. The present model remains stable up to $S = 16$, approaching near isothermal melting without oscillations. This improvement is attributed to the use of source-based latent heat model in this work, in contrast to the apparent heat capacity method employed by Kopp et al., as further discussed in Appendix B.

Results obtained with the Dirichlet and Robin substeppers are very similar, except at the fast-slow interface, where they exhibit slightly different oscillations in the same fashion as fig. 14b. These oscillations are negligible, particularly since they occur far away from the melt pool. Since results in the HAZ are effectively the same, the Robin substepper is adopted for the remainder of this section

Kopp et al. reports $S = 0.25$ as the best fit for the melt pool length, a relatively low value that is consistent with Figure 5 of Lane et al.. Both the models with and without an advected subdomain obtain similar results for $S = 0.25$, although the advection produces a slightly longer melt pool length, as shown in table 3 and fig. 18b. In addition, the melt pool is shifted slightly backward relative to the heat source motion when advection is included.

Case	Dataset	P [W]	V [mm s ⁻¹]	Calibrated parameters	Advected subdomain?	S	L [μm]	W [μm]	D [μm]
B3	Simulation	179.2	800.0	S, ν, R_z	✓	0.25	360.5	129.7	34.9
				S, ν, R_z	✗	0.25	354.7	128.3	34.0
				ν, R_z	✗	1	388.0	128.3	34.0
				ν, R_z	✗	4	396.5	128.3	33.9
				ν, R_z	✗	16	398.5	128.3	33.9
	Kopp et al.			S, ν, R_z	✗	0.25	356	129	34.8
	Experiment			—	—	—	359	132	36
C1	Simulations	179.2	1200.0	—	✗	0.25	298.8	106.8	24.6
				$\nu_{C1} = 0.366$	✓	0.25	362.6	117.9	28.5
	Experiment			—	—	0.25	370	113	29
A2	Simulations	137.9	400.0	—	✗	0.25	315.3	145.4	44.1
				$\nu_{A2} = 0.308$	✓	0.25	305.2	143.5	43.5
	Experiment			—	—	0.25	300	152	43

Table 3: Simulated and experimental melt pool dimensions (length L , width W , depth D) for tracks B3, C1 and A2. Calibrated parameters obtained for B3 fail to generalize to C1 and A2, and new absorptivities ν_{C1} and ν_{A2} are calibrated for these cases.

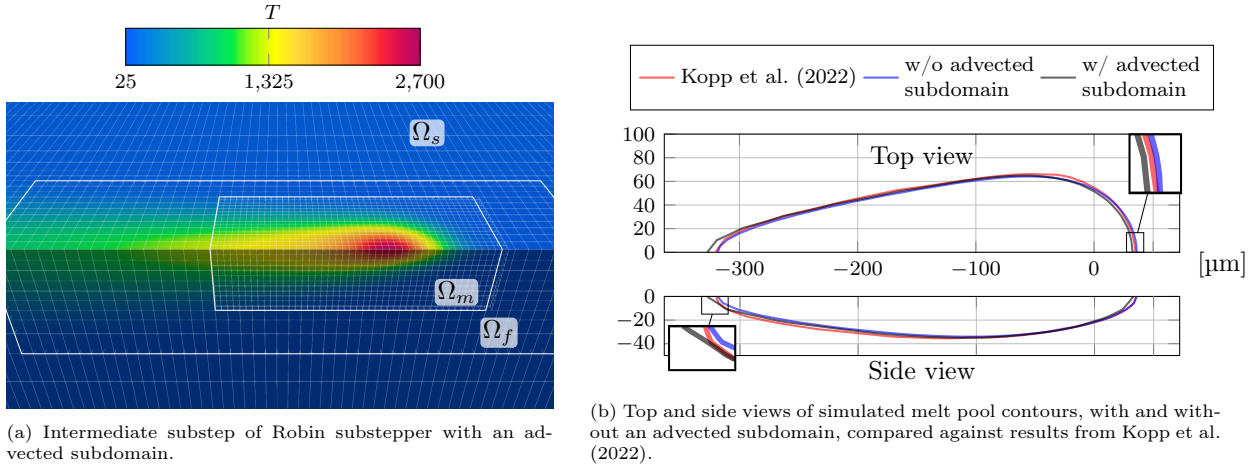


Figure 18: Solution and comparison with Kopp et al. (2022) of melt pool contours for experiment B3.

Figure 19: Left: Temperature field at an intermediate substep of the Robin substepper with an advected subdomain. Right: Comparison of simulated melt pool contours. Data from Kopp et al. obtained from https://gitlab.com/hpfem/publications/2021_spacetime_am/-/releases/Submission.

Using an advected subdomain with $S = 0.25, \nu = 0.32, R_z = 0.28R$ achieves slightly better results in predicting L , although the improvement is small, with all predictions lying within 1.2% of the experimental results. However, this parameter set fails to generalize to the other experiments, as shown by table 3. They lead to length prediction errors of 5% and 19.2% for tracks A2 and C1, respectively. These errors can be reduced to 0.5% and 2% by calibrating case-specific absorptivities $\nu_{A2} = 0.308$ and $\nu_{C1} = 0.366$, while keeping S and R_z fixed.

More importantly, the experiments measure a *longer* melt pool in C1 than in B3. They both apply the same laser power, with C1 going 1.5 times faster than B3. In contrast, the presented model predicts a *shorter* melt pool in C1 than in B3. Figure 20a plots melt pool lengths for absorptivities $\nu \in [0.3, 0.5]$: for a given

absorptivity, the melt pool length is always shorter in C1 than in B3.

Since a longer melt pool is observed experimentally in C1, the model is most likely overestimating temperatures in B3, indicating that an energy sink is missing in the model. As noted previously, convection and radiation cannot be the cause, as they act on much longer time scales.

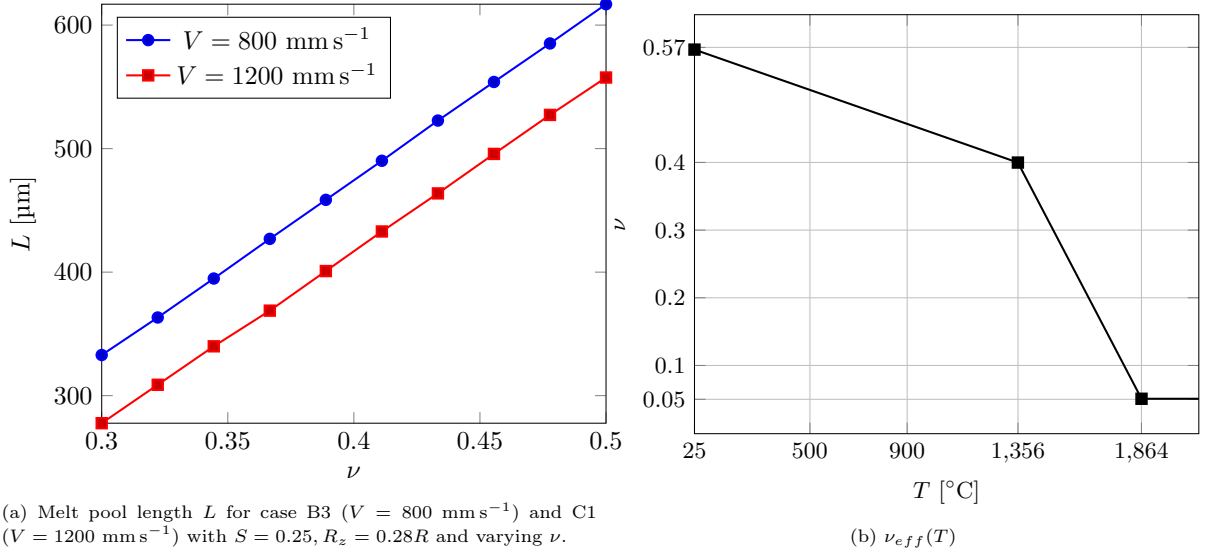
To compensate for the missing energy sink, a temperature-dependent absorptivity is introduced:

$$\nu_{eff}(T) = \begin{cases} \nu_0 + \frac{\nu_1 - \nu_0}{T_1 - T_0}(T - T_0) & T < T_1 \\ \nu_1 + \frac{\nu_2 - \nu_1}{T_2 - T_1}(T - T_1) & T_1 \leq T < T_2 \\ \nu_2 & T \geq T_2 \end{cases}$$

This corresponds to a two-segment piecewise linear function with a constant value ν_2 past a threshold temperature T_2 .

