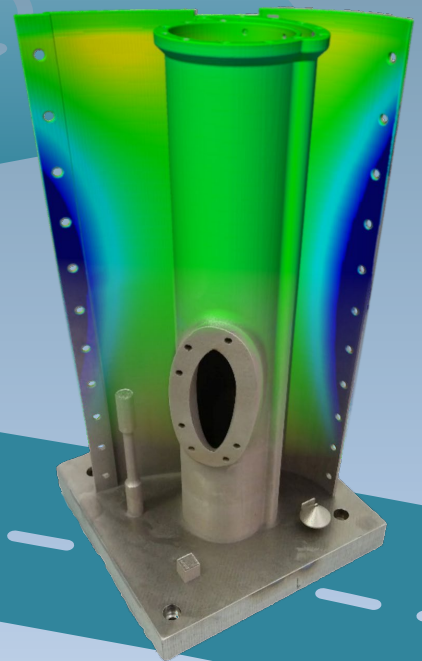
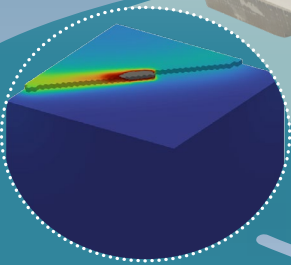
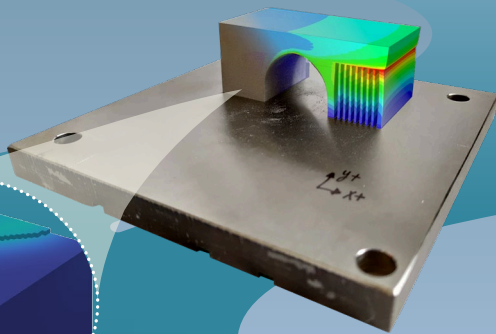
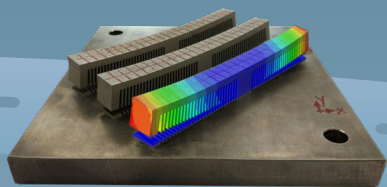


Enhanced Inherent Strain Modelling for Powder-based Metal Additive Manufacturing

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April 2025

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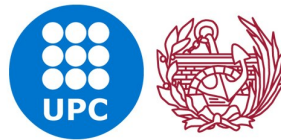


ENHANCED INHERENT STRAIN MODELLING FOR POWDER-BASED METAL ADDITIVE MANUFACTURING

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Doctoral Degree in Civil Engineering

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ABSTRACT

Metal additive manufacturing (MAM), particularly powder bed fusion using a laser beam (PBF-LB), has transformed manufacturing by enabling the production of intricate and optimised metal components directly from digital designs. This process offers major advantages such as material efficiency, high geometric flexibility, and the ability to produce lightweight, customised parts. However, its industrial adoption is hindered by challenges such as large residual stresses and distortions resulting from steep temperature gradients and rapid thermal cycles inherent in layer-by-layer manufacturing process. These issues compromise dimensional accuracy and structural integrity, posing barriers to the broader implementation of the technology.

High-fidelity thermo-mechanical finite element (FE) simulations can predict these phenomena but their high computational cost makes them impractical for large-scale industrial applications. The inherent strain method (ISM) has emerged as an efficient alternative, condensing complex thermal and mechanical phenomena into an inherent strain tensor applied in simplified elastic simulations. While ISM significantly reduces computational time, conventional implementations often lack robustness, requiring extensive recalibration for different geometries and scanning strategies and failing to capture spatial and temporal variations in thermal histories.

This thesis addresses these limitations by developing an enhanced inherent strain method (EISM) for powder bed fusion (PBF), improving ISM's predictive accuracy and extending its applicability to complex industrial geometries. By integrating a macro-scale thermal analysis into ISM, the method dynamically refines the precomputed inherent strain tensor based on part-scale temperature evolution. This enhancement better accounts for geometry- and boundary-specific thermal effects, improving distortion predictions compared to conventional ISM.

Additionally, this work tackles the fundamental challenge of determining inherent strain tensors necessary for ISM-based methodologies. Two complementary approaches are proposed: (1) an empirical calibration strategy using twin-cantilever beam coupons, where distortions measured after partial cutting are used to determine best-fit inherent strain tensors via inverse engineering, and (2) a numerical approach employing a meso-scale thermo-mechanical model within a multi-scale framework, computing local inherent strains and homogenising them to obtain macro-scale inherent strain tensors.

Comprehensive experimental calibration and validation were conducted using Ti-6Al-4V components manufactured via PBF-LB. Temperature histories were recorded with embedded thermocouples, while distortion and residual stress data were acquired using coordinate measuring machines (CMM), 3D scanning, and incremental hole-drilling, respectively. The empirical and numerical methodologies for inherent strain tensor determination, along with EISM, were validated across multiple geometries, including twin-cantilever beams, a non-symmetric bridge, and an industrial

aerospace component (the Steady Blowing Actuator). The results demonstrated that EISM significantly improved distortion predictions while maintaining computational efficiency, reducing errors by more than half compared to conventional ISM.

In conclusion, this thesis presents two methods for calculating the inherent strain tensor (empirical and numerical) and introduces the EISM methodology for distortion prediction, improving the accuracy of distortion prediction in PBF-LB. In this way, the dependence on trial-and-error-based experimental testing is reduced, moving towards an optimised simulation-based design and facilitating the industrial adoption of MAM.

RESUMEN

La fabricación aditiva de metales, en particular la fusión de lecho de polvo mediante láser (*PBF-LB*, por sus siglas en inglés, *Powder Bed Fusion - Laser Beam*), ha revolucionado la manufactura industrial al permitir la fabricación directa de componentes metálicos complejos y optimizados a partir de modelos digitales. Este proceso ofrece varias ventajas clave, como una mayor eficiencia en el uso de material, flexibilidad geométrica y la capacidad de producir piezas con diseños avanzados. No obstante, los rápidos ciclos térmicos inherentes a la fabricación aditiva capa por capa generan altos gradientes térmicos. Esto da lugar a tensiones residuales y distorsiones que comprometen la precisión dimensional y la integridad estructural de las piezas, limitando su adopción a nivel industrial.

Las simulaciones termo-mecánicas basadas en el método de elementos finitos (MEF) permiten predecir estos efectos con alta fidelidad, pero su elevado coste computacional restringe su aplicabilidad en entornos industriales. Como alternativa, el método de la deformación inherente (*ISM*, por sus siglas en inglés, *Inherent Strain Method*) simplifica el problema al condensar los efectos termo-mecánicos en un tensor de deformaciones aplicable en simulaciones elásticas. Sin embargo, la determinación de este tensor sigue siendo un desafío, lo que afecta la fiabilidad de sus predicciones en geometrías industriales complejas.

Esta tesis presenta un método mejorado de deformación inherente (*EISM*, por sus siglas en inglés, *Enhanced Inherent Strain Method*), que mejora la capacidad predictiva del ISM integrando un análisis térmico a escala macro con el ISM original. Así, el tensor de deformación inherente es modificado dinámicamente en función de la evolución térmica global de la pieza. Esta mejora permite incorporar los efectos térmicos específicos de la geometría y las condiciones de contorno.

Por otra parte, se desarrollaron dos estrategias complementarias para la determinación del tensor de deformación inherente: (1) una estrategia empírica, basada en la calibración con cupones de doble ménsula donde las distorsiones medidas tras un corte parcial permiten la determinación del tensor mediante ingeniería inversa, y (2) una metodología numérica basada en modelos locales termo-mecánicos detallados que aplican técnicas de homogenización dentro de un marco multiescala.

La calibración y validación experimental de las metodologías se realizó mediante componentes de Ti-6Al-4V fabricados mediante *PBF-LB*. Se llevaron a cabo mediciones de temperatura mediante termopares embebidos, así como mediciones de distorsiones y tensiones residuales utilizando máquinas de medición por coordenadas (MMC), escaneo 3D y perforación incremental (*HD*, por sus siglas en inglés, *Hole Drilling*), respectivamente. Se analizaron diferentes geometrías, incluyendo vigas de doble ménsula, un puente no simétrico y un componente aeroespacial industrial (*Steady Blowing Actuator*). Los resultados demostraron que el EISM mejora significa-

tivamente la predicción de distorsiones respecto al ISM convencional, reduciendo el error a menos de la mitad y con un coste computacional asumible.

En conclusión, esta tesis presenta dos métodos para calcular el tensor de deformación inherente (empírico y numérico) e introduce la metodología EISM para la predicción de distorsiones, mejorando la precisión en la predicción de distorsiones en PBF-LB. De este modo, se reduce la dependencia de ensayos experimentales basados en prueba y error, avanzando hacia un diseño optimizado mediante simulación y facilitando la adopción industrial de la fabricación aditiva de metales.

RESUM

La fabricació additiva de metalls, en particular la fusió de llit de pols mitjançant làser (*PBF-LB*, per les seves sigles en anglès, *Powder Bed Fusion - Laser Beam*), ha revolucionat la manufactura industrial en permetre la fabricació directa de components metàl·lics complexos i optimitzats a partir de models digitals. Aquest procés ofereix diversos avantatges clau, com una major eficiència en l'ús del material, flexibilitat geomètrica i la capacitat de produir peces amb dissenys avançats. No obstant això, els ràpids cicles tèrmics inherents a la fabricació additiva capa per capa generen alts gradients tèrmics. Això dona lloc a tensions residuals i distorsions que comprometen la precisió dimensional i la integritat estructural de les peces, limitant-ne l'adopció a nivell industrial.

Les simulacions termo-mecàniques basades en el mètode dels elements finits (MEF) permeten predir aquests efectes amb alta fidelitat, però el seu elevat cost computacional en restringeix l'aplicabilitat en entorns industrials. Com a alternativa, el mètode de la deformació inherent (*ISM*, per les seves sigles en anglès, *Inherent Strain Method*) simplifica el problema en condensar els efectes termo-mecànics en un tensor de deformacions aplicable en simulacions elàstiques. No obstant això, la determinació precisa d'aquest tensor continua sent un repte, fet que afecta la fiabilitat de les seves prediccions en geometries industrials complexes.

Aquesta tesi presenta un mètode millorat de deformació inherent (*EISM*, per les seves sigles en anglès, *Enhanced Inherent Strain Method*), que millora la capacitat predictiva de l'ISM integrant una anàlisi tèrmica a escala macro amb l'ISM original. Així, el tensor de deformació inherent es modifica dinàmicament en funció de l'evolució tèrmica global de la peça. Aquesta millora permet incorporar els efectes tèrmics específics de la geometria i les condicions de contorn.

D'altra banda, s'han desenvolupat dues estratègies complementàries per a la determinació del tensor de deformació inherent: (1) una estratègia empírica, basada en la calibració amb cupons de doble mènula on les distorsions mesurades després d'un tall parcial permeten la determinació del tensor mitjançant enginyeria inversa, i (2) una metodologia numèrica basada en models termo-mecànics locals detallats que apliquen tècniques d'homogeneïtzació dins d'un marc multiescala.

La calibració i validació experimental de les metodologies es va realitzar mitjançant components de Ti-6Al-4V fabricats amb *PBF-LB*. Es van dur a terme mesures de temperatura mitjançant termoparets embeguts, així com mesures de distorsions i tensions residuals utilitzant màquines de mesura per coordenades (MMC), escaneig 3D i perforació incremental (*HD*, per les seves sigles en anglès, *Hole Drilling*). Es van analitzar diferents geometries, incloent-hi bigues de doble mènula, un pont no simètric i un component aeroespacial industrial (*Steady Blowing Actuator*). Els resultats van demostrar que l'EISM millora significativament la predicció de distorsions

respecte a l'ISM convencional, reduint l'error a menys de la meitat i amb un cost computacional assumible.

En conclusió, aquesta tesi presenta dos mètodes per calcular el tensor de deformació inherent (empíric i numèric) i introdueix la metodologia EISM per a la predicció de distorsions, millorant la precisió en la predicció de distorsions en PBF-LB. D'aquesta manera, es redueix la dependència d'assajos experimentals basats en prova i error, avançant cap a un disseny optimitzat basat en simulació i facilitant l'adopció industrial de la fabricació additiva de metalls.

LABURPENA

Metalen fabrikazio gehigarriak, bereziki hauts-ohean oinarrituriko laser bidezko fusioak (*PBF-LB, ingelesezko sigletan, Powder Bed Fusion - Laser Beam*), fabrikazio industrialaren iraultza ekarri du, eredu digitaletatik abiatuta pieza metaliko konplexu eta optimizatuak zuzenean fabrikatzea ahalbidetu baitu. Prozesu horrek funtsezko abantailak eskaintzen ditu, hala nola materiala eraginkortasun handiagoz erabiltzea, malgutasun geometrikoa eta diseinu aurreratuak dituzten piezak ekoizteko gaitasuna. Hala ere, geruzaz-geruzako fabrikazio gehigarrian berezkoak diren ziklo termiko azkarrek tenperatura-gradiente handiak sortzen dituzte. Horren ondorioz, hondar-tentsioak eta distortsioak sortzen dira, piezen zehaztasun dimentsionala eta egitura osotasuna arriskuan jarritz, eta ondorioz prozesuaren industria-mailako hedapena mugatuaz.

Elementu finituen metodoan (*FEM, ingelesezko sigletan, Finite Element Method*) oinarritutako simulazio termo-mekanikoez fenomeno horiek fidagarritasun handiz aurreikustea ahalbidetzen dute, baina hauen kostu konputazional altuak ingurune industrialetan aplikatzeko aukera murrizten du. Alternatiba gisa, berezko deformazioaren metodoak (*ISM, ingelesezko sigletan, Inherent Strain Method*) arazoa sinplifikatzen du, efektu termo-mekaniko konplexuak deformazio-tentsore batean kondentsatuz, ondoren simulazio elastikoetan aplikatzeko. Hala ere, tentsore horren zehaztapenak erroka handia izaten jarraitzen du, eta horrek bere auresateko fidagarritasuna mugatzen du geometria konplexua duten pieza industrialetan.

Tesi honetan berezko deformazioaren metodo hobetu bat (*EISM, ingelesezko sigletan, Enhanced Inherent Strain Method*) aurkezten da, ISMren auresateko gaitasuna hobetzen duena berau eskala handiko analisi termiko batez aberastuz. Honela, berezko deformazio-tentsorea dinamikoki aldatzen da piezaren bilakaera termiko globalaren arabera. Hobekuntza honi esker, geometria eta muga-baldintzei lotutako efektu termiko espezifikoak kontuan hartzen dira.

Bestalde, berezko deformazio-tentsorea zehazteko bi estrategia osagarri garatu ziren: (1) estrategia enpirikoa, mentsula bikoitzeko kupoen bidezko kalibrazioan oinarritua, non ebaketa partzial baten ondoren neurtutako distortsioek alderantzizko ingeniartzaren bidez tenkagailua zehaztea ahalbidetzen duten, eta (2) eskala txikiko simulazio termo-mekaniko zehatzetan oinarritutako zenbakizko metodologia. Eskala anitzeko esparru baten barruan homogenizazio-teknikak aplikatuz deformazio-tentsore orokortua kalkulatzeko ahalbidetzen du.

Metodologiaren kalibrazio eta balidazio esperimentala *PBF-LB* bidez fabrikatutako Ti-6Al-4V lagin eta piezen bidez egin zen. Tenperatura-neurketak egin ziren termopare txertatuen bidez, bai eta distortsioen eta hondar-tentsioen neurketak ere, koordenatuen bidezko neurketa-makinak (*CMM, ingelesezko sigletan, Coordinate Measuring Machine*), 3D eskaneatzea eta zulaketa inkrementala (*HD, ingelesezko sigletan, Hole Drilling*) erabiliz, hurrenez hurren. Geometria desberdinak aztertu ziren,

mentsula bikoitzeko habeak, simetrikoa ez den zubi bat eta osagai aeroespazial industrial bat barne (*Steady Blowing Actuator*). Emaitzek erakutsi zuten EISMak nabarmen hobetzen duela ohiko ISMarekiko distortsioen aurreikuspena, errorea erdira baino gutxiagora murriztuz eta kostu konputazional onargarriarekin.

Laburbilduz, tesi honek berezko deformazio-tentsorea kalkulatzeko bi modu (enpirikoa eta zenbakizkoa) eta distortsioak iragartzeko EISM metodologia aurkezten ditu, PBF-LBko distortsioen iragarpenaren zehaztasuna hobetuz. Horrela, proba eta errorean oinarritutako saiakuntza esperimentalekiko mendekotasuna murrizten da, simulazioan oinarritutako diseinu optimizaturantz aurrera eginez eta metalen fabrikazio aditiboa industrialki hartzea erraztuz.

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ACRONYMS

AM	Additive Manufacturing
AMR	Adaptive Mesh Refinement
CA	Cellular Automata
CIMNE	International Center for Numerical Methods in Engineering
CMM	coordinate measuring machine
CWM	Computational Welding Mechanics
DED	Directed Energy Deposition
DED-Arc	Directed Energy Deposition - Arc
DED-LB	Directed Energy Deposition - Laser Beam
DIC	Digital Image Correlation
DVRT	Differential Voltage Reluctance Transducer
EISM	Enhanced Inherent Strain Method
FE	Finite Element
FEM	Finite Element Method
HAV	heat-affected volume
HPC	High-Performance Computing
IR	Infrared
IS	Inherent Strain
ISM	Inherent Strain Method
LDS	Laser Displacement Sensor
LVDT	Linear Variable Differential Transformers
MAPE	Mean Absolute Percentage Error
MAM	Metal Additive Manufacturing
MC	Monte Carlo
MISM	modified inherent strain method
ML	Machine Learning
PBF	Powder Bed Fusion
PBF-EB	Powder Bed Fusion - Electron Beam
PBF-LB	Powder Bed Fusion - Laser Beam
PDE	Partial Differential Equation

PF	Phase-Field
PIML	Physics-Informed Machine Learning
ROM	Reduced Order Modelling
SBA	Steady Blowing Actuator
SME	Small- and Medium-sized Enterprise
VED	Volumetric Energy Density
wEDM	wire electrical discharge machining

INTRODUCTION

1.1 Motivation and problem statement

Additive Manufacturing (AM), also known as 3D printing, has revolutionised the manufacturing industry by enabling the production of highly complex and customised parts directly from digital designs [23, 36]. This design flexibility, combined with the ability to optimise geometries for performance and material efficiency, has made AM a key technology for industries such as aerospace, automotive, and healthcare [40]. Among the various AM processes, Powder Bed Fusion - Laser Beam (PBF-LB) has emerged as one of the most precise techniques for manufacturing metallic components, particularly for applications where material properties and dimensional accuracy are critical.

PBF-LB employs a laser beam to selectively melt thin layers of metallic powder, enabling precise layer-by-layer fabrication. This AM approach provides exceptional control over the microstructure and mechanical properties of the final component [45].

One of the most widely used materials in PBF-LB is Ti-6Al-4V, a titanium alloy renowned for its excellent strength-to-weight ratio, corrosion resistance, and biocompatibility [66]. These properties make it particularly suitable for high-performance applications, including aerospace components, biomedical implants, and structural parts in demanding environments.

However, the adoption of PBF-LB faces significant challenges. During the manufacturing process, the highly localised and rapid heating and cooling cycles induce steep thermal gradients. These gradients generate large residual stresses and distortions, which can compromise the dimensional accuracy and mechanical integrity of the final part [44]. Addressing these issues often involves trial-and-error approaches that are costly, labour-intensive, and inefficient. For instance, corrective measures are typically applied after manufacturing, increasing scrap rates and overall production costs [12].

To overcome these challenges, predictive computational modelling has become an essential tool in AM [66]. Physics-based, high-fidelity finite element simulations provide detailed insights into the thermo-mechanical behaviour of the process, allowing for distortion and residual stress prediction. However, these models are computationally expensive, especially when applied to real-world parts involving thousands of layers.

To address this challenge, researchers have developed various strategies to reduce computational costs. These strategies include Adaptive Mesh Refinement (AMR) techniques, multi-scale modelling approaches, surrogate models or reduced-order models

and layer lumping [14]. However, while these approaches improve computational feasibility, they still require significant resources and remain impractical for routine industrial use.

An alternative approach is the *Inherent Strain Method (ISM)* [44, 75], a simplified modelling methodology that significantly reduces computational cost while retaining the ability to accurately predict distortions and, to a lesser extent, residual stresses. ISM replaces complex thermo-mechanical simulations with a sequence of linear elastic mechanical steps, where the accumulated thermal, plastic, and other inelastic deformations are condensed into an equivalent inherent strain tensor. This tensor is then systematically applied layer-by-layer to predict part-scale deformations [44].

A crucial aspect of ISM is the accurate determination of the inherent strain tensor. This can be achieved through empirical approaches (calibrating the inherent strains from experimental measurements) or through numerical techniques, particularly meso-scale thermo-mechanical simulations in a multi-scale modelling framework [44, 74]. However, despite its computational efficiency, the practical implementation of ISM is hindered by several key challenges:

- **Inherent strain tensor calculation:** There is no standardized procedure for obtaining inherent strain tensors from experimental trials using inverse engineering techniques. Such an approach would be highly suitable for industrial applications, as inverse engineering-based methodologies are well established in manufacturing and can be directly linked to empirical process data. Many industries rely primarily on experimental datasets due to the high sensitivity of process parameters in PBF-LB, which makes it difficult to adopt purely numerical methods.

On the numerical side, meso-scale thermo-mechanical models have been developed to calculate inherent strains, but they often have limited scope. Most models consider only a few layers to reduce the computational cost, which may lead to inaccuracies in representing thermal gradients, mechanical interactions, and boundary effects. This localized modelling approach fails to fully capture the cumulative stress buildup across an entire part, leading to discrepancies between predicted and actual distortions [12].

- **Generalization Issues:** Existing ISM methodologies frequently lack robustness when applied to parts featuring intricate geometries or complex scanning strategies due to the simplifications inherent to ISM. Many models rely on simplified assumptions about thermal gradients and deformation patterns, which may not generalize well to all configurations. Consequently, while ISM provides computational efficiency, its predictive accuracy remains highly dependent on calibration for specific process configurations, limiting its widespread industrial adoption.
- **Limited Validation and Scalability:** Despite its theoretical advantages, ISM implementations still lack extensive validation against experimental datasets, particularly for "full-scale industrial parts". Most studies focus on small-scale benchmarks, making it unclear how well the method performs for complex, real-world applications.

Despite its computational efficiency, the applicability of **ISM** in **PBF-LB** remains constrained by these challenges. Addressing these limitations would significantly enhance its predictive accuracy and reliability, making it a more effective tool for distortion prediction and, to a lesser extent, residual stress estimation.

1.2 Objectives

The main objective of this research is to **develop an efficient and validated numerical methodology based on the ISM to predict distortions in PBF-LB manufactured components**. The proposed methodology aims to enhance the predictive accuracy and industrial applicability of the **ISM**, bridging the gap between computational efficiency and modelling fidelity.

To achieve this, the following specific objectives are defined:

- **Objective 1: Development of an empirical approach for inherent strain calibration.** Establish a systematic methodology for determining inherent strain tensors through experimental measurements. This involves fabricating benchmark test coupons, measuring distortions and applying inverse engineering approaches to extract inherent strain values.
- **Objective 2: Calculation of inherent strain tensors using meso-scale thermo-mechanical simulations.** Develop a meso-scale numerical model that enables the accurate extraction of inherent strains from high-fidelity thermo-mechanical models. This requires simulating localized thermal and mechanical behaviour under realistic **PBF-LB** process conditions and ensuring that inherent strain tensors derived at the meso-scale are transferable to part-scale simulations.
- **Objective 3: Enhancement of the ISM for improved accuracy and generalization.** Refine the conventional **ISM** by incorporating corrections based on experimental data and meso-scale insights.
- **Objective 4: Validation of both high-fidelity and simplified models against experimental results.** Compare the predictions of high-fidelity thermo-mechanical simulations and the enhanced **ISM** with experimental measurements of temperature, distortion and residual stresses. Assess the accuracy of both detailed and simplified modelling approaches across different process conditions and geometries, ensuring confidence in their predictive capabilities.
- **Objective 5: Industrial validation and demonstration of the simplified methodology.** Demonstrate the applicability of the proposed **ISM**-based methodology in a real industrial use case. Validate the model's performance on complex geometries, ensuring its effectiveness in predicting distortions for full-scale parts. Assess the feasibility of integrating the methodology into industrial workflows to reduce reliance on costly trial-and-error manufacturing adjustments.

By achieving these objectives, this research aims to provide an improved predictive modelling framework for **PBF-LB**, enabling more reliable and cost-effective distortion prediction for industrial applications.

1.3 Significance

This research advances predictive modelling methodologies for [PBF-LB](#), addressing the need for computationally efficient and scalable distortion prediction techniques. By refining and validating the [ISM](#), it offers a more accurate and accessible alternative to high-fidelity simulations, facilitating wider adoption in both research and industry.

From an academic perspective, this study enhances multi-scale modelling by integrating meso-scale thermo-mechanical simulations with part-scale inherent strain methodologies. It also establishes a systematic experimental calibration framework, enabling empirical validation of simplified models. Furthermore, the improved [ISM](#) enhances generalisation by incorporating process-dependent corrections for scanning strategies, complex geometries, and boundary conditions. The validation of both high-fidelity and simplified models provides benchmark data, supporting future research in computational modelling for [MAM](#).

In an industrial context, this work reduces reliance on costly and time-consuming trial-and-error-based process optimisation. By enabling more accurate and rapid distortion prediction, it allows manufacturers to optimise process parameters before fabrication, minimising material waste and post-processing requirements. The enhanced [ISM](#) offers a computationally efficient alternative to high-fidelity simulations, making predictive modelling more accessible to industries with limited computational resources. Its validation on real [PBF-LB](#) components ensures applicability to full-scale manufacturing, supporting quality assurance and certification processes.

Beyond academia and industry, this research aligns with broader technological and economic trends. It contributes to the standardisation of distortion prediction methodologies, essential for advancing [AM](#) part certification and qualification. By improving process reliability and efficiency, it supports cost reduction and promotes sustainability in metal [AM](#) by minimising waste and optimising resource utilisation. Moreover, it facilitates the integration of simulation-driven [AM](#) workflows, accelerating the transition towards digital manufacturing and Industry 4.0.

1.4 Scope

This research focuses on the numerical modelling and experimental validation of distortion prediction methodologies for [PBF-LB](#) manufactured Ti-6Al-4V components. It encompasses the development and validation of both high-fidelity and simplified modelling approaches, including but not limited to the Inherent Strain Method ([ISM](#)). The scope of the study is defined as follows:

- The study is limited to the [PBF-LB](#) process and does not extend to other metal additive manufacturing techniques such as Powder Bed Fusion - Electron Beam ([PBF-EB](#)) or Directed Energy Deposition ([DED](#)).
- Only Ti-6Al-4V is considered, as it is widely used in high-performance applications.

- Support structures (typically used in [PBF](#)) are out of scope. Printed parts will only include solid-like supports (if required), while thin wall-like supports are excluded. Furthermore, their numerical modelling is not considered in this work.
- The study primarily focuses on distortion prediction using high-fidelity numerical simulations, meso-scale modelling, and simplified modelling approaches. The modelling of microstructural evolution, phase transformations, or mechanical properties is beyond the scope of this study.
- All experimental results are obtained in-house to ensure consistency in data acquisition and process conditions.
- The study includes both high-fidelity thermo-mechanical simulations and inherent strain-based methodologies, ensuring a multi-scale approach to distortion prediction.
- The methodology is validated using both simple test coupons and industrial-scale components to ensure its applicability to real-world manufacturing scenarios.
- While computational efficiency is evaluated, the study does not aim to develop new numerical solvers but rather to optimise existing modelling approaches for improved accuracy and industrial applicability.

By defining these constraints, this research maintains a balanced focus on numerical modelling, experimental validation, and real-world application, ensuring that the proposed methodologies are both scientifically rigorous and industrially relevant.

1.5 Thesis outline

This thesis is structured to reflect the integration of numerical modelling, experimental validation, and methodology development for distortion prediction in [PBF-LB](#). It follows a logical progression from background and state-of-the-art studies to numerical and experimental methodologies, followed by validation and implementation in real industrial use cases. The research contributions are documented in three published articles, which are incorporated into the thesis as individual chapters.

[Chapter 1](#) provides an overview of the research motivation, objectives, significance, scope, and dissemination of results. [Chapter 2](#) presents an overview of the state of the art, structured into three main areas: an introduction to metal additive manufacturing, a review of numerical modelling approaches for [PBF-LB](#), and an overview of experimental procedures used for model calibration and validation. It also identifies research gaps that this work aims to address.

[Chapter 3](#) presents the numerical modelling framework for [PBF-LB](#), detailing the computational approaches employed and developed in this research. It covers high-fidelity thermo-mechanical simulations, the Inherent Strain Method ([ISM](#)), and the En-

hanced Inherent Strain Method (EISM), providing a comprehensive discussion of their theoretical foundations, governing equations, and computational implementation.

Chapter 4 describes the experimental work conducted for calibration and validation, including the design and fabrication of test coupons and a larger demonstration component. It also outlines the measurement techniques applied to characterise temperature evolution, distortions, and residual stresses in the manufactured parts.

The core contributions of this research are structured into three chapters, each corresponding to a published article. **Chapter 5** presents an **empirical methodology for determining inherent strains**, developed through experimental measurements and calibration techniques. This chapter corresponds to **Paper 1**. **Chapter 6** introduces a **numerical approach for calculating inherent strains**, where meso-scale thermo-mechanical simulations are used to extract inherent strain tensors. This chapter is based on **Paper 2**. **Chapter 7** discusses an **enhanced inherent strain method**, which incorporates improvements to traditional ISM and is validated using both numerical and experimental results. This chapter corresponds to **Paper 3**.

Chapter 8 summarises the key findings of this research, highlights the main contributions, addresses its limitations, and outlines future work directions.

To illustrate the relationships between different thesis chapters, their methodological linkages, and their connection to the published articles, **Figure 1.1** provides a visual representation of the research framework. The diagram highlights how experimental and numerical methodologies contribute to the development of the enhanced inherent strain method, with each component feeding into the overall distortion prediction framework.

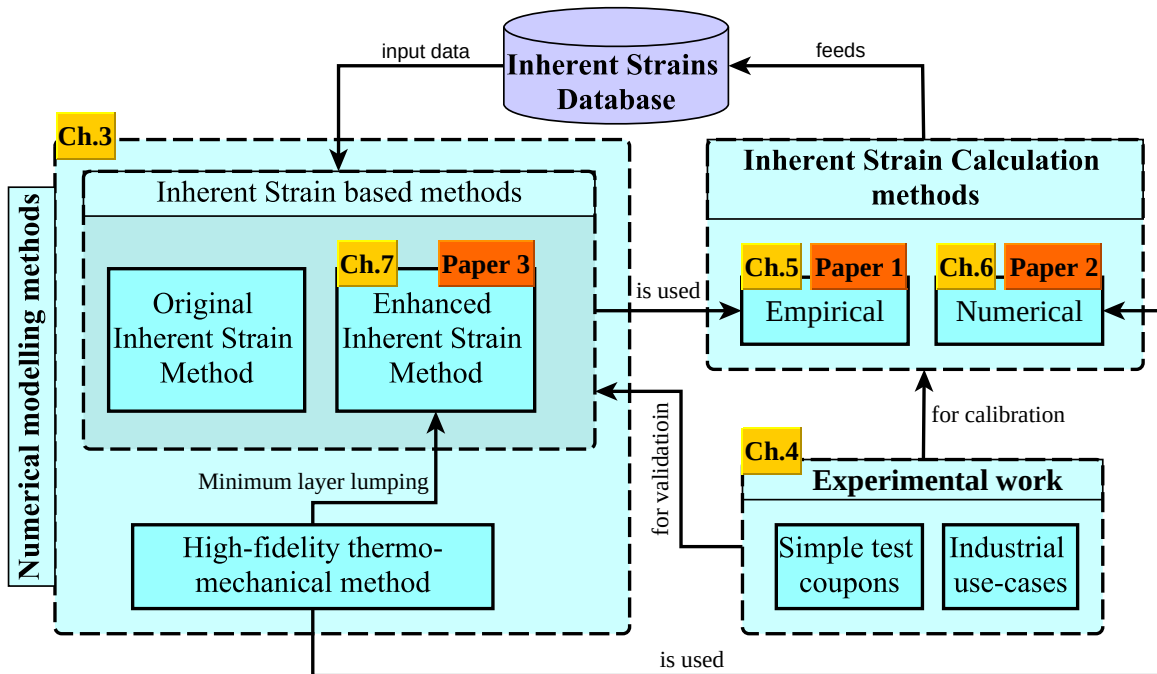


Figure 1.1: Conceptual map of the research workflow, linking numerical modelling, experimental work, and inherent strain methodologies across thesis chapters.

1.6 Research dissemination

The outcomes of this research have been disseminated through peer-reviewed journal publications and conference presentations, ensuring the visibility and validation of the findings within the scientific community. The dissemination strategy aligns with the structured approach of the thesis, with each core research contribution documented in a published article and presented at relevant international conferences.

1.6.1 Publications in peer-reviewed international journals

The key contributions of this research have been published in international peer-reviewed journals. Each publication corresponds to a specific aspect of the thesis, as outlined below:

- **Paper 1 [69]:**

Iñaki Setien, Michele Chiumenti, Sjoerd van der Veen, Maria San Sebastian, Fermín Garciandía, and Alberto Echeverría. “Empirical methodology to determine inherent strains in additive manufacturing.” In: *Computers & Mathematics with Applications*. Simulation for Additive Manufacturing 78.7 (Oct. 2019), pp. 2282–2295. ISSN: 0898-1221. DOI: [10.1016/j.camwa.2018.05.015](https://doi.org/10.1016/j.camwa.2018.05.015). URL: <https://www.sciencedirect.com/science/article/pii/S0898122118302839>

- **Paper 2 [67]:**

Iñaki Setien, Michele Chiumenti, Maria San Sebastian, Manuel A. Caicedo, and Carlos A. Moreira. “Defining and Optimising High-Fidelity Models for Accurate Inherent Strain Calculation in Laser Powder Bed Fusion.” en. In: *Metals* 15.2 (Feb. 2025), p. 180. ISSN: 2075-4701. DOI: [10.3390/met15020180](https://doi.org/10.3390/met15020180). URL: <https://www.mdpi.com/2075-4701/15/2/180>

- **Paper 3 [68]:**

Iñaki Setien, Michele Chiumenti, Maria San Sebastian, Carlos A. Moreira, and Manuel A. Caicedo. “Integrating Temperature History into Inherent Strain Methodology for Improved Distortion Prediction in Laser Powder Bed Fusion.” In: *Metals* 15.2 (2025). ISSN: 2075-4701. DOI: [10.3390/met15020143](https://doi.org/10.3390/met15020143). URL: <https://www.mdpi.com/2075-4701/15/2/143>

Each article has been peer-reviewed, ensuring the credibility and impact of the research within the additive manufacturing and computational modelling communities.

1.6.2 Presentations in international conferences

The findings of this research have also been presented at international conferences on additive manufacturing and computational mechanics. These presentations have facilitated discussions with experts in the field, contributing to the refinement of the methodologies. The major conference contributions include:

- **Chiumenti, M.; Salsi, E.; Cervera, M.; Setien, I.; Echevarría, A.,** *Numerical modelling of Selective Laser Melting in additive manufacturing and its experimental validation*, International Conference on Computational Plasticity, Barcelona, Spain, Sept. 2017.
- **Setien, I.,** *Simplified numerical methods for distortion prediction in Selective Laser Melting and their experimental validation*, International Conference on Simulation for Additive Manufacturing, Munich, Germany, Oct. 2017.
- **Setien, I.,** *Distortion Prediction in Selective Laser Melting: Methodology for Inherent Strain Determination*, Fraunhofer Direct Digital Manufacturing Conference, Berlin, Germany, Mar. 2018.
- **Setien, I.,** *Distortsioen aurreikuspena “Selective Laser Melting” prozesuan: inherent strain deformazioen kalkulurako metodologia*, Materialeen Zientzia eta Teknologia, San Sebastian, Spain, Jul. 2018.
- **Setien, I.,** *AM Inherent Strain Calibration Strategy based on High-Fidelity Finite Element Models*, NAFEMS NORDIC Seminar: Exploring the Design Freedom of Additive Manufacturing through Simulation, Helsinki, Finland, Dec. 2018.
- **Chiumenti, M.; Setien, I.; Echevarría, A.,** *Enhanced inherent strain method for Additive Manufacturing simulation*, Computational Methods for Coupled Problems in Science and Engineering, Sitges, Barcelona, Spain, Jun. 2019.
- **Setien, I.; Chiumenti, M.; Echevarría, A.,** *Additive Manufacturing inherent strain calibration strategy based on high-fidelity finite element models*, Computational Methods for Coupled Problems in Science and Engineering, Sitges, Barcelona, Spain, Jun. 2019.
- **Setien, I.; Chiumenti, M.; Echevarría, A.,** *Enhanced inherent strain method applied to a ‘bridge-like’ structure*, International Conference on Simulation for Additive Manufacturing, Pavia, Italy, Sep. 2019.

These dissemination efforts have ensured the broad communication of research findings while fostering collaborations and receiving critical feedback from the scientific and industrial communities.

STATE OF THE ART

2.1 Metal additive manufacturing

2.1.1 Introduction

Additive Manufacturing (AM) is an advanced manufacturing paradigm that enables the creation of three-dimensional (3D) objects by progressively adding material layer-by-layer based on a digital model. Unlike conventional subtractive methods, AM allows for the fabrication of complex geometries with minimal material waste, significantly reducing the need for traditional tooling.

Among the various AM processes, Metal Additive Manufacturing (MAM) is a specialised subset that focuses on metallic materials. It has gained increasing industrial and academic interest due to its capability to produce high-performance metal components with intricate designs that would be impossible or prohibitively expensive to manufacture using traditional techniques. Despite its advantages, challenges remain, particularly regarding adoption by Small- and Medium-sized Enterprise (SME)s, where cost, technical expertise, and scalability are key factors [65].

2.1.2 Metal additive manufacturing processes

MAM processes are classified under the ISO/ASTM 52900:2021 standard, which categorises AM into seven major techniques. However, only four of these processes are commonly applied to metals, as summarised in Table 2.1. These processes vary in their energy source, material deposition mechanism, and applicability. The operating principles of these four primary MAM techniques are illustrated in Figure 2.1.

Additionally, these MAM techniques can be further categorised based on the type of energy source employed, as depicted in Figure 2.2. This classification provides a clearer distinction between process sub-variants and their respective energy input mechanisms.

Each of these techniques has advantages and drawbacks, which affect their suitability for specific industrial applications.

Table 2.1: MAM processes, their operational modes, and typical applications [42].

Process	Mode	Typical Applications
Material Extrusion (ME)	Metal material is selectively extruded through a nozzle or orifice, typically using bound metal filaments.	Functional metal parts, prototyping.
Binder Jetting (BJ)	A liquid binder is selectively deposited onto a powder bed, forming a green part that is later sintered.	Functional metal parts, low-rate production of non-critical components.
Directed Energy Deposition (DED)	A focused heat source (laser or electron beam) melts and fuses metal feedstock (wire or powder) as it is deposited.	Functional metal parts, repairs, adding material to existing components.
Powder Bed Fusion (PBF)	A high-energy laser or electron beam selectively fuses regions of a powder bed to form a solid metal part.	Functional metal parts, high-precision prototyping.

2.1.3 Advantages and challenges

MAM is increasingly adopted in industry and academia due to its key advantages over conventional manufacturing methods. Its primary benefits are summarised as follows [5, 23]:

- **Rapid prototyping and low-volume production:** MAM enables the efficient and cost-effective fabrication of functional prototypes, reducing design iteration cycles and accelerating product development.
- **Complex geometries without additional cost:** Intricate internal structures, lightweight lattices, and optimised topologies can be directly manufactured without the constraints of conventional tooling.
- **Material efficiency:** Unlike subtractive methods, which generate significant waste, AM only consumes the necessary material, improving sustainability and cost-efficiency.
- **Customisation and personalisation:** AM facilitates the production of patient-specific implants, bespoke components, and tailored engineering solutions across multiple sectors.
- **Reduction in assembly requirements:** Complex assemblies can be consolidated into a single monolithic component, reducing part count and eliminating weak points associated with joining techniques.