Recognizing that multiple parameter sets can produce similar melt pool shapes, a joint calibration is performed on two experiments to reduce the risk of overfitting to a single experiment. Tracks B3 and C1 are chosen, since they exhibit the qualitative behavior missing from the model.

The calibration proceeds in two steps. First, a least-squares optimization loop is carried out to determine $\nu(T)$ and S , with additional weight assigned to the melt-pool length. Then, a second optimization loop is used to determine R_z , emphasizing the width and depth. The resulting parameters are $S = 0.31$, $R_z = 0.42R$ and the piecewise linear absorptivity shown in fig. 20b. Interestingly, the calibration produces an absorptivity dip past the melting point: a physically unrealistic feature which, in this case, compensates for the missing energy sink.



(a) Melt pool length L for case B3 ($V = 800 \text{ mm s}^{-1}$) and C1 ($V = 1200 \text{ mm s}^{-1}$) with $S = 0.25$, $R_z = 0.28R$ and varying ν .

(b) $\nu_{eff}(T)$

Figure 20: Left: Melt pool length as a function of absorptivity ν for cases B3 and C1. The simulations consistently predict a longer melt pool for B3 than for C1, in contrast with the experimental observations, which show the opposite trend. Right: Calibrated piecewise linear absorptivity $\nu_{eff}(T)$ found by the joint calibration on B3 and C1.

Results obtained with the newly calibrated parameters are shown in table 4. While the results are less accurate for B3, the errors remain well within 5 % of the experimental measurements. Similar accuracy is achieved for C1, and, critically, the model now predicts a longer melt pool length in C1 than in B3. The predictions for A2 also remain within 5 %.

Overall, the joint calibration is deemed successful: the model reproduces both the qualitative dependence of the melt pool length on the scanning speed and the quantitative melt pool dimensions of the independent test case A2, which was not included in the calibration.

Case	Dataset	P [W]	V [mm s ⁻¹]	Calibrated parameters	Advection subdomain?	L [μ m]	W [μ m]	D [μ m]
B3	Simulation	179.2	800.0	$S, \nu_{eff}(T), R_z$	✓	362.5	136.6	35.6
	Experiment			–	–	359	132	36
C1	Simulation	179.2	1200.0	$S, \nu_{eff}(T), R_z$	✓	366.2	118.5	29.8
	Experiment			–	–	370	113	29
A2	Simulation	137.9	400.0	–	✓	289.3	148.9	41.4
	Experiment			–	–	300	152	43

Table 4: Results for experiments B3, C1 and A2 with piecewise linear absorptivity $\nu_{eff}(T)$. Parameters found by joint calibration on B3 and C1 manage to generalize to A2.

4.3. 3D LPBF

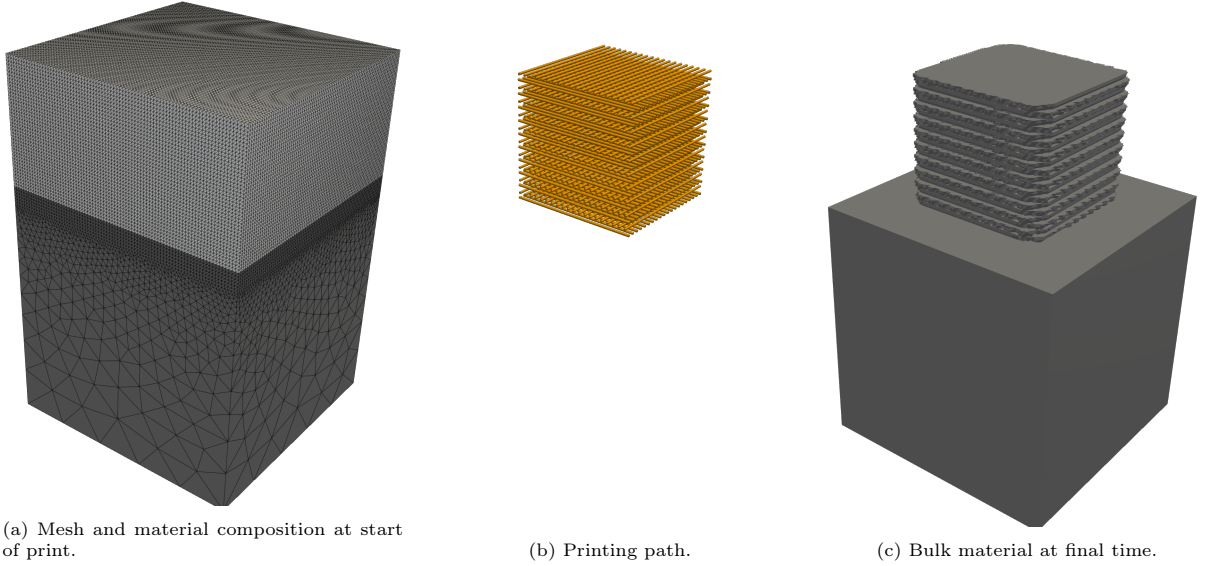


Figure 21: 1.0 mm cube. Powder elements corresponding to each layer are activated during recoating time-steps.

() Powder () Bulk

To assess performance in a controlled yet representative setting, the LPBF print of a cube geometry is considered. Similarly to Puso and Hodge (2023), the cube size is varied from 1.0 mm to 3.0 mm to study scaling effects and analyze the impact of domain size on the efficiency of the substepping schemes.

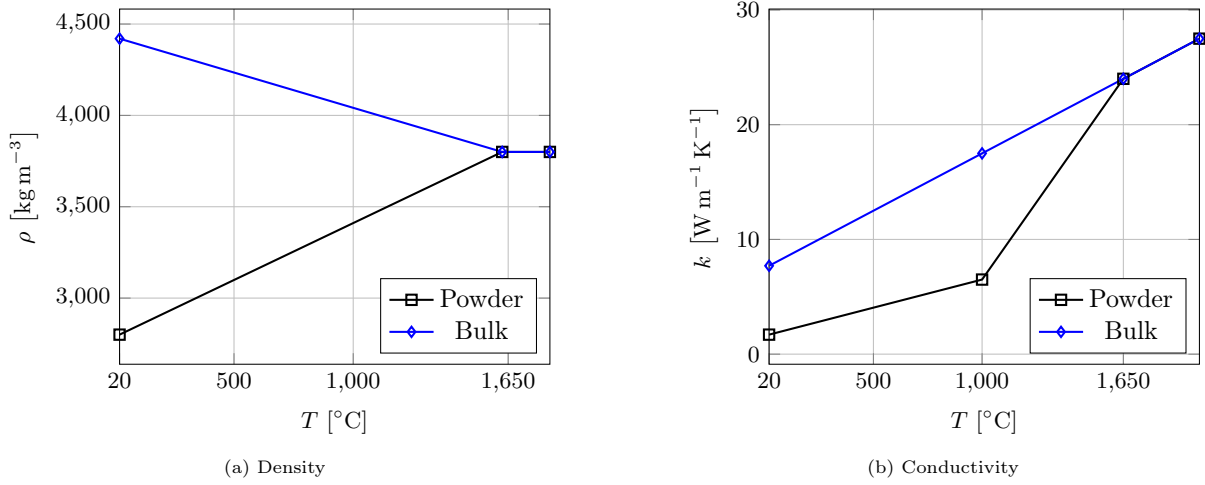


Figure 22: Thermally dependent material parameters for Ti-6Al-4V powder and bulk.

Property	Value	Unit
Solidus temperature T_s	1600	°C
Liquidus temperature T_l	1650	°C
Latent heat L	3.5×10^5	J kg ⁻¹
Environment temperature T_{env}	25	°C
Emissivity ε	0.35	
Convection coeff. h_{conv}	10	W m ⁻² °C ⁻¹
Specific heat c_p	560	J kg ⁻¹ °C ⁻¹
Density ρ	fig. 22a	
Conductivity k	fig. 22b	

Table 5: Ti-6Al-4V material parameters for 3D LPBF cube simulations.

The material considered is Ti-6Al-4V with thermally dependent density and conductivity. The adopted values are reported in table 5 and fig. 22. Although specific values vary across studies, and there is little data available for the powder phase, the chosen parameters are representative of those commonly employed in the literature.

The heat input is modeled using a Gaussian profile

$$r(\mathbf{x}, t) = \frac{6\sqrt{3}P}{\pi^{3/2}R^3} \exp\left(\frac{-3\|\mathbf{x} - \mathbf{x}_{\text{hs}}(t)\|_2^2}{R^2}\right) \quad \mathbf{x}_{\text{hs}} = \mathbf{x}_0 + \mathbf{V}(t)t$$

with a net laser power $P = 70.0$ W, radius $R = 100.0$ μm and speed $V = 1000.0$ mm s^{-1} .

The mesh, printing path and bulk material at the final time are shown in figs. 21a to 21c. The substrate is 2 mm thick, and 0.5 mm wider than the cube in the in-plane directions. A tetrahedral mesh is employed, with fine elements of size $\frac{R}{4}$ in the powder bed and coarse elements of size $4R$ at the bottom of the substrate. The scanning path is aligned with the axes and alternates direction from a layer to the next, with 10.0 s of cooling time in-between. The layer thickness and hatch spacing are both set to R . The fast subdomain is defined by padding the heating track by $3.5R$ in all directions. Figure 21c shows an example of the resulting bulk mesh after all layers have been printed and cooled.

The models compared are the Robin and Dirichlet substeppers without an advected subdomain, as well as the Robin substepper with an advected subdomain. For the advected subdomain case, both monolithic and staggered treatments of eq. (10) are considered. All speed-ups are reported relative to the unsubstepped standard model. Throughout this section, the fast time step Δt_f is fixed at $0.5T_{hs}$ for the models without

an advected subdomain, whereas in the advected subdomain case it is progressively increased as the melt pool approaches steady state, following the criterion in eq. (11).

Edge length [mm]	$\Delta t_s [T_{hs}]$	Fast DOF [%]	Speed-up			
			Robin No AS	Dirichlet No AS	Robin Monolithic AS	Robin Staggered AS
1.0	5.0	22.0	2.0	1.7	1.9	1.4
	10.0	31.0	1.8	1.7	1.8	1.3
1.5	5.0	14.0	2.7	2.5	2.7	2.2
	7.5	17.0	2.7	2.5	2.9	2.2
2.0	5.0	10.0	3.3	3.0	3.6	3.3
	10.0	14.0	3.3	3.1	4.4	3.2
2.5	5.0	7.4	3.8	3.4	4.2	3.5
	12.5	11.9	3.9	3.7	5.4	4.1
3.0	5.0	5.5	4.2	3.7	4.7	4.0
	7.5	6.6	4.7	4.2	5.7	4.7
	10.0	7.7	4.8	4.4	6.4	5.1

Table 6: Speed-up factors relative to the unsubstepped model for increasing edge lengths of the cubic domain. The models without an Advected Subdomain (AS) employ $\Delta t_f = 0.5T_{hs}$, while the models with an AS progressively increase their Δt_f . The maximum Δt_f reached ranges from $2T_{hs}$ for the 1mm cube to $3T_{hs}$ for the 3.0mm cube.

Substepper	Advected subdomain	$\Delta t_s = 5T_{hs}$			$\Delta t_s = 10T_{hs}$		
		Res.	Jac.	LS	Res.	Jac.	LS
-	No	45%	33%	22%	-	-	-
Robin	No	30%	45 %	25%	29%	51 %	20%
Dirichlet	No	31%	43%	26%	29%	51%	20%
Robin	Yes, monolithic	34%	41%	25%	35%	47%	18%
Robin	Yes, staggered	31%	41%	27%	30%	46%	24%

Table 7: Fractional breakdown of computational costs for the 2.0mm cube cases reported in table 6. Columns indicate the percentage of joint assembly-solve time spent in residual assembly (Res.), Jacobian assembly (Jac.), and the linear solve (LS). All solvers employ GMRES with HYPRE preconditioning and the default Newton-Raphson settings of PETSc’s SNES.

Table 6 reports the speed-ups obtained by the various substeppers for increasing cube sizes. The ratio of fast DOFs to total DOFs is given to contextualize the observed gains. Timings are collected in serial in order to factor out the effects of load imbalances, and prints are truncated to a single layer to make simulation times manageable.

Across all domain sizes considered, the Robin substepper consistently outperforms the Dirichlet substepper. This is expected, as the Dirichlet approach requires solving the joint system (16) at every substepping cycle, whereas the Robin substepper solves the two subdomains sequentially, leveraging the locality of the fast dynamics. For instance, in the 2 mm cube case, the assembly and solution of the joint system account for 38% of the total assembly-solve time for $\Delta t_s = 5T_{hs}$, and 20% for $\Delta t_s = 10T_{hs}$.

Table 7 reports additional details on the fractional breakdown of the computational costs. Assembly costs dominate the overall computational time, which explains why the staggered treatment of the advected subdomain does not lead to a significant cost reduction compared with the monolithic approach: even though the staggered approach isolates the asymmetric part of the Jacobian, the linear solve is only about a fifth of the total cost.

The staggered approach typically requires three to four iterations to converge each micro-step when using

the Robin coefficients proposed in Chen et al. (2014). Nonlinear convergence is generally more challenging for the monolithic approach, so the staggered formulation can occasionally be more efficient, for example, at the beginning of the print when the material is still cold. However, as the melt pool stabilizes nonlinear convergence becomes easier and the advantage of the staggered method diminishes.

When evaluating the effect of the advected subdomain on performance, it is found that its benefit increases with track length, yielding substantial speed-ups for cubes sizes over 2.0 mm. This behavior is expected: as the melt pool has more time to stabilize, the fast time-step can grow further.

Note from table 6 that the Dirichlet substepper tends to respond better to increases in Δt_s , since it decreases the number of joint solves required. Interestingly, for the 1.0 mm cube, all substeppers perform worse at $\Delta t_s = 10T_{hs}$ than at $\Delta t_s = 5T_{hs}$. As Δt_s increases, the communication overhead between the partitions decreases, but the fraction of DOFs in the fast subdomain also increases. Hence, for a Δt_s too large relative to the domain size, the fast DOF ratio may exceed the profitability threshold; Hodge (2021) suggests a value around 30%.