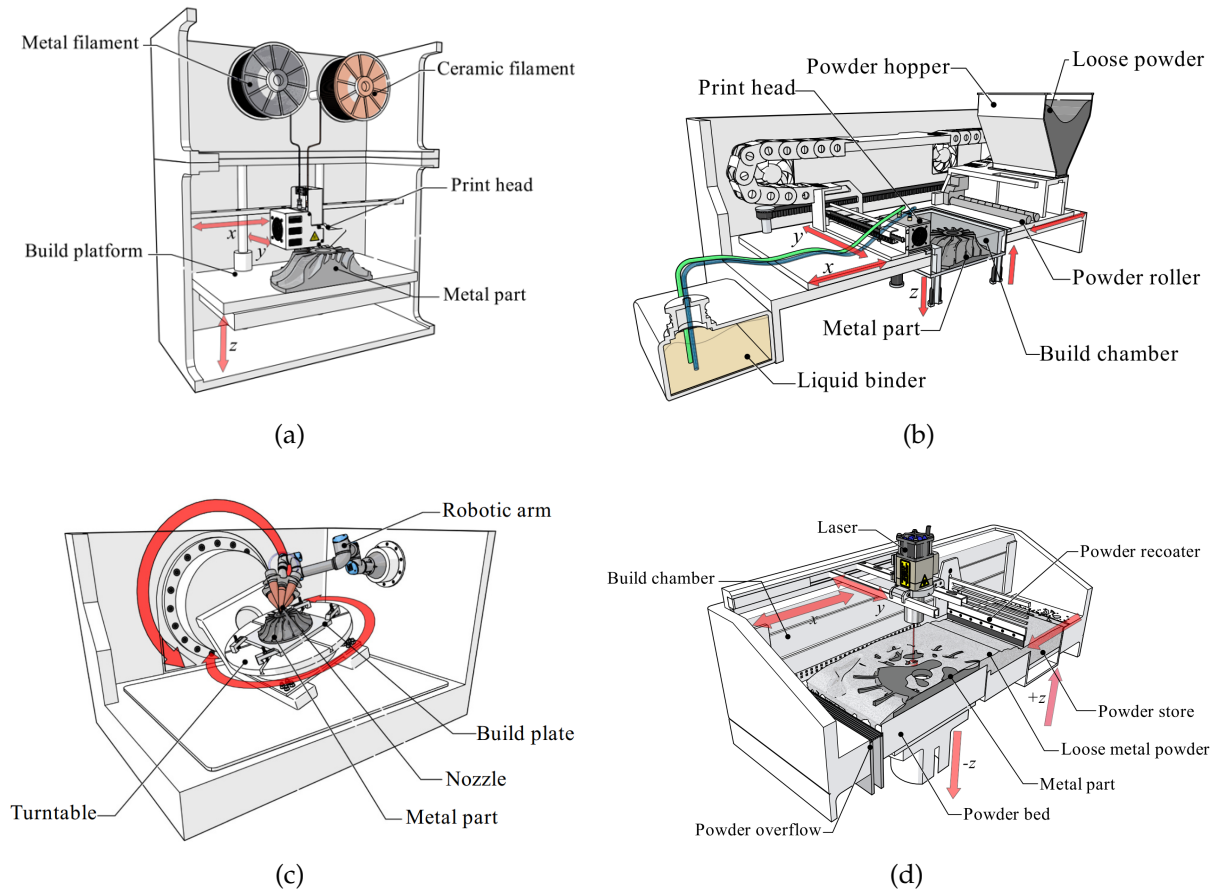


Figure 2.1: Schematic overviews of the four primary MAM processes: (a) Material Extrusion, (b) Binder Jetting, (c) Directed Energy Deposition, and (d) Powder Bed Fusion [5].

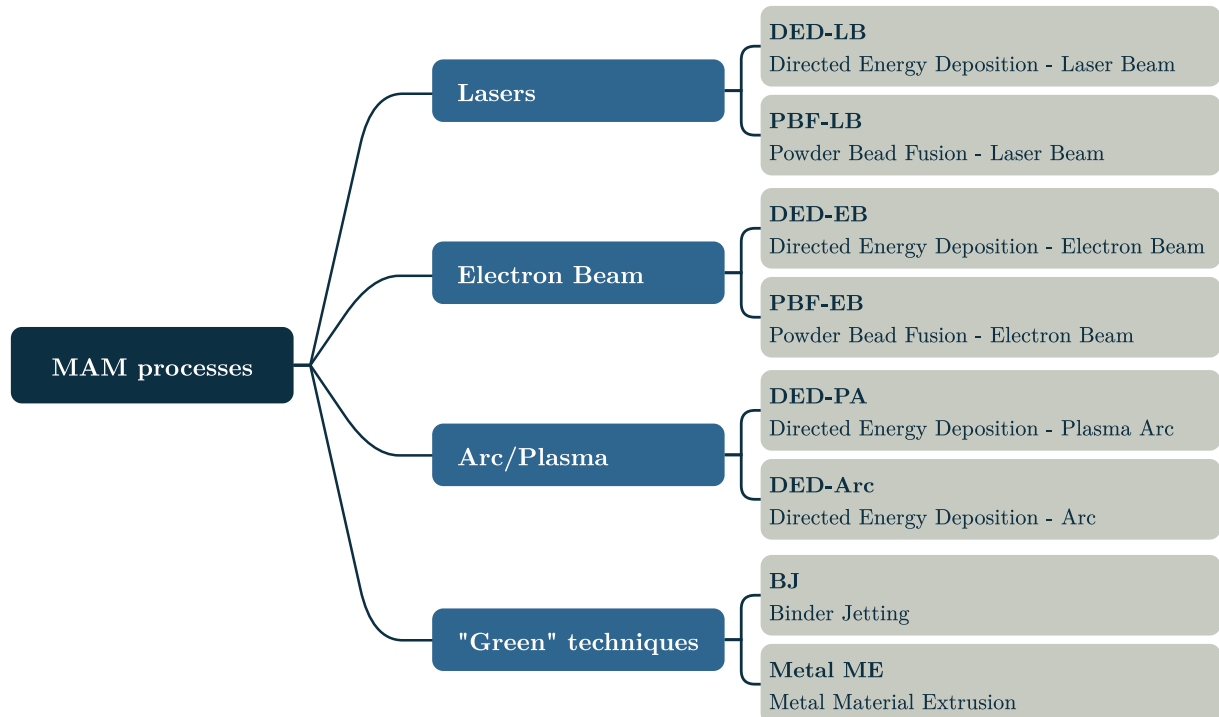


Figure 2.2: Classification of MAM techniques based on energy source. Adapted from [65].

However, significant challenges must be addressed for wider adoption, especially by [SMEs](#) [65]:

- **High initial investment:** Equipment and operational costs remain a barrier, particularly for high-end processes like [PBF](#).
- **Process complexity:** [PBF](#) and [DED](#) require stringent control of multiple parameters.
- **Material and part quality:** Issues like porosity, residual stresses, and surface roughness affect reliability.
- **Technical expertise:** Adoption is hindered by the need for skilled operators and post-processing requirements.

2.1.3.1 Applications

[MAM](#) is widely applied across multiple industries. Key application areas include [5, 23]:

- **Aerospace:** [MAM](#) enables the fabrication of lightweight, high-strength components such as turbine blades, fuel injectors, and structural parts. The GE9X engine for the Boeing 777X incorporates [AM](#)-produced parts, leading to significant weight reduction and improved efficiency.
- **Medical and dental:** The ability to manufacture patient-specific implants, prosthetics, and surgical guides is a major advantage of [MAM](#) in the healthcare sector. Customised implants offer better anatomical fit and enhanced biocompatibility.
- **Automotive:** [MAM](#) is utilised for rapid prototyping, spare part production, and end-use components in performance vehicles. Examples include titanium door handle frames and anti-theft wheel locks.
- **Energy sector:** [AM](#) is applied in the production of heat exchangers, turbine components, and parts for oil and gas industries, where efficiency and high-temperature resistance are critical.
- **Construction:** Large-scale [AM](#) has enabled projects like the world's first 3D-printed metal bridge in Amsterdam, demonstrating the feasibility of [AM](#) for architectural and infrastructural applications.
- **Defence:** The defence sector benefits from [MAM](#)'s ability to produce lightweight, durable parts for military vehicles, weapons systems, and customised equipment.

2.1.4 Powder Bed Fusion – Laser Beam (PBF-LB)

Among MAM techniques, PBF-LB continues to dominate the market, accounting for approximately 85% of the MAM market share in 2023 [4]. This widespread adoption is attributed to PBF-LB's high dimensional accuracy, material versatility, and suitability for complex geometries. Consequently, PBF-LB is extensively utilized in critical industries such as aerospace, biomedical, and automotive sectors. Representative examples of PBF-LB-produced parts in these industries are illustrated in Figure 2.3, demonstrating its versatility and growing adoption.

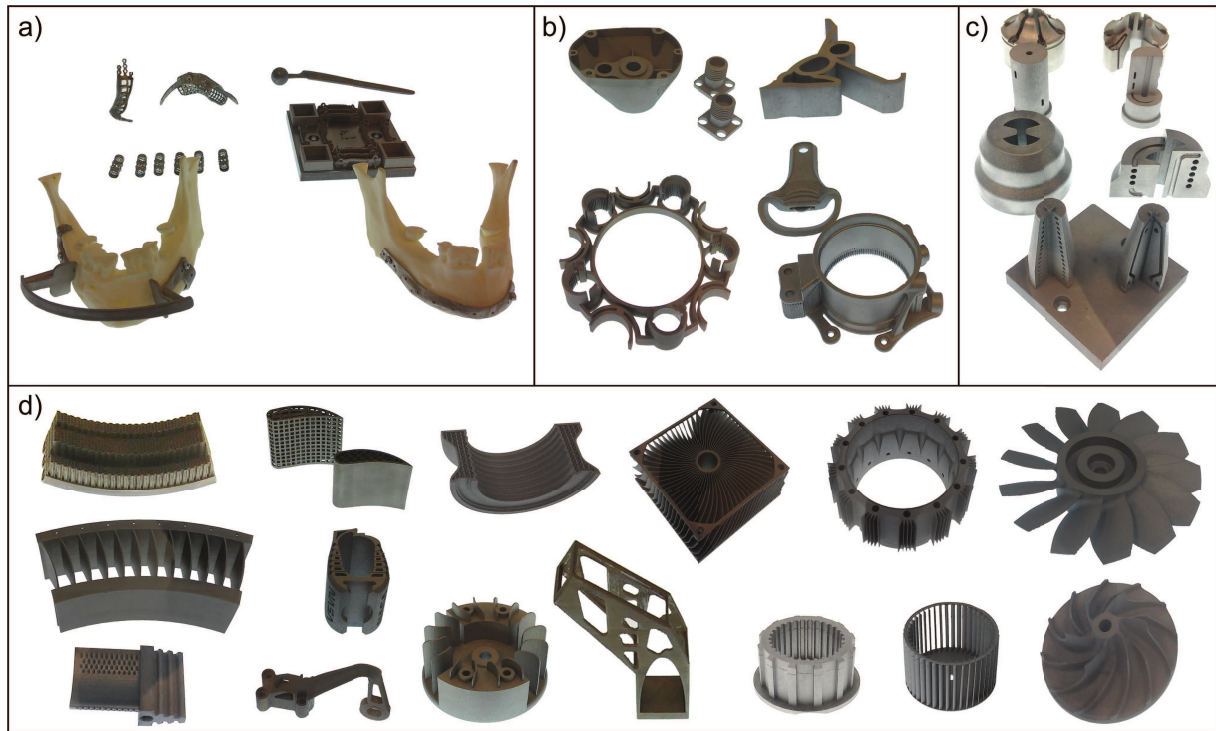


Figure 2.3: PBF-LB-manufactured components at LORTEK across various industries: (a) biomedical, (b) automotive, (c) tooling or moulds, and (d) aeronautics.

2.1.4.1 Advantages and challenges of PBF-LB

PBF-LB offers several advantages that make it a preferred choice for MAM applications. The process provides exceptional precision and dimensional accuracy, making it ideal for industries that demand high tolerances, such as aerospace and medical device manufacturing [5]. Furthermore, it supports a broad range of materials, including titanium, stainless steel, and nickel-based superalloys, allowing for versatility across various applications. Another key benefit is the near-net shape production, which minimises material waste and reduces the need for extensive post-processing [5].

A major advantage of PBF-LB is its ability to fabricate complex structures that are difficult to produce using traditional manufacturing techniques. The layer-wise approach enables the creation of intricate lattice structures and lightweight components, which are particularly beneficial in aerospace and automotive applications. Additionally, the process facilitates rapid prototyping, allowing for quick design

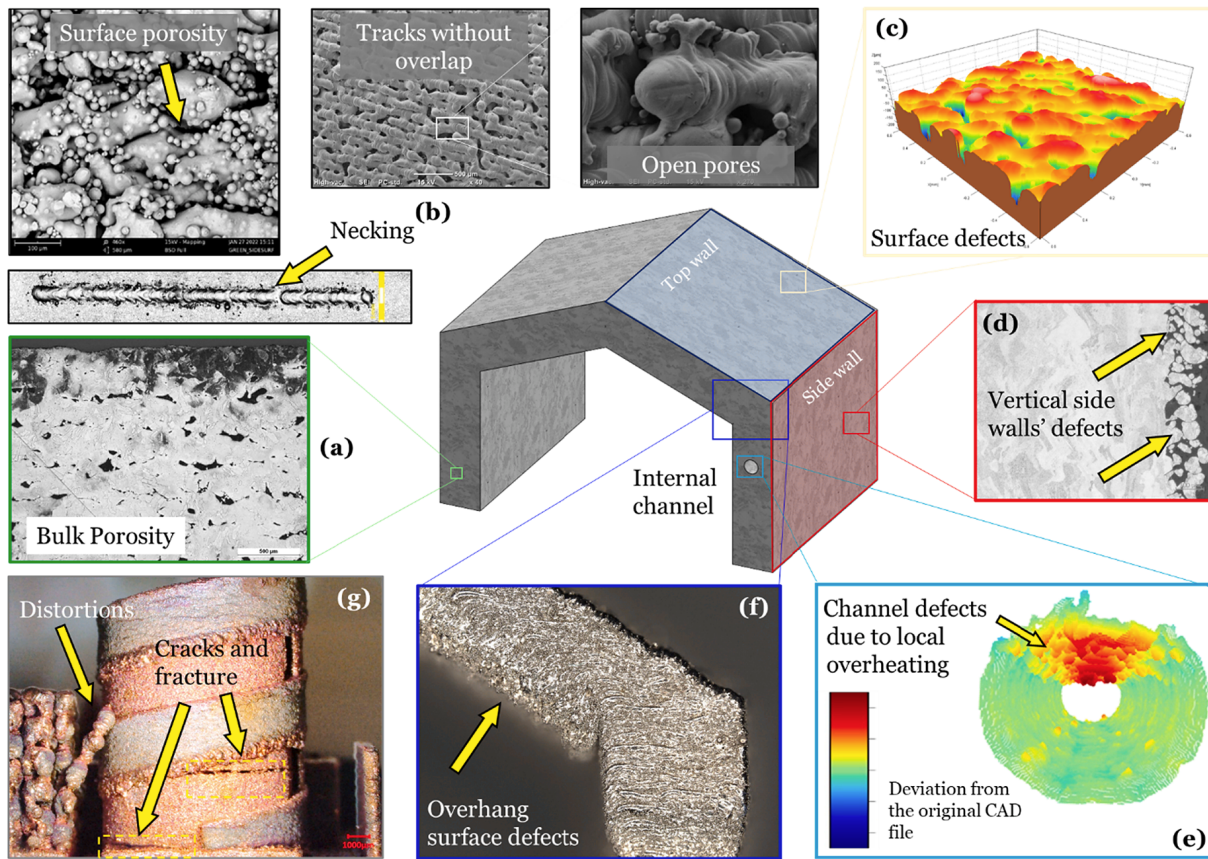


Figure 2.4: An overview of a number of most important defects in PBF-made metallic parts [14].

iterations and accelerated product development cycles. As a mature technology, **PBF-LB** benefits from extensive research and process optimization, leading to well-established manufacturing parameters and industrial adoption [23].

While **PBF-LB** offers numerous benefits, it still faces significant challenges due to the formation of undesirable defects (see Figure 2.4 for examples). One of the most significant issues is the generation of residual stresses due to the high thermal gradients involved in rapid laser melting and solidification. These stresses can lead to part distortion and, in extreme cases, cracking, necessitating mitigation strategies such as preheating the build platform and optimising scanning paths. Surface roughness is another limitation, arising from partially melted powder, layer-wise processing artefacts, and inconsistencies in powder spreading. Compared to conventionally machined surfaces, **PBF-LB** parts often require post-processing techniques, such as chemical etching or abrasive finishing, to achieve the desired surface quality.

Porosity formation is also a critical concern, affecting the structural integrity of **PBF-LB** components. Lack-of-fusion defects occur when insufficient energy input prevents full melting of the powder, while keyhole porosity arises when excessive energy causes unstable vaporisation, trapping gas pockets in the melt pool [13]. Additionally, process repeatability remains a challenge due to variations in powder morphology, laser beam stability, and environmental conditions. Research into in-situ monitoring and closed-loop control mechanisms is ongoing to enhance consistency and quality assurance in **PBF-LB**.

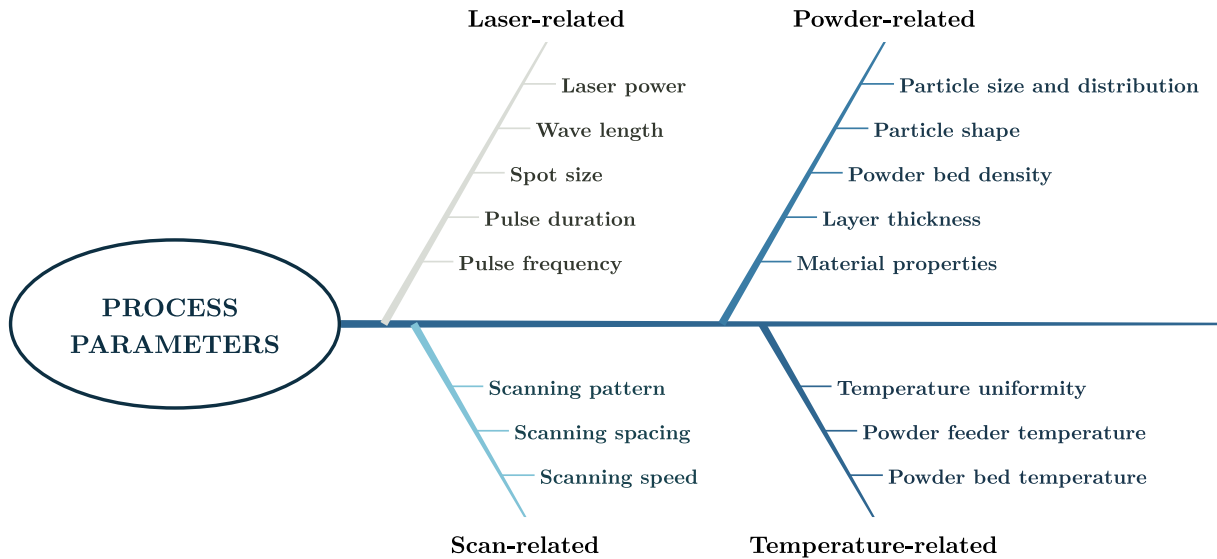


Figure 2.5: Key process parameters in PBF-LB. Adapted from [72].

2.1.4.2 Process parameters

The PBF-LB process involves numerous process parameters, with the most critical ones summarised in Figure 2.5.

The mechanical properties and structural integrity of PBF-LB components are significantly influenced by fundamental process parameters, including laser power, scanning speed, hatch spacing, and layer thickness. These parameters collectively determine the Volumetric Energy Density (VED), which is expressed as:

$$E_V = \frac{P}{v \cdot h \cdot t} \quad , \quad (2.1)$$

where P is the laser power, v is the scan speed, h is the hatch spacing, and t is the layer thickness.

Proper optimisation of these parameters is essential to ensure full powder fusion while minimising porosity and residual stresses, ultimately leading to high-quality printed components.

2.1.4.3 Recent developments and future trends

Recent advancements in PBF-LB include the introduction of multi-laser systems for improved productivity, in-situ monitoring for defect detection, and hybrid manufacturing approaches that integrate AM with conventional machining. The continued development of novel alloys tailored for AM and the integration of artificial intelligence for real-time process control are expected to further enhance its capabilities.

The increasing industrial adoption of PBF-LB is evident across multiple sectors, particularly in aerospace, medical, and automotive applications. Research into novel process strategies and material formulations is actively addressing the existing limitations, reinforcing PBF-LB's role as a transformative manufacturing technology [37].

2.2 Numerical modelling of PBF-LB

2.2.1 Introduction

Numerical simulations play an essential role in understanding and optimising the PBF-LB process, which is characterised by rapid melting and solidification, evolving free surfaces, potential evaporation, and large thermal gradients [12]. The inherent multi-physics nature of PBF-LB arises from a wide range of simultaneous phenomena occurring over extremely short time scales. Figure 2.6 illustrates some of these intricate physical interactions, including heat absorption, recoil pressure, surface tension, melting and solidification, multiphase gas flow, evaporation, laser-material interaction, and melt pool dynamics. This multi-physics complexity spans multiple scales: micro-scale (grain nucleation and phase transformations), meso-scale (powder-layer details and melt-pool flow), and macro-scale (part-scale temperature evolution, distortion, and residual stresses) [14].

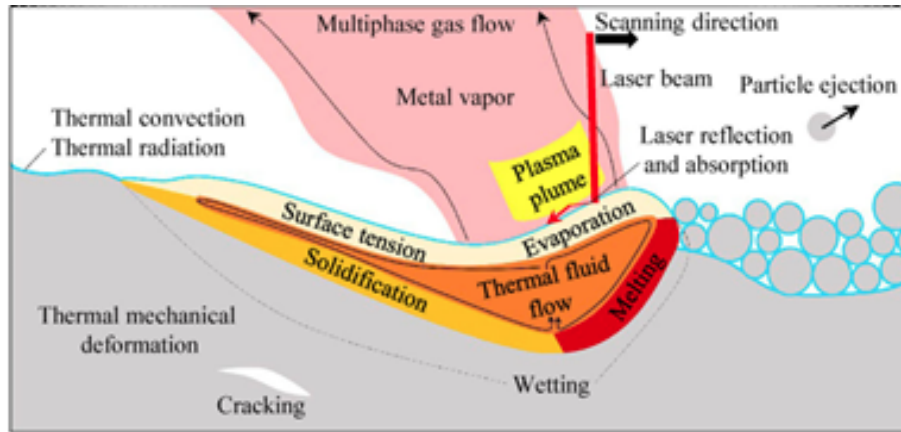


Figure 2.6: Key physical phenomena involved in PBF-LB: from the laser–powder interaction and potential vapour plume to melt-pool wetting and thermal convection, all contributing to microstructure evolution and part-scale deformations. Adapted from [1].

In PBF processes, the large ratio of melt-pool size to part dimensions, combined with high deposition speeds, leads to the simultaneous occurrence of these phenomena at widely differing length and time scales. Consequently, various modelling approaches have been developed to capture the essential physics at each level. Figure 2.7 (top) illustrates a high-level concept of how information can flow across scales: effective material properties or boundary conditions can be transferred from smaller-scale simulations (e.g., melt pool or microstructure) to larger-scale ones (e.g., part-level thermo-mechanics), and vice versa. Figure 2.7 (bottom) presents the conventional three-scale framework [58]:

- **Micro-scale:** Grain-level phase-field or cellular automaton models for studying solidification pathways, grain orientations, and phase fractions.

- **Meso-scale:** Single- or multi-track simulations, often including discrete powder particles and fluid-flow solvers for the melt pool, capturing porosity formation, track bonding, and local thermal behaviour.
- **Macro-scale:** Continuum-based models with homogenised powder layers, focusing on global temperature evolution, residual stresses, and part-scale distortion.

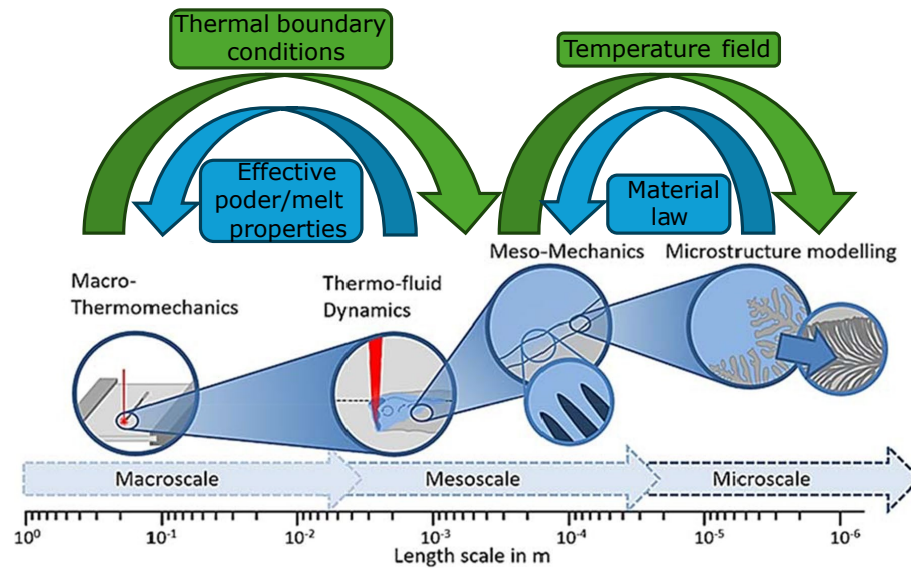


Figure 2.7: Coupling of macro-, meso-, and micro-scale models [52, 58].

The selection of modelling scale is dictated by both specific research objectives and computational resource constraints. At present, it is unfeasible to simulate every relevant physical phenomenon at the part scale. For instance, accurately predicting phenomena such as keyhole porosity or local bonding defects requires a meso-scale approach that resolves the detailed dynamics of the melt-pool free surface and the associated heat transfer [14]. In contrast, assessing residual stresses and distortions over an entire component typically relies on macro-scale models, in which the powder bed is treated as a homogenised continuum and the melt pool is represented by effective parameters to reduce computational cost. Consequently, hybrid or multi-scale strategies are often employed, where meso-scale simulations provide effective properties or strain fields that are integrated into macro-scale frameworks, and vice versa.

Despite their differing scopes, these multi-scale models share a common foundation in the underlying physical equations governing energy, mass, and momentum conservation, which are complemented by material constitutive laws.

Figure 2.8 further illustrates how different modelling strategies align with physics-based formulations at meso- and macro-scales. The left section of the diagram highlights the primary physical domains governing PBF and DED processes, including heat transfer, fluid dynamics, solid mechanics, and metallurgy. As observed, heat transfer is fundamental in all process modelling since it governs other physical phenomena. The right section shows the corresponding modelling approaches used at meso- and macro-scales, along with key outputs at each level. While meso-scale

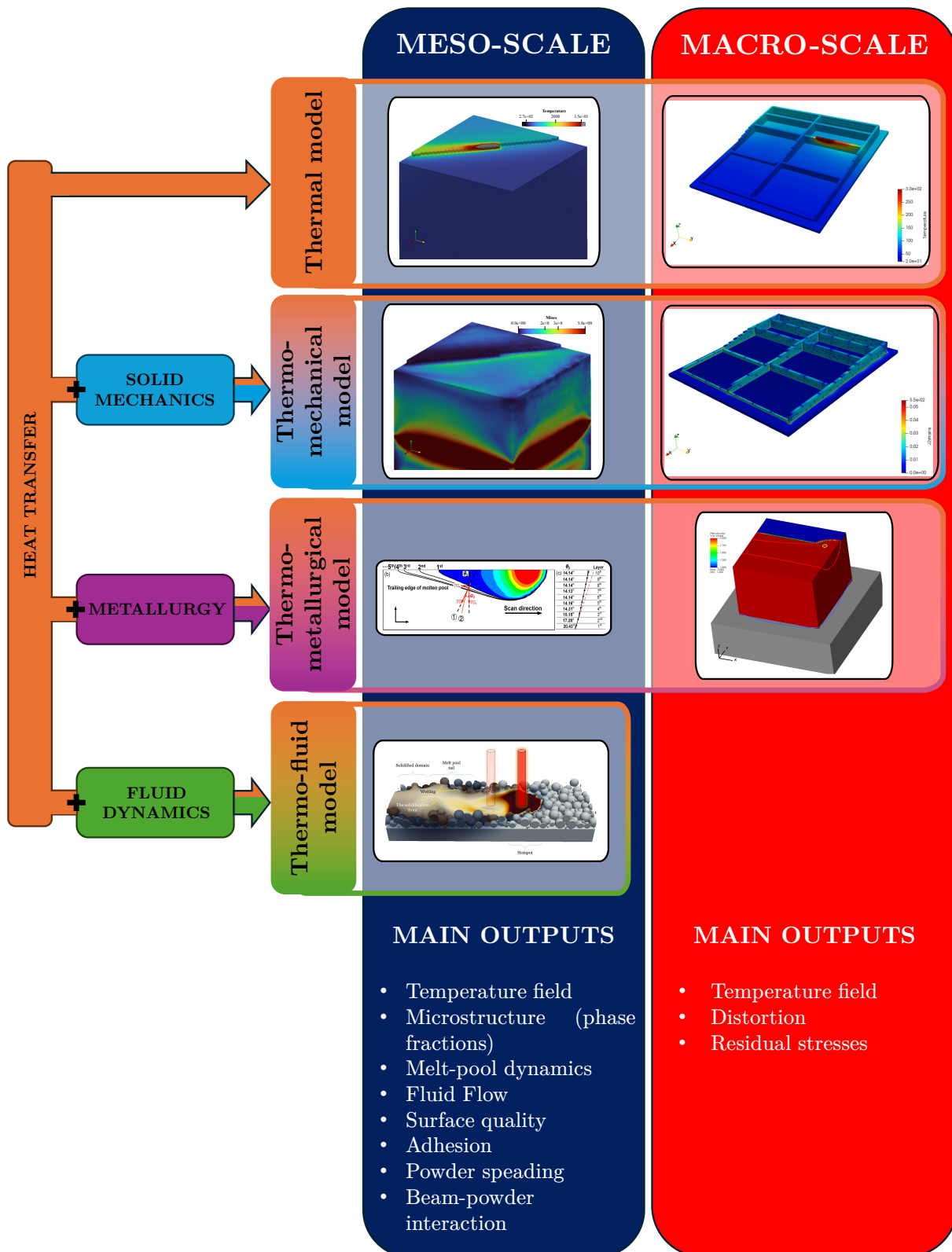


Figure 2.8: Overview of PBF-LB modelling strategies at meso- and macro-scales. The left side categorises physical fields that influence PBF-LB, while the right side illustrates modelling strategies and their respective key outputs.

models can capture detailed local features such as melt-pool dynamics, porosity, and powder spreading, macro-scale models focus on larger-scale predictions such as residual stresses and distortions.

To obtain numerical solutions, these physics-based models require discretisation techniques. Several numerical approaches have been employed in the literature. Table 2.2 summarises how these numerical techniques have been applied to PBF models. Additionally, Figure 2.9 illustrates the application of these techniques at various scales and modelling methodologies.

Table 2.2: Summary of numerical modelling techniques and their applications in PBF. Adapted from [70].

Numerical technique	Applications
Finite Element Method (FEM)	Heat transfer and mechanical characterization
Finite Volume Method (FVM)	Heat transfer and melt-pool dynamics
Lattice Boltzmann Method (LBM)	Heat transfer and melt-pool dynamics
Ray Tracing	Beam absorption and ray tracing
Discrete Element Method (DEM)	Powder bed preparation and heat transfer

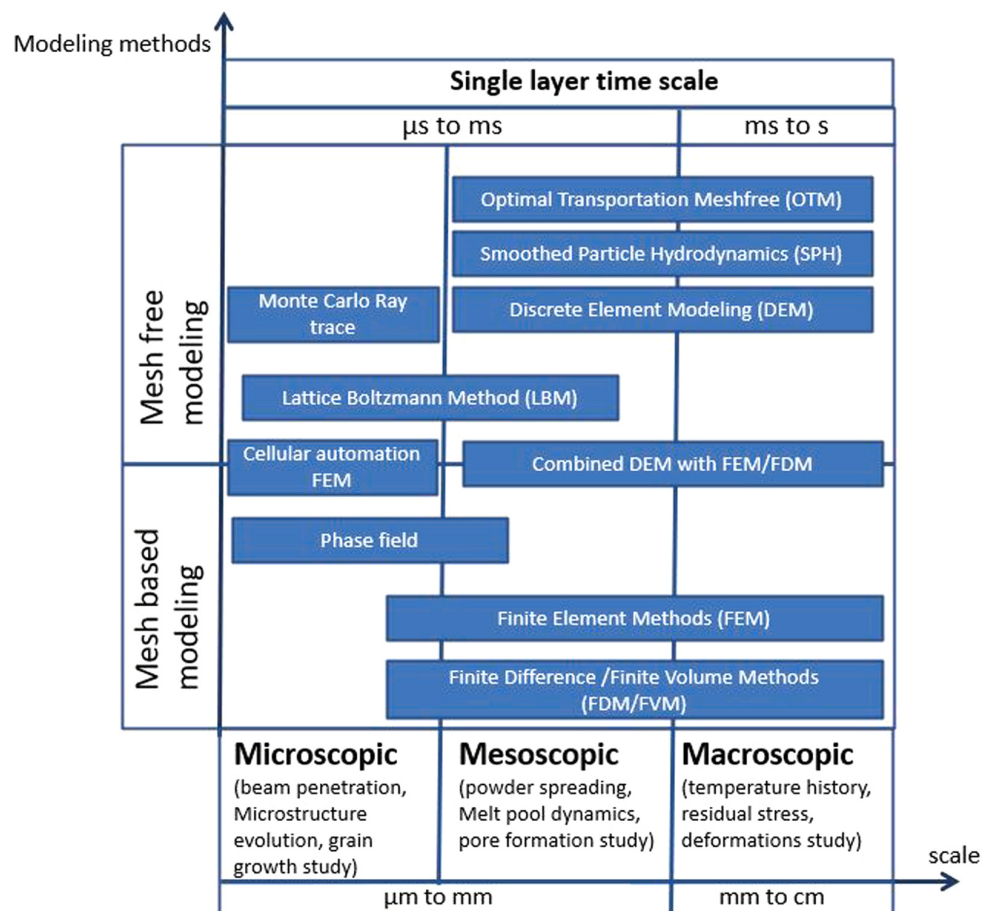


Figure 2.9: Classification of numerical simulation techniques applied to PBF across different scales and modelling methodologies [70].

By integrating different modelling strategies, numerical simulations improve process understanding, optimise scanning strategies, and mitigate defects in [PBF-LB](#). The following sections will explore the methodologies employed at these different scales, detailing their respective capabilities, limitations, and ongoing developments.

2.2.2 *Micro-scale modelling approaches*

Micro-scale models in [PBF-LB](#) provide fundamental insights into the metallurgical phenomena that occur during rapid melting and solidification. They capture processes such as grain nucleation, dendritic growth, and phase transformations that directly influence the microstructure (and hence the mechanical properties, anisotropy, and defect formation) of additively manufactured components [14]. Unlike meso- and macro-scale models, micro-scale approaches focus on local interactions at the grain level, investigating the evolution of grain boundaries, phase interfaces, and sub-melt pool phenomena to provide a detailed understanding of the local solidification process.

2.2.2.1 *Scope and relevance*

The extreme thermal cycling and steep temperature gradients characteristic of [PBF-LB](#) lead to non-equilibrium solidification conditions. As a consequence, the resulting microstructure (whether columnar or equiaxed, dendritic or globular) differs significantly from that produced by conventional processing techniques. These microstructural features have a significant impact on the final mechanical performance. However, due to computational limitations, micro-scale simulations are typically applied to small representative domains. The necessary local thermal history, which drives these phenomena, is usually supplied by higher-level simulations or in-situ measurements.

2.2.2.2 *Computational approaches*

A variety of numerical strategies have been developed to model micro-scale phenomena in [PBF-LB](#). Among the most widely used approaches are:

PHASE-FIELD MODELLING. The Phase-Field (PF) method is a powerful continuum-based approach that represents the interface between solid and liquid phases using a continuous order parameter. This method solves coupled thermodynamic and kinetic equations to simulate the evolution of complex microstructures, including dendritic growth and the transition between columnar and equiaxed grain morphologies. It provides a continuous and detailed description of interfacial dynamics and dendritic growth. However, the method requires fine spatial discretisation and is computationally demanding. [Figure 2.10](#) illustrates a phase-field simulation, where the interplay between interfacial energies and thermal gradients governs dendritic growth.

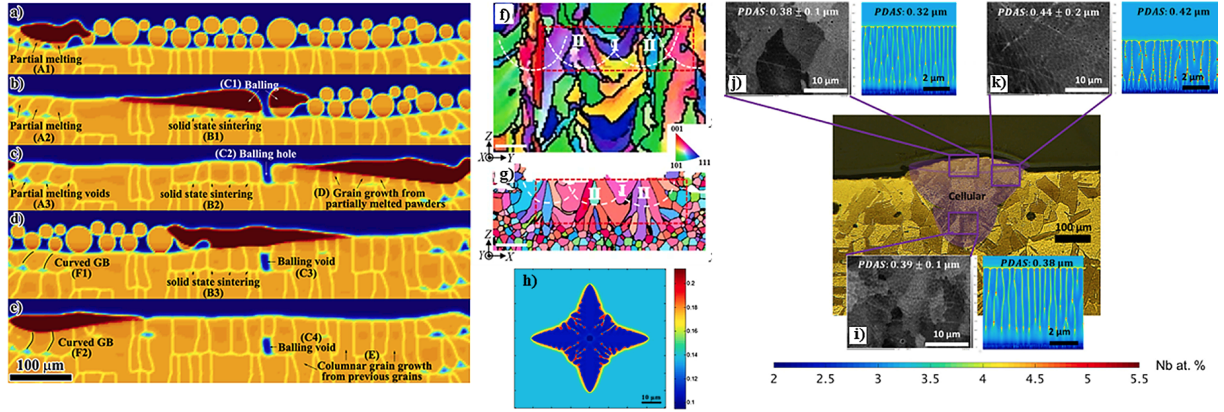


Figure 2.10: PF simulation of solidification in PBF-LB, capturing dendritic growth and the transition from columnar to equiaxed grains under high thermal gradients. Adapted from Figure 44 in [14].

CELLULAR AUTOMATA. Cellular Automata (CA) models discretise the simulation domain into a grid of cells, each representing a local crystallographic state or phase. Transformation rules, often derived from empirical data, dictate the evolution of these cells, enabling the simulation of grain nucleation, growth, and impingement. Due to their computational efficiency, CA models are well-suited for simulating large domains. However, the heuristic nature of the rules may oversimplify complex interfacial phenomena. Figure 2.11 illustrates a CA simulation that reproduces the evolution of grain structures under a prescribed thermal history.

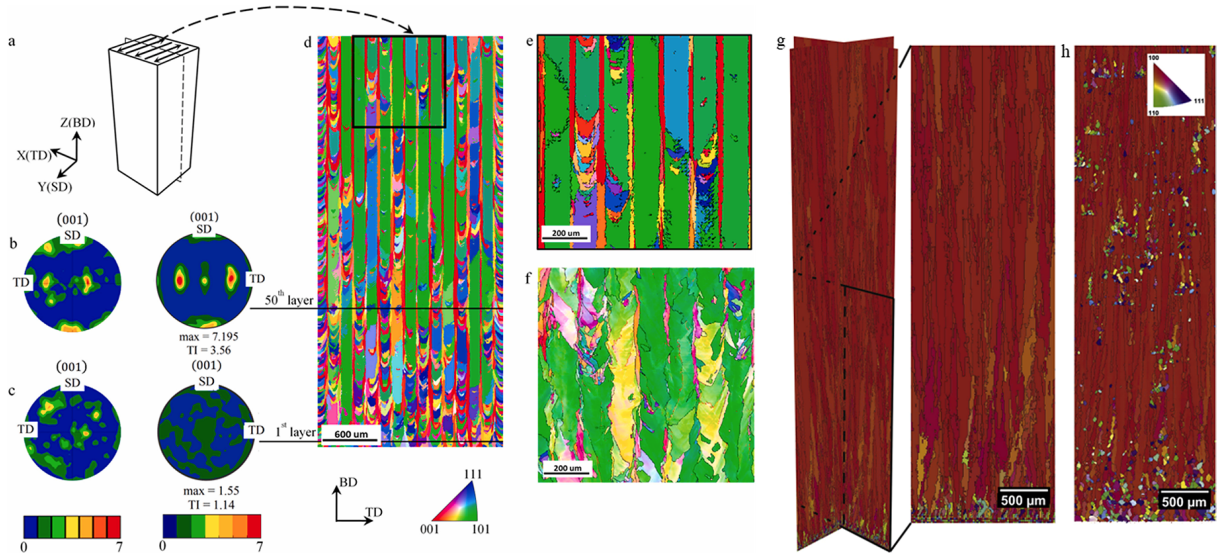


Figure 2.11: CA simulation of grain evolution in PBF-LB. The image shows how local transformation rules, driven by temperature history, result in the nucleation and growth of grains. Adapted from Figure 36 in [14].

KINETIC MONTE CARLO METHODS. Monte Carlo (MC) methods employ stochastic algorithms to simulate microstructural evolution through random sampling of grain boundary migration and coarsening events. These techniques are particularly useful

for predicting the statistical distribution of grain sizes and for exploring the influence of thermal fluctuations. However, they are generally computationally expensive for large systems and exhibit limited temporal resolution. Figure 2.12 shows an example of a Monte Carlo simulation that captures the evolution of grain boundaries through energy minimisation.

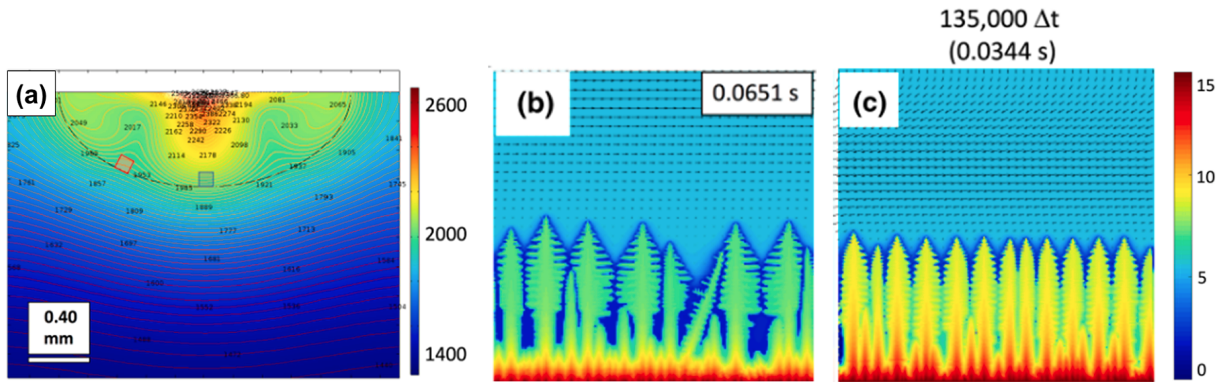


Figure 2.12: MC simulation of grain boundary evolution in PBF-LB, where stochastic rules based on local energy minimisation drive grain coarsening and migration. Adapted from Figure 41 in [14].