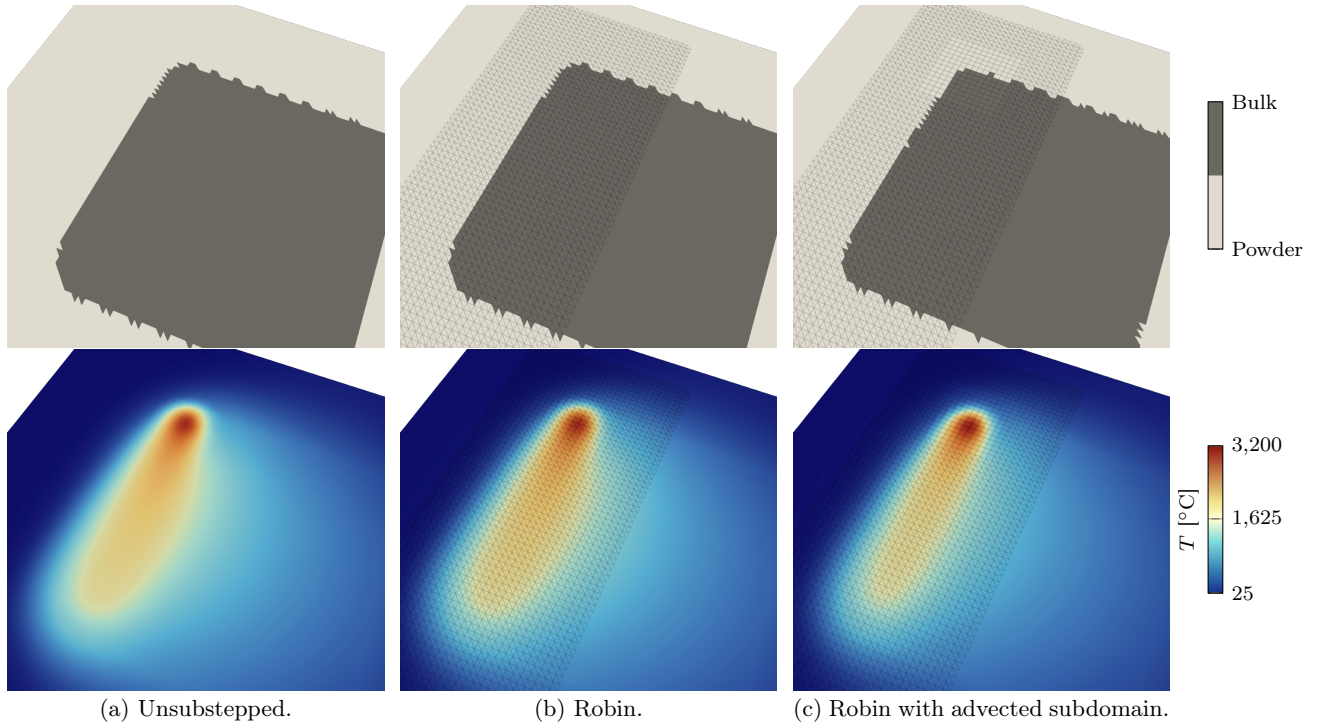


Figure 23: Temperature contour and material composition at intermediate time for the 1 mm cube case with $\Delta t_s = 10T_{hs}$. Tetrahedral elements correspond to the fast subdomain, and hexahedral elements to the advected subdomain.

After assessing the performance of the various substepping schemes, their solution fields are now compared. Figure 23 shows material composition and temperature contours at an intermediate time for the 1.0 mm cube with $\Delta t_s = 10T_{hs}$. The elements of the fast and advected subdomains, Ω_f (tetrahedra) and Ω_m (hexahedra), are highlighted in figs. 23b and 23c. Since the macro-step spans an entire track, the fast subdomain extends into the powder bed and does not intersect the thermal tail.

It is observed that, in the absence of an advected subdomain, the Robin and unsubstepped solutions are very similar. However, the presence of the advected subdomain leads to a visibly different thermal profile, with a thermal tail aligned with the scan direction.

This behavior occurs because the advected subdomain overlaps with the thermal tail left by the previous track: the interhatch spacing is $1R$, while the advected subdomain width is $1.5R$. The former is quite common in practice, and the latter is hard to further reduce without excluding part of the heat source from the advected subdomain. Consequently, the advection shears away the previous thermal tail, resulting in a

profile aligned with the current track, and ultimately underestimating the heat diffusion into the previously printed material.

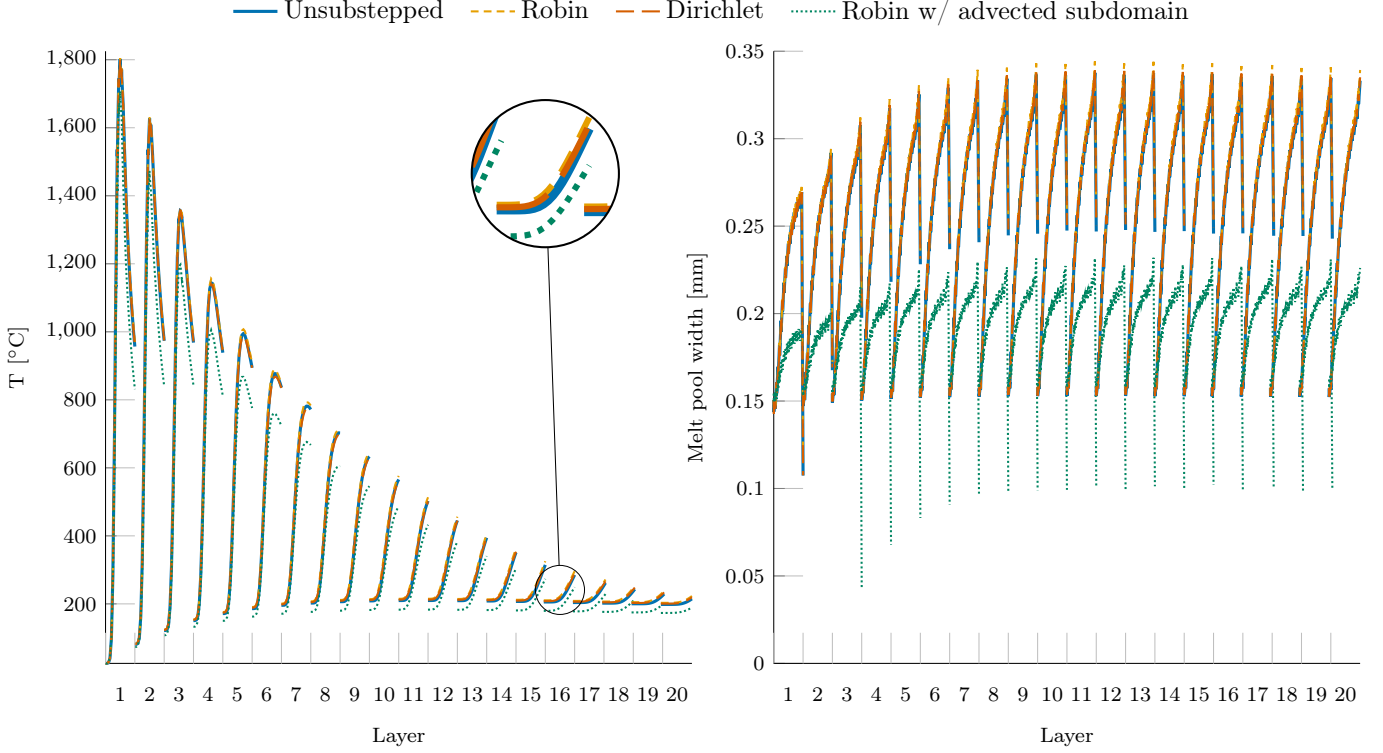


Figure 24: Temperature history at a point (left) and melt pool width (right) throughout the print of the 1.0 mm cube using $\Delta t_s = 10T_{hs}$. The probe is located at the center of the top surface of the substrate, that is, right below the first layer. Cooling intervals are excluded for clarity.

This is corroborated by fig. 24. The left panel shows the temperature history at a probe, and the right panel the melt pool width throughout the print. The latter further quantifies the aforescribed shearing effect, while the former shows that thermal diffusion in the depth direction is also affected by advection.

The other substeppers otherwise agree quite well with the unsubstepped solution. As shown by the temperature history, the Dirichlet substepper provides a slightly more accurate prediction than the Robin substepper in this case.

5. Conclusions

The current work presents a comprehensive study on substepping methods for LPBF modeling, and more generally, moving heat source problems with large contrasts in time scales.

- The proposed Robin-Robin scheme is shown to be relatively cheap in comparison to other methods in the literature, while being as or more accurate. More generally, a joint fast-slow solve in the substepping cycle does not appear to be required for accuracy, provided that the underlying domain decomposition scheme is well chosen.
- The Dirichlet substepper benefits from alternative predictor strategies, such as a purely diffusive step without the heat source. The latter is shown to be more accurate, especially for large Δt_s , and results in easier nonlinear solves during both the predictor and micro-steps; the original predictor can lead to unphysical temperature spikes at the fast-slow interface which grow worse with Δt_s .

A possible direction for future work is the development of a Robin variant of the semi-monolithic scheme. Such an approach would be less sensitive to the predictor choice than the Dirichlet scheme and could achieve higher overall accuracy than either of the schemes presented in this work.

- Results of the first numerical example indicate that the current bottleneck for larger macro-steps is the time integration scheme of the slow problem. Most references in the literature hover around similar macro-step sizes of $5 - 10T_{hs}$. The example also shows that the truncation of the substepping loop to a single iteration does not significantly impact accuracy.
- The underlying model is shown to be relevant, as it is able to reproduce experimental melt pool geometries. However, it required the use of an unphysical dip in absorptivity to do so, suggesting that a heat sink mechanism is missing from the model. Said mechanism could be related to evaporation or fluid flow.
- The advected subdomain approach can yield significant speed-ups, as demonstrated in the last numerical example, but these benefits are largely limited to cases with long tracks and few direction changes. Moreover, the model produces relatively large errors when a track overlaps with the thermal tail of previous tracks, reducing its general applicability. The moving mesh and advection terms add considerable complexity to both implementation and solver strategies. This approach is therefore best suited when high accuracy in the HAZ is required and the scan pattern is simple, rather than as a general-purpose speed-up technique.

To improve the advected subdomain approach, future work could investigate spatially and temporally varying advection velocities. The former can be achieved with an Arbitrary Lagrangian-Eulerian framework, and would allow the advected region to shrink dynamically and minimize its influence. The latter could be achieved by gradually ramping up the advection from zero to the laser speed at the start of a track, thereby smoothing the transition between the non-advected and advected regimes. This would likely mitigate the temperature spike observed when the switch occurs within a single time-step.

Taken together, these results show that substepping schemes offer a computationally efficient path for LPBF thermal simulations without a substantial loss of accuracy. Future work should investigate thermo-mechanical extensions, improved physical models for heat loss mechanisms, and improved time integration schemes for the slow problem to enable larger macro-steps.

6. Acknowledgments

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Appendix A. Weak forms of advected subdomain model

This appendix provides the weak forms of the moving and fixed subproblems of the advected subdomain approach. The latter is presented first, as it is comparatively simpler. After spatial discretization using FEM and temporal discretization using the Backward-Euler scheme, the residual form of eq. (5) with boundary and interface conditions is given by

$$\mathcal{R}_f = \int_{\Omega_f} \phi_f \rho c_p \frac{T_f^{n+1} - T_f^n}{\Delta t} + \int_{\Omega_f} \phi_f \rho L \frac{f_l(T_f^{n+1}) - f_l(T_f^n)}{\Delta t} + \int_{\Omega_f} \nabla \phi_f \cdot (k \nabla T_f^{n+1})$$

$$\begin{aligned}
& - \int_{\partial\Omega_{f,\text{conv}}} \phi_f h_{\text{conv}} (T_f^{n+1} - T_{\text{env}}) - \int_{\partial\Omega_{f,\text{rad}}} \phi_f \varepsilon \sigma (T_f^{n+1} - T_{\text{env}}^4) \\
& - \int_{\Gamma} \phi_f \left(k|_{T_m^{n+1}} \partial_n T_m + (T_m^{n+1} - T_f^{n+1}) \right) = 0 \quad \forall \phi_f \in V_f \quad (\text{A.1})
\end{aligned}$$

Conversely, the treatment of the moving subproblem is more involved, as the advection terms in eq. (4) require stabilization. In this work, *spatial-only* VMS (Variational MultiScale) stabilization is applied, as described in Codina (2000). To derive the corresponding terms, the PDE (4) is first rewritten in terms of a strongform residual R and a spatial differential operator $\mathcal{L}$:

$$R_T T = 0 \quad (\text{A.2})$$

$$\begin{aligned}
R_w u &:= \rho c_p \partial_t u + \rho L \partial_t f_l|_u + \mathcal{L}_w u - r \\
\mathcal{L}_w u &:= -(\rho c_p + \rho L f_l'|_w) \mathbf{v} \cdot \nabla_{\xi} u - k \Delta_{\xi} u
\end{aligned} \quad (\text{A.3})$$

VMS stabilization, like the Streamline Upwind Petrov-Galerkin method, adds residual-based diffusion in the advection direction to the weak form. The residual (A.2) is weighted by the test function, an elementwise stabilization parameter τ , and the adjoint operator $\mathcal{L}^*$, which reverses the sign of the advection term:

$$\begin{aligned}
\mathcal{R}_m &= \int_{\Omega_m} \phi_m \rho c_p \frac{T_m^{n+1} - T_m^n}{\Delta t} + \int_{\Omega_m} \phi_m \rho L \frac{f_l(T_m^{n+1}) - f_l(T_m^n)}{\Delta t} \\
& - \int_{\Omega_m} \phi_m (\rho c_p + \rho L f_l'(T_m^{n+1})) \mathbf{v} \cdot \nabla T_m^{n+1} + \int_{\Omega_m} \nabla \phi_m \cdot (k \nabla T_m^{n+1}) \\
& - \int_{\partial\Omega_{m,\text{conv}}} \phi_m h_{\text{conv}} (T_m^{n+1} - T_{\text{env}}) - \int_{\partial\Omega_{m,\text{rad}}} \phi_m \varepsilon \sigma (T_m^{n+1} - T_{\text{env}}^4) \\
& - \int_{\Gamma} \phi_m \left(k|_{T_f^{n+1}} \partial_n T_f + (T_f - T_m^{n+1}) \right) \\
& - \int_{\Omega_m} (\mathcal{L}_{T_m^{n+1}}^* \phi_m) \tau R_{T_m^{n+1}} T_m^{n+1} - \int_{\Omega_m} \phi_m r = 0 \quad \forall \phi_m \in V_m \\
\tau &= \left(\frac{4k}{h^2} + \frac{2\|\mathbf{v}\| \rho (c_p + L f_l'(T_m^{n+1}))}{h} \right)^{-1} \\
R_T T &= \rho c_p \partial_t T + \rho L \partial_t f_l|_T - (\rho c_p + \rho L f_l'(T_m^{n+1})) \mathbf{v} \cdot \nabla_{\xi} T - k \Delta_{\xi} T - r \\
\mathcal{L}_T^* v &= (\rho c_p + \rho L f_l'(T_m^{n+1})) \mathbf{v} \cdot \nabla_{\xi} v - k \Delta_{\xi} v \quad (\text{A.5})
\end{aligned}$$

Appendix B. Comparison of apparent heat capacity and source-based latent heat models

This section compares the performance of the apparent specific heat capacity (c_{app}) model and the source-based model introduced by Kollmannsberger et al. (2018); Celentano et al. (1994), focusing on nonlinear convergence and L2 error

For this study, the one-dimensional melting bar problem proposed by Kollmannsberger et al. (2018) is revisited. The setup consists of a semi-infinite rod, initially solid and at a uniform temperature T_s . At $t = 0$, the rod is suddenly heated at $x = 0$ with a Dirichlet boundary condition $T(0, t) = T_l$. The bar then undergoes isothermal melting with phase change occurring at the melting temperature $T_m < T_l$. The problem is illustrated in fig. B.25.