2.2.2.3 Coupling with meso- and macro-scale models

Although micro-scale models typically cover only small representative volumes due to computational limitations, their outputs are critical inputs for multi-scale frameworks. For example, grain orientation distributions, phase fractions, and local defect statistics derived from PF, CA, or MC simulations can be used to inform the anisotropic constitutive laws or effective properties in meso- and macro-scale thermo-mechanical models. In many cases, temperature histories obtained from part-scale finite element thermal simulations serve as boundary conditions for micro-scale models, thereby enabling realistic prediction of solidification pathways under industrial processing conditions [14].

2.2.2.4 Challenges and future perspectives

Despite significant advancements, several challenges remain in micro-scale modelling of PBF-LB. The high computational cost limits the domain sizes that can be realistically simulated, restricting their applicability to full-scale components. Furthermore, model calibration often relies on empirical parameters, leading to uncertainties in predictive accuracy. Another major challenge is experimental validation, as in-situ measurements of microstructural evolution during PBF-LB remain difficult to obtain.

Future research efforts are focused on improving scale-bridging methodologies, enhancing computational efficiency, and developing in-situ validation techniques. Integrating micro-scale predictions with in-process monitoring data and advanced experimental characterisation techniques, such as synchrotron-based X-ray diffraction, will be essential in further refining these models and increasing their industrial relevance.

2.2.3 Thermo-mechanical modelling for PBF-LB

Thermo-mechanical modelling plays a pivotal role in the numerical simulation of PBF-LB, as it enables the prediction of temperature distributions, residual stresses, and part distortions, key factors in assessing the mechanical integrity of printed components. Purely thermal models provide insights into heat transfer and phase transformations, whereas mechanical models capture the material's stress response. Consequently, these models aim to predict thermal histories, distortions, and residual stresses at both meso- (typically beyond the melt pool) and macro-scales.

The fundamentals of thermo-mechanical modelling for MAM build upon established principles from Computational Welding Mechanics (CWM) [38, 47, 75], since AM can be considered an extension of multi-pass welding. Both processes share similar heat source models and stress evolution mechanisms. However, compared to conventional welding, MAM introduces additional complexities such as prolonged processing times, repeated thermal cycling, and the cumulative effects of large material deposition [39].

Depending on the required accuracy and available computational resources, thermo-mechanical models may be implemented as either *weakly coupled* (where thermal analysis is performed first and then used to drive mechanical simulations) or *fully coupled* (where thermal and mechanical equations are solved simultaneously). In MAM simulations, a weakly coupled approach is often adopted (see Figure 2.13), based on the assumption that the mechanical response does not significantly influence the thermal history [48].

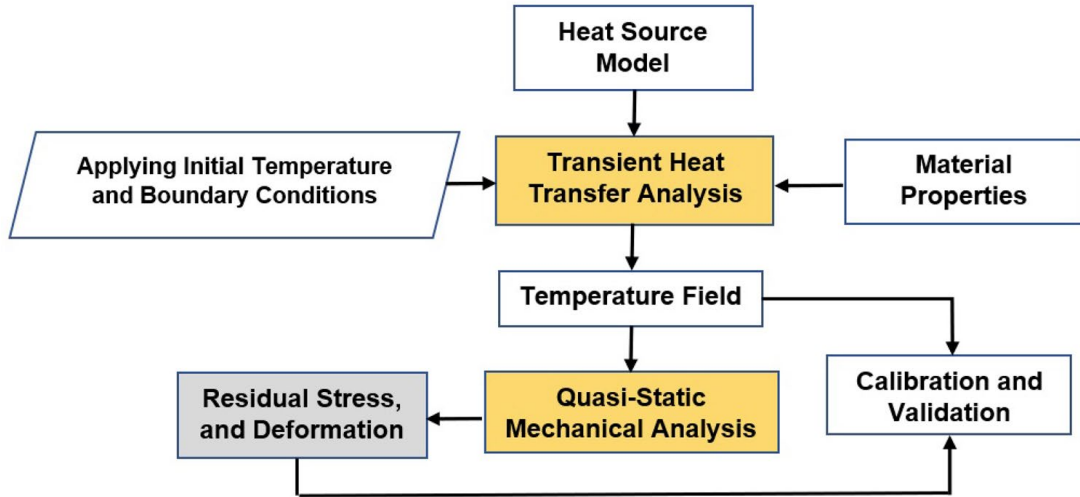


Figure 2.13: Flowchart of the weakly coupled thermo-mechanical model [54].

Significant contributions to the development of thermal and thermo-mechanical models for MAM are summarised in Table 2 and Table 6 in [12] and Table 1 in [10].

The following sections outline the fundamental governing equations, stress development mechanisms, and computational strategies employed in thermo-mechanical modelling of PBF-LB.

2.2.3.1 Thermal model

In the context of CWM, the thermal model is based on pure conduction model and the powder is assumed to be a continuum with averaged thermo-physical properties [52].

Temperature evolution is governed by an enthalpy-based heat equation, which implicitly accounts for latent heat effects due to melting and solidification. Table 2.3 summarises the basic heat conduction equation in enthalpy form, the inclusion of latent heat via $H(T)$, and common boundary and initial conditions used.

Table 2.3: Summary of thermal formulation (including phase change).

Equation/Condition	Mathematical formulation
Governing equation	$\dot{H} = \nabla \cdot (k \nabla T) + \dot{Q}(x, t)$
Enthalpy definition	$H(T) = \rho \int_{T_{\text{ref}}}^T c_p(T) dT + L f_{\text{liq}}(T)$
Dirichlet BC	$T(x, t) = T_0(x, t) \text{ on } \Gamma_D$
Neumann BC	$-k \nabla T \cdot \mathbf{n} = q(x, t) \text{ on } \Gamma_N$
Convective (Robin) BC	$-k \nabla T \cdot \mathbf{n} = h(T - T_\infty) \text{ on } \Gamma_C$
Radiative BC	$-k \nabla T \cdot \mathbf{n} = \epsilon \sigma [T^4 - T_\infty^4] \text{ on } \Gamma_R$
Initial condition	$T(x, 0) = T_{\text{init}}(x)$

In these equations, ρ denotes density, k is thermal conductivity, $T(x, t)$ represents temperature, and $\dot{Q}(x, t)$ is the volumetric heat source. The enthalpy $H(T)$ incorporates both sensible and latent heat, where c_p is the specific heat capacity, L is the latent heat of fusion, and $f_{\text{liq}}(T)$ describes the liquid fraction during phase transition. Additionally, ϵ denotes surface emissivity, σ is the Stefan–Boltzmann constant, and h is the convective heat transfer coefficient.

HEAT SOURCE MODELLING. In this class of models, laser–material interaction (the heat generation process) is simplified using a moving volumetric heat source, excluding all physics related to these phenomena [47].

A widely used heat input model is the *Gaussian volumetric heat source* due to its ability to approximate the laser beam profile effectively. This model assumes a three-dimensional Gaussian distribution of laser energy and has been widely adopted in finite element simulations of PBF-LB [12, 62].

Another well-known approach is the *Goldak double-ellipsoid heat source* model, originally developed for welding applications and later adapted for PBF-LB. Unlike the standard Gaussian approach, this model accounts for asymmetric heat distribution, with distinct front and rear ellipsoidal regions that better capture heat penetration effects [38, 47]. As a result, it is particularly useful for simulations that require higher fidelity in melt-pool depth predictions.

For macro-scale thermal analyses, the *uniform heat input model* [20] distributes laser power evenly within a defined heat-affected volume, prioritising computational efficiency over fine-scale melt pool resolution.

Additional volumetric heat input models are summarised in Table 3 of [12]. Some studies have also employed *Monte Carlo ray-tracing techniques* to estimate the laser absorption profile and integrate it into volumetric heat source models [70].

Each of these heat input models involves trade-offs between accuracy and computational cost. While Gaussian and Goldak-based sources remain widely used for detailed melt pool simulations, uniform heat input models are often preferred for computationally efficient part-scale analyses.

2.2.3.2 Mechanical model

Thermo-mechanical simulations use the temperature history from the thermal model as input to compute mechanical deformations caused by thermal expansion and contraction. Mechanical behaviour is typically modelled under quasi-static conditions with small-strain theory. Table 2.4 summarises the governing equations for mechanical equilibrium, strain decomposition, constitutive laws, and boundary conditions.

Table 2.4: Summary of the mechanical formulation.

Equation/condition	Mathematical formulation
Momentum balance (quasi-static)	$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0}.$
Small-strain kinematics	$\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T).$
Strain decomposition	$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \boldsymbol{\varepsilon}^p + \boldsymbol{\varepsilon}^{th} + \boldsymbol{\varepsilon}^{tr}.$
Constitutive law (general)	$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}^e.$
Boundary condition: Dirichlet	$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_0(\mathbf{x}, t) \quad \text{on } \Gamma_u.$
Boundary condition: Neumann	$\boldsymbol{\sigma} \cdot \mathbf{n} = \boldsymbol{\tau}_0(\mathbf{x}, t) \quad \text{on } \Gamma_t.$
Initial conditions	$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_{init}(\mathbf{x}), \quad \dot{\mathbf{u}}(\mathbf{x}, 0) = \mathbf{v}_{init}(\mathbf{x}).$

Here, $\mathbf{u}$ is the displacement field, $\boldsymbol{\sigma}$ is the Cauchy stress tensor, and $\mathbf{b}$ represents body forces such as gravity. The strain tensor $\boldsymbol{\varepsilon}$ is decomposed into elastic ($\boldsymbol{\varepsilon}^e$), plastic or viscoplastic ($\boldsymbol{\varepsilon}^p$), thermal ($\boldsymbol{\varepsilon}^{th}$), and transformation-induced ($\boldsymbol{\varepsilon}^{tr}$) components. The boundary $\partial\Omega$ is partitioned into Γ_u (where displacements are prescribed) and Γ_t (where tractions are specified).

MATERIAL CONSTITUTIVE MODELS. Various material models have been employed in the literature to describe the mechanical response of materials under the complex thermal and mechanical loading conditions of PBF-LB:

- *J2-elasto-plastic models:* Based on von Mises yield criteria, these models assume isotropic plasticity and are widely used for residual stress prediction [24, 29].
- *J2-thermo-elasto-visco-plastic models:* These models account for strain hardening, thermal shrinkage, and stress relaxation at elevated temperatures, making them suitable for high-fidelity simulations [19, 55]. At room temperature, the material exhibits an elasto-plastic response, while at temperatures above the melting

point, it behaves as a pure viscous material. Additionally, the constitutive law incorporates phase-change effects by computing the solid/liquid fraction.

- *Johnson-Cook model*: A widely used strain-rate and temperature-dependent plasticity model that captures the effects of high strain rates and thermal softening in [MAM](#) [39].

KEY FACTORS INFLUENCING MECHANICAL BEHAVIOUR. In addition to constitutive laws, several key factors influence the mechanical response:

- *Cut-off temperature*: A threshold temperature above which the material is assumed to be in a softened or liquid state, preventing the computation of mechanical stresses [47].
- *Relaxation temperature*: The temperature at which stress relaxation becomes significant due to creep-like effects, which affects the evolution of residual stresses over time [27].
- *Temperature-dependent material properties*: Mechanical properties such as yield strength, elastic modulus, and thermal expansion coefficient evolve with temperature and must be accurately modelled [14].
- *Phase transformation effects*: Some metals undergo martensitic transformation during rapid cooling, significantly affecting the development of residual stresses [12].

CONSIDERATIONS FOR Ti-6Al-4V. Ti-6Al-4V is one of the most widely studied materials in [PBF-LB](#), requiring special considerations in mechanical modelling:

- *Phase transformation modelling*: Some models incorporate transformation-induced strains, while others assume a purely elasto-plastic response, neglecting phase transformation effects [18, 61].
- *Anisotropic mechanical properties*: Columnar β -grains aligned along the build direction introduce mechanical anisotropy, requiring advanced material models [39].
- *Strain-rate sensitivity*: Due to the rapid thermal cycling in [PBF-LB](#), the mechanical response of Ti-6Al-4V is highly strain-rate dependent [7].
- *Relaxation or annealing*: To avoid overestimating distortion and residual stress, stress relaxation effects should be incorporated into simulations [27].

RESIDUAL STRESS AND DISTORTION EVOLUTION. Residual stresses in [PBF-LB](#) arise due to rapid thermal cycling and constrained thermal expansion. Key findings from existing studies include:

- *Higher scanning speeds* reduce residual stresses by minimising heat accumulation [62].
- *Phase transformations* significantly may alter stress distributions [14].
- *Scanning patterns* affect stress magnitudes, with out-in patterns producing higher stresses compared to alternating scan paths [12].

COMPUTATIONAL CONSIDERATIONS. Although thermo-mechanical modelling provides critical insights into stress evolution and deformation mechanisms, the high computational cost of detailed simulations typically limits their application to small domains, such as track-level or layer-level analyses. Full-scale part simulations using detailed thermo-mechanical models remain impractical due to the computational resources required. Consequently, multi-scale approaches, such as the [ISM](#) and [AMR](#) techniques, are commonly employed for part-scale predictions. In this context, high-fidelity thermo-mechanical models primarily serve as calibration tools to inform and validate more computationally efficient strategies.

2.2.4 Thermo-metallurgical modelling

Thermo-metallurgical models aim to predict phase transformations, microstructural evolution (phase fractions, grain morphology), and material property variations based on the thermal history obtained from the thermal model. Using this thermal data, the solidification cooling rate and temperature gradient are first computed. Unlike other coupled models, thermo-metallurgical models do not solve additional field equations; instead, they rely on empirical or phenomenological relationships to determine phase fractions, grain growth, and metallurgical transformations [47].

Metallurgical models typically use temperature-dependent transformation kinetics, such as the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation for diffusion-controlled transformations or the Koistinen-Marburger equation for diffusionless martensitic transformation.

[Figure 2.14](#) illustrates a common output of thermo-metallurgical models, where the temperature field from the thermal simulation is used to compute grain morphology evolution.

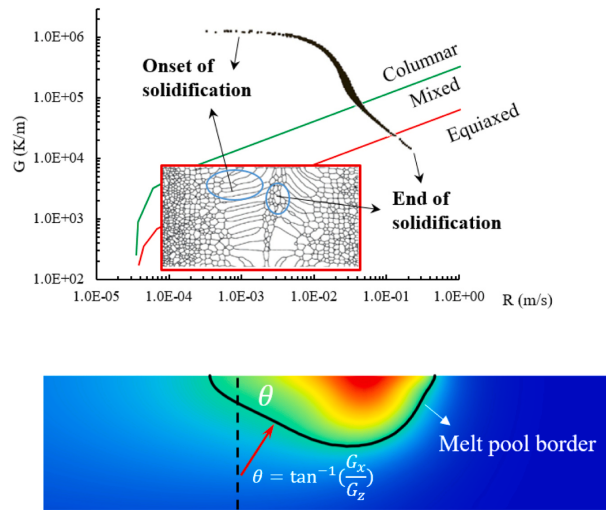


Figure 2.14: Calculated grain morphology for Ti-6Al-4V [76].

One of the most studied aspects in [PBF-LB](#) is the solid-state phase transformation in materials such as Ti-6Al-4V, where rapid cooling rates induce a martensitic $\beta \rightarrow \alpha'$ transformation [76].

Despite advancements in thermo-metallurgical modelling, challenges remain in accurately predicting microstructure heterogeneity, grain morphology, and phase transformations under cyclic heating and cooling conditions.

2.2.5 Thermo-fluid (multi-physics) modelling

Many macro-scale PBF-LB simulations assume that the melt pool can be approximated by conduction-only models. However, it is well established that fluid flow within the melt pool significantly influences local thermal transport, melt pool geometry, and defect formation mechanisms such as keyholing, spatter generation, and lack of fusion [14, 52].

Thermo-fluid (or multi-physics) models explicitly capture molten metal flow by coupling momentum conservation (Navier–Stokes equations) with heat conduction and surface thermodynamics. While these approaches enhance local accuracy, they are computationally expensive and are therefore typically applied to meso-scale domains, such as single-track or multi-track studies [12].

GOVERNING EQUATIONS. Thermo-fluid models for PBF-LB simultaneously solve the following fundamental equations:

- *Mass conservation:* Ensures the incompressibility of molten metal flow:

$$\nabla \cdot \mathbf{v} = 0 \quad . \quad (2.2)$$

- *Momentum conservation (Navier–Stokes equation):*

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p + \mu \nabla^2 \mathbf{v} + \mathbf{F}_{\text{surface}} + \mathbf{F}_{\text{other}} \quad , \quad (2.3)$$

where ρ is the density, $\mathbf{v}$ is the velocity field, p is the pressure, and μ is the dynamic viscosity. The term $\mathbf{F}_{\text{surface}}$ accounts for interfacial forces such as surface tension (γ), Marangoni stresses ($\partial\gamma/\partial T$), recoil pressure, and buoyancy effects [12, 14].

- *Energy conservation:*

$$\dot{H} + \rho c_p \mathbf{v} \cdot \nabla T = \nabla \cdot (k \nabla T) + \dot{Q}_{\text{laser}} \quad , \quad (2.4)$$

which includes convective heat transfer ($\mathbf{v} \cdot \nabla T$) and heat sources such as laser energy input ($\dot{Q}_{\text{laser}}$). The enthalpy $H(T)$ incorporates both sensible and latent heat as in Table 2.3.

FREE SURFACE TRACKING. Tracking the free surface of the melt pool is performed using Volume of Fluid (VoF), level-set, or marker-and-cell approaches. These handle the topological changes as powder particles melt, coalesce, and eventually resolidify [14].

Appropriate boundary conditions must also be defined to capture laser absorption at the liquid-gas or solid-gas interface, often incorporating local angle-dependent

absorption models. Convective and radiative heat losses at the free surface further influence melt pool dynamics [52].

By explicitly modelling molten metal flow, these thermo-fluid simulations capture phenomena difficult to represent in purely conduction-based approaches, such as Marangoni effects, recoil pressure, keyhole formation, and spatter and ejections.

NUMERICAL APPROACHES. Thermo-fluid **PBF-LB** models are typically implemented using one of the following numerical approaches:

- *Finite Volume Method (FVM)*: Commonly used in computational fluid dynamics (CFD) software such as FLUENT, OPENFOAM, and FLOW-3D for solving free-surface flow problems using VoF or level-set methods [12].
- *Lattice Boltzmann Method (LBM)*: Efficient for handling complex free surfaces and suitable for high-performance parallel computing [70].
- *Meshless Methods*: Smoothed Particle Hydrodynamics (SPH) and related particle-based methods are highly effective for capturing free-surface physics and large deformations [52].

CHALLENGES AND FUTURE PERSPECTIVES. Thermo-fluid simulations are highly computationally demanding, limiting their application to small local domains (single track or a few tracks). Extremely refined meshes and small time steps are required, preventing layer- or part-scale simulations. Further difficulties include accurate calibrations of surface tension, recoil pressure, beam absorption, and powder packing characteristics. Relying heavily on large High-Performance Computing (HPC) resources, future advances will likely integrate local, high-fidelity melt-pool predictions into multi-scale frameworks for part-scale simulation [12].

2.2.6 Material deposition modelling: element activation strategies

Accurate modelling of the layer-by-layer material deposition process is essential in **PBF-LB** simulations for predicting thermal histories, stress evolution, and part distortions. Since the computational domain evolves as new material is added, element activation strategies are employed to ensure that only the material corresponding to the deposited layers contributes to the finite element equations at any given time.

Historically, activation strategies have been adapted from **CWM** methods (originally developed for multi-pass welding) to simulate the progressive deposition of filler material [47]. In **PBF-LB**, these strategies enable the gradual inclusion of new elements in the model as the build process advances.

Two main approaches have been widely adopted for element activation in **PBF** simulations: the quiet element method and the element birth-death method (see Figure 2.15).

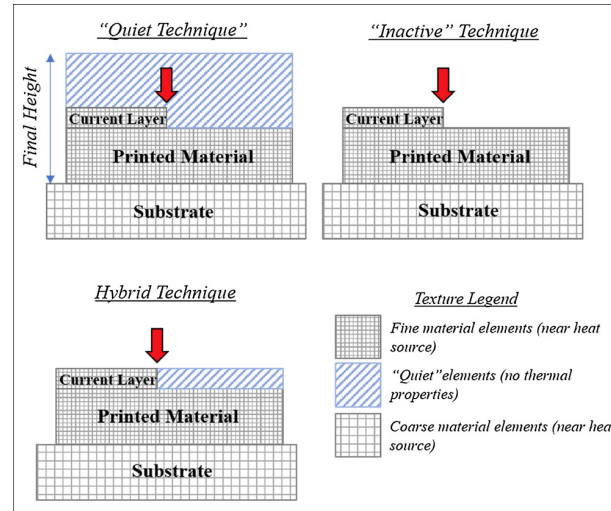


Figure 2.15: Element activation strategies: Quiet element method and element birth-death method (inactive element method) [39].

2.2.6.1 Quiet element method

In this approach, the entire part geometry is meshed at the beginning of the simulation. However, elements corresponding to not-yet-deposited material are assigned artificially modified material properties to minimise their influence on the solution. In thermal analyses, the thermal conductivity and specific heat capacity of these quiet elements are significantly reduced, ensuring negligible heat transfer through inactive regions [47]. In mechanical simulations, Young's modulus is typically downscaled.

The primary advantage of this method is that it maintains a constant system of equations throughout the simulation, eliminating the need for frequent global matrix reassembly. However, improper calibration of the scaling factors used to suppress quiet elements can lead to numerical errors, including ill-conditioning or unintended heat conduction through inactive regions [53].

2.2.6.2 Element birth-death method

In contrast, the element birth-death method initially excludes inactive elements from the finite element system, activating them explicitly as the deposition process progresses [49]. At the beginning of the simulation, all elements are deactivated, and they are progressively activated to simulate material addition.

This method ensures that only active elements contribute to the computations, making it more memory-efficient. However, it requires reassembling the stiffness matrix at each activation step, introducing additional computational overhead.

2.2.6.3 Hybrid approach

A hybrid approach that combines these two methods has been explored in the literature. For example, Denlinger et al. [28] proposed treating newly activated elements initially as quiet elements (minimising their impact on the system) before

fully integrating them into the active domain once thermal equilibrium is reached. This strategy enhances numerical stability while preserving computational efficiency.

2.2.6.4 Comparison of methods

Both activation strategies have been successfully applied in the thermo-mechanical modelling of PBF-LB. The choice between methods depends on the trade-offs between numerical efficiency and ease of implementation:

- The *quiet element method* is straightforward to implement in many commercial Finite Element (FE) codes but requires careful calibration of scaling factors.
- The *birth-death method* offers better numerical conditioning by excluding inactive elements until needed but incurs additional computational cost due to frequent matrix reassembly.
- *Hybrid approaches* combine the benefits of both strategies but require more complex implementation.

Additional factors to consider when modelling material deposition include:

- *Thermo-mechanical decoupling*: It is generally advisable to activate elements first in the thermal analysis, allowing them to reach appropriate temperatures before coupling with the mechanical simulation [47].
- *Element shape and deformation*: Ensuring that activated elements deform realistically without excessive distortion is critical, particularly in complex geometries.
- *Energy conservation*: Care must be taken to prevent artificial energy introduction when inactive and active elements share nodes [39].

2.2.7 Efficient simulation strategies and model order reduction

Despite advancements in numerical formulations and state-of-the-art computational resources, simulating the PBF-LB process remains highly computationally demanding. The high computational cost arises due to:

- *High spatial and temporal resolution* required to capture steep thermal gradients and rapid melt pool dynamics;
- *Large domain sizes*, often involving hundreds or thousands of layers;
- *Complex non-linearities* arising from phase changes, free-surface flows, and repeated thermal cycling.

To mitigate these computational challenges, various *efficiency strategies* and *model order reduction* techniques have been developed to reduce computational cost while retaining sufficient fidelity. These strategies include **inherent strain methods**, which bypass detailed thermo-mechanical transient models, **adaptive meshing** approaches, **flash-lumped** or **layer-equivalent** methods, and more recently, **Machine Learning (ML)-based** approaches. The most widely adopted techniques are discussed below.

2.2.7.1 Inherent Strain Method (ISM)

The distortions and residual stresses in [MAM](#), as well as in welding, primarily arise from inelastic strains. These strains are usually a combination of thermal strains, plastic strains, creep-like effects at high temperatures, and, in some materials, transformation strains due to phase changes. The [ISM](#) leverages the fact that these inelastic strains remain after cooling, thereby bypassing the need to perform a full thermo-mechanical transient analysis for each deposition pass or track.

ORIGINAL INHERENT STRAIN THEORY. The [ISM](#) was first introduced by Ueda et al. in the field of [CWM](#) during the 1970s and 1980s [75]. In welding applications, a small-scale reference problem (e.g., a bead-on-plate weld) is either simulated in detail or measured experimentally to extract the final inelastic strains that develop after cooling. These extracted strains, known as *inherent strains*, are then applied to a larger structure in a single-step elastic [FE](#) simulation, recovering the residual stresses and deformations without requiring a full transient analysis. Mathematically, the inherent strain tensor is defined as:

$$\epsilon^{\text{inherent}} = \epsilon^{\text{total}} - \epsilon^{\text{elastic}} \quad , \quad (2.5)$$

which is applied as an eigenstrain to the region of interest.

ADAPTATION TO PBF-LB. With the emergence of multi-layer metal [MAM](#), Keller et al. [44] adapted the [ISM](#) concept from welding under the assumption that all material points within a part experience a comparable thermo-mechanical history due to the highly localised and rapid nature of the process. Although [PBF-LB](#) involves many more passes and faster scanning speeds than typical welding operations, the fundamental principle remains unchanged: a high-fidelity local simulation or experimental measurements provide the final inherent strains, which are then applied at the part scale analysis (see [Figure 2.16](#)).

In practice, this method consists of a sequence of mechanical, linear-elastic simulation steps combined with a prescribed activation strategy, typically executed on a layer-by-layer basis. To further improve computational efficiency, multiple layers are often lumped and activated simultaneously, reducing both the number of simulation steps and the overall computational cost. This approach ultimately yields the final residual stress and distortion distributions.

REFINEMENTS TO THE ISM FOR PBF-LB. Recent studies have introduced several modified versions of the [ISM](#) to improve its accuracy in [PBF-LB](#), particularly in capturing rapid thermal cycling, layer reheating effects, and local geometry variations [17, 30, 31]. These refinements primarily focus on improving the derivation of inherent strains from local thermo-mechanical models:

- *Modified inherent strain method (MISM).* Liang et al. [46] introduced a variant of the inherent strain calculation that accounts for both *intermediate* compressive plastic strains (which occur at elevated temperatures when the material exhibits reduced yield strength) and a *steady-state* tensile stress that develops upon

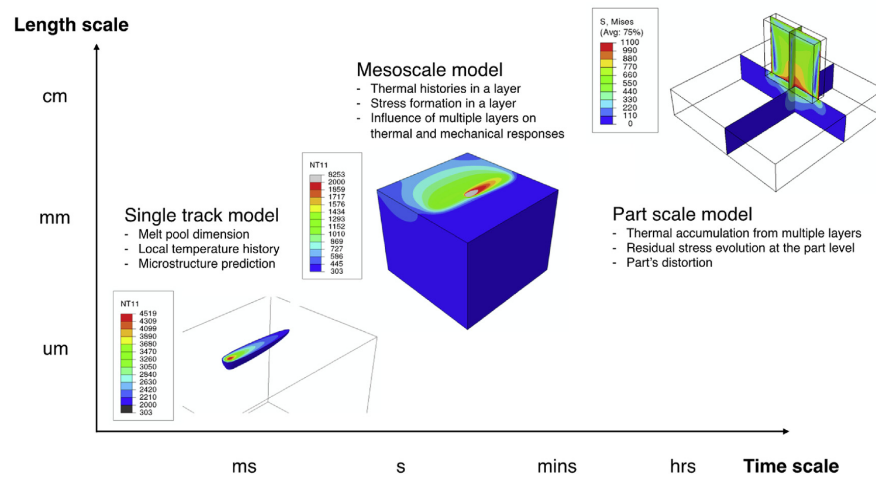


Figure 2.16: Multi-scale framework for estimating distortions and residual stresses [64].

cooling. *MISM* thus splits the total inherent strain into two components (e.g. “intermediate” and “steady” or “cooling-stage”) to better match the real residual stress distribution in the final part.

- *Improved MISM for residual stress.* A further extension of *MISM* addresses the tendency to overestimate residual stresses when assuming a constant elastic modulus at ambient temperature. By incorporating temperature-dependent material properties and high-temperature elastic moduli, this approach improves accuracy in final stress predictions.
- *Temperature-dependent MISM.* Another refinement allows the inherent strain distribution to vary with scanning speed or local thermal conditions, capturing the influence of process parameters on plastic strain accumulation. Dong et al. [30] proposed a *temperature-dependent* scheme in which multiple strain tensors are calibrated for different temperature regimes or process conditions. Although computationally more complex, this approach enhances predictive accuracy when scanning parameters vary significantly across a part.

ADVANTAGES AND LIMITATIONS. The *ISM* enables significant reductions in computational time, making it especially attractive for simulating large, complex builds that would otherwise be infeasible using fully transient thermo-mechanical analyses. However, its effectiveness depends on accurate calibration:

- The scanning parameters and process conditions must remain consistent to ensure that the local inelastic strain distribution is valid.
- Variations in geometry, boundary conditions, or machine settings may necessitate additional calibrations or an expanded inherent strain library.
- While *ISM* is effective for distortion predictions, its accuracy in capturing localised residual stresses is limited without further refinements.

Despite these limitations, the **ISM** has become one of the most widely used model reduction strategies for part-scale **PBF-LB** simulations. It demonstrates strong predictive capabilities for distortions and, to a reasonable extent, residual stresses, at a fraction of the computational cost of fully coupled simulations [54].

2.2.7.2 Adaptive mesh refinement (AMR)

AMR is a widely adopted strategy for managing large computational domains in **PBF-LB**. Rather than using a uniform fine mesh throughout the build volume, **AMR** refines the mesh dynamically in regions where high accuracy is needed (e.g. near the melt pool or in newly deposited layers) and maintains a coarser mesh elsewhere. This method captures steep gradients in temperature or stress more efficiently, lowering the total number of degrees of freedom and consequently reducing runtime [14, 55, 62].

Historically, adaptive refinement techniques were developed for **CWM**, where temperature and plastic strain fields evolve dynamically along the weld path [47, 75]. Early **MAM** simulations extended these concepts to multi-layer deposition, refining the mesh only around the laser-material interaction region [62]. Compared to globally fine-meshed models, this localised refinement significantly reduces computational complexity.

FUNDAMENTAL MECHANISMS OF AMR. **AMR** dynamically modifies the mesh resolution during simulation through two primary operations (see Figure 2.17 for an example):

- *Refinement*: Increasing local mesh density in regions with high temperature and stress gradients, such as the active melt pool or newly deposited layers.
- *Coarsening*: Reducing mesh density in already solidified or thermally stable regions where high resolution is no longer required.

By dynamically balancing refinement and coarsening, **AMR** maintains the required accuracy for local physics while minimising computational cost and memory usage [57, 62].

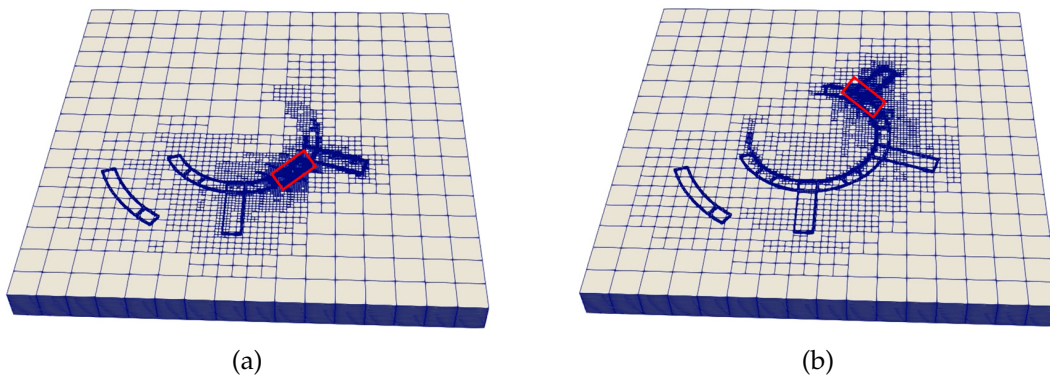


Figure 2.17: Illustration of **AMR** application using a multi-criteria approach. The evolution of the mesh is shown between (a) and (b) [55].

IMPLEMENTATION OF AMR IN PBF-LB SIMULATIONS. In a typical AMR scheme, mesh refinement and coarsening occur dynamically at each time step or deposition layer. The process consists of:

1. *Indicator-based refinement.* A local error *indicator* (e.g., temperature or stress gradient) is computed at each element or node. If the indicator exceeds a predefined threshold, that zone is marked for refinement; if it is well below a threshold, it is marked for coarsening. Common choices include Zienkiewicz–Zhu (ZZ) estimators for temperature or displacement, or simpler geometric criteria (e.g., proximity to the current melt region).
2. *Refinement operations.* These are typically implemented by splitting each element into 4 (in 2D) or 8 (in 3D) elements. Octree or quadtree data structures are particularly popular for PBF-LB part-scale analyses [55].
3. *Coarsening operations.* Once fine resolution is no longer necessary (e.g., far below the current build layer), elements are merged to reduce mesh density. This helps keep the total problem size manageable. To avoid "hysteresis", a minimum number of time steps or layers is often required before coarsening is allowed.
4. *Data transfer (projection).* After re-meshing, the solutions (temperature, displacement, internal variables, etc.) are projected from the old mesh to the new one. Specific *coarsening correction* strategies can preserve strain energy or equilibrium [57].

ADAPTIVE REFINEMENT CRITERIA. In PBF-LB simulations, as the laser moves in each layer, the high-temperature zone shifts with every time step or scanning pass. AMR can track this region by:

- *Geometry-based refinement:* Placing a bounding box (or oriented volume) around the instantaneous heat-input applied volume; elements intersecting it are refined, while elements further away are coarsened [62].
- *Solution-based refinement:* Computing gradients (temperature or stress) and refining regions where the indicator is large while coarsening where it is small. Although this method can be more accurate, it typically triggers more frequent mesh updates [55].

Many approaches combine both geometric and error-based criteria in a *multi-criteria* scheme (see Figure 2.17), yielding robust solutions with minimised computational overhead [12].

CHALLENGES. Although AMR significantly reduces the overall system size, each adaptation cycle involves data transfer, partial system reassembly, and potential complications at the interfaces between refined and coarsened regions. Techniques have been proposed to correct stress fields near these refinement boundaries [55]. Moreover, careful scheduling of adaptation steps (e.g., after every layer) can help limit computational overhead [28].

AMR is often combined with other model reduction strategies, such as *inherent strain methods* (Section 2.2.7.1) or *flash heating approaches* (Section 2.2.7.3), to further enhance computational efficiency.

CONCLUSION. AMR remains one of the most effective approaches for bridging the gap between small-scale phenomena (such as melt pool dynamics) and large part-scale analysis in PBF-LB. Improved error indicators, mesh data structures, and parallel algorithms for HPC environments continue to expand its feasibility for large or complex builds [14]. However, challenges remain, including robust solution transfer, repeated load balancing, and the extension of AMR-based approaches to more complex multi-physics simulations that incorporate fluid flow and free-surface tracking.

2.2.7.3 Flash or lumped heating approaches

An alternative strategy to detailed thermo-mechanical modelling in PBF-LB simulations is the use of flash or lumped heating approaches [10, 14, 60]. Instead of explicitly simulating the movement of the heat source along individual tracks with fine time steps, these methods approximate heat deposition on a larger scale (e.g., at the layer, hatch, or meta-layer) [22], thereby significantly reducing computational cost. By aggregating the thermal response over a macro-volume, flash heating models capture the overall bulk thermal history, neglecting the finer details of the scanning process.

CONCEPT AND IMPLEMENTATION. Flash or lumped heating approaches simplify thermal modelling by applying the required energy uniformly over a defined macro-volume rather than resolving individual scan paths. The procedure typically involves:

1. *Definition of a macro-volume unit:* A characteristic deposition volume is identified, such as a hatch, a full layer, or a group of layers (meta-layer).
2. *Energy calculation:* The total energy input from the heat source is computed for the selected macro-volume.
3. *Uniform energy application:* The computed energy is applied uniformly over the macro-volume during a specified heating period (ON-time).
4. *Cooling or dwell phase:* If necessary, a cooling period is introduced to allow for heat diffusion, mimicking the thermal history of actual laser scanning.

FLASH HEATING VARIANTS. Different flash heating strategies exist to control energy application (see Figure 2.18):

- *Basic flash heating:* A single, short-duration heat pulse is applied to rapidly raise the temperature within the macro-volume.
- *Multi-shot heating:* Energy is delivered in discrete pulses rather than a single application, reducing thermal discontinuities.
- *Gradual heating:* Energy is applied progressively over time, creating a more gradual and continuous temperature rise.

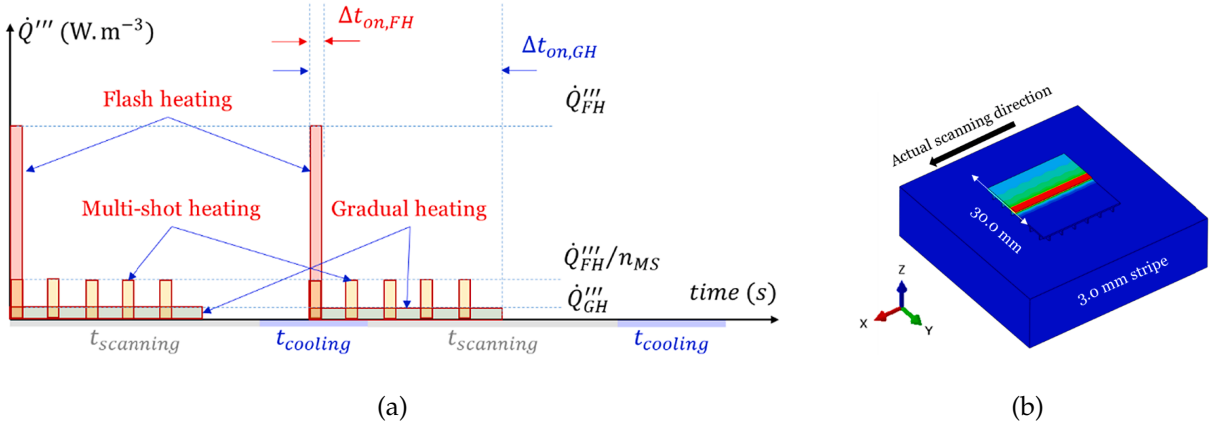


Figure 2.18: Illustration of flash heating and its variants (adapted from Fig. 66(a) and (b) in [14]). These methods condense multiple scanning passes per layer into a single or a minimal number of heating steps.

By consolidating multiple scanning passes into a single conduction event, these approaches eliminate the need for high temporal resolution at the track level. This trade-off between simulation detail and computational efficiency allows for significant speed-ups, although this comes at the expense of lowered precision in detecting local thermal gradients.

APPLICATION TO THERMAL AND MECHANICAL SIMULATIONS. Flash heating approaches are primarily employed in thermal simulations to predict bulk temperature evolution and overall heat accumulation in part-scale domains, where detailed melt pool dynamics are not the primary concern [12]. In thermo-mechanical simulations, these methods have been used for residual stress predictions. However, due to the simplified temperature gradients, these methods tend to underestimate localized strain accumulation and residual stress magnitudes, particularly in regions with steep thermal gradients.

ADVANTAGES AND LIMITATIONS. Flash heating approaches offer significant computational speed-ups by reducing the number of time steps per layer and lowering the overall computational burden. This enables simulations of large parts that would otherwise be infeasible with fully track-resolved models. Nevertheless, the reduced level of detail may compromise the accuracy of local melt pool phenomena predictions, and the smoothing of temperature gradients can lead to an underestimation of localised strains and residual stresses.

In summary, flash heating methods provide a practical compromise between computational efficiency and predictive accuracy, making them attractive for large-scale PBF-LB simulations where the global thermal behaviour is of primary interest.

2.2.7.4 Machine learning-based approaches

A more recent direction in PBF-LB simulation seeks to bypass (at least partially) the heavy computational burden of standard physics-based models through ML or *data-driven* techniques [14]. Instead of fully solving the governing equations at every time step or for every parameter set, an ML model (trained on offline high-fidelity simulations or on experimentally measured data) aims to predict certain fields (e.g. temperature, distortion) in real-time or with minimal additional computation.

In practice, researchers create a sufficiently large *training dataset* by running a range of parametrised physics-based simulations (or by gathering in situ sensor data from the PBF-LB machine). The ML method then *learns* the mapping from input parameters (laser power, scan speed, geometry, etc.) to outputs of interest (peak temperature, residual stress, final distortion). Models range from simple regression (polynomial fits) to more advanced methods such as neural networks or Gaussian process regressions, each with varying complexity and interpretability.

Some works adopt *Reduced Order Modelling* (ROM) in conjunction with ML, projecting the full Partial Differential Equation (PDE) system onto a small set of basis functions (e.g. via Proper Orthogonal Decomposition), and then using a trained neural network to approximate the evolution of these basis coefficients. This approach retains some physical consistency while yielding predictions that are orders of magnitude faster than a full finite element model.