The analytical solution was originally derived by Neumann, and is described in Hu and Argyropoulos (1996); Kollmannsberger et al. (2018). The solid-liquid interface $X(t)$ advances in the positive x direction according to

$$X(t) = 2\lambda\sqrt{\alpha t}$$

where α is the thermal diffusivity and λ is the solution of the transcendental equation

$$\frac{St}{\exp \lambda^2 \operatorname{erf} \lambda} - \frac{St\sqrt{\alpha}}{\sqrt{\alpha} \exp \lambda^2 \operatorname{erfc} \lambda} = \lambda\sqrt{\pi} \quad St = \frac{c_p (T_l - T_m)}{L} \quad (\text{B.1})$$

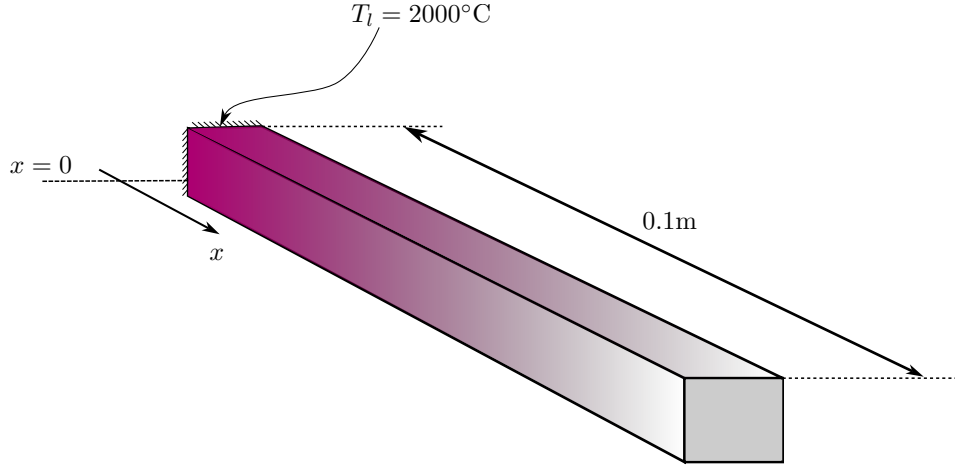


Figure B.25: Schematic of the one-dimensional melting bar model with a Dirichlet boundary condition at $x = 0$.

where St is the Stefan number. The analytical solution is then given by

$$T_{ex}(x, t) = \begin{cases} T_l - (T_l - T_m) \frac{\text{erf}\left(\frac{x/2\sqrt{\alpha t}}{2}\right)}{2} & x \leq X(t) \\ T_s + (T_m - T_s) \frac{\text{erfc}\left(\frac{x/2\sqrt{\alpha t}}{\lambda}\right)}{\lambda} & x > X(t) \end{cases}$$

where erf and erfc are the error function and its complement, respectively. Material parameters resembling Ti-6Al-4V are used, as listed in table B.8. A value $\lambda = 0.30568105$ is computed numerically by applying a root-finding algorithm to eq. (B.1) with the given parameters.

Parameter	Value	Unit	Parameter	Value	Unit
ρ	4510.0	kg m^{-3}	T_s	1500	$^{\circ}\text{C}$
c_p	520.0	$\text{J kg}^{-1} \text{K}^{-1}$	T_l	2000	$^{\circ}\text{C}$
k	16.0	$\text{W m}^{-1} \text{K}^{-1}$	T_m	1750	$^{\circ}\text{C}$
			L	3.3×10^3	J kg^{-1}

Table B.8: Material parameters for the melting bar problem. Values are taken from Kollmannsberger et al. (2018).

Equation (2) is solved using both the apparent specific heat capacity and the source-based methods to treat the latent heat terms. Note that, while the original problem involves strictly isothermal phase change, the regularized liquid fraction f_l introduces a narrow mushy region between T_s and T_l , which shrinks as S increases. Hence, the robustness of both models is assessed by progressively increasing S until the nonlinear solvers cease to converge. Figure B.26 shows f_l and its derivative for representative values of S considered in this section.

The problem is marched in time from $t = 0$ to $t = 120\text{s}$ using the Backward-Euler method with $\Delta t = 1\text{s}$. A uniform mesh with linear elements of size $h = 0.01\text{mm}$ is employed, and a high order quadrature rule (degree 4) is used to capture the subgrid variations in the regularized liquid fraction f_l . The implementation uses **FEniCSx** (Baratta et al., 2023) with the default **SNES** nonlinear solver from **PETSc** to solve the Newton–Raphson problems.

The authors find that the apparent specific heat capacity model fails to converge beyond $S_1 = 43$, whereas the source-based model reaches $S_2 = 394$. As seen in fig. B.26, it is clear that S_2 is practically indistinguishable from the isothermal phase change limit.

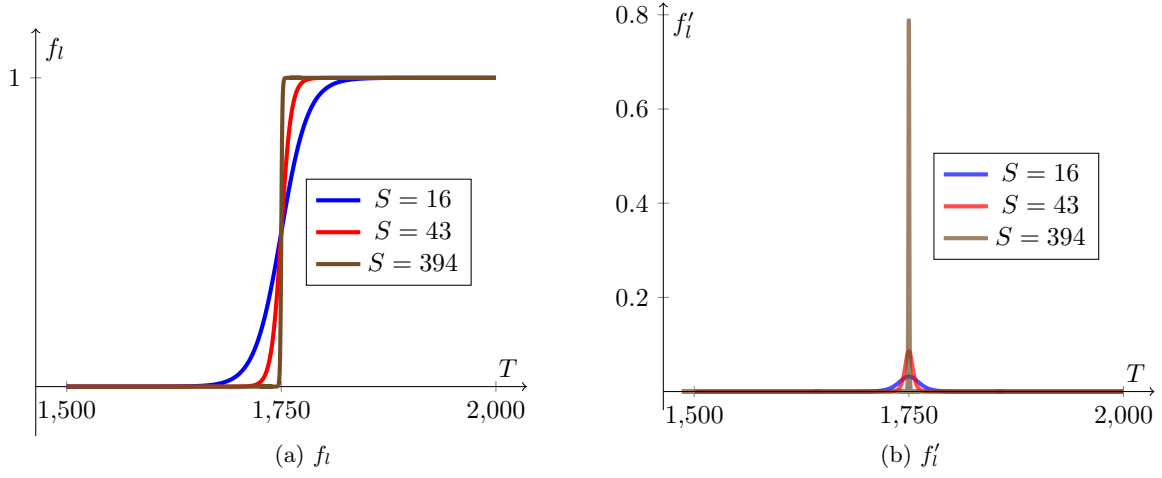


Figure B.26: Liquid fraction f_l and its derivative f'_l for various S values.

Figure B.27a compares the temperature profiles predicted by both models at various times. Small differences are visible at $t = 1$ s and $t = 10$ s, but by $t = 30$ s both solutions are in good agreement with the analytical result. Interestingly, despite the lower S value, the apparent specific heat capacity model achieves slightly lower L2 error, as shown in fig. B.27b.

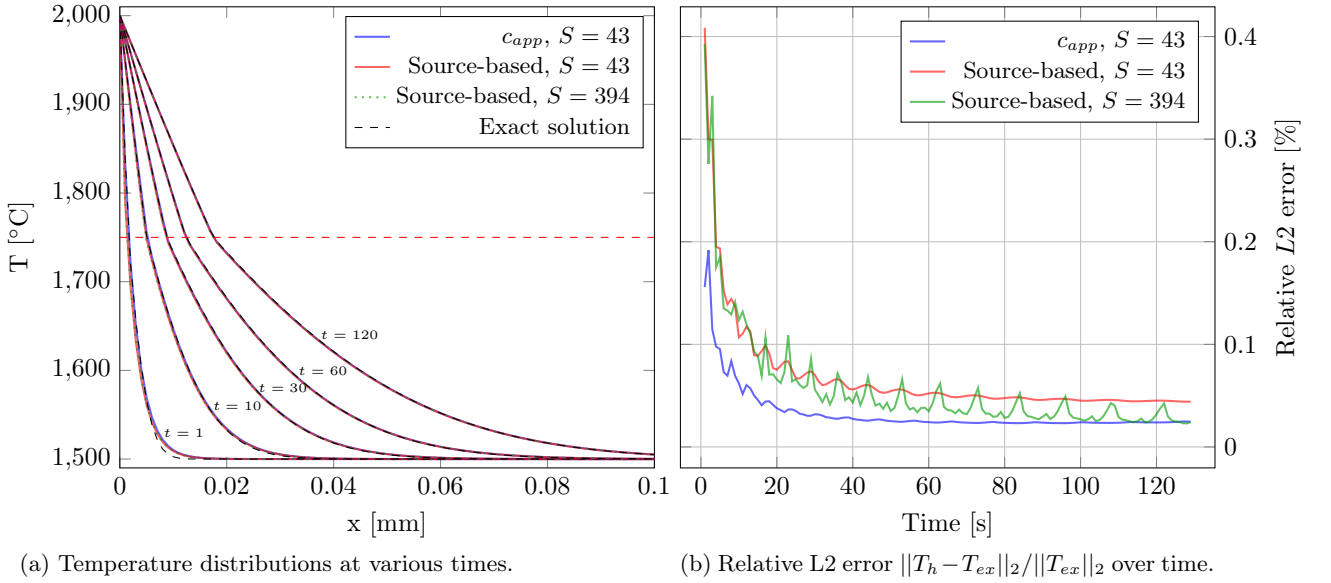


Figure B.27: Temperature distributions and comparison of relative L_2 error for $h = 0.01$ m and $\Delta t = 1$ s. The apparent heat capacity and source-based models reach $S_1 = 43$ and $S_2 = 394$, respectively. Errors obtained by the apparent specific heat capacity model are slightly lower.

However, the picture changes with finer discretizations. After refining the mesh size by a factor of 10, the apparent specific heat capacity and source-based models are able to converge $S_1 = 9$ and $S_2 = 708$, respectively. Likewise, after refining the time-step by a factor of 10 while keeping the original mesh size, they converge up to $S_1 = 16$ and $S_2 = 637$. Moreover, the source-based model achieves lower errors in both cases, as shown by fig. B.28, with the difference becoming more pronounced for the larger S values.

In conclusion, it is difficult to declare a clear winner in terms of accuracy: for the base discretization, the

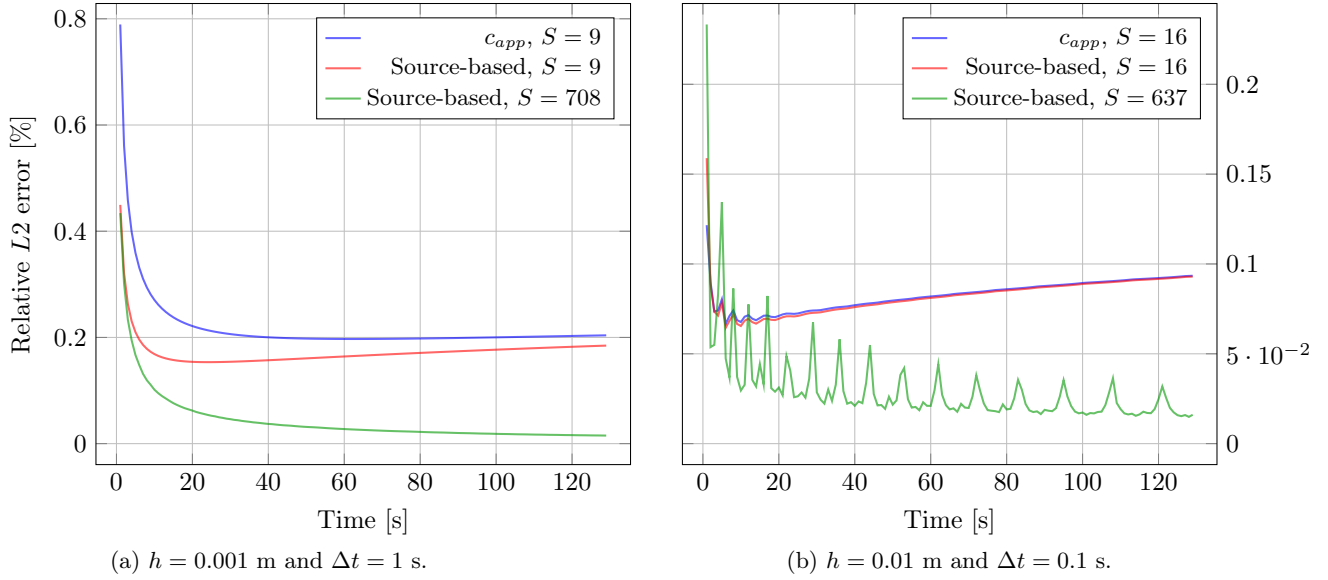


Figure B.28: Relative L_2 errors over time for refined mesh size (left) and refined time-step (right). The source-based models reaches much higher S values and achieves lower errors.

c_{app} model fares better, whereas for finer discretizations the source-based model is preferred.

Nevertheless, the source-based model is clearly more robust, as it can approximate the isothermal phase change limit much more closely. Based on the authors' experience, the apparent specific heat capacity model often fails to converge for low values of S when applied to LPBF problems. For this reason, the source-based model is employed in this work. The authors further note that the adoption of an apparent heat capacity formulation may explain why some references (Hodge, 2021; Puso and Hodge, 2023; Elahi et al., 2025) report the need for very fine time-steps ($\Delta t < 0.1T_{hs}$).

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CONCLUSIONS

This chapter lists the main contributions and conclusions of this thesis, as well as ideas for future lines of research that could build upon it.

9.1 MAIN CONTRIBUTIONS

The primary scientific contributions of this thesis lie in the development of novel computational methods to accelerate part-scale LPBF simulations without compromising accuracy, presented in chapters 7 and 8. These frameworks were developed to address the time-scale disparity inherent in LPBF simulations, a challenge that has received considerably less attention in the literature compared to its spatial counterpart. These contributions include the development of two complementary and composable computational frameworks, along with several methodological advances:

- The **advected subdomain** method introduces a moving subdomain attached to the heat source, where the problem is posed in the reference frame of the heat source. The method is presented with both Dirichlet–Neumann (chapter 7) and Robin–Robin (chapter 8) couplings. Both staggered and monolithic variants are explored, with support for distributed-memory architectures.
- The complementary *steadiness workflow*, which adaptively increases the time-step size by monitoring solution steadiness.
- A systematic overview of existing substepping approaches for LPBF, synthesizing common patterns, guidelines, expected speed-ups, accuracy trade-offs, and open challenges.
- A novel **Robin–Robin substepping** scheme based on custom Robin coefficients from Chen et al. [2014], achieving mesh-independent convergence behavior.
- New predictor-step strategies for substepping, motivated by time-scale reasoning, that improve accuracy for the Hodge [2021] substepper.
- Integration of the advected subdomain method into the substepping framework, demonstrating compounded speed-ups in favorable scenarios.

In addition, chapters 5 and 6 present applied contributions focused on the mitigation of warpage and residual stresses in MAM processes. Novel substrate designs and modeling of recoater-induced failure provided insight into practical strategies for reducing process-induced defects:

- Chapter 5 introduces a **slotted substrate design**, which reduces the structural stiffness of the substrate to alleviate the constraint imposed on the part.
- Chapter 6 proposes a modeling framework to analyze **recoater-induced distortion** in LPBF.

Taken together, these contributions establish both practical mitigation techniques and a computational toolbox that enhance the efficiency and predictive capability of high-fidelity part-scale modeling.

9.2 CONCLUSIONS

This thesis addressed two central challenges in **MAM**: (i) mitigating warpage and residual stresses, and (ii) developing computational methods to enable accurate part-scale simulations.

The principal conclusions from the first challenge, tackled in chapters 5 and 6, are summarized as follows:

- Slotted substrate designs demonstrated a significant reduction in residual stresses in **DED**, with only marginal influence on microstructure, although a slight increase in warpage was observed. This effect could potentially be mitigated through geometric compensation.
- The proposed volumetric loading was able to capture the effects of the recoater on both warpage and residual stresses. Thin-walled open structures oriented perpendicularly to the recoater motion were found to be particularly susceptible to recoater-induced failure. Component agglomeration and geometric compensation were proposed as potential mitigation strategies.