Although ML-based approaches can be extremely fast once trained, their reliability depends heavily on the quality and diversity of the training data. Extrapolation beyond the training range (for instance, printing a material or geometry not represented in the data) can produce poor or unphysical predictions. Another challenge is capturing local phenomena such as keyholing or partial re-melting, which require sufficiently fine resolution in both the training simulations and the ML model. Nevertheless, for parameter sweeps, design optimization, or real-time process monitoring, ML-based surrogates have shown promise in significantly accelerating PBF-LB simulations without requiring the memory and computational resources of classical high-fidelity models [14].

In summary, data-driven techniques can complement or even replace full-scale thermal or thermo-mechanical analyses for certain tasks, provided that adequate training data are available. They may be coupled with either inherent strain or flash/lumped approaches to produce quick, approximate solutions across a wide parameter space, thereby supporting iterative design or online control strategies. The ongoing research challenge lies in expanding these techniques to multi-physics processes and complex geometries while maintaining accuracy and robustness outside the training regime.

2.2.7.5 Concluding remarks on model reduction.

In summary, several efficient strategies have been developed to handle the extreme computational demands of PBF-LB simulations:

- **Inherent strain methods** skip repeated transient thermo-mechanical analyses by imposing precomputed inelastic strains in an elastic model,

- **Adaptive meshing** concentrates refinement only where necessary,
- **Flash/lumped approaches** approximate entire layer scans by single conduction steps,
- **Machine learning** surrogates exploit data-driven models to predict responses with minimal PDE solves.

All of these approaches aim to reduce computational time and memory footprints, making large or complex parts tractable to simulate while still retaining sufficient fidelity to guide process design, control, and part qualification.

2.3 Experimental procedures for model calibration and validation

Numerical modelling inherently involves approximations, simplifications, and assumptions. In the context of PBF-LB processes, experimental measurements play a pivotal role in both establishing model credibility and refining computational frameworks [3].

In general, experimental data serve two distinct but complementary purposes:

1. **Calibration:** Adjusting uncertain parameters in numerical models to align with measured data.
2. **Validation:** Independently assessing whether the model can accurately predict physical behaviour without additional adjustments.

According to AWS A9.5:2013 [3] and Babuska et al. [8], a rigorous calibration and validation process ensures that models are not overfitted but generalisable across varying conditions.

Each experimental measurement provides a specific and necessary benchmark for different aspects of numerical modelling:

- **Temperature evolution:** This is essential for calibrating heat source parameters, such as laser absorptivity and heat transfer coefficients. Moreover, it ensures accurate thermal gradient predictions, which directly influence stress formation.
- **Distortion and deformation:** Accurate prediction of part distortion is essential for ensuring reliable numerical models. Furthermore, understanding distortion helps optimise various factors, such as scan strategies, support structures, and printing orientations, to minimise geometric deviations.
- **Residual stress:** Residual stress is crucial for validating mechanical models that predict stress accumulation. Additionally, it provides insights into failure mechanisms such as cracking and delamination.

However, temperature, distortion, and residual stresses are not standalone values. They directly influence the predictive accuracy of thermal and mechanical models used in PBF-LB simulations.

2.3.1 Temperature evolution measurements

Understanding the thermal history in [PBF-LB](#) is fundamental for both calibrating heat transfer models and validating temperature predictions. The rapid heating and cooling cycles inherent to [PBF-LB](#) generate complex thermal gradients that influence melt pool behaviour, phase transformations, and residual stress development.

Among the experimental techniques employed, thermocouples remain the most widely used method for tracking in-situ temperatures in [PBF-LB](#). They offer high-accuracy, real-time local temperature readings, making them essential for benchmarking and refining numerical models.

Dunbar et al. [33] developed an enclosed instrumentation system within an LPBF machine to measure in-situ temperature evolution (see [Figure 2.19](#)). In their study, K-type thermocouples were embedded in the build plate to capture transient temperature profiles, enabling the refinement of numerical models through adjustments in thermal conductivity, absorptivity, and convection coefficients. Their results demonstrated good agreement with finite element predictions.

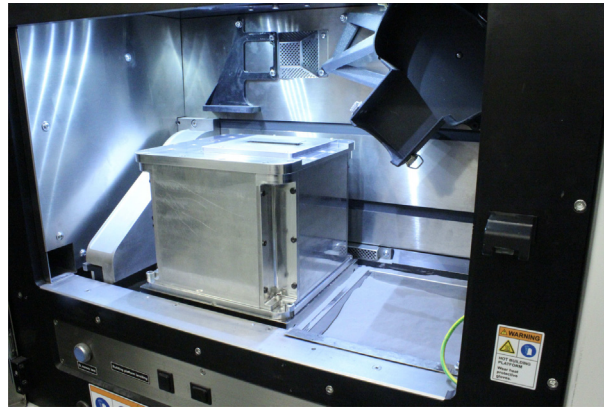


Figure 2.19: Experimental setup for in-situ temperature measurements (using K-type thermocouples) and distortion measurements (using a [DVRT](#)) in [PBF-LB](#). Adapted from [33].

Similarly, Chiumenti et al. [22] conducted temperature measurements by embedding thermocouples into Ti-6Al-4V [PBF-LB](#) components. In an EOS M280 system, the thermocouples were positioned in pre-drilled holes within the build to study heat accumulation effects across multiple layers. Although challenges related to thermal lag and air gaps affected the readings, high-speed data acquisition improved the accuracy of the heat source models, achieving predicted temperature fields within 10% accuracy.

In the study by Chen et al. [17], thermocouples were strategically placed on the substrate to capture the thermal history during layer deposition. Temperature measurements were performed using K-type thermocouples in an EOS M290 [PBF-LB](#) machine. Specifically, three Omega SA1XL-K-72 thermocouples were mounted on the underside of the substrate to monitor temperature changes at various points during the build process. Their findings validated a finite element thermal model for predicting the thermal history in [PBF-LB](#) and underscored the significant influence of heat accumulation on temperature gradients across layers.

Denlinger et al. [26] integrated K-type thermocouples into a PBF-LB build to investigate temperature evolution during Inconel 718 deposition. Their measurements revealed that newly deposited layers experienced the highest temperature fluctuations, while lower layers gradually accumulated residual heat. These results emphasise the importance of effective thermal management strategies in minimising process-induced stresses.

While thermocouples remain widely used, alternative methods offer distinct advantages. Infrared (IR) thermography and pyrometry facilitate full-field, non-contact temperature monitoring; however, their accuracy is susceptible to emissivity variations, necessitating careful calibration [39]. In contrast, single-pixel pyrometers provide precise high-temperature tracking but require multiple sensors to capture comprehensive thermal fields [39].

Lu et al. [51] combined thermocouples with IR thermal imaging to achieve full-field thermal data acquisition during Directed Energy Deposition - Laser Beam (DED-LB). Their study demonstrated strong agreement between imaging and thermocouple readings, refining numerical models.

The selection of a measurement technique ultimately depends on several factors, including spatial resolution, calibration feasibility, and the applicable temperature range.

2.3.2 *Distortion and deformation measurements*

Understanding distortion and deformation in PBF-LB is essential for ensuring the dimensional accuracy and mechanical integrity of printed components. The cyclic heating and cooling inherent to PBF-LB generate thermal gradients, leading to residual stresses that cause warping and deviations from the intended geometry. To quantify these effects, researchers employ various experimental measurement techniques that capture distortion and deformation both during and after the build process.

Measurement techniques for distortion and deformation in PBF-LB can be broadly classified into contact-based and non-contact-based methods. Contact-based techniques such as coordinate measuring machine (CMM), Differential Voltage Reluctance Transducer (DVRT), and Linear Variable Differential Transformers (LVDT) provide high-precision data, but they require physical interaction with the component. Non-contact methods, including Digital Image Correlation (DIC), Laser Displacement Sensor (LDS), and laser scanning, allow deformation or displacement tracking without direct contact but may be affected by surface reflectivity, powder adherence, or scanning errors. Additionally, each technique differs in whether it acquires data from a single point or provides full-field (area) measurements.

2.3.2.1 *Contact-based methods*

Coordinate measuring machine (CMM) is a contact-based method that uses a mechanical probe to scan a part's surface, providing highly precise measurements of geometric deviations compared to a CAD reference. It is commonly used for post-process validation due to its micrometer-level accuracy. However, its main drawback

is low scanning speed, point-based data at discrete locations and cannot track deformation in real-time.

Gouge et al. [39] used a Core RS-50 CMM to measure point-wise distortion in Inconel 718 parts produced via PBF-LB. They performed scans at four separate XY positions, recording height deviations in increments of 0.05 mm along the Z-axis.

Both **Linear Variable Differential Transformers (LVDT)** and **Differential Voltage Reluctance Transducer (DVRT)** are point-based sensors designed for tracking real-time displacement during printing, though their operating principles differ. LVDTs operate via electromagnetic induction, while DVRTs rely on variable reluctance sensing. Despite this difference, their usage is functionally similar. They are ideal for substrate warping measurement but do not provide spatial deformation maps as they both measure displacement at a single point.

Dunbar et al. [32] deployed an M-DVRT-3 Lord Microstrain sensor inside a sealed protective vault (see Figure 2.19) to monitor Z-direction displacement during printing. This setup provided real-time insight into substrate warping but was limited to a single measurement location. Denlinger et al. [26] used LVDT sensors to track build-plate deformation, correlating displacement trends with thermal stress accumulation.

2.3.2.2 Non-contact methods

Laser Displacement Sensor (LDS) is a non-contact, high-speed measurement technique that tracks height variations at a single point. It is useful for monitoring cyclic deformations but suffers from line-of-sight requirements and powder interference.

Dunbar et al. [32] tested LDS for in situ distortion tracking, but powder adherence significantly impacted reliability.

Laser scanning is a non-contact, high-resolution technique that reconstructs a 3D geometric model by analysing laser beam reflections across a surface. It provides full-field distortion data, enabling comprehensive post-process deformation analysis.

Chen et al. [17] employed a FARO Laser ScanArm V3 to scan entire double cantilever beams, comparing measured distortions to numerical predictions with an error below 11%.

Lu et al. [50] used a Breuckmann SmartSCAN3D laser scanner to capture warpage in thin-walled Ti-6Al-4V structures. Their approach enabled full-field distortion analysis, revealing critical deformation zones in thin-walled geometries and supporting numerical model calibration.

Digital Image Correlation (DIC) is a non-contact, optical technique that captures full-field deformation data by comparing sequential high-resolution images. This makes it ideal for tracking strain evolution across an entire surface, though it requires surface preparation to ensure contrast.

Strantz et al. [71] used DIC with high-speed cameras to analyse strain evolution in Ti-6Al-4V components produced via PBF-LB. Their study provided full-field deformation maps, validating thermo-mechanical models.

Lu et al. [51] utilised displacement sensors and DIC cameras with optical filters to obtain full-field deformation data. Their findings showed that the warpage initially peaked and gradually stabilised over subsequent layers.

2.3.3 Residual stress measurements

Residual stresses in PBF-LB originate from the rapid thermal expansion and contraction inherent to the process. If not properly managed, these stresses can lead to part distortion or failure, making accurate experimental validation critical for reliable mechanical modelling.

Residual stress measurement techniques can be broadly classified into destructive and non-destructive methods. Destructive cutting methods determine stress distributions by removing material and quantifying the resulting strain relief. Two commonly used destructive approaches are:

- Hole-drilling method: A small hole is drilled into the material, and the relieved strains are measured to back-calculate the original stress state. Although widely adopted, this technique is generally limited to surface measurements and offers moderate accuracy (± 50 MPa) [39].
- Contour method: The component is sectioned along a predefined plane, and the deformation of the cut surface is measured to reconstruct the original residual stress distribution. This method provides full-field stress data with high accuracy.

Ahmad et al. [2] investigated residual stresses in Ti-6Al-4V and Inconel 718 fabricated by PBF-LB using the contour method. Their experimental setup involved wire electrical discharge machining (wEDM) to slice the samples, followed by CMM scanning to map surface deformations. Their study revealed high tensile stresses near the surface and compressive stresses in the core, validating an inherent strain-based numerical model with strong agreement between simulation and experiment. Similarly, Swain et al. [73] employed the incremental hole-drilling method to measure residual stresses in Ti-6Al-4V components produced via PBF-LB on an MTS-3000 RS measurement system (see Figure 2.20). Their work evaluated stress distributions before and after annealing heat treatment, demonstrating that annealing effectively reduces tensile residual stresses and highlighting the importance of post-processing.

In another study, Denlinger et al. [25] investigated residual stress evolution in electron beam additive manufacturing of Ti-6Al-4V by combining blind hole-drilling measurements with in situ distortion tracking. Their results suggested that stress relaxation occurs during deposition, and they proposed a method to incorporate this phenomenon into thermo-elasto-plastic finite element models.

Non-destructive diffraction-based techniques provide an alternative approach by employing high-energy beams to measure lattice strains without altering the part. The most common diffraction methods include:

- X-ray Diffraction (XRD): A well-established technique for near-surface stress measurements. Although effective, XRD requires careful calibration and relies on assumptions about material properties.
- Neutron Diffraction (ND): This method enables depth-resolved stress measurements, making it particularly valuable for assessing bulk materials.

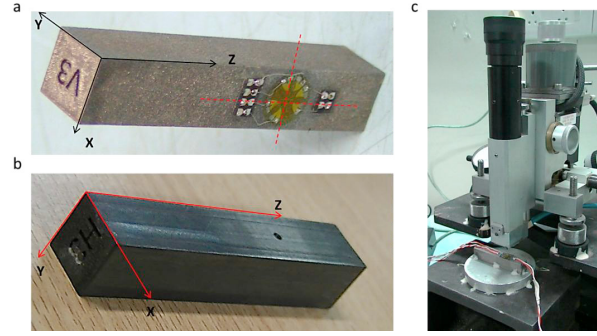


Figure 2.20: Incremental hole drilling for residual stress measurement in a Ti-6Al-4V sample. The figure illustrates the experimental setup and specimen configuration [73].

Compared to cutting methods, diffraction-based techniques offer higher accuracy, providing residual stress fields rather than single-point data. They also allow for non-destructive analysis, preserving part integrity for further testing, and enable depth-resolved measurements, particularly in the case of neutron diffraction. However, these techniques require specialized equipment and extensive calibration, which can limit their accessibility [71].

For instance, Strantz et al. [71] conducted a combined experimental and computational study on Ti-6Al-4V components manufactured by PBF-LB. Using high-energy XRD at the Cornell High Energy Synchrotron Source (CHESS), they obtained three-dimensional residual stress fields with high-resolution lattice strain mapping. This enabled a detailed assessment of stress gradients and potential failure regions, and the experimental data served to validate computational thermo-mechanical models.

More recently, Dong et al. [30] employed XRD to validate residual stress predictions in Ti-6Al-4V thin-walled structures fabricated via PBF-LB. Their measurements, taken at multiple locations along the build, revealed that mid-wall regions experienced the highest stress concentrations (an effect significantly influenced by scan strategies and cooling rates).

In summary, the choice of a residual stress measurement technique is influenced by several factors, including the desired spatial resolution, measurement depth, calibration feasibility, and access to specialized facilities. Both destructive and non-destructive methods offer distinct advantages that are essential for developing and validating robust numerical models for additive manufacturing processes.

2.3.4 Conclusion

Experimental validation is a cornerstone in the development of robust numerical models for PBF-LB. By clearly distinguishing between calibration (where experimental data are used to tune model parameters) and validation (where independent measurements assess predictive accuracy) researchers can mitigate overfitting and enhance model generalizability.

The reviewed experimental techniques illustrate that:

- **Thermal measurements**, using both contact-based sensors (e.g., thermocouples) and non-contact methods (e.g., infrared thermography), are crucial for calibrating heat transfer models and predicting thermal gradients.
- **Distortion and deformation assessments** through contact-based methods (e.g., CMM, LVDT, DVRT) and non-contact techniques (e.g., DIC, laser scanning) provide complementary insights into part geometry and warpage.
- **Residual stress evaluations**, achieved by both destructive (hole-drilling and contour methods) and non-destructive (XRD, ND) approaches, underpin the validation of mechanical models and help identify potential failure mechanisms.

Together, these methodologies establish a validation framework that not only refines numerical simulations but also guides the optimisation of processing conditions. Moving forward, integrating these diverse experimental approaches will be essential to overcome measurement challenges and improve the predictive accuracy of PBF-LB models.

In summary, a comprehensive experimental strategy ensures that numerical models effectively capture the complex phenomena inherent in additive manufacturing, ultimately leading to enhanced model reliability and process optimisation.

2.4 Material Ti-6Al-4V

Ti-6Al-4V is the most commonly used titanium alloy in MAM. It offers an excellent combination of strength, low density, and corrosion resistance, making it especially attractive for high-performance applications in aerospace, automotive, and biomedical industries. Numerous AM-specific standards include Ti-6Al-4V. In particular, ASTM F2924 [6] is a widely recognized specification that addresses additively manufactured Ti-6Al-4V components built via PBF.

2.4.1 PBF-LB processing of Ti-6Al-4V

In PBF-LB, the build chamber is typically maintained in an inert gas environment (e.g., argon) to prevent oxidation. This is particularly crucial for titanium alloys due to their high reactivity. Additionally, some manufacturers and customers require compliance with standards such as ASTM F2924 [6], which specifies requirements for powder feedstock, process parameters, post-processing treatments (e.g., stress relieving, hot isostatic pressing), and the final mechanical properties of Ti-6Al-4V components, including yield strength, ultimate strength, and ductility.

When the laser spot fuses the powder, the local region experiences extremely high thermal gradients (on the order of 10^6 K/m) and cooling rates. These gradients can favor the formation of a dominant α' martensitic microstructure when the cooling rate exceeds a threshold (often near 10^3 – 10^5 K/s for Ti-6Al-4V) [11]. Such microstructures typically exhibit high strength but limited ductility, and post-build heat treatments may be required to produce the desired balance of mechanical properties.

2.4.2 Material model requirements for simulation

Predictive simulations of [PBF-LB](#) for Ti-6Al-4V require a comprehensive set of temperature-dependent material properties. In addition to standard thermo-physical parameters (density, specific heat, thermal conductivity), the following aspects are often considered:

- **Solidus and Liquidus temperatures:** Ti-6Al-4V melts at around 1878 K (solidus) up to 1923 K (liquidus). Accurate representation of latent heat effects in this range is crucial for capturing melt pool sizes [39].
- **Phase transformation thresholds:** The β -transus (about 1260–1300 K) delineates $\alpha + \beta \rightarrow \beta$ upon heating. For rapid cooling, the α' -martensite start temperature (often in the range 600–800 K) becomes relevant [35]. Both phase boundaries are critical for simulating microstructural evolution in Ti-6Al-4V.
- **Temperature-dependent mechanical properties:** The Young's modulus, yield stress, ultimate tensile strength, Poisson's ratio, and coefficient of thermal expansion are typically required [11]. Because of the steep thermal gradients inherent to [PBF-LB](#), thermal expansion properties can dominate the generation of residual stress [25]. Thus, an accurate coefficient of thermal expansion curve is critical.
- **Anisotropy or isotropic assumption:** Although columnar grains can introduce anisotropy at the microstructure scale, many macro-scale simulations assume isotropic material behaviour. If strong texture arises from particular scanning strategies, modelling anisotropy may be necessary for better fidelity.
- **Relaxation or annealing:** High-temperature stress relaxation during the build should be accounted for to avoid exaggerated residual stress predictions [27].

2.4.2.1 Material properties used for simulation work

The temperature-dependent material properties of the Ti-6Al-4V alloy were defined based on the literature [35]. This source provides averaged data from multiple references and includes additional experimental tests, offering a reliable initial guess for these properties. This comprehensive dataset ensures accurate and reliable material behaviour modelling under varying thermal conditions.

For mechanical behavior, the small-strain material model described in [Chapter 3](#) incorporates these temperature-dependent properties. As part of that model, plastic flow, isotropic hardening, flow stress thermal softening as well as stress relaxation are included. [Figure 2.21](#) presents the thermophysical and mechanical property curves used in the simulations, each plotted as a function of temperature.

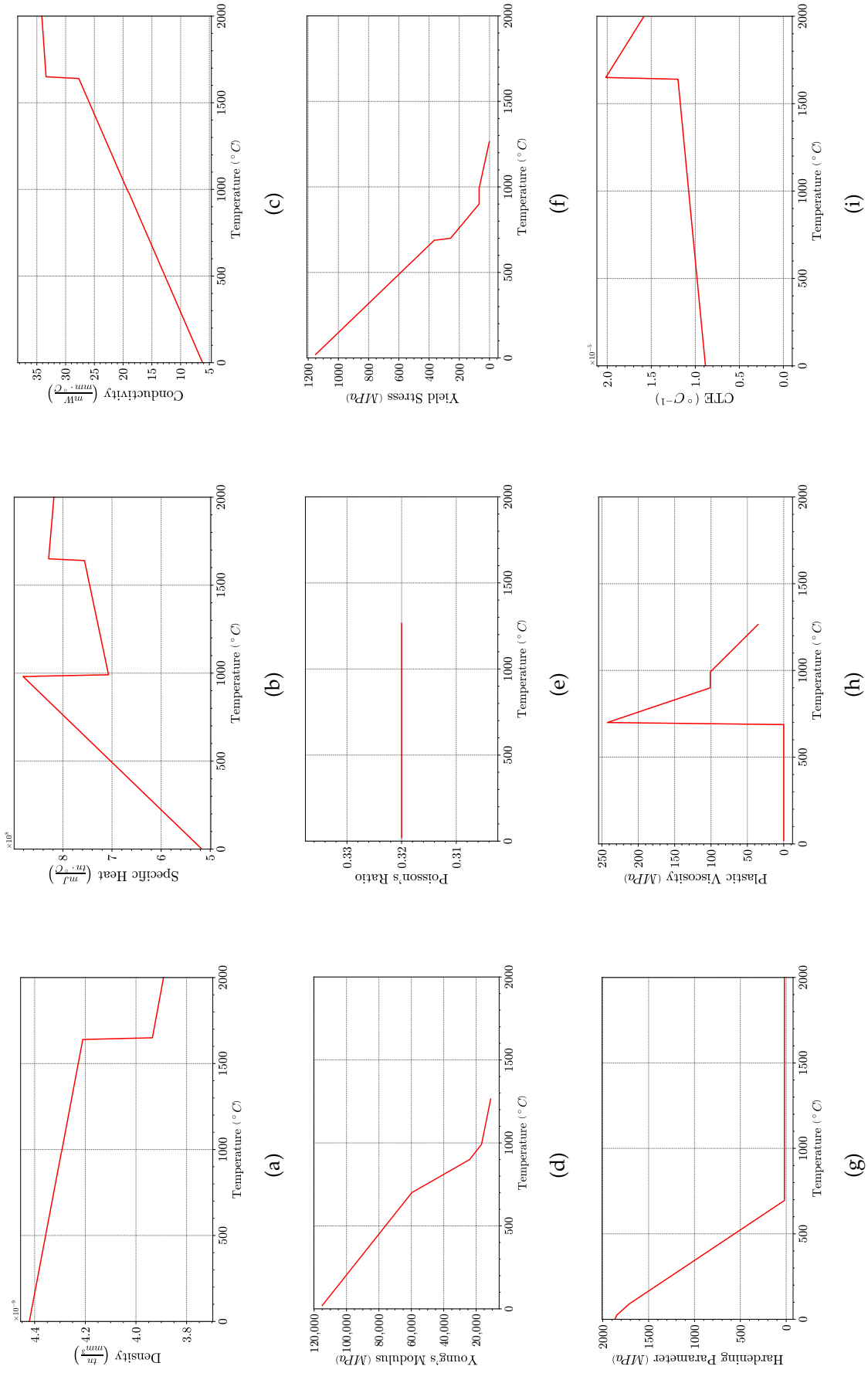


Figure 2.21: Temperature-dependent thermo-mechanical properties of Ti-6Al-4V material: (a) Density, (b) Specific heat, (c) Thermal conductivity, (d) Young's modulus, (e) Poisson's ratio, (f) Yield stress, (g) Isotropic linear hardening parameter, (h) Plastic viscosity, (i) Thermal expansion coefficient.

2.5 Summary and research gaps

In this chapter, an overview of **MAM** has been provided, with a focus on **PBF-LB** processes. The fundamental challenges, including distortion, residual stresses, and complex multi-physics phenomena, have been shown to require robust numerical modelling and experimental validation. From the preceding sections, several conclusions can be drawn:

1. **MAM**, particularly **PBF-LB**, unlocks unprecedented design freedom but faces challenges such as steep thermal gradients, residual stresses, distortion, and defects like porosity or poor bonding. These issues can undermine part quality and limit broader industrial adoption.
2. *Multi-scale numerical simulations* (micro-, meso-, macro-) are indispensable for understanding and predicting the thermo-mechanical behaviour of **PBF-LB**. However, coupling these scales remains difficult, as computational demands become prohibitive when trying to capture both local and global phenomena.
3. *Efficient simulation strategies* (e.g. **AMR**, flash/lumped heating, **ISM**, and **ML**-based methods) have been proposed to ease the high computational burden. While each of these techniques reduces computational cost compared to traditional high-fidelity approaches, they introduce their own approximations and require careful validation.
4. Among these *efficient techniques*, the **ISM** stands out as a well-established but still evolving simplification framework. It is widely used for its ability to bypass detailed thermo-mechanical analysis, enabling large-scale distortion predictions to be handled with acceptable computational resources.

Research gaps

Despite the progress outlined above, various open questions remain:

- **Standardising the inherent strain calculation.** The literature provides no universally accepted procedure for calculating inherent strain tensors:
 - *Experimental (inverse) approaches* often lack a robust, systematic methodology for converting measured distortions into consistent strain tensors, hindering straightforward industrial application.
 - *Meso-scale thermo-mechanical models*, can accurately reflect local conditions but in many examples remain too localised or ad-hoc, without fully capturing the integrated thermal and mechanical history.
- **Balancing efficiency and accuracy in large-part simulations.** While **ISM** provides computational efficiency, reliable validation under industrially relevant geometries and scan parameters remains insufficiently explored. Many published studies are restricted to smaller test cases.

- **Refining the ISM methodology.** The ISM itself, despite proven benefits, makes certain assumptions (e.g., uniform inherent strains, lumps of layers) that can limit accuracy or generalisability. There is scope to incorporate corrections based on experimental data and local meso-scale insights, extending the method's predictive capability to more complex or large-scale PBF-LB parts.

Overall, although there is a clear trend toward *efficient* predictive modelling, including the use of inherent strain and other reduced-order methods, further research must refine and unify inherent strain calculation procedures, expand experimental validation for industrial geometries, and enhance the simplified methodology itself.

3

COMPUTATIONAL MODELS AND METHODS

This chapter provides a comprehensive description of the [FE](#)-based numerical methodologies that have been employed or developed to simulate the [PBF-LB](#) process in Ti-6Al-4V. Three modelling strategies are presented, which together form the foundation for the [Chapters 5](#) to [7](#) (each corresponding to the one of the articles published in this thesis). In particular, this chapter covers:

- The *high-fidelity thermo-mechanical analysis*, which captures the local thermo-mechanical behaviour;
- The standard *Inherent Strain Method* ([ISM](#)), which facilitates efficient part-scale predictions using a predefined inherent strain tensor;
- The *Enhanced Inherent Strain Method* ([EISM](#)), which further refines the [ISM](#) approach by incorporating a macro-scale thermal analysis to adjust the inherent strain tensor based on the part-scale temperature history.

Each section also discusses how these methods interact with practical modelling considerations such as material deposition, boundary conditions, layer lumping, time discretization, and other relevant factors.

3.1 High-fidelity thermo-mechanical analysis

High-fidelity thermo-mechanical analysis aims to capture the local physics of [PBF-LB](#), including the effects of the moving heat source, rapid heating and cooling cycles, and development of elasto-visco-plastic strains. The thermo-mechanical coupling is implemented in a staggered (weakly coupled) manner, whereby the thermal problem is solved first, followed by the mechanical problem (see [Figure 2.13](#)).

3.1.1 Thermal analysis

3.1.1.1 Governing equation and boundary conditions

Temperature evolution can be described by the energy balance equation. A common form of the governing equation is

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \dot{Q}(\mathbf{x}, t) \quad \text{on } \Omega. \quad (3.1)$$

where $\rho = \rho(T)$ is the density, $c_p = c_p(T)$ is the specific heat capacity, $k = k(T)$ is the thermal conductivity, $T = T(\mathbf{x}, t)$ is the temperature field, and $\dot{Q}(\mathbf{x}, t)$ is a volumetric heat source.

The contribution of latent heat to the enthalpy is neglected, assuming that melting and solidification occur significantly faster than thermal diffusion and that the heat absorbed and released during the process is equivalent and takes place within the same time step [21].

Equation (3.1), together with initial and boundary conditions, defines the problem to be solved. Boundary conditions are imposed on different portions of the domain boundary Γ . A Dirichlet (temperature) condition prescribes

$$T(\mathbf{x}, t) = T_0(\mathbf{x}, t) \quad \text{on } \Gamma_D, \quad (3.2)$$

and a Neumann (heat flux) condition enforces a specified flux,

$$-k \nabla T \cdot \mathbf{n} = q_n(\mathbf{x}, t) \quad \text{on } \Gamma_N. \quad (3.3)$$

Convective and radiative boundary conditions are more complex Robin-type conditions. Convection can be modelled as

$$-k \nabla T \cdot \mathbf{n} = h(T - T_\infty) \quad \text{on } \Gamma_C, \quad (3.4)$$

where h is the heat transfer coefficient, and radiative loss is introduced via

$$-k \nabla T \cdot \mathbf{n} = \epsilon \sigma (T^4 - T_\infty^4) \quad \text{on } \Gamma_R, \quad (3.5)$$

where ϵ is the surface emissivity and σ the Stefan–Boltzmann constant.

An initial condition must also be specified for the temperature field, for example, at $t = 0$:

$$T(\mathbf{x}, 0) = T_{\text{init}}(\mathbf{x}), \quad (3.6)$$

ensuring a well-posed problem.

3.1.1.2 Heat source model

As discussed in Chapter 2, in CWM, the heat generation process is typically simplified by prescribing a heat input distribution, thereby excluding the underlying physics of heat generation and the complex phenomena occurring within the melt pool. In this context, Gaussian and double-ellipsoid (Goldak) heat source models are widely

employed in welding and additive manufacturing simulations [38]. These models are particularly advantageous when accurate resolution of local temperature gradients and melt pool dimensions is required, necessitating extremely small time increments and highly refined meshes in the heat application zone.

In the present work, however, as the focus is on a broader scale rather than local melt pool physics, the external heat input per unit volume is assumed to be uniformly distributed over a box-shaped volume [21, 22]. The applied volumetric heat flux is computed as:

$$\dot{Q} = \frac{\eta W}{V_{\text{pool}}^{\Delta t}}, \quad (3.7)$$

where W is the laser power, η is the heat absorption coefficient, and $V_{\text{pool}}^{\Delta t}$ is the heat-affected volume (HAV), calculated as the sum of the volumes of all finite elements intersected by the moving heat source during the current time increment:

$$V_{\text{pool}}^{\Delta t} = \sum_{e=1}^{n_e} V^{(e)}|_{e \in \text{HAV}}. \quad (3.8)$$

Here, $V^{(e)}$ represents the volume of element e , and HAV denotes the set of all elements intersected by the moving heat source during the current time step Δt .

The size of HAV depends on the time discretisation criterion and the scanning path. The methodology for identifying the intersected finite elements is detailed in Section 3.1.3.5. Regardless of the specific elements affected, this power distribution ensures that the total energy input remains conserved.

3.1.2 Mechanical analysis

3.1.2.1 Governing equation and boundary conditions

The mechanical equilibrium is governed by the quasi-static balance of momentum equation:

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = 0 \quad \text{on } \Omega, \quad (3.9)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, and $\mathbf{b}$ represents body forces per unit volume.

To fully define the problem, appropriate mechanical boundary conditions must be imposed. The boundary Γ of the domain is partitioned into regions Γ_u , where displacements are prescribed, and Γ_t , where traction forces are applied:

- Dirichlet (displacement) boundary condition:

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_0(\mathbf{x}, t) \quad \text{on } \Gamma_u. \quad (3.10)$$

- Neumann (traction) boundary condition:

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t}_0(\mathbf{x}, t) \quad \text{on } \Gamma_t. \quad (3.11)$$

The stress-strain relationship of the material is given by:

$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}^e , \quad (3.12)$$

where $\mathbf{C}$ is the fourth-order constitutive tensor, and $\boldsymbol{\varepsilon}^e$ is the elastic strain tensor.

Under the assumption of small-strain theory, the elastic strain tensor is computed as:

$$\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{th} - \boldsymbol{\varepsilon}^{vp} , \quad (3.13)$$

where $\boldsymbol{\varepsilon}$ is the total strain tensor, $\boldsymbol{\varepsilon}^{th}$ is the thermal strain tensor (accounting for the strain induced by temperature changes), and $\boldsymbol{\varepsilon}^{vp}$ is the visco-plastic strain tensor.

The total strain tensor $\boldsymbol{\varepsilon}$ and the displacement field $\mathbf{u}$ are related through the linear strain-displacement kinematics:

$$\boldsymbol{\varepsilon}(\mathbf{u}) = \nabla^s(\mathbf{u}) , \quad (3.14)$$

where ∇^s denotes the symmetric gradient operator of the displacement field $\mathbf{u}$.

The temperature history obtained from the heat transfer analysis is used to compute the thermal strain as follows:

$$\boldsymbol{\varepsilon}^{th} = [\alpha(T) \cdot (T - T_{ref}) - \alpha(T_0) \cdot (T_0 - T_{ref})] \mathbf{I} , \quad (3.15)$$

where T is temperature, $\alpha(T)$ is the temperature-dependent secant thermal expansion coefficient, T_{ref} is the reference temperature for the expansion coefficient, and T_0 is the initial temperature of the material at the beginning of the simulation.

To regulate thermal strain effects at high temperatures, a cut-off temperature T_{anneal} is introduced:

$$T = \begin{cases} T_{\text{anneal}} , & \text{for } T \geq T_{\text{anneal}} , \\ T , & \text{for } T < T_{\text{anneal}} . \end{cases} \quad (3.16)$$

As a result, the deposited material, initially in a liquid-like state with a temperature of $T_0 \geq T_{\text{anneal}}$, does not undergo thermal strain.

3.1.2.2 Constitutive model

The material model for Ti-6Al-4V must account for strain-rate dependency at elevated temperatures and accurately capture stress and strain relaxation behaviour [7].

A suitable constitutive model for these characteristics is the J2 thermo-elasto-viscoplastic formulation under the small-strain assumption, as detailed in [20]. This model incorporates phase change effects and effectively represents the elasto-plastic material behaviour at low temperatures as well as the purely viscous response observed near and above the melting point.

Although conventional phase transformation models define three states (solid, mushy, and liquid-like), this study adopts a simplified approach, considering only two states (solid and liquid-like), as described in [57]. The transition between these states is regulated by the annealing temperature threshold T_{anneal} , as illustrated in Figure 3.1.

The constitutive behaviour is defined as follows:

- **Solid state:** The thermo-elasto-visco-plastic constitutive model incorporates both isotropic hardening and thermal softening effects. Strain-rate-independent plasticity and visco-plasticity are combined, governed by temperature-dependent parameters. The volumetric (p) and deviatoric (s) components of the stress tensor are computed as follows:

$$\begin{cases} p = K (\nabla \cdot \mathbf{u} - \varepsilon^{th}) , \\ s = 2G (\mathbf{e} - \mathbf{e}^{vp}) , \end{cases} \quad (3.17)$$

where K and G are the temperature-dependent bulk and shear moduli, respectively, while $\mathbf{e}$ and $\mathbf{e}^{vp}$ denote the deviatoric total strain and visco-plastic strain tensors.

The constitutive model employs a temperature-dependent J2 yield surface $\Phi(s, q, T)$, defined as:

$$\Phi(s, q, T) = ||s|| - R(q, T) \leq 0 , \quad (3.18)$$

where $R(q, T)$ is the temperature-dependent yield surface radius, given by:

$$R(T, q) = \sqrt{\frac{2}{3}} \left(\sigma_y(T) - q(T, \xi) \right) , \quad (3.19)$$

where $\sigma_y(T)$ is the temperature-dependent elastic limit, ξ is the equivalent plastic strain, and q is a stress-like internal variable controlling the *isotropic hardening* of the model.

The visco-plastic strain evolution laws are defined as:

$$\dot{\mathbf{e}}^{vp} = \dot{\gamma}^{vp} \mathbf{n} , \quad (3.20)$$

$$\dot{\xi} = \dot{\gamma}^{vp} \sqrt{\frac{2}{3}} , \quad (3.21)$$

where $\mathbf{n} = \frac{\mathbf{s}}{||\mathbf{s}||}$ is the normal to the yield surface. The visco-plastic multiplier $\dot{\gamma}^{vp}$ is computed from the following rate-dependent evolution law:

$$\dot{\gamma}^{vp} = \left\langle \frac{\Phi(s, q, T)}{\eta} \right\rangle^{\frac{1}{m}} , \quad (3.22)$$

where $\langle \cdot \rangle$ denotes the Macaulay brackets, and $\eta(T)$ and $m(T)$ are the temperature-dependent plastic viscosity and rate sensitivity, respectively.

- **Liquid-like state:** No elastic or thermal strains are generated. The material behaviour is governed by a purely viscous Norton–Hoff model:

$$\begin{cases} \nabla \cdot \mathbf{u} = 0 , \\ s = \eta \dot{\mathbf{e}}^{vp} . \end{cases} \quad (3.23)$$

Thus, stress relaxation in Ti-6Al-4V is accounted for by modelling the material as if it were in a liquid-like state.

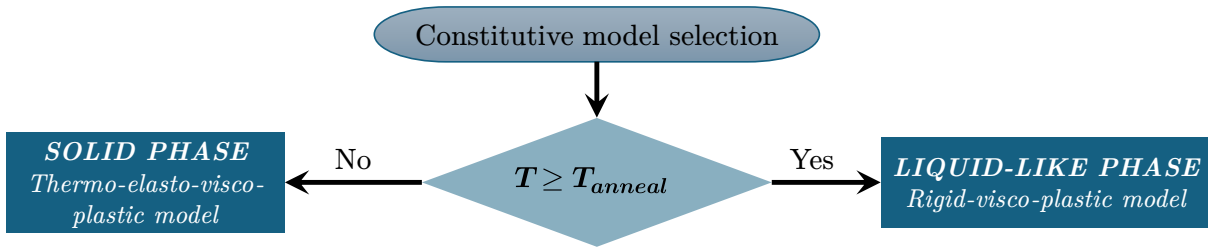


Figure 3.1: Constitutive model selection flowchart.

3.1.3 Finite element modelling

3.1.3.1 Finite Element technology

The selection of FE technology depends on the specific requirements of the process simulation. The standard irreducible FE formulation can suffer from volumetric locking when applied to nearly incompressible materials. This issue arises particularly in PBF-LB simulations when employing a J2 plasticity model to describe metallic materials, especially in their liquid-like state, where deformation is predominantly deviatoric (i.e., isochoric).

To address this problem, the stress and strain tensors are decomposed into their volumetric and deviatoric components, as detailed in Section 3.1.2.2. This leads to a system of equations with two unknown fields: displacement ($\mathbf{u}$) and pressure (p). This approach, known as the mixed $\mathbf{u}/p$ formulation, alleviates the artificial stiffness introduced by standard FE methods [15, 16].

As an alternative, Q1Po-type elements can be employed to consider quasi-incompressible material behaviour [16].

3.1.3.2 Material deposition modelling

Material deposition modelling is a crucial aspect of additive manufacturing simulations. Numerically, this requires handling evolving computational domains, where some regions contain active (deposited) material while others remain inactive (yet-to-be-deposited material). The thermo-mechanical phenomena occur exclusively within the active domain, where temperature and displacement fields are computed within the active finite elements.

A well-established approach for simulating material deposition in PBF-LB is the birth-death element activation strategy [22]. This method accurately represents the progressive addition of material as the printing process advances. In this framework, inactive elements remain in their initial state until they are activated based on the scanning path (illustrated in Figure 3.2). Once a layer is deposited, the build plate is lowered by the nominal layer thickness, and a fresh powder layer is spread. However, distortions in the top surface of previously deposited layers can lead to variations in the actual thickness and distribution of the newly spread powder. The birth-death activation approach inherently accounts for such variations, as illustrated in Figure 3.2 at $t = t_3$. Here, inactive elements (blue) deform due to the displacement of active elements (red), while ensuring that the new powder layer aligns with the nominal height.

Moreover, this approach captures transient deformations caused by the thermal expansion and contraction of melted material within each layer. As an example, Figure 3.2 shows the progressive deformation of elements 2 and 3 during activation at $t = t_1$ and $t = t_2$, respectively.

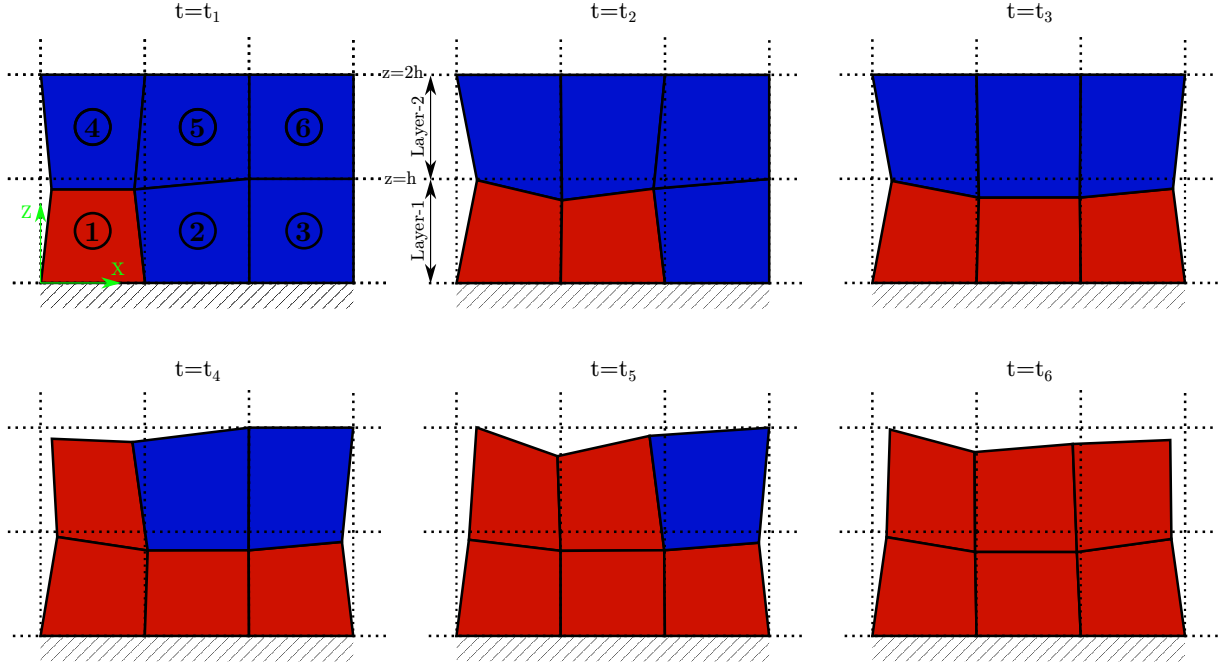


Figure 3.2: Illustration of the birth-death material deposition modelling strategy through activation steps in a domain composed of six elements. Red elements are activated and subjected to shrinkage, while blue elements remain inactive but deform due to node displacements shared with active elements. Activation strains are incorporated to account for these pre-activation deformations.

To ensure precise modelling of the interaction between inactive and active elements during both heat transfer and mechanical analysis, particular attention is given to the activation strategy.

In the heat transfer analysis, the temperature at the integration points of inactive elements remains equal to the initial temperature specified at the nodes. This ensures a smooth thermal transition and prevents unrealistic temperature gradients upon activation.

Similarly, in the mechanical analysis, inactive elements may experience initial deformations due to the displacement of nodes shared with active elements. To counteract this, activation strains are introduced, following the approach in [9, 57]. These strains compensate for the deformations, ensuring that the newly activated elements are in a stress-free configuration upon activation. This approach maintains consistency in the mechanical response and avoids introducing spurious residual stresses into the model. The activation strains are computed as:

$$\boldsymbol{\varepsilon}^{act} = \nabla^s(\mathbf{u}_0), \quad (3.24)$$

where $\nabla^s(\cdot)$ denotes the symmetric gradient operator of $\cdot$, and $\mathbf{u}_0$ are the initial displacements of the newly activated elements.

Including activation strains, the constitutive equation becomes:

$$\sigma = \mathbf{C} : (\varepsilon - \varepsilon^{vp} - \varepsilon^{th} - \varepsilon^{act}) . \quad (3.25)$$

Activation strains are history-dependent because they rely on u_0 , which is calculated at each activation step based on the scanning path and time-stepping accuracy. This highlights the importance of accurately implementing the scanning sequence to correctly model activation strains and their effect on the thermo-mechanical behaviour.

3.1.3.3 Time discretization

The choice of time step (Δt) is dictated by the scale and physical phenomena of interest. Since the thermo-mechanical model developed in this thesis focuses on local physics and the evolution of thermo-elasto-visco-plastic strains, selecting an appropriate time increment is crucial.

The time increment parameter is user-defined and typically requires iterative tuning to balance computational efficiency and accuracy. A large time step reduces computational cost but may compromise accuracy, while an excessively small time step can lead to unnecessary computational overhead.

When the speed of the heat source is significantly higher than the rate of thermal diffusion, it is possible to increase the time increment without sacrificing accuracy. This reference time increment serves as a guideline for determining an appropriate time step for the simulation. Based on the work of Irwin et al. [41] and considering the employed heat input model (see Equation (3.7)), the reference time increment is given by:

$$\Delta t_{ref}^{LI} = \frac{0.5 \cdot \alpha}{v_s^2} \cdot \left(\frac{v_s \cdot c}{\alpha} \right)^{1.92} \simeq 0.5 \cdot \frac{c^2}{\alpha} , \quad (3.26)$$

where α is the thermal diffusivity at ambient temperature, v_s is the heat source speed, and c is the length parameter of Goldak's ellipsoid.

The time increment Δt varies depending on whether the power input is active (*on*) or inactive (*off*) (e.g., during hatch jumps, recoating times, and final cool-down). During *off* periods, the time step is adjusted based on predefined criteria, such as a target cooling rate or temperature threshold.

3.1.3.4 FE mesh and adaptive refinement

FE mesh generation within FEMUSS is semi-automated, designed to minimize user effort while ensuring high-quality discretization. The process begins with an initial mesh, typically a coarse discretization of the baseplate and part bounding boxes. Unlike conformal meshing, a voxel-based approach is employed, embedding the geometry within a structured mesh.

A hybrid layer-wise AMR strategy is applied, closely linked to the element activation algorithm. Elements intersecting the deposition path, as defined by the HAV, are refined, while coarsening is delayed in the build direction at the layer level. The user must specify three key AMR parameters:

- Maximum refinement level ($Lev_{\max}$),
- Minimum refinement level ($Lev_{\min}$),
- Refinement height (h_{ref}).

For details on these parameters, refer to [57].

Proper selection of the bounding-box mesh dimensions is crucial for optimal solver performance. The final octree partitioning should yield an isotropic mesh with an aspect ratio close to 1.0. However, voxel-based meshing results in sharp boundaries, which can lead to a staircase effect, manifesting as oscillations in stress fields. The severity of this effect depends on the geometry resolution and mesh refinement.

3.1.3.5 Toolpath-mesh intersection

In the finite element modelling of additive manufacturing processes, it is essential at each time step to determine:

- The elements to be activated,
- The elements to which the heat input is applied, and
- The update of free surfaces that represent the current geometry of the build part, which is necessary for accurately computing convection and radiation heat losses.

These data are critical for simulating material deposition, heat input application and the associated heat losses, and adaptive meshing. To this end, a geometry-based element search engine is employed. This engine takes the scanning path and a set of geometric parameters as inputs and intersects them with an arbitrary mesh to identify the relevant elements.

The search engine is based on a rectangle attached to a reference point moving along the scanning path (see Figure 3.3). The scanning path is defined by connecting a series of points in space and time. Suppose a path located on top of a deposited layer is defined by the points $(X_1, X_2, X_3, \dots, X_m)$ at times $(t_1, t_2, t_3, \dots, t_m)$, with the assumption that the tool travels at a constant velocity between any two successive points.

For a given time step $\Delta t = t^{n+1} - t^n$, the heat source moves along the sub-segment from $X(t^n)$ to $X(t^{n+1})$. The search engine constructs a box by extruding a rectangle (oriented perpendicular to the segment) of dimensions $b_{\text{pool}} \times h_{\text{pool}}$ along the sub-segment of length Δl , as the *red box* illustrated in Figure 3.3. The heat input, as defined in Equation (3.7), is applied to the elements intersected by the red box, while the newly activated elements are those intersected by the green box, whose height corresponds to the layer height. Once these intersected elements are identified, the surfaces subject to convection and radiation heat losses are updated accordingly.

This search engine works in conjunction with the AMR engine to automatically generate and manipulate the mesh. For more details, see [56].

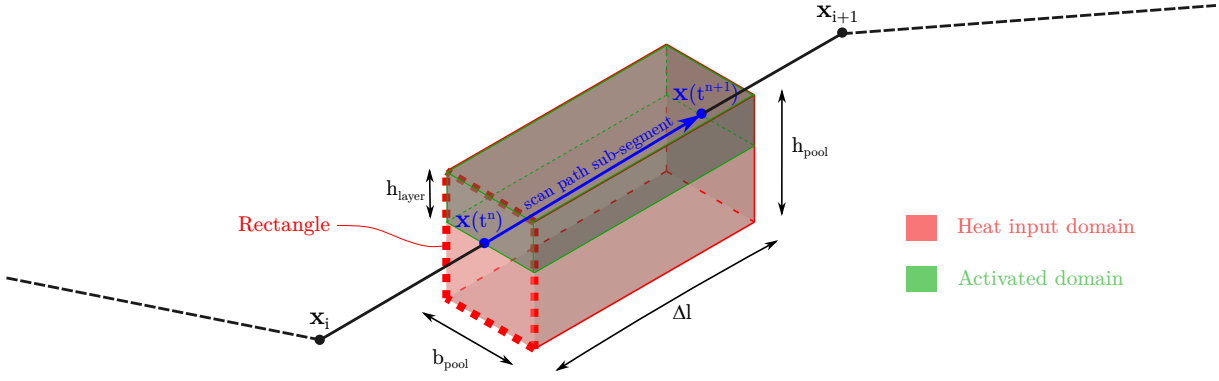


Figure 3.3: Box-shaped toolpath used for searching elements.

3.2 Original inherent strain method (ISM)

3.2.1 General principles

The original and most widely employed *ISM* is a computationally efficient approach for predicting distortions and, to a lesser extent, residual stresses by assigning a prescribed "shrinkage" strain (inherent strain) in a quasi-static, purely elastic *FE* analysis [43, 69, 75]. Despite minor variations, the method is based on the assumption that all material points within the domain experience the same thermo-plastic history. This assumption is justified by the highly localised and rapid nature of the *PBF-LB* process, where the melt pool is typically small compared to the overall component size.

A key aspect of *ISM* is defining the **inherent strain tensor**, which can be identified through:

1. Direct empirical approaches [69], or
2. Meso-scale thermo-mechanical simulations followed by homogenization [67].

The mechanical equilibrium is governed by the quasi-static balance of momentum equation:

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \mathbf{0} , \quad (3.27)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, and $\mathbf{b}$ represents body forces per unit volume.

The constitutive relationship of the material is:

$$\boldsymbol{\sigma} = \mathbf{C} : \boldsymbol{\varepsilon}^e , \quad (3.28)$$

where $\mathbf{C}$ is the fourth-order constitutive tensor, and $\boldsymbol{\varepsilon}^e$ is the elastic strain tensor.

Under the assumptions of small strain theory, the elastic strain tensor is computed as:

$$\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon}^{total} - \boldsymbol{\varepsilon}^{inh} , \quad (3.29)$$

where $\boldsymbol{\varepsilon}^{total} = \nabla^s(\mathbf{u})$ is the total strain tensor, and $\boldsymbol{\varepsilon}^{inh}$ is the inherent strain tensor.

The inherent strain tensor includes all non-elastic strain components:

$$\boldsymbol{\varepsilon}^{inh} = \boldsymbol{\varepsilon}^{total} - \boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon}^{th} + \boldsymbol{\varepsilon}^{pl} + \boldsymbol{\varepsilon}^{act} \quad , \quad (3.30)$$

where $\boldsymbol{\varepsilon}^{th}$ is the thermal strain tensor, $\boldsymbol{\varepsilon}^{pl}$ is the plastic strain tensor and $\boldsymbol{\varepsilon}^{act}$ is the activation strain tensor.

The decomposition of inelastic strains may vary depending on the specific phenomena considered.

In the original ISM, $\boldsymbol{\varepsilon}^{inh}$ is assumed to be constant at each material point and applied upon material deposition. The precomputed inherent strain tensor, denoted as $\boldsymbol{\varepsilon}^{inh,0}$, is used as input:

$$\boldsymbol{\varepsilon}^{inh} = \boldsymbol{\varepsilon}^{inh,0} \quad . \quad (3.31)$$

3.2.2 Modelling approach

The ISM is a layer-by-layer elastic analysis method. At each time step, a new layer is added to the computational domain. A common practice is to use a lumping strategy in which multiple layers are grouped and activated simultaneously. This approach reduces the computational burden by decreasing both the number of steps required and the total number of elements in the model.

A schematic of this procedure is shown in Figure 3.4. For each layer $\ell = 1, \dots, N$, the following steps are executed sequentially:

1. *Activation*: The FEs corresponding to the current layer are activated.
2. *Application*: The inherent strain $\boldsymbol{\varepsilon}^{inh,0}$ is applied.
3. *Solution*: A linear-elastic problem is solved under appropriate boundary conditions, typically a fully constrained baseplate.

Since the problem is linear-elastic, each step requires solving a linear system, which is computationally inexpensive compared to fully coupled thermo-plastic simulations.

3.2.3 Inherent strain tensor calculation

The inherent strain tensor can be determined using either empirical calibration or meso-scale thermo-mechanical models via a multi-scale approach. These methods are detailed in Chapters 5 and 6, respectively.

3.2.3.1 Empirical inverse method

In this method, characteristic test coupons (e.g., simple cantilever structures) are printed, and distortions are measured post-build and after support removal. By iteratively comparing measured distortions with linear elastic FE simulation predictions, the inherent strain tensor that best reproduces experimental observations is identified. The calibration procedure is illustrated in Figure 3.5 and is detailed in the paper included in Chapter 5.

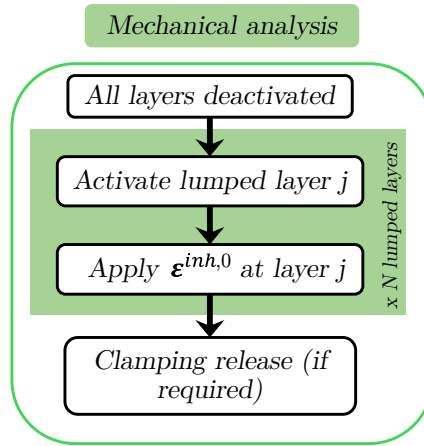


Figure 3.4: Overview of the ISM methodology, illustrating the sequence of layer activation and inherent strain application.

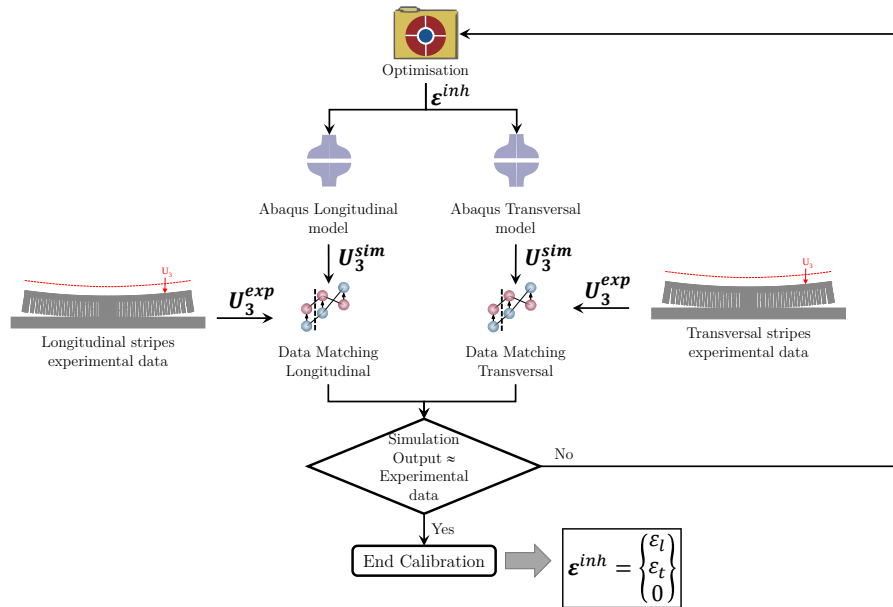


Figure 3.5: Iterative loop for inherent strain calibration.

3.2.3.2 High-fidelity local simulation

Alternatively, a meso-scale thermo-mechanical model can be employed. This model explicitly resolves both the laser scanning sequence and the associated thermo-mechanical response of the material. A representative subdomain is selected, within which up-scaled variables (i.e., the inherent strain tensor) are extracted using homogenisation techniques (see Figure 3.6). The computed inherent strain tensor is then used for part-scale simulations.

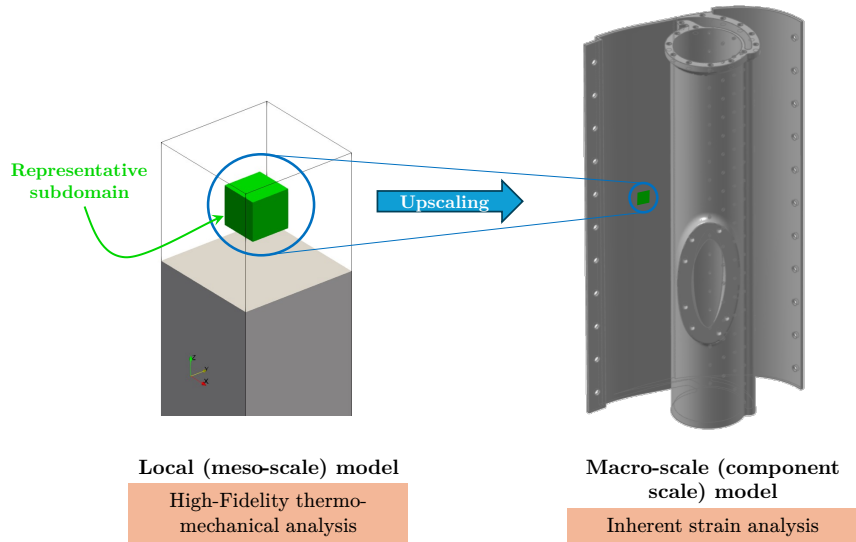


Figure 3.6: Illustration of multi-scale modelling.

3.2.4 Material deposition modelling

In *ISM*, material deposition is simulated using the birth–death element technique, as described in Section 3.1.3.2. With this approach, all elements are initially inactive and are activated in sequence according to the build process.

Unlike high-fidelity moving heat source models, *ISM* operates at a *layer-level* resolution: in each time step, elements corresponding to an entire layer (or a lumped set of layers) are activated simultaneously. Consequently, the *element search algorithm* used for element activation is relatively simple. The new layer is defined by a plane normal to the build direction, and elements intersecting this plane (as well as those directly below) are selected for activation. This approach reduces computational overhead compared to more fine-grained scanning-based strategies.

3.2.5 FE mesh considerations

An effective *FE* mesh for the inherent strain method should balance geometric accuracy with computational efficiency. A common approach is ensuring at least one element per lumped layer, enabling sequential activation. Voxel-based meshes naturally facilitate this strategy, as each "slice" of elements corresponds to a lumped layer, simplifying layer-wise activation and node compatibility.

However, if the *FE* framework supports advanced activation techniques, such as partial element activation or level-set methods, strict adherence to a layered mesh becomes less critical. In such cases, flexible meshing strategies can be used to better capture geometric details.

3.2.5.1 FE technology used

Since *ISM* relies on linear-elastic simulations, the standard irreducible *FE* formulation is sufficient, eliminating the need for specialized incompressibility treatments.

3.2.6 Time discretization

ISM simulations are not physically time-dependent; "time" is merely a layer index. Each step activates a layer (or a lumped set of layers) and solves a linear-elastic equilibrium problem. This sequence is repeated until the full part is simulated, meaning the total number of time steps equals the number of simulated layers.

3.3 Enhanced inherent strain method (EISM)

3.3.1 General principles

Although the original ISM can effectively predict distortions for many PBF-LB applications, its simplifying assumptions can cause discrepancies in components involving steep thermal gradients, non-uniform geometries, or intricate scanning strategies. To address these limitations, an *Enhanced Inherent Strain Method (EISM)* was developed (Chapter 7).

In the original ISM, each deposited layer inherits a constant inherent strain state upon activation, often neglecting transient temperature histories. While this simplification reduces computational cost, it can lead to inaccurate distortion predictions in geometrically complex regions.

By contrast, the EISM retains the core principle of prescribing a precomputed inherent strain tensor but augments it with the computed part-scale thermal history. In other words, the inherent strain tensor is dynamically adjusted on a layer-by-layer basis, accounting for temperature-dependent expansion and contraction effects. This refinement enables a more accurate representation of geometry- and boundary-condition-induced thermal effects.

3.3.2 Modelling approach

The EISM follows a sequentially coupled layer-by-layer thermo-mechanical workflow. Figure 3.7 provides an overview: instead of applying a single, constant *inherent strain* at the moment of layer activation, the EISM first computes the *average thermal history* of each (lumped) layer using a simplified heat transfer analysis. Based on this thermal history, the effective inherent strain tensor is dynamically updated to reflect temperature-dependent strain.

Thus, the methodology integrates the thermo-mechanical analysis outlined in Section 3.1 with the inherent strain approach described in Section 3.2.

3.3.2.1 Thermal analysis

The layer-by-layer part-scale thermal model follows the approach outlined in previous studies [59]. In this work, it is used to calculate the average temperature field evolution of the printed domain before the subsequent (lumped) layer is deposited.

The heat transfer analysis generally follows the approach described in Section 3.1.1. However, rather than explicitly modelling the movement of the heat source, a gradual

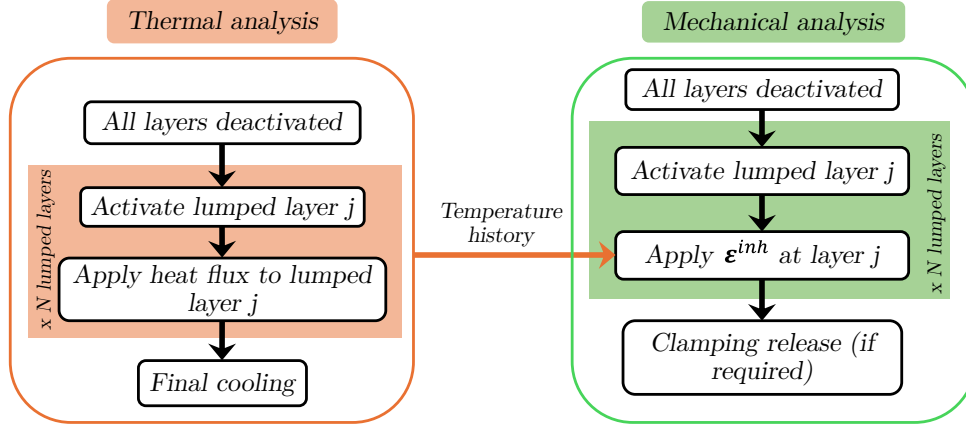


Figure 3.7: Overview of the EISM methodology, illustrating the sequential coupling between part-scale thermal and mechanical analyses.

heating strategy is applied over a macro-volume. This consists of imposing a time-averaged volumetric heat source on each lumped layer during an equivalent time step. The heat input for the j -th lumped layer is computed as:

$$\dot{Q}_j = \frac{\sum_{i=n \cdot (j-1)+1}^{n \cdot j} (\dot{Q}_i \cdot t_i^{\text{laser}})}{\sum_{i=n \cdot (j-1)+1}^{n \cdot j} (t_i^{\text{laser}} + t_i^{\text{recoater}})} , \quad (3.32)$$

where i is the layer index, n denotes the number of layers in each lump, and t_i^{laser} and t_i^{recoater} represent the laser exposure and recoating times for layer i , respectively.

This approach ensures energy equivalence with the actual process, while keeping the total simulation time unchanged.

The proposed thermal analysis captures the *global* temperature evolution at part scale, assuming certain simplifications that are not critical for this methodology:

- *Smeared-out scanning path*: In reality, the laser scanning pattern moves rapidly across the powder bed, causing localised heating and cooling cycles. By contrast, the lumped volumetric approach averages the total heat input across each macro-layer, thereby smoothing out local temperature peaks and gradients.
- *Geometric sensitivity*: Thin walls, overhangs, and complex features may undergo sharp local thermal gradients. These localized effects are only partially captured in the macro-scale model.
- *Boundary conditions*: While boundary heat losses can be specified to reflect different cooling conditions, localized boundary effects (e.g., around supports or small contact areas) may not be fully resolved by the time-averaged approach.

3.3.2.2 Mechanical analysis

The mechanical formulation follows [Section 3.1.2](#), with the key distinction that the inherent strain tensor is now temperature-dependent.

The inherent strain tensor includes all non-elastic strain components:

$$\boldsymbol{\varepsilon}^{inh} = \boldsymbol{\varepsilon}^{total} - \boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon}^{th} + \boldsymbol{\varepsilon}^{pl} + \boldsymbol{\varepsilon}^{act} \quad , \quad (3.33)$$

where $\boldsymbol{\varepsilon}^{th}$ is the thermal strain tensor, $\boldsymbol{\varepsilon}^{pl}$ is the plastic strain tensor, and $\boldsymbol{\varepsilon}^{act}$ is the activation strain tensor.

In the original [ISM](#), $\boldsymbol{\varepsilon}^{inh}$ is assumed constant for each material point and applied upon material deposition. This precomputed inherent strain tensor, denoted as $\boldsymbol{\varepsilon}^{inh,0}$, is subsequently used as input data in methodologies based on inherent strain theory.

The [EISM](#) enhances the original approach by incorporating temperature dependence. The scope is to make $\boldsymbol{\varepsilon}^{inh}$ both temperature- and time-dependent, using the average temperature of the deposited domain. Consequently, $\boldsymbol{\varepsilon}^{inh,0}$ is enhanced with the thermal strain history calculated in the layer-by-layer macro-scale thermal analysis (as detailed in [Section 3.3.2.1](#)). Thus, the inherent strain $\boldsymbol{\varepsilon}^{inh}$ applied in [EISM](#) is expressed as:

$$\boldsymbol{\varepsilon}^{inh} = \boldsymbol{\varepsilon}^{inh,0} + \Delta\boldsymbol{\varepsilon}^{th} \quad . \quad (3.34)$$

The thermal strain depends on the thermal field and is computed as:

$$\boldsymbol{\varepsilon}^{th} = [\alpha(T) \cdot (T - T_{ref}) - \alpha(T_0) \cdot (T_0 - T_{ref})] \mathbf{I} \quad , \quad (3.35)$$

where T is the current temperature, $\alpha(T)$ is the temperature-dependent secant thermal expansion coefficient, T_{ref} is the reference temperature for the expansion coefficient and T_0 is the initial temperature of the material at the start of the simulation.

Note that $\boldsymbol{\varepsilon}^{inh,0}$ typically accounts for the total thermal deformation during the cooling procedure. Thus, for $T = T_{ref}$, the deformation reaches its maximum value:

$$\boldsymbol{\varepsilon}^{th,0} = [-\alpha(T_0) \cdot (T_0 - T_{ref})] \mathbf{I} \quad . \quad (3.36)$$

However, the thermal analysis provides the temperature field of the component just before the deposition of the next (lumped) layer. Therefore, the actual thermal deformation is recovered by [EISM](#) by including the missing contribution $\Delta\boldsymbol{\varepsilon}^{th}$, defined as:

$$\Delta\boldsymbol{\varepsilon}^{th} = [\alpha(T) \cdot (T - T_{ref})] \mathbf{I} \quad . \quad (3.37)$$

Thus, the $\boldsymbol{\varepsilon}^{inh}$ applied in [EISM](#) is:

$$\boldsymbol{\varepsilon}^{inh} = \boldsymbol{\varepsilon}^{inh,0} + [\alpha(T) \cdot (T - T_{ref})] \mathbf{I} \quad , \quad (3.38)$$

where T is the current temperature at the component.

At the end of the process, when all material points reach T_{ref} , $\Delta\boldsymbol{\varepsilon}^{th}$ reduces to zero, making the applied $\boldsymbol{\varepsilon}^{inh}$ identical to that of the original [ISM](#).

Additionally, unlike the [ISM](#), the [EISM](#) considers *temperature-dependent material properties*, leading to different thermo-mechanical behaviour as the process progresses.

3.3.3 Time discretization

Time discretization in the EISM is directly linked to the layer lumping strategy, with implications for spatial and temporal resolution. Based on the gradual heating approach described in Section 3.3.2.1, the time step for the j -th lumped layer is:

$$\Delta t_j = \sum_{i=n \cdot (j-1)+1}^{n \cdot j} \left(t_i^{\text{laser}} + t_i^{\text{recoater}} \right), \quad (3.39)$$

where i is the layer index, n is the number of layers in each lump, and t_i^{laser} and t_i^{recoater} correspond to the laser exposure and recoating times for layer i , respectively.

The layer lumping strategy must be carefully selected, as plastic strain typically stabilizes only after several layers have been deposited, as shown in [67]. Since the objective is to enhance $\epsilon^{\text{inh},0}$ while preserving the plastic and activation components unchanged, the minimum number of layers considered in the calculations must be thoughtfully chosen. Conversely, excessive lumping should also be avoided, as it may compromise the accuracy of the temperature field. This consideration is also closely related to mesh resolution, as finer lumping necessitates smaller elements.

3.3.4 Other modelling aspects

The same birth-death (element activation) approach described in Section 3.1.3.2 is employed.

No specialised element formulation beyond the standard irreducible FE formulation is required, as a temperature-dependent thermo-elastic material model is employed, meaning that plasticity-related issues do not arise.

The mesh generation requirements are identical to those of the ISM.

3.3.5 Comparison with temperature-dependent and extended inherent strain approaches

In recent years, several researchers have proposed *extended* or *modified* Inherent Strain (IS) techniques to address the limitations of the classic approach. This section compares the EISM proposed in this thesis with two notable alternatives:

1. A temperature-dependent modified ISM developed by Dong et al. [30] for Directed Energy Deposition - Arc (DED-Arc), and
2. A new variant of ISM introduced by Pourabdollah et al. [63] for PBF-EB.

Dong et al. (Temperature-dependent modified ISM for DED-Arc). Dong et al. proposed a segment-wise inherent strain assignment strategy, in which each deposited DED-Arc layer is subdivided, and each segment is assigned a distinct inherent strain derived from the interpass temperature computed through a *flash-heating* thermal simulation. While this method effectively captures heat accumulation effects typical of the DED-Arc process, it applies a single inherent strain value per segment based solely on the temperature at the moment of deposition. As a result, subsequent temperature

changes do not modify the inelastic strain field, which remains piecewise constant throughout the simulation.

In contrast, the **EISM** presented in this thesis begins with a baseline tensor, $\epsilon^{\text{inh},0}$, obtained from a high-fidelity, meso-scale multi-layer simulation (see [Chapter 6](#)). This baseline strain is then *continuously updated* on a layer-by-layer (or lumped-layer) basis, using the evolving part-scale thermal field. In this way, any temperature variations due to geometry or boundary conditions can influence the final distortion by dynamically modifying the inherent strain field.

Pourabdollah et al. (New variant ISM for PBF-EB). Pourabdollah et al. proposed a new variant of **ISM** intended to account for both compressive plastic strains near the melt pool and macro-scale thermal strains evolving during an **PBF-EB** build. They adopted a time-averaged volumetric heat input and layer agglomeration for the thermal simulation to reduce computational cost. While this approach successfully captures global thermal mismatches (similar in spirit to the macro-scale thermal analysis in **EISM**), they prescribe a single arbitrary plastic strain value per (lumped) layer. Their study also tests until acceptable agreement with measured out-of-plane distortion in an overhang region is achieved. However, this trial-and-error calibration leaves the physical origin and magnitude of the imposed plastic strain values somewhat empirical.

By contrast, **EISM** combines (i) a physically motivated baseline inherent strain tensor from detailed meso-scale simulation, and (ii) an evolving part-scale thermal correction. The mechanical equilibrium is solved each time a new (lumped) layer is activated, incorporating spatially varying thermal effects. Therefore, geometric regions subject to part-scale thermal gradients receive updated inherent strain corrections. This synergy allows **EISM** to capture the resulting distortions in a manner more tightly grounded in physical process data.

3.4 Implementation in computational tools

The finite element methodologies developed in this thesis were implemented in two different software frameworks: **FEMUSS** and **Abaqus®**. Both platforms were employed at various stages of the research, depending on the specific requirements of each simulation.

FEMUSS

FEMUSS (Finite Element Method Using Sub-grid Scales) is an advanced computational framework developed at the International Center for Numerical Methods in Engineering (**CIMNE**) [57]. Designed for high-fidelity numerical simulations, **FEMUSS** integrates **AMR**, thermo-mechanical coupling, and high-performance computing capabilities, making it particularly suited for addressing complex multi-physics problems in research and engineering. All modules implemented within **FEMUSS** interact in an optimized manner to deliver fast and accurate numerical simulations based on the Finite Element Method (**FEM**).

FEMUSS has been tailored to support various [AM](#) technologies, enabling both high-fidelity thermo-mechanical analyses and simplified inherent strain-based simulations. Additionally, its automatic mesh generation from scanning-path data and its multi-criteria approach for [AMR](#) significantly enhance its usability.

Although FEMUSS offers powerful features such as adaptive meshing (critical for reducing computational costs in computationally demanding thermo-mechanical models), certain capabilities, such as material removal for partial cutting operations, were not available at the outset of this doctoral project. However, FEMUSS evolved substantially throughout the course of this research. Consequently, it became the primary tool for large-scale and detailed thermo-mechanical simulations, particularly in cases where automatic meshing and adaptive mesh refinement were essential for ensuring accuracy while minimizing computational time.

Abaqus

Abaqus® is a widely used commercial finite element platform that provides a general-purpose environment with some specialized features for additive manufacturing simulation, such as predefined material deposition frameworks. Its ease of setup and robust solver make it suitable for various engineering analyses. However, Abaqus lacks a built-in adaptive meshing strategy comparable to the one required for the most advanced high-fidelity thermo-mechanical simulations presented in this thesis. Additionally, it does not include an automatic mesh generation tool for [AM](#).

For simulations that did not require adaptive refinement (such as certain simplified models or smaller-scale analyses), Abaqus served as a reliable option. In addition, it was used for analyses that required cutting of supports. Nevertheless, the absence of real-time adaptive meshing limited its applicability for the most computationally demanding simulations discussed in this work.

Summary

Both FEMUSS and Abaqus were employed at different stages of this research. FEMUSS became the principal framework for high-fidelity, adaptive thermo-mechanical simulations due to its advanced meshing and refinement capabilities. In contrast, Abaqus provided a convenient platform for smaller problems and specialized tasks where adaptive refinement was not required. The complementary use of these two tools ensured that the numerical methodologies developed in this thesis were effectively implemented across a wide range of computational scenarios.

4

EXPERIMENTAL WORK

This chapter provides a detailed description of the experimental campaign conducted to support the calibration and validation of the proposed numerical models. The experiments were carried out at LORTEK using its [PBF-LB](#) facilities and measurement equipment. Three different geometries were investigated, each serving a specific purpose:

- **Twin-cantilever beams:** Small-scale specimens designed to measure distortion after partial cutting from the baseplate. Primarily used for *calibration*.
- **Non-symmetric bridge:** A mid-sized geometry for capturing both *temperature history* and *distortion data*, including partial support removal and residual stress measurements. Used for *both calibration and validation*.
- **Steady Blowing Actuator (SBA):** A large, complex industrial component selected to assess the model's applicability to real-world geometries. Used for *validation*.

All specimens were fabricated using the [PBF-LB](#) process with Ti-6Al-4V powder. The experiments were designed to capture *temperature evolution*, *distortion*, and *residual stress*, ensuring a comprehensive dataset for model calibration and validation.

After manufacturing, geometric deviations were recorded using both [CMM](#) probing and high-resolution 3D scanning. Residual stress measurements were conducted on the bridge using the incremental hole drilling method. Additionally, partial cutting via [wEDM](#) was performed on some coupons to measure net distortion as residual stress was released.

4.1 Test geometries and materials

4.1.1 *Twin-cantilever beams*

A well-established geometry for studying distortion in PBF-LB is the "twin-cantilever" coupon, schematically illustrated in Figure 4.1. This geometry consists of two cantilever beams connected by a narrow central column attached to the baseplate. Once printing is complete, the support legs connecting the cantilever beams to the baseplate on each side are removed via wEDM, causing the beams to bend upward due to the redistribution of residual stress. Therefore, the twin-cantilever geometry has been widely used for developing, calibrating, and validating simulation frameworks.

Figure 4.2 presents a set of as-built twin-cantilever beams prior to partial wEDM cutting.

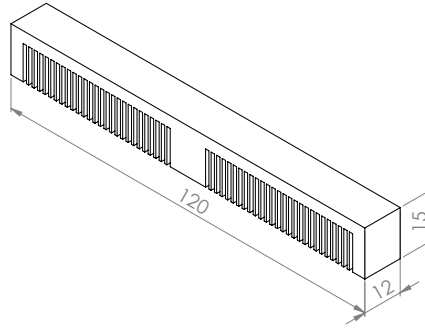


Figure 4.1: Schematic of the twin-cantilever geometry (dimensions in mm).

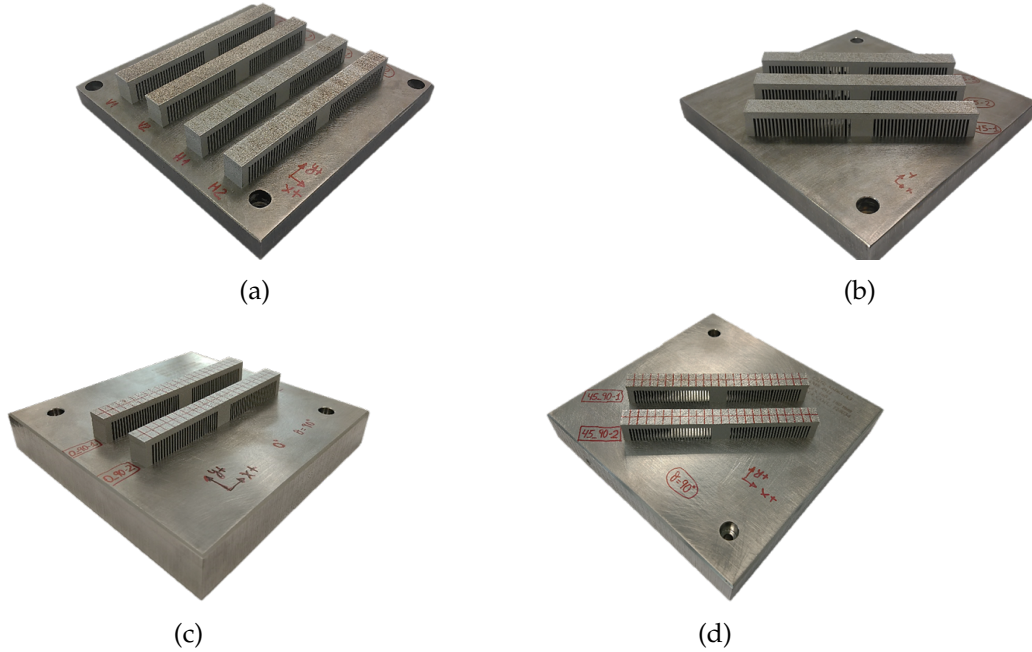


Figure 4.2: As-built twin-cantilever beams on a $150 \times 150 \times 15$ mm baseplate: (a) Baseplate-1, (b) Baseplate-2, (c) Baseplate-3, and (d) Baseplate-4.

4.1.2 Non-symmetric bridge

The second geometry, referred to as the "non-symmetric bridge" and illustrated in Figure 4.3, was designed to capture both in-process and post-manufacturing distortion using partial cutting to release residual stresses, following a similar principle as the twin-cantilever beams. Additionally, this geometry:

- Facilitates the installation of thermocouples in the baseplate beneath various regions,
- Allows for simplified distortion measurements along front and top surfaces, and
- Enables a partial cut release operation on one side to measure distortion changes due to residual stress relief.

Figure 4.4 shows the manufactured non-symmetric bridge immediately after printing.

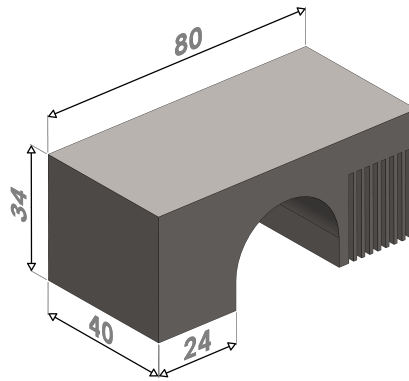


Figure 4.3: CAD model of the non-symmetric bridge geometry (dimensions in mm).

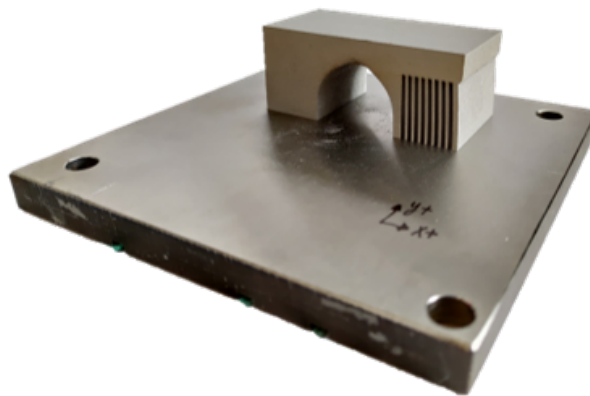


Figure 4.4: As-built non-symmetric bridge on a $150 \times 150 \times 24$ mm baseplate.

4.1.3 Steady Blowing Actuator (SBA)

The third and most complex geometry investigated was a *Steady Blowing Actuator (SBA)*, shown in Figure 4.5. Its bounding box measured approximately $101 \times 137 \times 306 \text{ mm}^3$ and featured internal holes, a tall tube-like structure, and two wing-like fins protruding from the main body. This aeronautical component is used in active flow control applications, typically mounted on an aircraft structure to delay flow separation. The SBA was designed without internal supports. This component was developed as part of the FLOWCAASH project [34], a European Union H2020 research initiative aimed at manufacturing flow control actuators for aircraft using PBF-LB.