The extreme simplifications required to run the **LPBF** models in chapter 6 (meta-layers spanning ten physical layers) underscored the strongly multiscale nature of the **LPBF** process compared to **DED**.

This accuracy–feasibility trade-off highlighted the need for computational frameworks that directly target the time-scale disparity inherent in **LPBF**. The **advected subdomain** and **substepping** approaches, explored in chapters 7 and 8, were shown to significantly accelerate part-scale simulations while preserving fidelity at the heat source scale.

The performance of the advected subdomain method was examined across chapters 7 and 8. The main conclusions regarding this approach are as follows:

- The advected subdomain method demonstrated significant speed-ups in favorable scenarios (long tracks) by bypassing the constraint $\Delta t \leq 1T_{hs}$. Chapter 7 showcases time-steps of up to $8T_{hs}$.
- Each time-step is roughly 2 to 3 times more computationally expensive than a standard time-step, due to the loss of the **SPD** property of the system matrix and the additional operations required per step. This overhead can be amortized in long tracks, where the step size can be increased significantly.
- Accuracy is increased in the **HAZ**: thermal gradients are steeper at the heat-front and smoother at the heat-tail, consistent with the observations of Goldak et al. [1984] who introduced the double-ellipsoid heat source model to replicate these features.
- Accuracy is greatly reduced by direction changes and adjacent tracks. The advection tends to shear away thermal tails left behind by previous tracks, resulting in a loss of accuracy that greatly limits the method’s applicability.

Turning off advection can temporarily mitigate this issue, but for complex scan patterns, favorable conditions may never arise. In its current form, the method is best suited for long, isolated tracks, or melt pool specific studies.

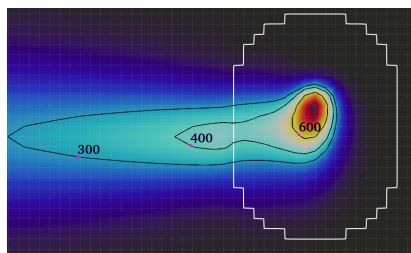


Figure 42: Shearing of thermal tail at sharp turn due to advected subdomain. Advected subdomain has a tendency to straighten the thermal tail in the direction of motion.

In contrast, the **substepping** methods presented in chapter 8 proved more general and robust, and their implementation is comparatively straightforward. By partitioning the domain into fast and slow regions Ω_f and Ω_s , and integrating them with different time-steps Δt_f and $\Delta t_s \gg \Delta t_f$, substepping directly addresses the time-scale disparity in LPBF in a less roundabout manner than the advected subdomain method.

Key findings include:

- The main driver of cost reduction is the DOF ratio in the fast and slow domains, with the time-step ratio $\Delta t_s/\Delta t_f$ playing a secondary role in reducing the frequency of expensive slow steps. Too large a $\Delta t_s/\Delta t_f$ can increase computational cost by increasing the size of Ω_f .
- Both fully staggered and semi-monolithic structures were identified and explored. A novel fully-staggered Robin-Robin scheme with mesh-independent convergence was proposed and achieved similar or marginally better accuracy than the semi-monolithic approach of Hodge [2021]. Both schemes clearly outperformed the fully staggered Dirichlet-Neumann formulation. These results indicate that the choice of DD interface coupling is more critical than the presence or absence of joint-solves.
- Additional iterations in the staggered substepping loop were found to have a negligible impact on accuracy, suggesting that a single iteration is sufficient.
- Literature comparison and numerical tests indicated that the main accuracy bottleneck for large macro-steps lies in the time-integration scheme employed in Ω_s , rather than in the accuracy of the predictor step or the slow-fast interpolation.
- For large macro-steps with the Hodge [2021] substepper, the choice of predictor strategy significantly affected accuracy. Predictors focusing on diffusion rather than heat input improved both accuracy and stability.
- When compounded with the advected subdomain method, substepping yields additional speed-ups in long-track scenarios, although the aforementioned limitations and lack of robustness of the advected subdomain still apply.

In addition, chapter 8 examined the treatment of latent heat during the powder-to-solid transition. The enthalpy-based method of Celentano et al. [1994], Kollmannsberger et al. [2018] was found to be significantly more robust than the commonly used apparent heat capacity method.

Parenthetically, the relevance of the underlying thermal model was assessed against experimental melt pool measurements from Lane et al. [2020]. The model could not reproduce the observed increase in melt pool length with scanning speed unless a thermally dependent absorptivity was introduced and calibrated. However, the calibrated absorptivity implied a power dip beyond the melting point, an unphysical result that suggests the model is missing a heat-loss mechanism, most likely associated with melt pool dynamics and fluid flow.

Taken together, advected subdomain and substepping methods form a versatile computational toolbox for accelerating high-fidelity part-scale LPBF simulations, advancing the feasibility of predictive modeling in MAM.

9.3 FUTURE WORK

The work presented in this thesis opens several promising avenues for further research, both on the physical modeling of LPBF and on computational strategies for cost reduction. In line with the thesis' main contributions, the discussion below centers on algorithmic and modeling aspects.

Future research on the advected subdomain could focus on improving its robustness and applicability to complex scan patterns:

- To improve robustness to direction changes, one could consider a non-uniform advection field, that varies in space and/or time.

Spatially, an ALE formulation could be employed to define a smooth velocity field that gradually fades to zero away from the heat source, ensuring a more continuous transition and decreasing the risk of shearing effects.

Temporally, the advection velocity could ramp up from zero at the start of a new track to the full heat source velocity after a few steps, mitigating the temperature overshoot observed when advection is abruptly switched on.

- Since accuracy losses occur when thermal gradients in the HAZ are not aligned with the heat source motion, an adaptive controller could detect and deactivate advection under these conditions.

Substepping is certainly the most promising method for the robust acceleration of part-scale LPBF simulations, and several lines of research can be pursued to improve it:

- A more detailed study on the time-scales involved in LPBF would provide valuable quantitative insights to guide the choice of time-steps Δt_f and Δt_s .
- The presented framework is modular, and decouples the choice of DD scheme from other aspects of the substepping algorithm.

In particular, one could explore a semi-monolithic Robin scheme, substituting the Dirichlet condition of Hodge [2021] with a Robin condition. The latter is inherently more general, as it can be tuned to behave like a Dirichlet or a Neumann condition by changing the Robin coefficient. Moreover, foregoing the Dirichlet condition would make the method less sensitive to the predictor step.

- The exploration of higher-order time integration schemes for the slow partition is a promising avenue to improve accuracy for large Δt_s . Although an increase in computational cost is expected, this is likely worthwhile: each macro-step advances the solution over a large physical time interval, maximizing the impact of improved accuracy.
- Refining the predictor step and the slow-fast interpolation scheme during micro-steps is another possibility. This would further reduce the modeling error introduced by the substepping algorithm for large macro-steps and the early stages of the micro-steps, respectively. Options include data-driven predictors and higher order interpolation schemes.
- The development of a more sophisticated criterion for defining the fast partition Ω_f . Currently, a fixed padding around the path of the heat source is used. Criteria based on temperature gradients or error indicators, rather than heuristics, would minimize the number of fast DOFs while ensuring accuracy.
- To improve scalability in distributed memory settings, dynamic load rebalancing of the fast partition could be implemented using partitioning libraries such as ParMETIS or Zoltan, thereby avoiding processor idling during micro-steps.

Further investigation is needed to identify the missing heat-loss mechanism suggested in chapter 8. The goal should be to determine whether this mechanism can be modeled without resorting to fully coupled thermo-fluidic simulations. Importantly, such work should aim to reproduce a consistent set of experimental results with a single calibrated parameter set, avoiding case-by-case recalibration.

Overall, these directions aim at making part-scale LPBF simulations feasible without compromising accuracy, ultimately enabling the virtual design of parts with minimal physical testing.

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