Figure 4.6 depicts the as-built SBA. Additional control samples were printed in the same batch to assess mechanical properties, powder oxygen levels, and other characteristics.

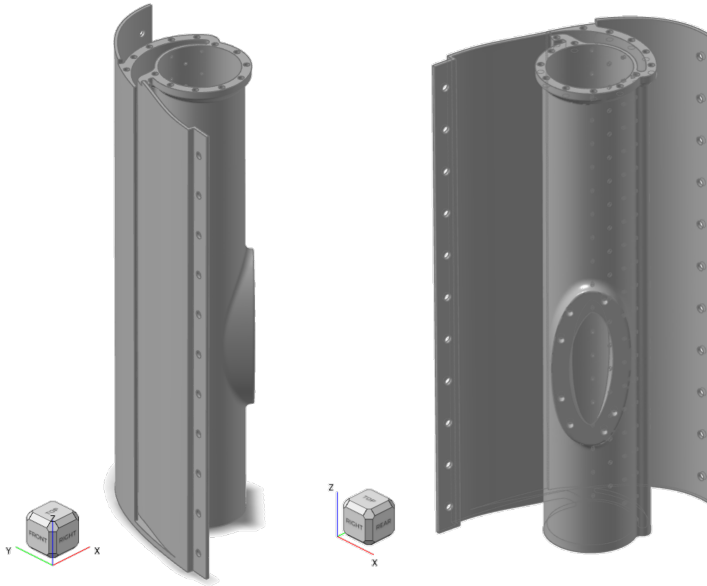


Figure 4.5: Two views of the CAD model of the SBA geometry (dimensions in mm).



Figure 4.6: As-built SBA on a $160 \times 160 \times 30 \text{ mm}$ baseplate.

4.1.4 Material: Ti-6Al-4V powder

All specimens were printed using gas-atomised Ti-6Al-4V Grade 23 powder ($\text{O} < 1300 \text{ ppm}$). The powder composition, listed in Table 4.1, meets ASTM F3001-14 specifications for Ti-6Al-4V ELI (Extra Low Interstitial) in PBF-LB applications.

The powder was characterised to confirm compliance with requirements for composition, morphology, humidity, flowability, particle size distribution, and internal porosity (Table 4.2).

Prior to each build, the powder was sieved to remove agglomerates and oversized particles, ensuring a reproducible layer deposition.

Oxygen control is critical in preventing embrittlement, maintaining ductility, and ensuring mechanical reliability. Excess oxygen destabilises the microstructure and

Table 4.1: Composition of as-atomised Ti-6Al-4V Grade 23 powder (wt.%).

Ti	Al	V	Fe	C	S	H	N	O
Bal.	6.30	3.93	0.045	0.012	<0.005	0.0056	0.0105	0.085

Table 4.2: Summary of Ti-6Al-4V powder characteristics.

Powder characteristics	Value
Humidity (as-received)	8.9 %
Apparent density	2.383 g/cm ³
Flowability (Hall flowmeter)	Continuous flow, 53 s required for 50 g
Internal porosity	0.06 %
Particle size distribution	D10: 24 µm; D50: 40 µm; D90: 54 µm

reduces fatigue resistance. To mitigate this, a protective argon atmosphere was maintained inside the build chamber, ensuring an oxygen content of no more than 0.2%.

4.2 Manufacturing equipment

4.2.1 PBF-LB machines

Two different **PBF-LB** machines were used in this study, selected based on machine availability, component geometry, and specific experimental requirements.

4.2.1.1 SLM 250 (MCP-ReaLizer)

The twin-cantilever coupons were fabricated using an *SLM 250* (MCP-ReaLizer GmbH, Germany) machine, shown in [Figure 4.7a](#). This system is compatible with a wide range of metallic powders, including titanium alloys, aluminium alloys, stainless steel (306L), tool steels, and nickel-based superalloys such as Inconel. Technical specifications of the *SLM 250* are summarised in [Table 4.3](#).

4.2.1.2 SLM 280 HL (SLM Solutions)

The non-symmetric bridge and the SBA components were fabricated using an *SLM 280 HL* (SLM Solutions, Lübeck, Germany) machine, shown in [Figure 4.7b](#). This advanced **PBF-LB** machine also supports a broad spectrum of metallic powders, including cobalt-chromium alloys, aluminium alloys, stainless steels, titanium alloys, and nickel-based superalloys. Detailed specifications for the *SLM 280 HL* are listed in [Table 4.3](#).

Table 4.3: Technical specifications of the SLM 250 and SLM 280 HL LPBF machines.

Technical specifications (units)	SLM 250	SLM 280 HL
Build volume (mm ³)	250 × 250 × 300	280 × 280 × 365
Laser power (W)	200 (IPG fibre laser)	400 (IPG fibre laser)
Build rate (cm ³ /h)	2 – 10	≤ 55
Layer thickness (μm)	20 – 100	20 – 75
Minimum feature size (μm)	≈ 100	150
Beam focus diameter (μm)	30 – 300	80 – 115
Maximum scan speed (m/s)	10	10
Maximum preheating temperature (°C)	200	200



(a)



(b)

Figure 4.7: PBF-LB equipment used in this study, belonging to LORTEK: (a) SLM 250 (MCP-Realizer GmbH, Germany); (b) SLM 280 LH (SLM Solutions, Lübeck, Germany).

4.3 Measurement equipment and instrumentation

4.3.1 Dimensional metrology: CMM and 3D scanning

4.3.1.1 Coordinate-measuring machine (CMM)

Dimensional inspections were conducted using a CMM Mitutoyo CRYSTA APEX S 7106 (Mitutoyo Corporation, Kawasaki, Japan) (see Figure 4.8). The CMM was used to quantify distortions at predefined points along all twin-cantilever beam specimens and the non-symmetric bridge. This equipment provides a measurement accuracy of approximately ± 0.002 mm in the X, Y, and Z axes, making it suitable for precise inspection tasks of manufactured components.

4.3.1.2 *Structured light 3D scanning*

Full-field measurements of geometries, specifically the non-symmetric bridge and the [SBA](#) actuator, were performed using a structured-light stereo vision scanner *Ensensio X36* (IDS Imaging Development Systems GmbH, Obersulm, Germany). This scanner offers robust depth data acquisition even under challenging surface conditions, such as low contrast or uniform texture, which are common in parts produced by the [PBF-LB](#) process. The resulting dense point clouds were post-processed and subsequently compared against reference geometries, allowing for comprehensive full-field deviation analyses.

4.3.2 *Thermocouple-based temperature measurement*

Temperature measurements were conducted using K-type thermocouples (*5SRTC-GG-KI-30-2M*, Omega Engineering, Norwalk, CT, USA) with a probe diameter of approximately 0.5 mm. These thermocouples were embedded into the baseplate of the non-symmetric bridge to monitor temperature evolution during the build process. Data acquisition was performed using a high-speed data logger with adjustable sampling frequencies ranging from 10 to 1000 Hz, tailored to the specific experimental requirements.

4.3.3 *Residual stress measurement*

Incremental hole-drilling residual stress measurements were performed using a *Restan MTS-3000* system (SINT Technology, Calenzano, Italy) (see [Figure 4.9](#)) in accordance with the ASTM E837 standard. This equipment comprises high-precision strain-gauge rosettes (*CEA-062UL-120*, Micro-Measurements, Vishay Precision Group) and an automated drilling head fitted with a tungsten carbide milling cutter of diameter 1.6 mm, resulting in final hole diameters of approximately 1.8 mm. Data acquisition and residual stress calculations were conducted using dedicated analysis software (*EVAL*), employing Tikhonov regularisation to improve the stability and accuracy of residual stress results.

4.3.4 *Wire electrical discharge machining (wEDM)*

Partial cutting operations were performed using [wEDM](#). While the specific equipment details were unavailable, cutting parameters were carefully selected to minimise thermal and mechanical effects during machining. This precaution was essential to ensure that the residual stress state of the specimens remained unaffected. The primary objective of the [wEDM](#) operation was to release accumulated stresses, leading to measurable elastic spring-back deformations that serve as indirect indicators of residual stress distribution.

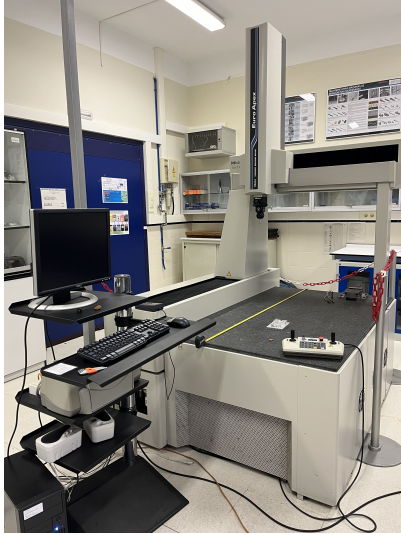


Figure 4.8: Mitutoyo CRYSTA APEX S 7106 CMM.

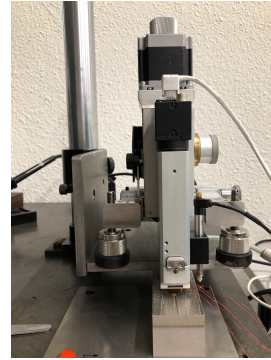


Figure 4.9: Restan MTS-3000 system used for incremental hole-drilling residual stress measurements.

4.4 Experimental procedure

This section provides a detailed overview of the manufacturing processes and measurement procedures implemented for each geometry. The main objectives were to accurately quantify distortions, record temperature histories, and characterise residual stresses. The specific methodologies employed to achieve these objectives are outlined below. Routine preparation steps, such as general CAD modelling, slicing, or standard machine setup operations, are considered conventional and thus not detailed explicitly.

4.4.1 *Twin-cantilever beams*

A total of eleven twin-cantilever beams were manufactured across four Ti-6Al-4V baseplates ($150 \times 150 \times 15 \text{ mm}^3$) using five distinct scanning strategies. These experiments were conducted to measure residual stress-induced distortions for the calibration of the inherent strain tensor.

4.4.1.1 *Manufacturing procedure*

Twin-cantilever beams were printed using the SLM 250 system under an argon atmosphere, with a preheating temperature of 200°C and a nominal layer thickness of $50 \mu\text{m}$. The calibrated process parameters are provided in [Table 4.4](#). These parameters were optimised to ensure quality requirements such as high density, low surface roughness, suitable microstructure, and optimal mechanical properties.

Five scanning strategies were investigated: longitudinal (0°), transverse (90°), diagonal (45°), 90° rotating, and 45° rotating scan patterns, as illustrated in [Figure 4.10](#). These strategies were tested to assess their influence on final distortion.

Table 4.4: Calibrated process parameters used for printing all components in SLM 250.

Parameter	Hatch	Boundary	Contour
Laser power (W)	200	200	200
Scanning speed (mm/s)	950	1100	1100
Beam diameter (mm)	0.18	0.18	0.18
Hatch spacing (mm)	0.12	–	–

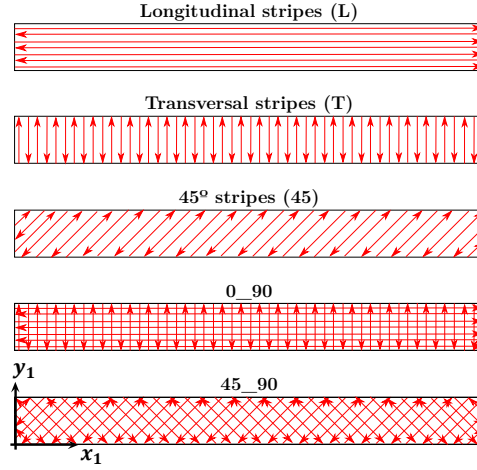


Figure 4.10: Illustration of different scanning strategies investigated for twin-cantilever coupons.

4.4.1.2 *wEDM partial cutting*

After manufacturing, the twin-cantilever coupons remained in the as-built state on the baseplate until they were partially cut using *wEDM*, leaving only the central column attached to the baseplate (see Figure 4.11). Upon release, the beam tips bent upward due to residual stress redistribution.

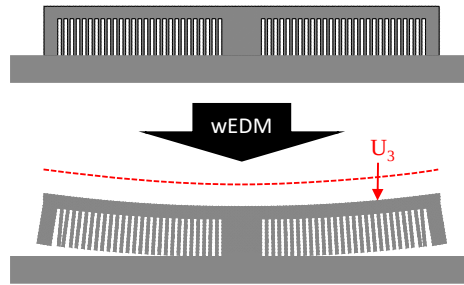


Figure 4.11: Twin-cantilever cutting and vertical distortion measurement.

4.4.1.3 *Distortion measurement*

Following *wEDM* cutting, distortions along the top centreline of each beam were measured at regular intervals of 5 mm using the *CMM* system described earlier (see Figure 4.12 for an example).

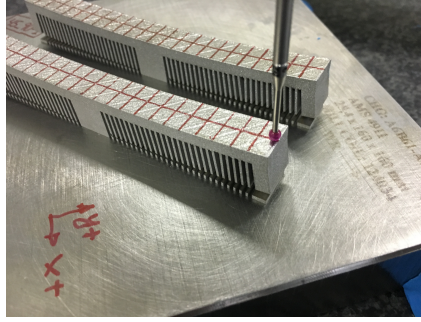


Figure 4.12: Probe of the CMM measuring a point on the upper surface of a twin-cantilever beam.

4.4.2 Non-symmetric bridge

A single non-symmetric bridge specimen was fabricated, specifically designed to measure temperature evolution, distortions, and residual stresses for both calibration and validation purposes.

4.4.2.1 Baseplate preparation and thermocouple installation

Six K-type thermocouples (Omega 5SRTC-GG-KI-30-2M) were embedded in machined blind holes as close as possible to the top surface of the baseplate ($150 \times 150 \times 24 \text{ mm}^3$), as shown in Figure 4.13. Additional details on the thermocouple placement are provided in the technical drawing in Figure 4.14.

The thermocouple wires were routed externally through the main door of the SLM 280 HL machine, as illustrated in Figure 4.15, and connected to a high-speed data logger. The sampling rate was dynamically adjusted, starting at 1000 Hz when the laser was near the measurement points, decreasing to 100 Hz as the process progressed, and finally reducing to 10 Hz during the cooling phase.

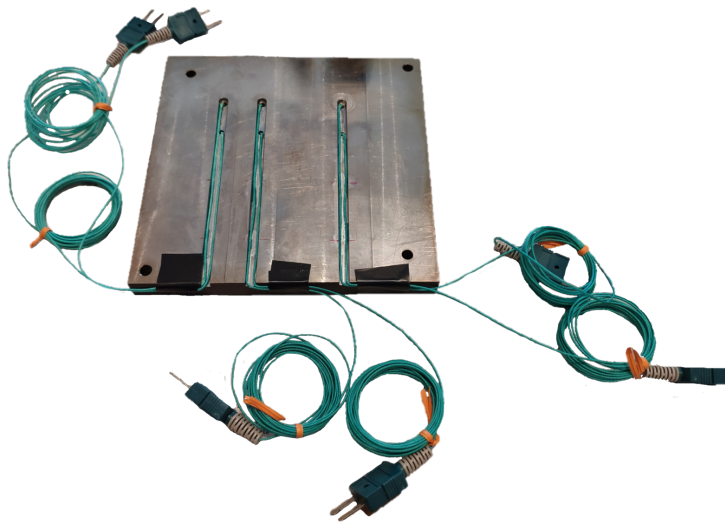


Figure 4.13: Thermocouple-integrated baseplate prepared for printing the non-symmetric bridge.

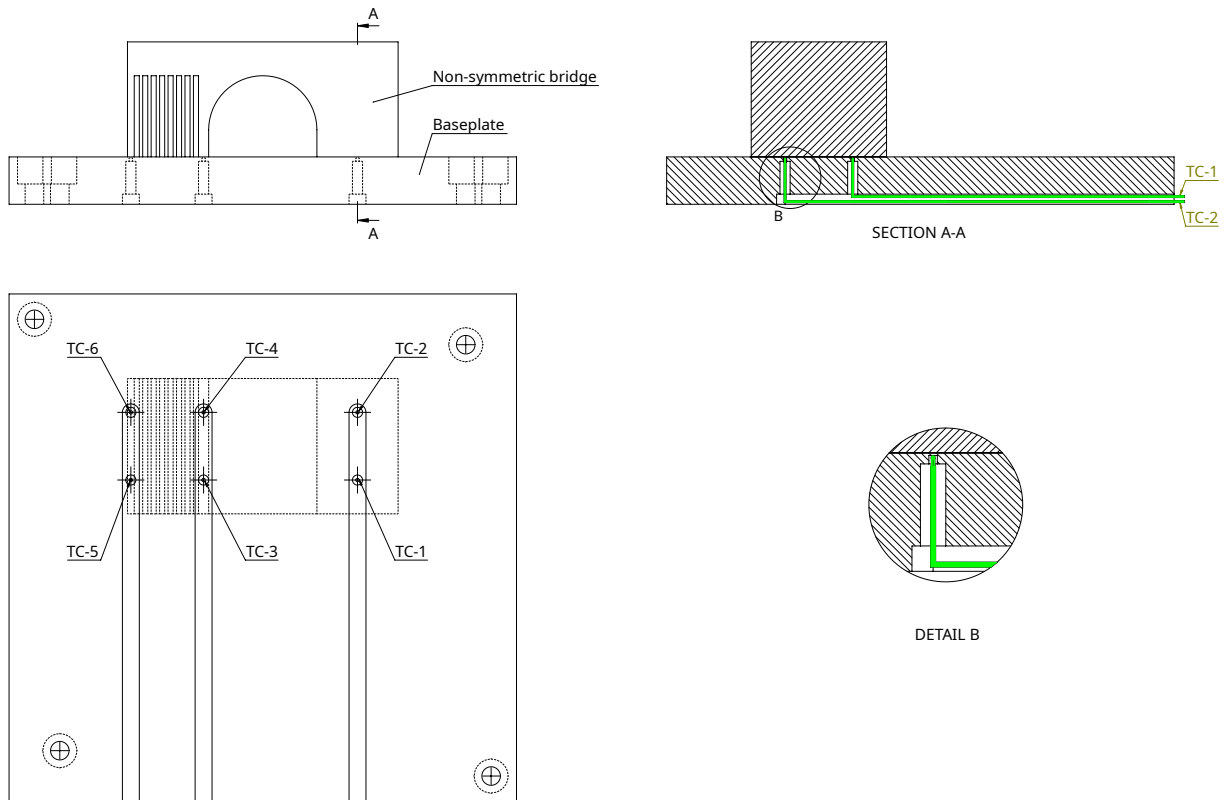


Figure 4.14: Draft of thermocouple (TC) locations within the baseplate. Each thermocouple is labelled as TC-x, indicating its specific position. The detail view provides a detailed representation of the thermocouple arrangement, highlighting their placement within machined blind holes to measure temperatures as close as possible to the top surface of the baseplate.

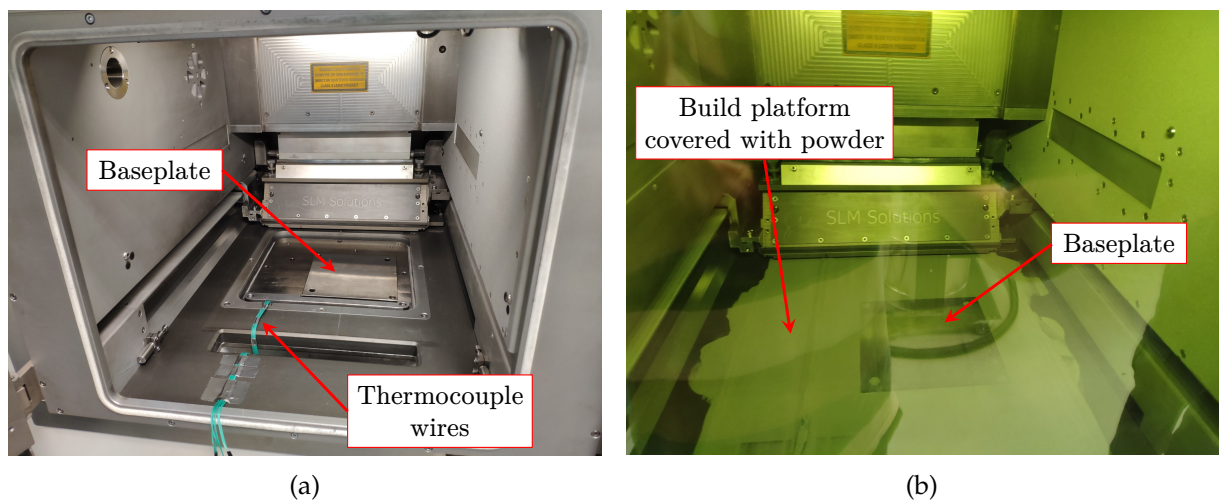


Figure 4.15: Experimental setup illustrating: (a) the installation of the wired baseplate within the build chamber, highlighting the routing of wires through the main door and (b) the initial setup before starting the printing process.

4.4.2.2 Manufacturing procedure

The non-symmetric bridge was manufactured on the SLM 280 HL machine under an argon atmosphere, with a preheating temperature of 200 °C and a nominal layer thickness of 60 μm . The calibrated process parameters for hatch, boundary and contour are provided in Table 4.5.

For the scanning strategy, an alternating laser scanning pattern with a rotational angle of 66.7° was employed (see Figure 4.16). This strategy is widely adopted to evenly distribute thermal stresses, thereby minimising the risk of warping and residual deformations in the printed component.

Table 4.5: Calibrated process parameters used for printing all components in SLM 280 HL.

Parameter	Hatch	Boundary	Contour
Laser power (W)	350	150	150
Scanning speed (mm/s)	1100	650	650
Beam diameter (mm)	0.08	0.08	0.08
Hatch spacing (mm)	0.12	—	—

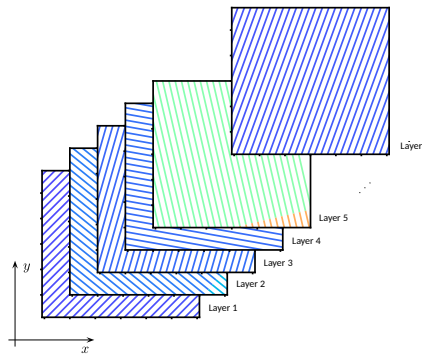


Figure 4.16: Schematic of the 66.7° scanning strategy used.

4.4.2.3 wEDM partial cutting

A partial wEDM cut was performed to release residual stresses from the overhanging region of the bridge. Figure 4.17 illustrates the state of the bridge before and after cutting.

4.4.2.4 Distortion and residual stress measurement

Initial distortion was measured along the vertical face (*front path* in Figure 4.18) using the CMM. After partial wEDM cutting, additional distortion measurements were taken along the upper surface (*top path* in Figure 4.18) at 5 mm intervals.

Residual stress measurements were conducted using incremental hole-drilling in accordance with the ASTM E837-13a standard. Measurements were taken at three carefully selected locations, as shown in Figure 4.19. Figure 4.20 provides a snapshot of the hole drilling process at point-1.

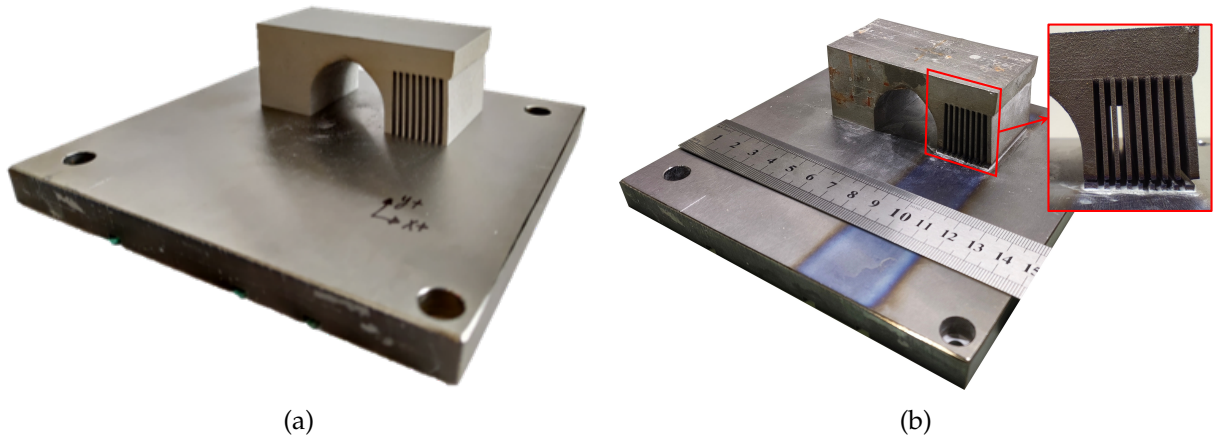


Figure 4.17: State of the bridge geometry before and after partial cutting to release residual stress: (a) before the cut, and (b) after the cut. The detailed view highlights the cut zone where the bridge was partially released from the baseplate.

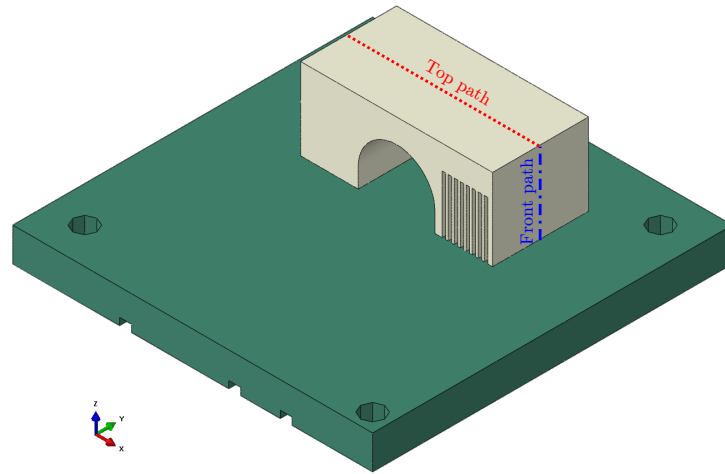


Figure 4.18: Schematic showing front and top paths where distortion measurements were taken for the non-symmetric bridge.

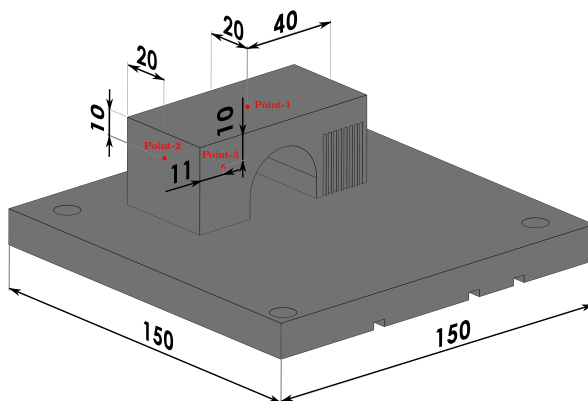


Figure 4.19: Locations of the three measurement points for residual stress analysis on the non-symmetric bridge.

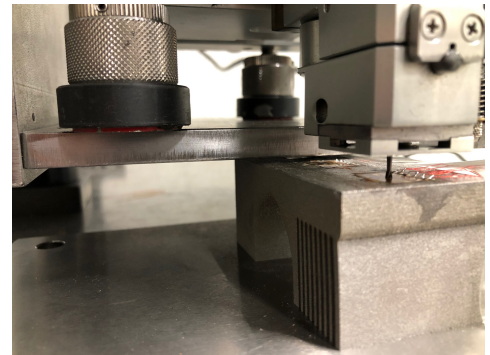


Figure 4.20: Hole drilling process at point-1.

4.4.3 *Steady Blowing Actuator (SBA)*

A single [SBA](#) geometry was manufactured as a validation case to demonstrate the applicability of the calibrated numerical models to complex industrial components.

4.4.3.1 *Manufacturing procedure*

The [SBA](#) was manufactured using the SLM 280 HL machine under an argon atmosphere, with a preheating temperature of 200 °C and a nominal layer thickness of 60 μm. To accommodate its taller geometry and minimise distortions caused by baseplate flexibility, the part was printed on a thicker Ti-6Al-4V baseplate (160 × 160 × 30 mm³), which also served to enhance heat dissipation. The same rotating scanning strategy (see [Figure 4.16](#)) and optimised process parameters (see [Table 4.5](#)) as those used for the non-symmetric bridge were employed.

4.4.3.2 *Distortion measurement*

The completed SBA geometry was measured using structured-light 3D scanning (Ensenso X36). The resulting dense point cloud was processed, aligned, and compared to the nominal CAD model to generate full-field deviation maps. This analysis provided a detailed quantification of distortions induced during the build process, serving as a key validation metric for numerical simulations.

4.4.4 *Summary of the experimental programme*

A concise overview of the key steps, sample quantities, and measurements performed for each geometry is presented in [Table 4.6](#). This structured experimental programme generated datasets necessary for calibrating and validating the numerical methods.

Table 4.6: Summary of experimental procedures for each geometry.

	Twin-Cantilever	Non-Symmetric Bridge	SBA Actuator
Machine	SLM 250	SLM 280 HL	SLM 280 HL
Number of samples	11	1	1
Thermocouples	None	6 positions	None
Scanning strategy	5 strategies	Rotating (66.7°/layer)	Rotating (66.7°/layer)
Distortion measurements	CMM	CMM	3D scanning
Residual stress measurements	Indirect (distortion)	Incremental hole drilling	None
w-EDM cutting	Partial support release	Partial support release	None

EMPIRICAL METHOD FOR INHERENT STRAIN CALCULATION

5.1 Introduction

This chapter presents one of the core articles integrated into this thesis. As outlined in previous sections, while high-fidelity thermo-mechanical simulations provide detailed insights into process physics, their high computational cost makes them impractical for iterative design processes and industrial applications. To address this, simplified modelling methodologies such as the [ISM](#) have been developed. However, a key challenge of [ISM](#) is that it requires an inherent strain tensor as input.

The article presented in this chapter tackles this issue by introducing an empirical procedure for inherent strain calibration based on inverse engineering techniques and experimental measurements conducted on twin-cantilever specimens. This approach not only provides reliable inherent strain values but also establishes a direct link between experimental observations and simplified numerical models.

5.2 Scientific contribution

This work makes several key contributions to the field of inherent strain modelling for [PBF-LB](#). First, it introduces an empirical calibration methodology adapted from welding mechanics to determine inherent strains in [PBF-LB](#). This procedure allows for the systematic derivation of inherent strain values based on experimentally measured distortions.

Second, the study provides a detailed analysis of the impact of scanning strategies on inherent strain formation, revealing that periodic scanning strategies yield in-plane isotropic inherent strains, simplifying numerical modelling. This insight facilitates more efficient simulation workflows by reducing anisotropy-related uncertainties in predictive models.

Finally, the proposed methodology is validated through an experimental campaign using twin-cantilever specimens. The results confirm that the inherent strain-calibrated numerical model predicts distortions within a 10% margin of error compared to experimental measurements. These findings establish a robust foundation for subsequent simulation studies and practical applications in industrial-scale process optimisation.

5.3 Summary and conclusions

This study demonstrates that an inverse engineering approach, combined with experimental data, can effectively calibrate inherent strains in PBF-LB processes. Through twin-cantilever specimen testing, it is shown that different scanning strategies result in distinct patterns of residual stress and distortion, with longitudinal scanning producing larger deformations than transversal or periodic strategies.

Using the determined inherent strain values, the numerical model successfully reproduces the experimentally observed distortions, with discrepancies remaining below 10%. These results validate the proposed empirical methodology and highlight its practical applicability for process simulation and optimization.

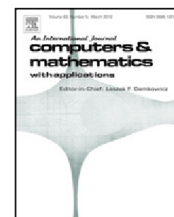
In the broader context of this thesis, this work not only provides a robust, experimentally validated calibration strategy but also lays the groundwork for the development of advanced simulation tools aimed at optimising additive manufacturing processes and reducing manufacturing costs.

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Empirical methodology to determine inherent strains in additive manufacturing



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ABSTRACT

Part distortion is a critical issue during Additive Manufacturing (AM) of metallic parts since it prevents this technology from being implemented at industrial level. To this regard, distortion prediction even from design stage has become crucial. Actually, numerical modelling methodologies play an important role here. Different modelling approaches have been developed but one of the most computationally efficient methodology to predict distortion is the so called inherent strain method. In this work an empirical methodology to determine inherent strains is presented. This is the input data in simplified Finite Element (FE) models in order to predict distortion and residual stress fields. These inherent strains are calculated considering layer lumping strategies that might be adopted in the numerical model as well. The procedure has been developed and validated using the well-known twin-cantilever beam structure. Ti-6Al-4V beams have been manufactured by LPBF technology following different scanning strategies. Distortion after support removal has been measured in order to be compared against numerical results. The methodology has been applied at coupon level giving accurate results and providing a preliminary validation.

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1. Introduction

Additive Manufacturing (AM) gathers various techniques for building three dimensional objects in a layer by layer sequence starting from a digital model [1,2]. This incomparable characteristic allows the production of complex, customised and fully optimised parts directly from the design stage, avoiding the need of expensive and restrictive conventional manufacturing processes. Therefore, it is nowadays widely considered that AM is the new paradigm for design and production of high performance components.

Laser Powder Bed Fusion (LPBF) is one of the most widespread powder-bed technology for metallic components. In these processes, the material is locally and rapidly heated and then allowed to solidify in order to form a dense geometry. The temperature history experienced by the material determines the microstructure and therefore the mechanical properties. Large thermal strains are involved in the process, generating residual stresses and distortions [3], affecting significantly the mechanical properties and causing dimensional inaccuracies to the final part. Henceforth, there are still serious obstacles toward its wider acceptance and establishment into modern industrial practice.

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The issues above are unknowns for the designer each time a part is manufactured by AM. Currently, they are tackled by expensive trial and error experiments until all requirements are fulfilled. This implies high manufacturing costs, increased even more due to the waste and scrap generated when quality inaccuracies between the designed and built components occur. Therefore, predictive methods such as the computational simulation are essential in an attempt to predict and control the aforementioned phenomena even at the design stage. Thermo-mechanical and thermo-microstructure behaviour modelling of AM processes is increasingly useful and necessary to deal with these challenges efficiently [4].

AM process modelling has its own challenges due to the multiphysics and multiscale character of the process. Its physical fundamentals are very similar to those of multi-pass welding processes. Thus, Finite Element Method (FEM) based on welding modelling techniques developed so far, can be adapted to develop AM simulations [5–8]. Accurate coupled thermo-mechanical simulations are considered as high-fidelity numerical models where the real weld pool moving along the scan path is modelled in detail according to Computational Welding Mechanics (CWM). Many researchers have successfully applied and validated this method in order to predict thermal, mechanical and microstructural histories [9–16]. Nevertheless, these high-fidelity modelling approaches have only been applied at coupon level since they are computationally impracticable for real size parts. Added difficulties such as longer process time, higher number of time-steps, etc. are the reasons behind this limitation. Particularly, AM processes like LPBF, where the weld pool size is very small compared to part size, are affected by these issues.

Consequently, several simplified methodologies have been developed in order to model this process at industrial scale level with the main aim of predicting distortions and residual stresses [17–21].

These methods can be classified into two categories. On the one hand, there are methods focused on reducing the computational effort by making more efficient and scalable the algorithms and the numerical methods required to solve the Finite Element (FE) problem [22], or by reducing the model size applying adaptive meshing techniques [23].

On the other hand, there are engineering approaches which make assumptions to simplify the physics behind the metal deposition process with the purpose of simulating distortions and/or residual stresses at part level. Some researchers [9] have simplified the heat source modelling, i.e. applying equivalent energy input at hatch, layer or even layer-compound level. Others have avoided even the heat transfer problem through applying equivalent shrinkage load in a purely mechanical analysis [21,24,25]. One of the most promising and efficient approach is the inherent strain method [25,26]. This well-known methodology has already been successfully applied to both CWM and AM processes [19]. It allows for replacing computationally costly thermo-mechanical simulations by a linear-elastic-mechanical one. The key point in this simplified analysis is to define which is the inherent strain or shrinkage load to apply in the model in order to capture the mechanical response of the fabricated component.

There are two approaches to determine these inherent strains as proposed in CWM [27]: (a) Multi-scale or local-global modelling; (b) Empirical approach.

The multi-scale modelling option consists of solving micro and/or meso-scale models to determine inherent strains at local level whereas in the second option, they are calibrated by means of experimental tests and calculations.

The work presented in this paper is focused on the development of an empirical methodology to determine inherent strains. In Section 2 all the experimental work carried out to develop the methodology and its validation is explained. The FE model based on the inherent strain methodology to predict distortions and residual stresses fields in LPBF is described in Section 3. The model is then calibrated looking for the most suitable inherent strains to be used. Section 4 is dedicated to the detailed description of the empirical procedure to determine inherent strains. Section 5 gathers both experimental and numerical results achieved for both calibration and validation stages. Finally, Section 6 presents the main conclusions of this work.

2. Experimental work

An overview of the experimental work carried out is provided here.

2.1. Experimental set-up

Several experimental trials were conducted in order to obtain data for the calibration phase described in Section 4. Different coupons were manufactured using a LPBF process. A SLM 250 (from MCP-Realizer) machine equipped with 200 W fibre laser was used. The machine has a construction space of 250 mm × 250 mm × 300 mm which can accommodate the production of components with maximum size. It must also be noted that the machine works with a protective atmosphere, being 0.2% the maximum oxygen allowable, in order to prevent titanium parts from oxidation.

Twin-cantilever type structures made of Ti-6Al-4V were fabricated over several thick baseplates (150 mm × 150 mm × 15 mm). Fig. 1 shows the geometry of the sample and its dimensions.

As shown in Fig. 2, 3 different scanning strategies with respect to the baseplate's reference system (xy) were employed to print the twin-cantilevers. A total number of 11 twin-cantilevers were manufactured in 4 baseplates and different batches. Their distribution and the scanning strategy assigned to each baseplate is represented in Fig. 3. The orientation of twin-cantilevers with respect to the main reference system (xy) leads to 5 different scanning strategies (see Fig. 4). The local coordinate system x_1y_1 attached to the beam is shown in Fig. 3. Hence, on the one hand 3 sets of twin-cantilevers were manufactured with longitudinal, transversal and 45° stripes without any rotation between layers. On the other hand, 2 more

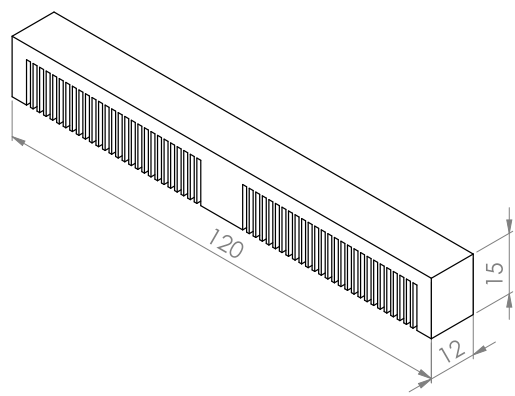


Fig. 1. Twin-cantilever specimen with dimensions in mm.

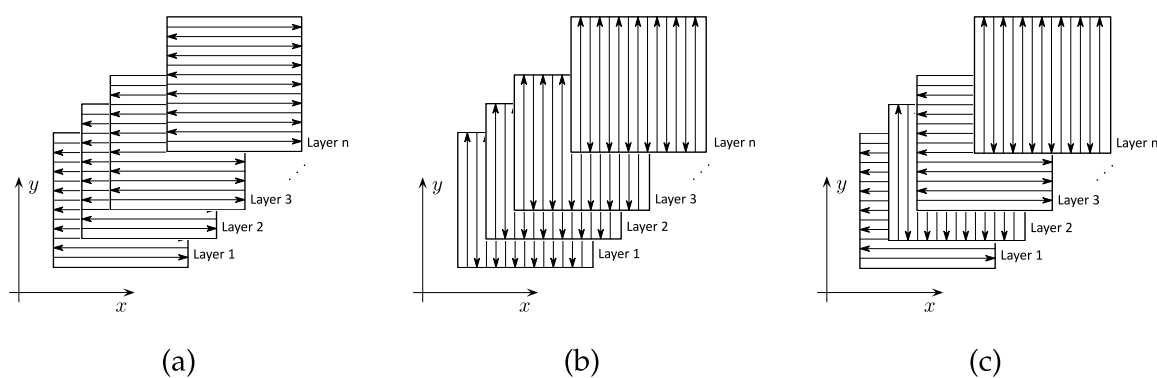


Fig. 2. Considered scanning strategies taking as reference the baseplate. (2(a)) 0° line constant scan pattern. (2(b)) 90° line constant scan pattern. (2(c)) 90° rotating scan pattern.

	Baseplate 1	Baseplate 2	Baseplate 3	Baseplate 4
Perspective view of the baseplate				
Top view of the baseplate				
Scanning strategy	 (b) (a)	 (a)	 (c)	 (c)

Fig. 3. Manufactured baseplates and corresponding scanning strategies used in each baseplate.

sets of beams were manufactured with 90° rotating scan pattern with different initial offset of the rotation angle (0° and 45°).

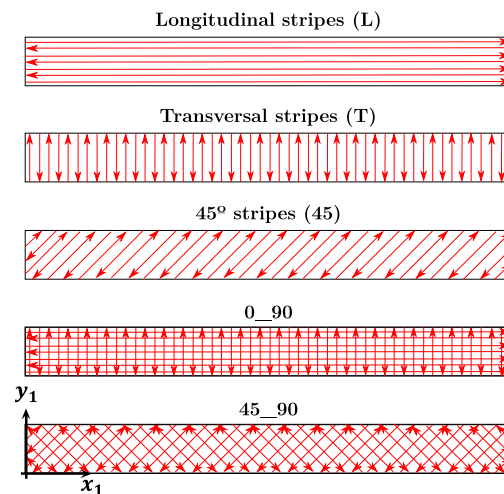


Fig. 4. Scanning strategies summary taking as reference the local coordinate system of the beam.

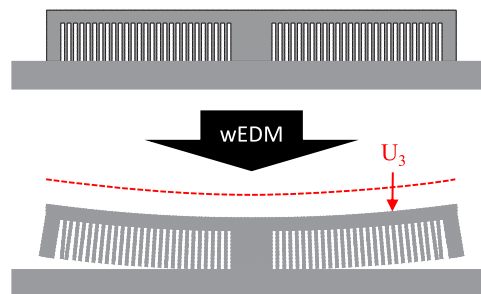


Fig. 5. Twin-cantilever cutting and vertical distortion measurement.

Table 1
LPBF process parameters.

	Hatch	Boundary	Contour
Laser power (W)	200	200	200
Scanning speed (mm/s)	950	1100	1100
Hatch distance (μm)	120	–	–
Beam diameter (μm)	180	180	180

The use of optimum process parameters is extremely important for producing satisfactory parts using these processes. In our particular case, previously optimised Ti-6Al-4V process parameters were employed (see Table 1). These parameters were adjusted for hatch, boundary and contour zones. The preheating temperature was 200 °C and the nominal layer thickness was 50 μm .

2.2. Measurement equipments

After manufacturing and without any stress relaxation treatment, the specimens were partially cut from the baseplate by wire Electrical Discharge Machining (wEDM), leaving the middle column attached to the baseplate. Thus, residual stress field cumulated during the manufacturing process was redistributed leading to the bending of the part. The final vertical distortion was measured on the top surface centre-line along the x_1 direction as illustrated in Fig. 5. Measurements were carried out by means of a Coordinate-Measuring Machine (CMM) every 5 mm along the centre-line in x_1 direction. This bending deformation is an indirect way of assessing the magnitude of residual stresses. Therefore, it has been used for the calibration of the inherent strains.

3. Finite element modelling of AM process by LPBF

3.1. Inherent strain method

The inherent strain method is an efficient method which enables a fast prediction of the residual stresses and distortions. The origin of the inherent strain method is directly related to Computational Welding Mechanics and it has been widely

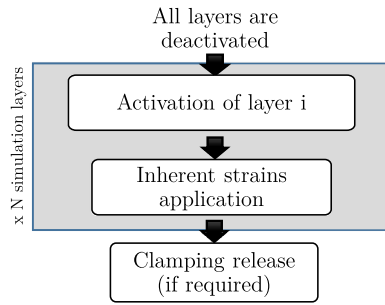


Fig. 6. Simulation steps required by the inherent strain based simplified model.

used [25]. Briefly, it consists of an elastic FE quasi-static analysis where the deformation is induced by user-defined inherent strains. This approach is very compelling from a computational point of view since time-consuming thermo-mechanical simulations are avoided.

During the heating and cooling cycles of the AM process, the total strains ϵ^{total} can be split into elastic strains $\epsilon^{elastic}$, thermal strains $\epsilon^{thermal}$, plastic strains $\epsilon^{plastic}$, strains induced by the phase transformation ϵ^{phase} and creep strains ϵ^{creep} [28]. Hence:

$$\epsilon^{total} = \epsilon^{elastic} + \epsilon^{thermal} + \epsilon^{plastic} + \epsilon^{phase} + \epsilon^{creep} \quad (1)$$

The inherent strains ϵ^{inh} are defined as:

$$\epsilon^{inh} = \epsilon^{total} - \epsilon^{elastic} = \epsilon^{thermal} + \epsilon^{plastic} + \epsilon^{phase} + \epsilon^{creep} \quad (2)$$

The balance of momentum equation for a quasi-static analysis is:

$$\nabla \cdot \sigma + b = 0 \quad (3)$$

where σ is the stress tensor and b are the body forces.

The stresses can be calculated by:

$$\sigma = D^e \epsilon^{elastic} = D^e (\epsilon^{total} - \epsilon^{inh}) \quad (4)$$

where D^e is the elastic constitutive tensor.

The inherent strain method has been successfully adapted to Powder Bed Fusion (PBF) processes in a multi-scale simulation framework [19]. Typically, the building strategy is approximated by layer-by-layer sequence. Hence, at each time-step a new layer is added to the computational domain. In fact, it is a common practice to discretise a part into layers with a thickness which is multiple of the real layer thickness referred to as lumping strategy.

Hence, according to the definition of the inherent strain tensor components, it is possible to take into account the “effects” of the actual scanning strategy.

Material deposition modelling must also be addressed in this methodology. From the numerical point of view, this implies the use of a FE activation strategy. At each time step a new layer must be activated and the AM building process is simulated as a sequence of mechanical calculations, one for each manufacturing layer.

The layer activation strategy is based on the so called “born and death elements” technique. According to this activation strategy, elements are not part of the model until they are activated according to the nominal height due to the powder feeding in PBF processes [15,16,29].

Thus, this simplified model consists of a mechanical linear elastic problem complemented with the activation strategy and user defined inherent strains. As a result, the whole analysis requires several simulation steps which are summarised in the flowchart depicted in Fig. 6. Initially, the slicing of the mesh is defined automatically according to the layer thickness and orientation defined in the input data. In the first step, all layers are removed from the computational domain. A new layer is added in each step together with the corresponding inherent strains. Finally, the boundary conditions corresponding to the clamping on the base-plate can be removed (cutting stage). Fig. 7 shows an intermediate state of a simulation where the building evolution can be observed. The key factor in this simplified methodology is how inherent strains are determined considering also the effect of the layer lumping. This is detailed in Section 4.

3.2. Finite element modelling

A 3D purely mechanical model was developed using the commercial software ABAQUS to simulate the deformation of the twin-cantilever beams under different scanning strategies. The modelling methodology and particularly the layer lumping enables to use a relatively coarse FE mesh. It consists of a structured cartesian mesh of 15,552 hexahedral elements

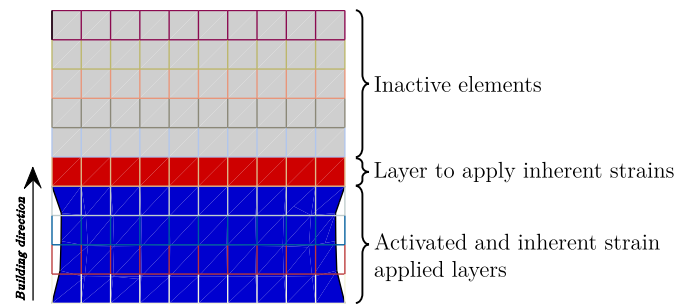


Fig. 7. Intermediate state of the simulation based on inherent strain methodology.

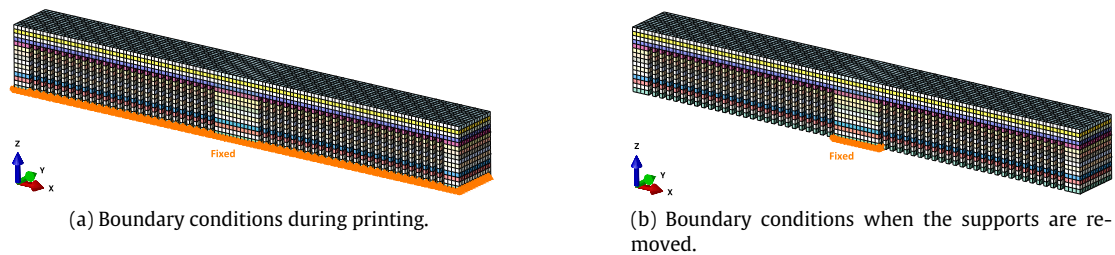


Fig. 8. Twin-cantilever finite element mesh and boundary conditions.

and 26,416 nodes. Moreover, symmetry boundary conditions were used when the scanning strategy presents symmetry, reducing the model size to a quarter.

Fig. 8 shows the entire mesh. Each simulation layer, which can be identified in the figure by the different colours, is 1 mm thick. The lumping ratio was 20:1. Thus, 20 real layers were represented by 1 simulation layer. Moreover, each layer was discretised by 1 element through the building direction.

The building platform was not considered in the model since it was represented by a fully constrained bottom region (Fig. 8(a)). Moreover, supports removal by wEDM was modelled as a simple change of boundary conditions (Fig. 8(b)). After the wEDM, only the bottom surface of the middle column was fixed, releasing all clamping belonging to the supporting structures.

The Ti-6Al-4V material properties used to characterise the constitutive tensor are: Young modulus ($E = 113,340$ MPa) and Poisson ratio ($\nu = 0.3$). The wall-clock time required, exploiting 12 Intel Xeon E5 cores, was about 20 s.

4. Inherent strains calibration

As pointed out in Section 3.1, the key factor at the methodology is to characterise the prescribed deformations responsible for the formation of both residual stresses and the distortions (after the stress release by cutting operation).

Two methods can be distinguished for this purpose:

- Reduced order methods.
- Empirical methods.

4.1. Reduced order methods

This multiscale modelling approach proposed by different authors [19,20,30] is a promising and fully predictive way of determining the inherent strain tensor with a reduced dependency from experimental data. It consists of an hierarchical procedure whereby inherent strains are predetermined through high-fidelity FE models. A coupled thermo-mechanical analysis is carried out considering the actual scanning strategy sequence by a moving heat source representing the power input. As a result, both thermal and visco-plastic deformations can be accurately computed. Hence, the corresponding inherent strains can be identified. Note that this procedure can be repeated at local level for different scanning strategies so that an off-line database of inherent strains can be constructed according to different process parameters. Later, this input can be used for the actual parts (global parts). Hence, a local–global analysis is carried out (see Fig. 9).

However, the definition of representative local models able to take into account all the fundamental process parameters is not straightforward. Neither the model set-up nor the mapping between high-fidelity local and global analysis are not completely clear yet. Henceforth, we do not choose this option for determining inherent strains.

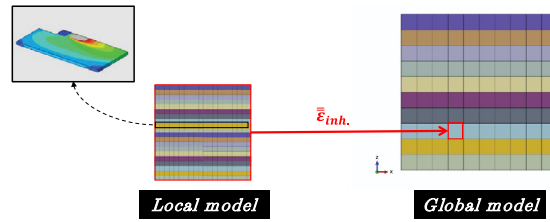


Fig. 9. Multiscale simulation based inherent strain determination scheme.

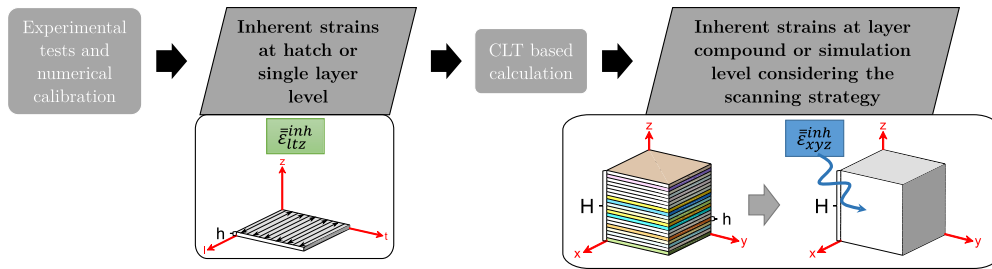


Fig. 10. Inherent strain determination strategy based on experimental tests.

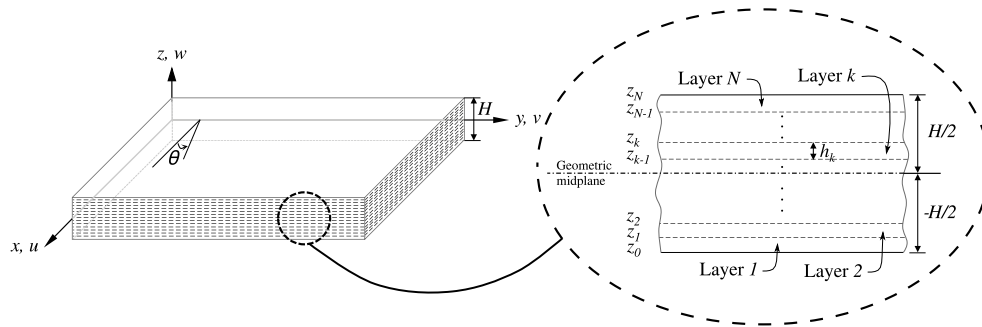


Fig. 11. Schematic representation of layers.

4.2. Empirical method

The empirical strategy adopted to obtain the inherent strains is presented in the flowchart shown in Fig. 10. According to this flowchart, the characteristic inherent strains which belong to each single layer are obtained by experimental tests and by iterative fitting. In this regard, according to the layer thickness used in the simulation, the equivalent inherent strain is calculated. This methodology is very similar to the one used for Classical Laminate Theory (CLT) to characterise the behaviour of composite laminates [31,32]. In fact, the layer-by-layer manufacturing using PBF technology has many similarities with the technology used to produce composite laminates. In both cases, the final structure is made layer-wise and it exists an induced anisotropy. In AM, the hatching sequence generates the same effects as due to fibres orientation.

The following definitions are necessary:

- It is assumed that the layer thickness used for the simulation (H) is composed by N deposited layers, being h the thickness of each one of them (see Fig. 11).
- (l, t, z) is the local coordinate system, following the orientation of the local hatching defined for each layer.
- (x, y, z) is the global coordinate system, attached to the building platform and used to define the hatches' orientation for each layer (see Fig. 11).
- The scanning strategy can be represented using the same nomenclature as for the stacking sequence of composite laminates [31]. Therefore, the orientation of hatches is established for each layer by defining the rotation angle (θ) , with respect to the reference x -axis (see Fig. 11). (i.e. a scanning strategy of 90° is represented as $[0/90]_N$).

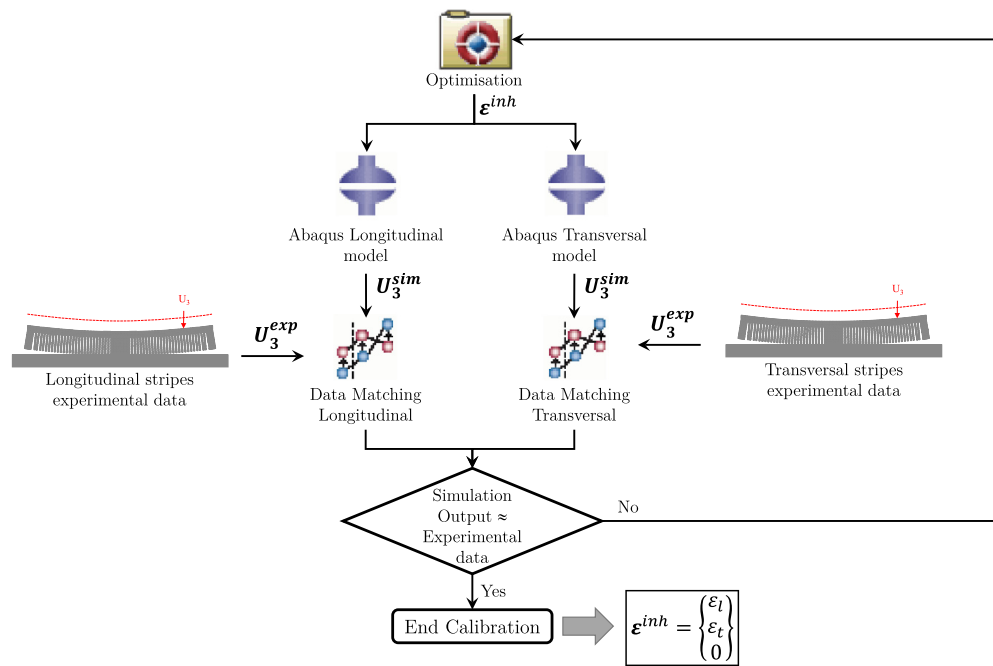


Fig. 12. Isight data matching optimisation loop for characteristic inherent strain calibration.

4.2.1. Inherent strains at hatch or single layer level

In order to determine the inherent strains at layer level, the following two basic hypotheses are made:

- The inherent strain tensor is orthogonal due to the actual nature of hatches.
- The inherent strain component in the building direction is zero. Hence, only in-plane components are taken into account. This hypothesis assumes that the vertical shrinkage of the deposited layer is compensated by the recoating phase of the PBF process. Therefore, from the modelling point of view, the inherent strain component in the building direction can be neglected.

The iterative calibration process employed is presented in Fig. 12. The residual stresses are proportional to the inherent strains applied to the structure. Therefore, an indirect measurement of this residual stress state enables to calculate the inherent strain field through inverse analysis. In our particular case, the twin-cantilever beam geometry (see Fig. 1) is proposed since it allows for a simple indirect measurement of the residual stresses as a function of its bending deformation after the cutting phase.

According to the aforementioned hypothesis, two inherent strain components must be determined only. Thus, at least two experiments are required. Taking advantage of the orthogonal nature of hatches, two orthogonal scanning strategies are set-up for the same twin-cantilever beam: longitudinal and transversal hatching as depicted in Fig. 4. Thus, 2 different residual stress state and consequently 2 different final bending deformation are obtained. An additional scanning strategy, with a orientation of 45° , is used to validate the model.

The relationship between inherent strains and distortion is determined through an optimisation loop where the objective function is the difference between the numerical results and the experimental measurements.

The optimisation problem has been solved via Isight commercial framework, combining: Abaqus FE model, data matching algorithm and experimental data input (see the flowchart in Fig. 12). Hooke–Jeeves direct penalty technique is used to solve this optimisation problem.

As a result, the inherent strain tensor at layer level is obtained and then used as a reference data for similar scanning strategies. It must be noted that the obtained inherent strain tensor is dependent on the process parameters used to manufacture the twin-cantilever beam.

Moreover, a simple verification of calibrated results is done by applying the obtained inherent strain tensor to 45° scanning strategy and comparing the numerical results against the experimental data.

4.2.2. Inherent strains for the numerical model

Although inherent strains can be obtained at layer level, some extra hypotheses are needed to account for the layer lumping used in the model. According to Kirchhoff hypothesis (CLT theory), strains vary linearly through the thickness of

the laminate structure as:

$$\begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \end{Bmatrix} = \begin{Bmatrix} \varepsilon_x^0 \\ \varepsilon_y^0 \\ \gamma_{xy}^0 \end{Bmatrix} + z \begin{Bmatrix} \kappa_x \\ \kappa_y \\ \kappa_z \end{Bmatrix} = \{\varepsilon^0\} + z \{\kappa\} \quad (5)$$

where ε_x^0 , ε_y^0 , ε_z^0 are the midsurface strains and κ_x , κ_y , κ_z are the curvatures due to bending and twisting.

An analogous hypothesis can be used for AM processes where the equivalent inherent strains can be calculated by Eqs. (6) and (7), summing the inherent strains of all the layers defining the lumped structure:

$$\varepsilon^{0Inh} = \frac{1}{N^2} \sum_{k=1}^N \begin{Bmatrix} \varepsilon_x^{Inh} \\ \varepsilon_y^{Inh} \\ \varepsilon_{xy}^{Inh} \end{Bmatrix}_k (4N - 6k + 3) = \frac{1}{N^2} \sum_{k=1}^N \varepsilon_k^{Inh} (4N - 6k + 3) \quad (6)$$

$$\kappa^{Inh} = \frac{-6}{hN^3} \sum_{k=1}^N \begin{Bmatrix} \varepsilon_x^{Inh} \\ \varepsilon_y^{Inh} \\ \varepsilon_{xy}^{Inh} \end{Bmatrix}_k (N - 2k + 1) = \frac{-6}{hN^3} \sum_{k=1}^N \varepsilon_k^{Inh} (N - 2k + 1) \quad (7)$$

where N is total number of lumped layers and ε_k^{Inh} is the characteristic inherent strain at layer k (see Fig. 12).

Both expressions are general. In case the scanning strategy presents a periodic rotation angle, the equivalent inherent strain of the lumped structure reduces to:

$$\varepsilon_{periodic}^{0Inh} = \frac{\varepsilon_l + \varepsilon_t}{2} \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix} \quad (8)$$

where ε_l and ε_t are the longitudinal and transversal components of inherent strains calibrated at layer level.

Interestingly, periodic scanning strategies result in in-plane isotropic inherent strains which do not depend on the rotation angle as long as periodicity is fulfilled. Consequently, the application of such inherent strain load is straightforward since the material orientation definition is not needed. In order to be periodic, the rotation angle must satisfy the condition rule in Eq. (9). Furthermore, the layer thickness to be considered in the simulation is determined by Eq. (10).

$$\frac{\pi}{\theta} \in \mathbb{N}; (\theta < \pi) \quad (9)$$

$$\exists n \in \mathbb{N}, H = n \frac{\pi}{\theta} h \quad (10)$$

5. Results and discussion

5.1. Experimental results

The final manufacturing of all twin-cantilevers fabricated following the procedure explained in Section 2 is shown in Fig. 13. The front view provided for each type of twin-cantilever reveals the effect of the chosen scanning strategy.

As shown in Fig. 3, two twin-cantilevers were fabricated for each scanning strategy except for 45° case, where one extra sample was manufactured. These repetitions enable a good experimental error estimation. Moreover, each twin-cantilever can be seen as two simple cantilever beams. Therefore, distortion data gathered from each structure is double (see Fig. 14) allowing for a better error distribution. All distortion curves are presented along the longitudinal axis [$0 \leq x \leq 60$ mm].

Distortion results for all types of cantilevers according to the scanning strategies defined in Fig. 4 are plotted in Fig. 15. In both graphs the vertical distortion results is normalised with respect to the longitudinal scanning. A clear influence of the scanning strategy can be noticed in the final distortion. Longitudinal stripes lead to the largest distortions whereas transversal stripes to the less pronounced ones. It is also remarkable the fact that the magnitude of the distortion corresponding to 45° stripes is the average of the longitudinal and transversal distortions respectively. Observe that the scanning patterns defined with a periodic rotation with respect to the reference system, show very similar results as depicted in Fig. 15(b). This result is in accordance with Eq. (8) which states that scanning strategies with periodic rotation lead to in-plane isotropic inherent strains.

In addition, the aforementioned curves are also very similar to the results obtained for the 45° stripes case.

5.2. Calibrated inherent strains

The calibration of the characteristic inherent strains was conducted following the methodology described in Section 4.2.1. The normalised inherent strain tensor obtained after the iterative data matching, can be observed in Eq. (11). The normalisation of the strain tensor was done with respect to its longitudinal component.

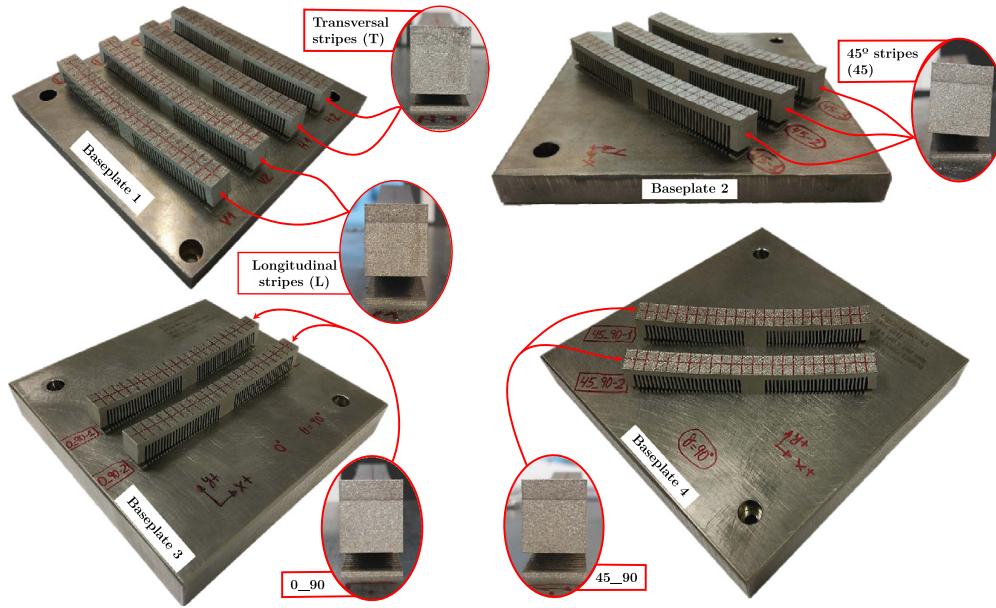


Fig. 13. Final state (after support removal) of all manufactured twin-cantilever beams.

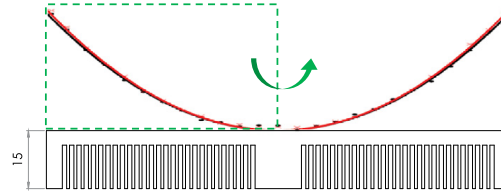


Fig. 14. Distortion data reflected with respect to the middle length of the twin-cantilever.

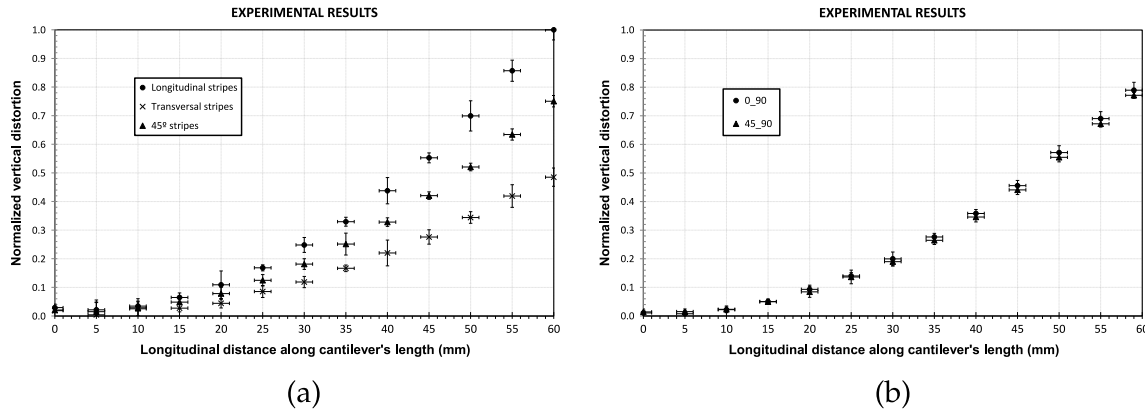


Fig. 15. Distortion measurement results along the top surface for all twin-cantilevers. (15(a)) No rotation between layers. (15(b)) 90° rotation between layers.

Around 50 iterations were performed to fit numerical results with experimental data until the sum of the squared difference was lower than 10%. To this regard, Figs. 16(a)–16(c) show the quality of the fitting carried out.

The vertical distortion obtained by FEM after applying the calibrated inherent strain can be observed in Figs. 17(a)–17(c). The deformed shape of twin-cantilevers is also in agreement with experimental results. It is remarkable how the numerical model is able to predict non-symmetrical deformations of the 45° stripes twin-cantilever (see Fig. 17(c)).

$$\boldsymbol{\varepsilon}^{inh} = \begin{Bmatrix} \varepsilon_l \\ \varepsilon_t \\ 0 \end{Bmatrix}_{ltz} = \begin{Bmatrix} -1 \\ -0.33 \\ 0 \end{Bmatrix}_{ltz} \quad (11)$$

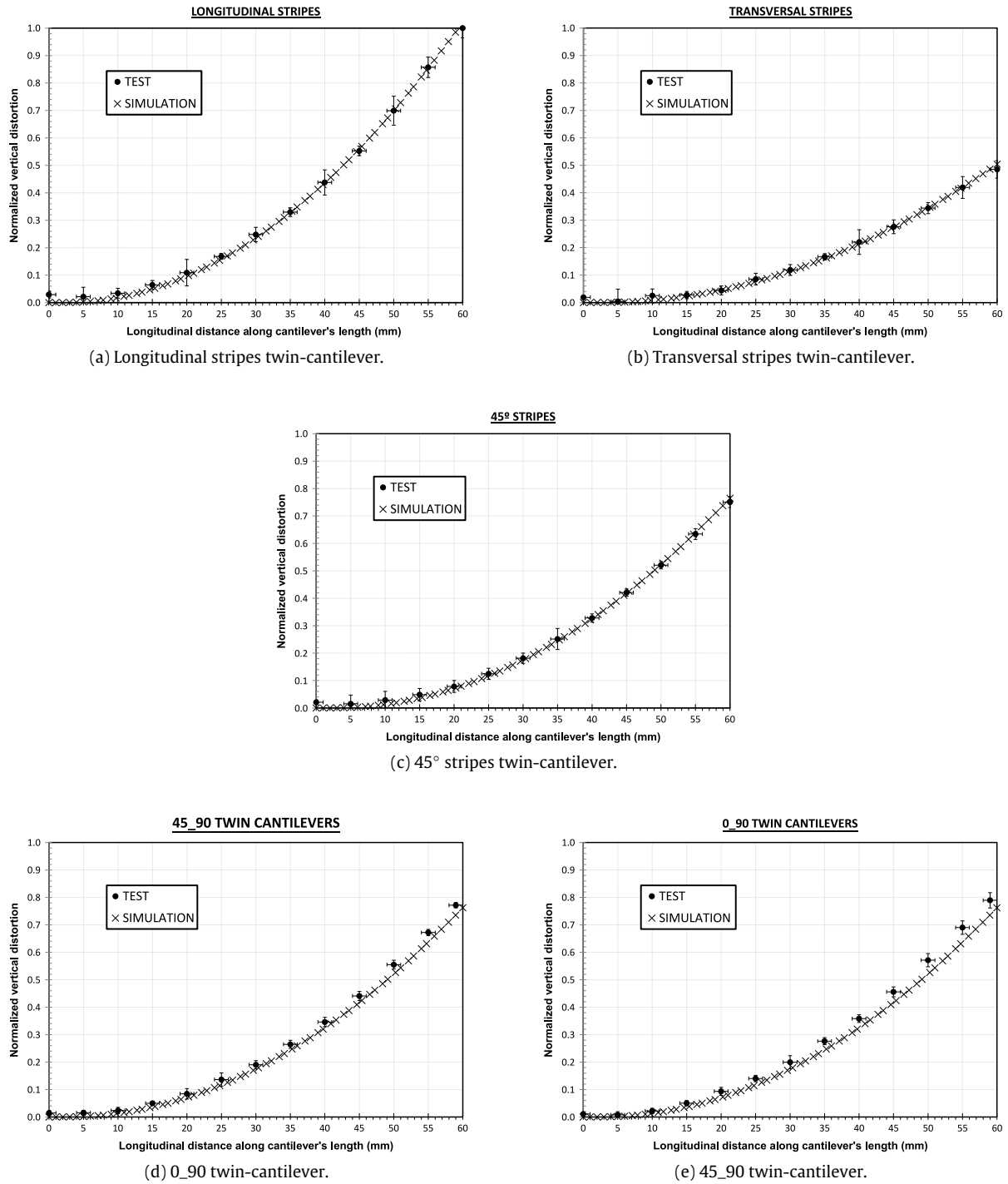


Fig. 16. Comparison of experimental and numerical results for distortion after the iterative inherent strain determination process.

5.3. Validation of results

The validation of the calculated inherent strains as well as the methodology explained in Section 4.2.1 was carried out observing the behaviour of the remaining twin-cantilevers which present a scanning rotation of 0_90 and 45_90 (see Fig. 4). Both scanning strategies are periodic so that Eq. (8) was used to calculate the normalised inherent strain tensor to be applied in the numerical model:

$$\epsilon_{periodic}^{0Inh} = \frac{\epsilon_l + \epsilon_t}{2} \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix} = -0.67 \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix}_{xyz} \quad (12)$$

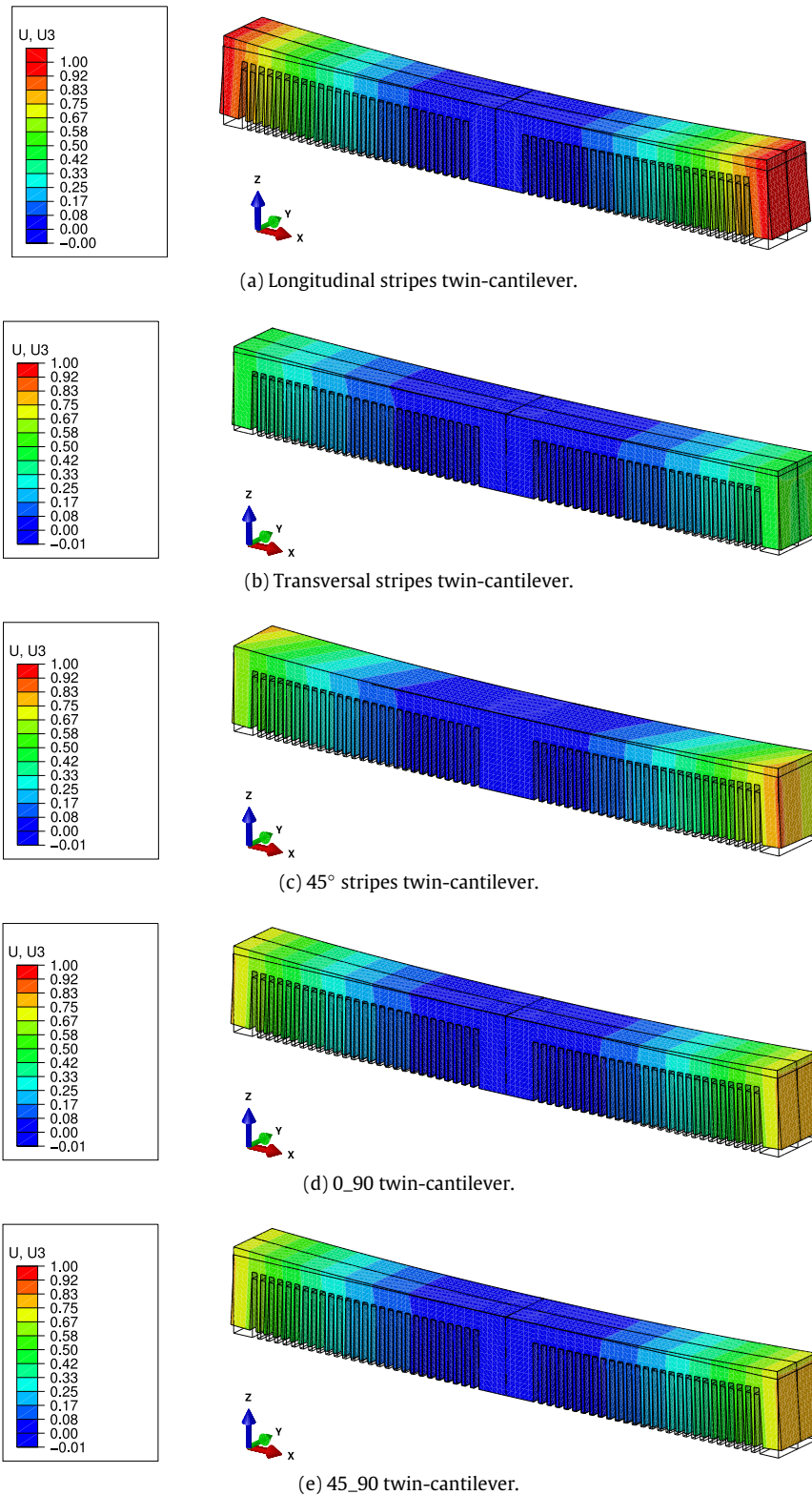


Fig. 17. Predicted normalised vertical distortion field (scaled $\times 2$) after twin-cantilevers were cut-down.

The comparison between numerical and experimental results in terms of vertical distortion of the top surface can be observed in Figs. 16(d) and 16(e). The FEM results match the experimental measurements quite well since the largest difference is less than 10%. The vertical distortion of the deformed structures in Figs. 17(d) and 17(e) is also consistent with experimental results.

6. Conclusions

An empirical methodology to determine characteristic inherent strains for a given scanning strategy is detailed. This result is used as input data for a linear-elastic analyses in order to obtain distortion and residual stress field caused by LPBF processes. Moreover, when the scanning strategy is periodic, the equivalent inherent strains can be assumed as in-plane isotropic, simplifying the implementation of the numerical model.

The development and validation of the methodology have been carried out by manufacturing twin-cantilever coupons following different scanning strategies. Thus, suitability of this methodology is proved at coupon level.

The following practical conclusions can be drawn:

- The distortion is clearly influenced by the chosen scanning strategy and the geometry of the structure. For the twin-cantilever geometry, longitudinal pattern leads to the largest distortions whereas the transversal pattern to the lowest. Finally, 45° pattern and 90° rotating stripes are in-between.
- Inherent strain tensor can be assumed as orthogonal. This result should be checked for other more complex geometries.
- Periodic scanning strategies lead to in-plane isotropic inherent strains.

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HIGH-FIDELITY NUMERICAL MODEL FOR INHERENT STRAIN CALCULATION

6.1 Introduction

This chapter presents the second article in this thesis series, which develops and optimises high-fidelity thermo-mechanical models for calculating inherent strains in [PBF-LB](#). While the first article focused on empirically calibrating the inherent strain tensor through experimental trials, this work offers an alternative approach based on high-fidelity meso-scale models. By employing a multi-scale thermo-mechanical modelling framework, the method provides significant flexibility for parametric studies. It enables the systematic variation of parameters such as scan strategy, dwell times, process conditions, and powder layer thickness, thereby predicting how these factors influence inherent strains and reducing the need for costly experimental campaigns.

This article provides a comprehensive analysis of local high-fidelity thermo-mechanical models and outlines a robust procedure for calculating the inherent strain tensor. In doing so, it investigates the contributions of thermal, plastic, and activation strains while identifying optimal control volume sizes and boundary conditions to minimise numerical artifacts. The resulting guidelines facilitate the definition of local models that reliably feed into macro-scale inherent strain analyses, ultimately enhancing the predictive capability of the overall simulation framework. Furthermore, rigorous validation against experimental data increases the industry reliability of simulation-driven predictions.

6.2 Scientific contribution

This work makes several novel contributions to the field of inherent strain modelling in [PBF-LB](#). First, it addresses a key limitation in current meso-scale thermo-mechanical models (which typically consider only a few layers to control computational cost and, as a consequence, fail to capture the complex thermal and mechanical interactions and boundary effects) by employing a sufficiently large local model. This expanded model encompasses many more layers, enabling a detailed control volume analysis

and the extraction of a homogenised inherent strain tensor that better represents the process physics.

Second, the study investigates and clarifies the appropriate definition of boundary conditions in the local model. By performing a comprehensive sensitivity analysis, it identifies an optimal control volume size (approximately equivalent to four deposited layers) that minimises the influence of surrounding boundary effects. This analysis not only ensures the accurate computation of inherent strains but also demonstrates that, under the adopted scanning strategy, the inherent strain tensor can be effectively approximated as isotropic in the XY plane.

Finally, by comparing the high-fidelity derived inherent strain tensor with those obtained through empirical methods, the work shows that (although the high-fidelity approach demands higher computational resources) it delivers improved accuracy and deeper insight into the contributions of thermal, plastic, and activation strains. These advancements provide a robust basis for simulation-driven process optimisation and offer practical guidelines for the application of high-fidelity models in industrial-scale additive manufacturing.

6.3 Summary and conclusions

This study presents a high-fidelity, multi-scale modelling approach for accurately calculating the inherent strain tensor in [PBF-LB](#) processes. By developing detailed local thermo-mechanical model that was calibrated using experimental temperature data, the methodology successfully quantifies the individual contributions of thermal, plastic, and activation strains to the inherent strain tensor. The research identifies an optimal control volume (approximately equivalent to four deposited layers) that minimizes boundary effects and enables a reliable homogenization of the inherent strain tensor. Under the adopted scanning strategy, the inherent strain tensor can be effectively approximated as isotropic in the XY plane.

Validation on a complex [SBA](#) actuator geometry confirms that the inherent strain tensors obtained with the proposed high-fidelity model are consistent with empirically derived tensors, thus reinforcing the robustness of the approach. These findings not only enhance our understanding of the fundamental mechanisms underlying inherent strain development but also provide a solid foundation for macro-scale inherent strain analyses.

Ultimately, this work contributes to the advancement of simulation-driven process optimisation in metal additive manufacturing by delivering a reliable computational method for inherent strain calculation.

6.4 Article data

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6.5 Article as published

The following pages reproduce the published article exactly as it appeared in the journal. The article begins on the next page.

Article

Defining and Optimising High-Fidelity Models for Accurate Inherent Strain Calculation in Laser Powder Bed Fusion

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Abstract: Powder Bed Fusion–Laser Beam (PBF-LB) is a leading technique in metal additive manufacturing, yet it continues to face challenges related to residual stresses and distortions. The inherent strain method has emerged as a valuable predictive tool, offering early assessments of part behaviour due to its simplicity and manageable computational demands. However, accurately defining the inherent strain tensor, which is critical for these models, remains a challenge. This study provides a comprehensive analysis of the local meso-scale model definition and inherent strain calculation procedure in the PBF-LB process using a multi-scale modelling approach. The primary objective is to guide the definition of local high-fidelity thermo-mechanical models. This research investigates the contributions of thermal, plastic, and activation strains (strains due to Finite Element (FE) activation) to the inherent strain tensor, demonstrating the significant impact of activation strains. A sensitivity analysis identified an optimal control volume size to ensure minimal boundary effects. An optimised local high-fidelity model is proposed to efficiently calculate inherent strain tensor, significantly reducing computational costs without compromising accuracy. The method was validated by applying it to a complex SBA actuator geometry, which showed good agreement between predicted and experimental distortions. The consistency of the proposed method with empirically derived tensors further reinforces its potential to improve predictive capabilities in the PBF-LB process, ultimately enhancing part quality.

Keywords: additive manufacturing; high fidelity; thermo-mechanical model; inherent strain; finite element modelling; multi-scale modelling; powder bed fusion; Ti-6Al-4V



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1. Introduction

Additive Manufacturing (AM) has significantly transformed modern manufacturing processes, particularly in the production of complex and high-precision components that are challenging or impossible to achieve using traditional manufacturing methods [1]. Among the various metal AM techniques, PBF-LB stands out due to its ability to produce high-precision and high-strength components directly from digital models. This process is particularly advantageous for industries such as aerospace, automotive, and biomedical, where the demand for custom, high-performance parts continues to grow [2,3].

The PBF-LB process involves spreading a thin layer of metal powder on a build platform, which is then selectively melted using a high-energy laser beam. This process is repeated layer by layer until the entire part is constructed. The ability to control the microstructure and mechanical properties of manufactured parts by adjusting process parameters, such as laser power, scan speed, and hatch spacing, makes PBF-LB a versatile and powerful manufacturing technology [4,5]. These parameters are critical as they influence the thermal history, microstructure, and mechanical properties of the final parts [6–8].

Despite its advantages, PBF-LB faces several challenges that need to be addressed to fully realise its potential. One of the primary issues is the development of residual stresses and distortions during the manufacturing process, which can lead to part failure or require additional post-processing steps [4]. These residual stresses arise due to the rapid heating and cooling cycles inherent in the PBF-LB process, creating steep thermal gradients and lead to uneven thermal expansion and contraction. Understanding and mitigating these residual stresses are crucial for ensuring the structural integrity and dimensional accuracy of manufactured parts [9].

The definition of optimal processing windows commonly involves a trial-and-error procedure to guarantee the desired quality of the printed components. However, these process parameters often require further tuning when applied to real geometries to maintain quality standards. This discrepancy arises because the conditions used to determine the process window are not identical to those encountered in real printing cases. Furthermore, all the experimental techniques employed to evaluate quality during the trial-and-error stage are labour-intensive and costly [4].

Predictive methods, particularly computational simulations, have become essential to address these challenges. These methods enable the prediction and control of thermal and mechanical behaviours during the design stage, reducing the need for extensive experimental trials. Computational simulations can provide detailed insights into the effects of process parameters on the final part, facilitating optimisation of manufacturing conditions to minimise residual stresses and distortions [10].

AM processes are inherently complex due to their multi-physics and multi-scale nature. The detailed modelling, and particularly PBF-LB technologies, require the solution of a multi-physics problem due to the interplay between various physical phenomena within very short periods. Despite significant increases in computational capacity in recent years [11], such simulations remain unaffordable at the part scale and, in some cases, even at the meso-scale.

When the main focus is on predicting distortion, residual stress, and microstructure, the Computational Welding Mechanics (CWM) approach, originally developed for welding process simulations, is applicable to additive manufacturing [12]. In this case, the objective is not to accurately predict temperature fields within the melt-pool but rather outside of it. This approach involves solving only the thermo-mechanical problem. The phenomena occurring inside the melt-pool are not solved; instead, the heat generation process is replaced with a prescribed heat input distribution. This simplification enables the models to efficiently simulate the laser beam movement and analyse the effects of scanning strategy on residual stresses at a local level [13].

While this approach reduces computational requirements by simplifying the underlying physics, CWM-based models still require a fine domain discretization (of the order of the melt-pool size). When the ratio between the part size and the melt-pool size is significant, solving these problems at the part scale remains computationally expensive and often unfeasible due to the enormous computational demands [14].

To address this challenge, researchers have developed various strategies to reduce computational cost while maintaining acceptable accuracy. These strategies include adap-

tive mesh refinement and coarsening (AMR) techniques, multi-scale modelling approaches, surrogate models or reduced-order models, and layer lumping [10]. AMR techniques, for instance, allow for finer resolution in critical regions of the printed component, enhancing the precision of the simulation without significantly increasing computational cost [15].

In this way, a promising approach is the Inherent Strain Method (ISM). This approach simplifies complex thermo-mechanical simulations by replacing them with linear-elastic mechanical simulations, making it more computationally efficient. The original ISM has undergone multiple improvements to enhance the accuracy of final deformation and residual stress predictions [16,17]. In ISM, the key point relies on the definition of the inherent strain tensor, which can be obtained through empirical approaches or meso-scale thermo-mechanical models using a multi-scale-based approaches [18]. Current meso-scale thermo-mechanical models developed to calculate inherent strain in PBF-LB often fall short due to their limited scope, particularly the insufficient number of layers considered. These models typically focus on a very small domain with a few layers to keep the computational cost controlled, which may not accurately capture the complex thermal and mechanical interactions and boundary effects [4].

Furthermore, in the community still remains some discussion about the proper definition of the boundary conditions in the local model or how the inherent strains should be calculated without perturbation from the surroundings. This is a critical point when using multi-scale approaches [4].

Bridging this gap is a key motivation for this study. This article presents a thorough analysis of the local meso-scale model definition and inherent strain calculation procedure. The primary objective of this research is to provide guidance for defining local models and generate knowledge for applying these models to calculate inherent strain, which can then be used in simplified analyses based on the inherent strain methodology at the part scale level.

This paper is structured as follows:

- Section 2 presents the multi-scale modelling approach, including the local high-fidelity thermo-mechanical model and the macro-scale inherent strain methodology. The computation of inherent strains from the local high-fidelity model and the averaging strategy used are also defined.
- Section 3 describes the experimental work conducted for model calibration and validation, including test geometries, manufacturing process, and measurement techniques.
- Section 4 details how the multi-scale modelling approach was applied to the defined local and global models.
- Section 5 presents and discusses the results of the numerical simulations and their comparison with experimental measurements. This section critically analyses the effects of the control volume size, boundary conditions and surrounding areas, and the nature of the calculated inherent strains.
- Section 6 summarises the main conclusions of this research and suggests directions for future work.

This structured approach aims to provide a comprehensive understanding of the challenges and solutions related to calculating inherent strains in the PBF-LB process, ultimately contributing to the advancement of additive manufacturing technologies.

2. Multi-Scale Modelling Approach

The multi-scale model used in this study follows the methods proposed by various authors [16,18–21]. Although the proposed model can be interpreted as a multi-scale model, it differs from the standard FE^2 and concurrent multi-scale approaches. In this case,

two meso-scale domains are considered. The first is a local model that accurately represents the meso-scale, capturing both the laser printing sequence and the thermal behaviour of the printed material. The second is a representative subdomain of the local model, where the up-scaled variables are computed. By defining this representative domain, the approach ensures that the up-scaled variables remain unaffected by the thermal and mechanical boundary conditions of the local model. This approach is conceptually similar to FE^2 methods, as both aim to create sufficiently large domains to ensure a statistically representative meso-scale while minimising potential noise from boundary conditions.

As a result of introducing this representative subdomain, the approach differs from standard multi-scale methods. However, it can be demonstrated that the results obtained with this approximation are in close agreement with macro-scale high-fidelity simulations. The size of this representative subdomain is defined based on experimental observations, taking into account the influence of the heat source on the temperature field.

The cornerstone of this approach lies in defining a proper meso-scale representation suitable to compute the inherent strains. Although various local models have been proposed in the literature, they are generally constrained by the number of layers and the dimensions of the local domain considered in the detailed analysis.

Therefore, the interplay of the meso- and macro-scale models is managed in the following way (see Figure 1). Firstly, a local meso-scale high-fidelity thermo-mechanical FE model is solved. In this, a staggered coupled thermo-mechanical analysis is performed, incorporating current process parameters and the scanning strategy sequence. This allows for accurate computation of thermal, visco-plastic, and activation strains, from which the corresponding inherent strains are computed.

Next, a macro-scale (component scale) simulation is conducted using the original inherent strain methodology in a layer-wise manner. The inherent strains computed from the local model are used as input data for this larger-scale simulation.

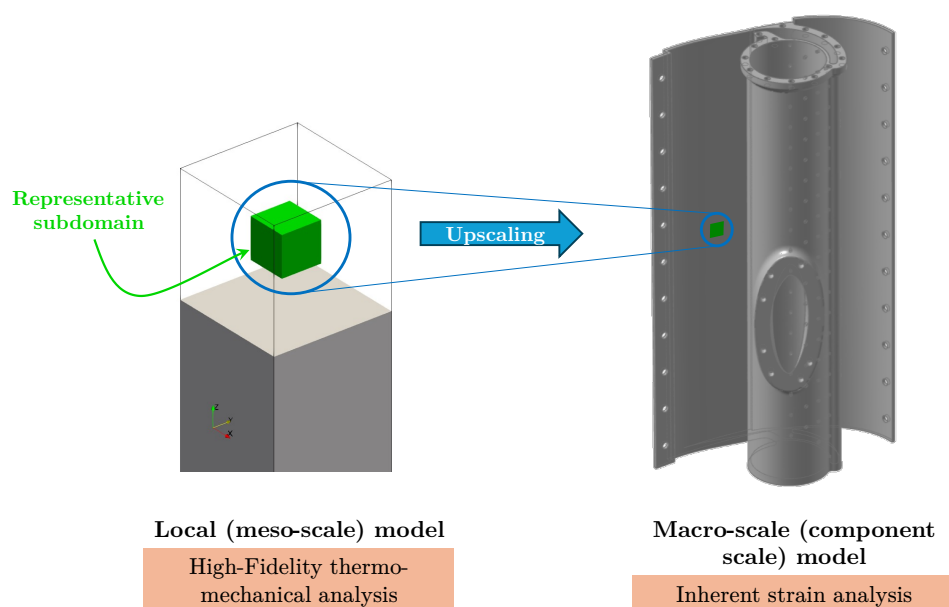


Figure 1. Multi-scale modelling illustration.

2.1. High-Fidelity Thermo-Mechanical Analysis

In this approach, a staggered solution is employed where the heat transfer problem is solved first, and then the resulting temperature history is used as input data for solving the mechanical problem.

2.1.1. Governing Equations Heat Transfer Analysis

The heat transfer in additive manufacturing processes is governed by the transient heat conduction equation, expressed as follows:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \dot{Q} \quad (1)$$

where ρ is the material density, c_p is the specific heat capacity, T is the temperature, t is time, k is the thermal conductivity, and $\dot{Q}$ represents internal heat rate generation per unit volume, including heat input from the laser or other energy sources.

As mentioned before, in CWM, the heat generation process is simplified by replacing it with a prescribed heat input distribution, thereby excluding all physics related to heat generation and the phenomena occurring within the melt-pool from the analysis. In this sense, Gaussian or double ellipsoid heat source models are extensively used in welding and additive manufacturing simulations [22]. These models are particularly beneficial when local temperature gradients are of interest, requiring very small time increments. In this case, the external heat input per unit volume was considered as a uniform distribution over a box-shaped volume [23,24]:

$$\dot{Q} = \frac{\eta W}{V_{pool}^{\Delta t}} \quad (2)$$

where W is the laser power, η is the heat absorption coefficient, and $V_{pool}^{\Delta t}$ is the heat-affected volume, which is the sum of the volumes of finite elements intersected with the moving box across the scanning path at the current time increment. This power distribution preserves the total energy input, regardless of the intersected elements.

Boundary conditions are essential for solving this equation and typically include the following:

- Convective Heat Loss: Described by Newton's law of cooling, $q = h(T - T_\infty)$, where h is the heat transfer coefficient and T_∞ is the ambient temperature.
- Radiation Heat Loss: Described by the Stefan–Boltzmann law, $q = \epsilon \sigma (T^4 - T_\infty^4)$, where ϵ is the emissivity and σ is the Stefan–Boltzmann constant.

These equations ensure that the thermal effects in the material due to the heat source and environmental interactions are accurately captured. However, in real applications, it is challenging to distinguish between these two heat loss mechanisms. As a result, it is common practice to use an equivalent heat transfer coefficient [24], h_{equ} , which encompasses both mechanisms: $q = h_{equ}(T - T_\infty)$.

The contribution of the effect of latent heat due to phase change is neglected, assuming that the heat absorbed during melting and the heat released during solidification are equivalent and occur within the same time step [24].

Mechanical Problem

The mechanical problem in additive manufacturing involves solving the linear momentum equations under quasi-static conditions:

$$\nabla \cdot \sigma + b = 0 \quad (3)$$

where σ is the Cauchy stress tensor and b represents body forces per unit volume.

The relationship between stress and strain is defined through a constitutive model as follows:

$$\sigma = C : \epsilon^e = C : (\epsilon - \epsilon^{th} - \epsilon^{vp}) \quad (4)$$

where C is the fourth-order elasticity tensor, ϵ is the total strain tensor, ϵ^e is the elastic strain tensor, ϵ^{vp} is the visco-plastic strain tensor, and ϵ^{th} is the thermal strain tensor, which accounts for the strain due to temperature changes.

The material is described via the constitutive model, which describes the evolution between stresses and strains under mechanical loads and thermal effects. In what follows, a full description of the constitutive model is presented.

2.1.2. Constitutive Model

The material model for Ti-6Al-4V should capture the dependency of strain rate at elevated temperatures, as well as describe the stress and strain relaxation behaviour [25].

A constitutive model capable of describing the behaviour of Ti-6Al-4V is the J2 elasto-visco-plastic constitutive law under a small strains regime, as detailed in [26]. This model, which incorporates the phase change effect, can accurately represent its mechanical behaviour.

The phase change is controlled via temperature thresholds, defining three different states:

- **Solid:** the elasto-visco-plastic constitutive model, including both isotropic hardening and thermal softening. Strain-rate-independent and strain-rate-dependent plasticity are combined and controlled through temperature-dependent parameters. The volumetric and deviatoric components of the stress tensor are computed as follows:

$$\begin{cases} p = K(\nabla \cdot \mathbf{u} - \epsilon^{th}) \\ s = 2G(e - e^{vp}) \end{cases} \quad (5)$$

where K and G are the bulk and shear temperature dependent modulus, respectively. e and e^{vp} are deviatoric total strain and visco-plastic strain tensors, respectively.

- **Liquid:** no elastic and thermal strains are produced. The material behaviour is described by a purely viscous (Norton–Hoff) model:

$$\begin{cases} \nabla \cdot \mathbf{u} = 0 \\ s = \eta \dot{e}^{vp} \end{cases} \quad (6)$$

where η is the temperature-dependent viscosity parameter.

- **Mushy:** provides a smooth transition from liquid to solid state. The elastic strains become negligible compared to visco-plastic strains and therefore, it is mainly governed by visco-plastic flow.

The FE technology used according to this constitutive model is based on the mixed u/p formulation. For more information, see [27].

Thus, the stress relaxation in Ti-6Al-4V can be accounted for by treating the material as if it were in a liquid state. In this particular case, the states of the material can be controlled via definition of two temperatures as shown in Figure 2. The most important temperature is the *relaxation or annealing temperature* (T_{anneal}).

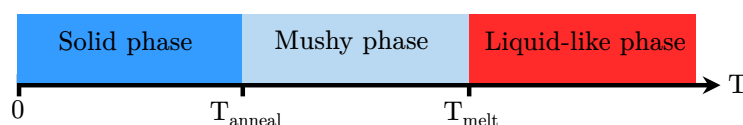


Figure 2. Definition of material state transitions based on temperature thresholds.

The temperature history obtained from the heat transfer analysis allows for the calculation of the thermal strain as follows:

$$\boldsymbol{\varepsilon}^{th} = [\alpha(T) \cdot (T - T_{ref}) - \alpha(T_0) \cdot (T_0 - T_{ref})] \mathbf{I} \quad (7)$$

where T is temperature, $\alpha(T)$ is the temperature-dependent secant thermal expansion coefficient, T_{ref} is the reference temperature for the expansion coefficient, and T_0 is the initial temperature of the material at the beginning of the simulation.

Regarding the temperature used to calculate thermal strains, T_{anneal} has been defined as a cut-off temperature (see Equation (8)).

$$T = \begin{cases} T_{anneal} & \text{for } T \geq T_{anneal} \\ T & \text{for } T < T_{anneal} \end{cases} \quad (8)$$

2.1.3. Material Deposition Modelling: Building Strains

Material deposition modelling is a critical aspect of additive manufacturing processes. Numerically, this requires finite element discretizations with evolving domains, comprising both active (deposited material) and inactive (not yet deposited material) regions. The thermo-mechanical phenomena occur exclusively within the active domain, generating temperature and displacement fields within the active finite elements (FEs).

The birth–death element activation approach is particularly well suited for PBF-LB [23], as it effectively mimics the progressive addition of material during the printing process. In this strategy, the inactive domain remains in its initial state until activated according to the scanning path (illustrated in Figure 3). After a layer is deposited, the build plate is lowered by the nominal layer thickness, and a new powder layer is spread by the recoater. However, distortions on the top surface of previously deposited layers introduce variability in the thickness and distribution of the newly spread powder. The birth–death activation approach inherently accounts for this variability in powder layer thickness, as shown in Figure 3 at $t = t_3$. At this stage, inactive elements (blue) deform in response to displacements in active elements (red), while ensuring that the top surface of the next powder layer remains at the nominal height.

Moreover, this approach captures transient deformations caused by thermal expansion and contraction of melted material during deposition within a given layer. For example, Figure 3 illustrates the evolution of deformation in elements 2 and 3 during the activation process at $t = t_1$ and $t = t_2$, respectively.

To ensure precise modelling of the interaction between inactive and active elements during both heat transfer and mechanical analysis, particular attention is given to the activation strategy. For mechanical analysis, activation strains (also referred to as building strains) are applied as outlined in [15,26]. These strains account for pre-activation deformations caused by volume adjustments in the filler material, ensuring that newly activated elements remain stress-free upon activation. The activation strains are computed as follows:

$$\boldsymbol{\varepsilon}^{act} = \nabla^s(\mathbf{u}_0) \quad (9)$$

where $\nabla^s(\cdot)$ denotes the symmetric gradient operator of $\cdot$, and $\mathbf{u}_0$ are the initial displacements of the newly activated FEs.

Incorporating activation strains, the constitutive equation becomes

$$\boldsymbol{\sigma} = \mathbf{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{vp} - \boldsymbol{\varepsilon}^{th} - \boldsymbol{\varepsilon}^{act}) \quad (10)$$

Activation strains are history-dependent because they rely on u_0 , which is calculated at each activation step based on the scanning path and time-stepping accuracy. This highlights the importance of accurately implementing the scanning sequence to correctly model activation strains and their effect on the thermo-mechanical behaviour.

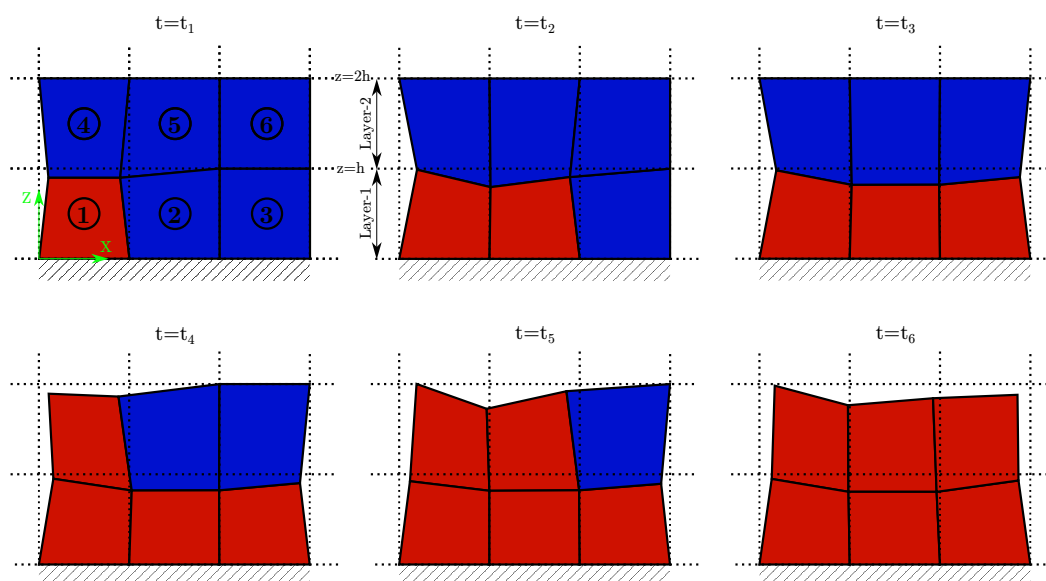


Figure 3. Illustration of the birth–death material deposition modelling strategy through activation steps in a domain composed of six elements. Red elements are activated and subjected to shrinkage, while blue elements remain inactive but deform due to node displacements shared with active elements. Activation strains are incorporated to account for these pre-activation deformations.

2.1.4. Time Discretization

When the speed of the heat source is much faster than the heat conduction, it is possible to increase the time increment without compromising the thermo-mechanical behaviour [28]. This time increment serves as a reference to determine the appropriate time increment for the simulation. Based on the work by Irwin et al. [28] and considering the heat input model employed here, the reference time increment is given by

$$\Delta t_{ref}^{LI} = \frac{0.5 \cdot \alpha}{v_s^2} \cdot \left(\frac{v_s \cdot c}{\alpha} \right)^{1.92} \simeq 0.5 \cdot \frac{c^2}{\alpha} \quad (11)$$

where α is the thermal diffusivity at ambient temperature, v_s is the heat source speed, and c is the length of Goldak's ellipsoid.

2.2. Inherent Strain Computation

The inherent strain includes all strain components but the elastic strain. It is commonly assumed that the inherent strain is equivalent to the plastic strain; however, this assumption may not hold true depending on the approach employed.

Considering the high-fidelity modelling approach previously defined, the inherent strain is defined as follows:

$$\epsilon^{inh} = \epsilon^{total} - \epsilon^e = \epsilon^{th} + \epsilon^{vp} + \epsilon^{act} \quad (12)$$

The definition of the size of the local model is not straightforward because it depends on several aspects like the inherent strain method, which is applied at macro-scale model, the process parameters employed, the material, boundary conditions, etc. Therefore, each case study should require special care when defining the size of the local model.

Moreover, the calculation of inherent strain requires a homogenisation strategy. This is because macro-level inherent strain models seldom employ an activation strategy based on actual layer thickness due to computational constraints. Instead, these models typically adopt a layer lumping strategy, which aggregates multiple layers into a single thicker layer to reduce computational time. Additionally, the original inherent strain methodology imposes limitations on the layer thickness that can be used in the simplified model. This limitation arises from the hypothesis that plastic strain is constant throughout the entire volume, which may not hold true for thinner layers.

In this study, the inherent strain tensor is proposed to be extracted from the central part of the local model. The control volume is carefully defined to ensure that boundary conditions and transient phenomena do not affect the results. Therefore, it should not suffer from the influence of the baseplate or the free top surface. Once the control volume is established, the volume-weighted average of the field variable is used to calculate the inherent strain tensor:

$$\bar{f} = \frac{1}{V} \sum_i f_i V_i \quad (13)$$

where V_i is the volume of cell i , f_i is the value of the field variable in cell i , and V is the total volume of the dataset, which is the sum of all cell volumes: $V = \sum_i V_i$.

This expression ensures that each cell's contribution is weighted by its volume. Thus, the average inherent strain tensor is then upscaled to be used to solve the macro-scale model.

2.3. Macro-Scale Inherent Strain Analysis

The classical and most commercially employed inherent strain method, despite minor variations, is based on the assumption that all material points within the domain undergo the same thermo-plastic history. This implies that each material point shares an identical thermal and plastic strain tensor at the time of activation. This assumption is particularly suitable for powder bed additive manufacturing processes, as the melt-pool (MP) is typically small compared to the size of the printed part.

The detailed implementation of this method is well documented in the literature [18,19,29]. This simplified approach involves a sequence of mechanical linear elastic steps, wherein an activation strategy is employed in combination with user-defined inherent strains.

Typically, the building strategy is approximated by a layer-by-layer sequence, where at each time step, a new layer is added to the computational domain. However, a common practice is to use a lumping strategy, in which multiple layers are grouped and activated simultaneously. This approach reduces the computational burden by decreasing both the number of steps required and the total number of elements in the model.

Material deposition is modelled using the birth–death approach. At each time step, a new layer is activated and the AM process is simulated as a sequence of mechanical calculations.

As noted in [18], the inherent strain tensor can be obtained either through experimental calibration or from meso-scale local models. In this study, where the main focus is on the calculation of inherent strain from detailed numerical models, the macro-scale inherent strain methodology will take as input the numerically calculated inherent strain tensor.

3. Experimental Campaign for Model Calibration and Validation

3.1. Description of Geometries

While the primary focus of this study is on modelling, it is essential to have experimental results for better understanding, model calibration, and validation. To this

end, two different geometries made of Ti-6Al-4V were defined using the same printing process parameters.

The first geometry is a non-symmetric bridge (see Figure 4), which is a benchmark that facilitates local data monitoring and reduces the complexity of the distortion analysis.

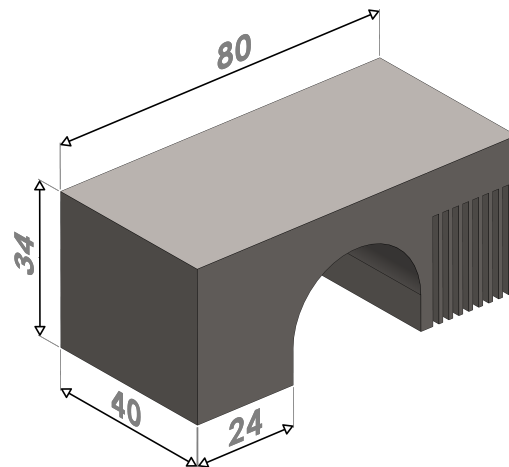


Figure 4. CAD model of the non-symmetric bridge geometry (units: mm).

The second geometry is a more complex and larger structure: Steady Blowing Actuator (SBA) (see Figure 5). This is an active flow control actuator that may be installed in the engine-wing union, wing leading edge, and/or engine pylon. It injects a continuous air stream to control airflow, reducing separation and improving the aerodynamic performance. Thus, it has the potential to delay local separation to higher angles of attack and increase maximum lift [30]. The design of this actuator was optimised in the framework of the FLOWCAASH project. The complex design of this actuator makes it ideal for studying the effects of distortion in industrial geometries.

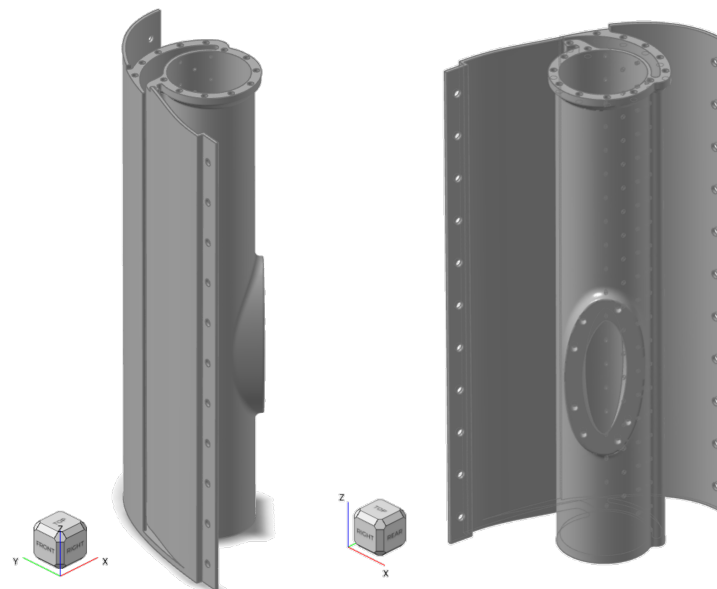


Figure 5. CAD model of the SBA actuator geometry. Bounding box dimensions: $101 \times 137 \times 306$ (mm³).

3.2. Manufacturing Process

Both geometries were manufactured using an SLM 280 HL machine (SLM Solutions, Lübeck, Germany), equipped with a 400 W fiber laser. The as-built state of both is shown in Figure 6. The main process parameters applied for both geometries are summarised

in Table 1. These parameters were determined through an optimisation process to meet quality requirements such as high density, low surface roughness, adequate microstructure, and optimal mechanical properties. All geometries were produced in an inert argon gas chamber to prevent powder oxidation during printing. The oxygen content was kept below 0.2% to ensure safety and quality. The preheating temperature was set to 200 °C, and the nominal layer thickness was 60 µm.

All previously mentioned process parameters are nominal values, but it is well known that these do not reflect the real values during printing. In numerical modelling, it is crucial to consider the real values of laser exposure and recoating time, especially if the goal is to calibrate the model against experimental data. Figure 7 illustrates the discrepancies between theoretical and measured laser exposure times, stressing the variability in recoating times. The differences in laser exposure times arise from variations between nominal and actual scanning speeds. Additionally, the non-constant recoating time significantly impacts the temperature history, particularly during the cool-down stage between layers. Therefore, these monitored data were incorporated into the numerical model to minimise uncertainties related to process parameters.

Table 1. PBF-LB process parameters.

Parameter	Hatch	Boundary	Contour
Laser power [W]	350	150	150
Scanning speed [mm/s]	1100	650	650
Hatch distance [mm]	0.12	-	-
Beam diameter [mm]	0.08	0.08	0.08

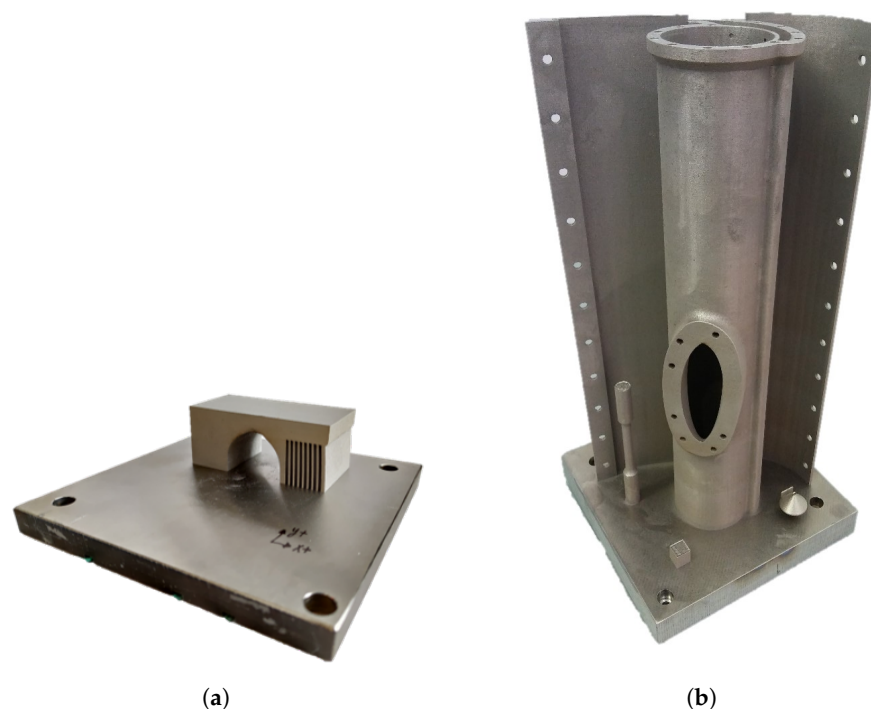


Figure 6. Printed parts: (a) Non-symmetric bridge and (b) SBA actuator.

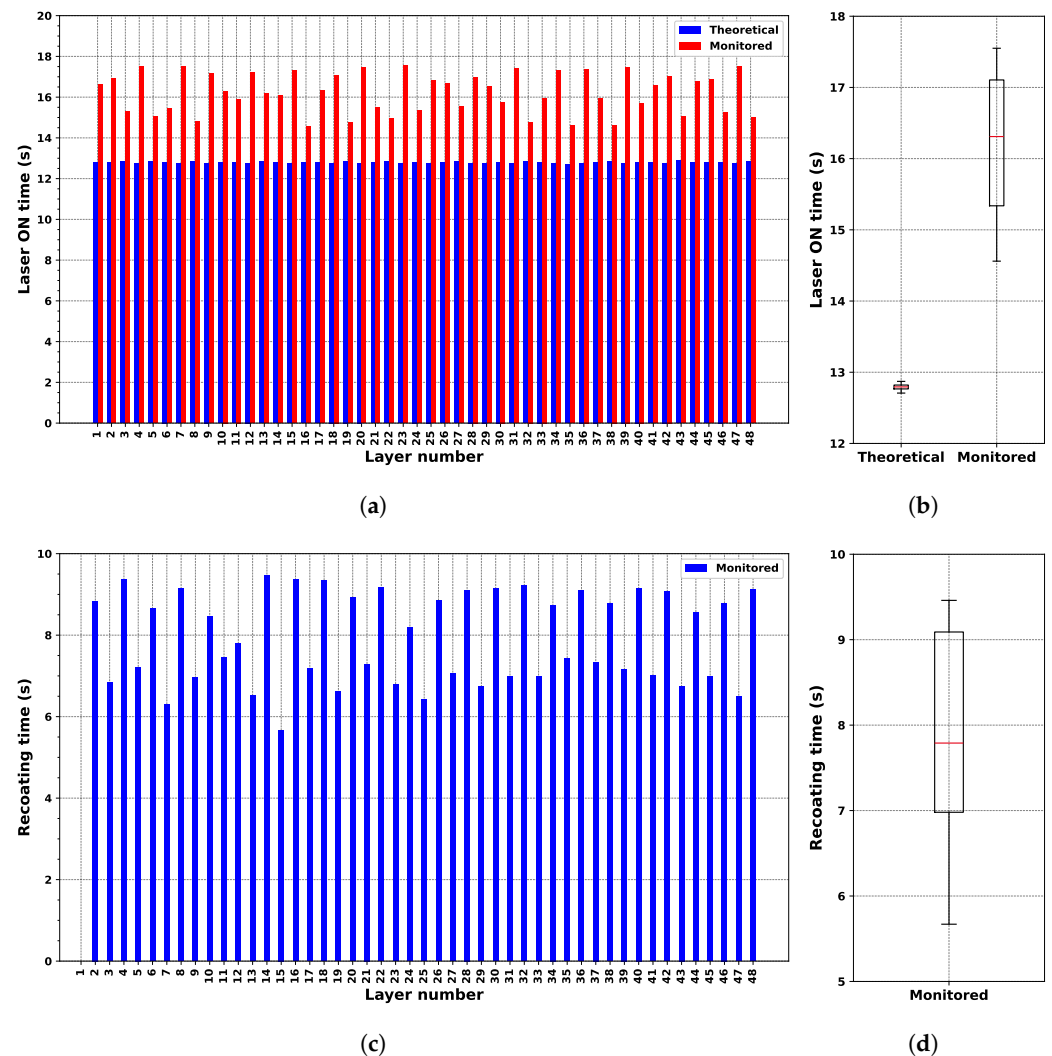


Figure 7. Laser exposure and recoating time data: (a) Comparison of theoretical and monitored laser exposure time per layer, (b) box plot comparing theoretical and monitored laser exposure time, (c) monitored recoating time per layer during printing, and (d) box plot of monitored recoating time during printing.

To ensure dimensional stability and effective heat dissipation throughout the machine, the parts were printed on sufficiently thick Ti-6Al-4V baseplates. These baseplates mitigate distortions and facilitate efficient heat transfer.

Regarding the scanning strategy, the alternating laser scanning strategy with a rotational angle of 66.7° was employed (see Figure 8). This strategy is widely adopted to evenly distribute thermal stresses, thereby minimising the risk of warping and residual deformations in the printed components.

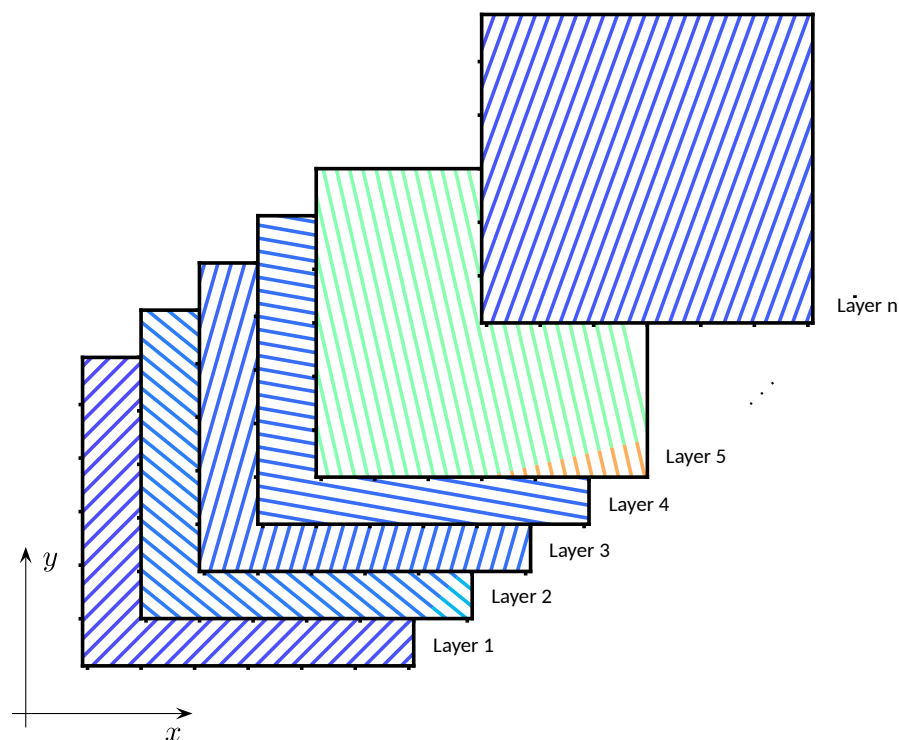


Figure 8. Schematic of the 66.7° scanning strategy used.

3.3. Temperature and Distortion Measurements

Temperature measurements were conducted at six specific locations of the bridge using K-type thermocouples. The thermocouples were positioned within blind holes machined in the baseplate where the part was printed, as depicted in Figure 9. They were strategically placed close to the top surface to capture peak temperatures accurately. To ensure accurate and fast data acquisition without aliasing, a high-speed data logger was employed. Careful consideration was given to the selection of thermocouple diameter to balance response time with ease of manipulation.

While contact-based temperature measurement sensors such as thermocouples are generally preferred for their accuracy in providing precise temperature data, their integration into the printing chamber and connection to the acquisition system can be challenging. In this case, the acquisition system was placed outside the machine, requiring meticulous routing of thermocouple wires through the main door, as depicted in Figure 10. The recoater blade was also modified by machining a small groove to prevent collisions with wires. Additionally, tight measures were implemented to prevent oxygen leakage, which is crucial for ensuring the integrity and quality of Ti-6Al-4V parts.

Distortion measurements were conducted on the SBA after the printing process, capturing the as-built part's geometry using a high-precision 3D scanner. An Ensensio X36 3D stereo vision camera (IDS Imaging Development Systems GmbH, Obersulm, Germany), utilising infrared structured light, was employed to obtain detailed point-cloud data. These data were subsequently compared with the nominal geometry to calculate geometric deviations and assess the accuracy of the printed part.

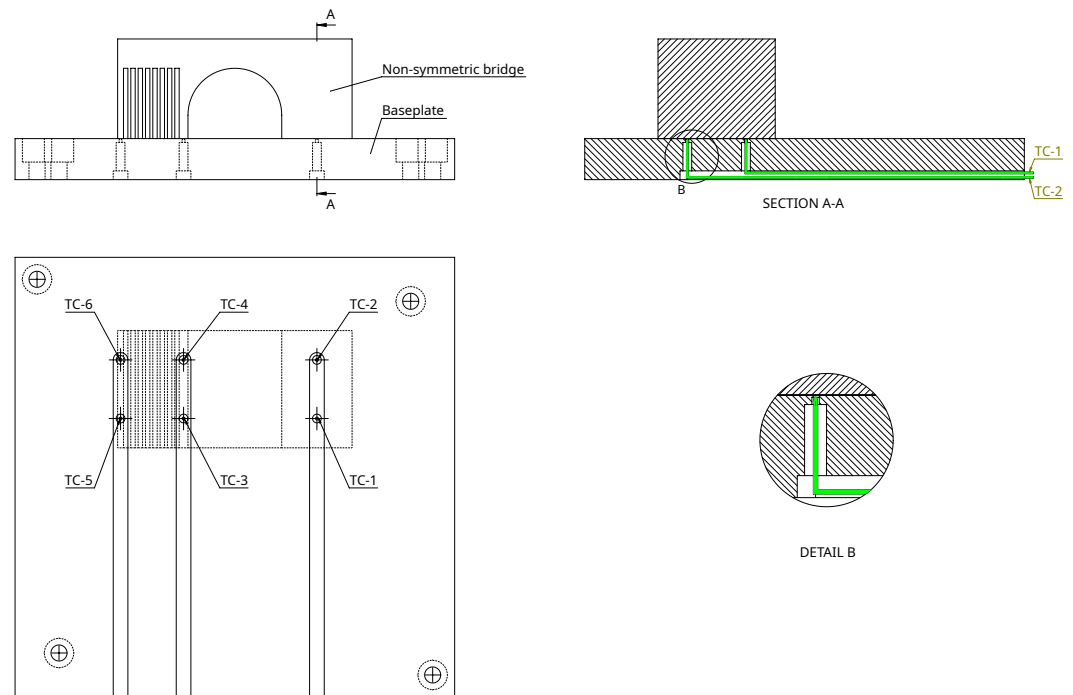


Figure 9. Technical draft of thermocouple (TC) locations within the baseplate. Each thermocouple is labeled as TC-x, indicating its specific position. The figure includes multiple standard drafting views: a front view showing the non-symmetric bridge and the baseplate, a bottom view displaying the thermocouple positions, a cross-section illustrating the groove and holes for thermocouple wiring, and a detail view highlighting thermocouple placement within the blind holes to measure temperatures near the top surface of the baseplate.

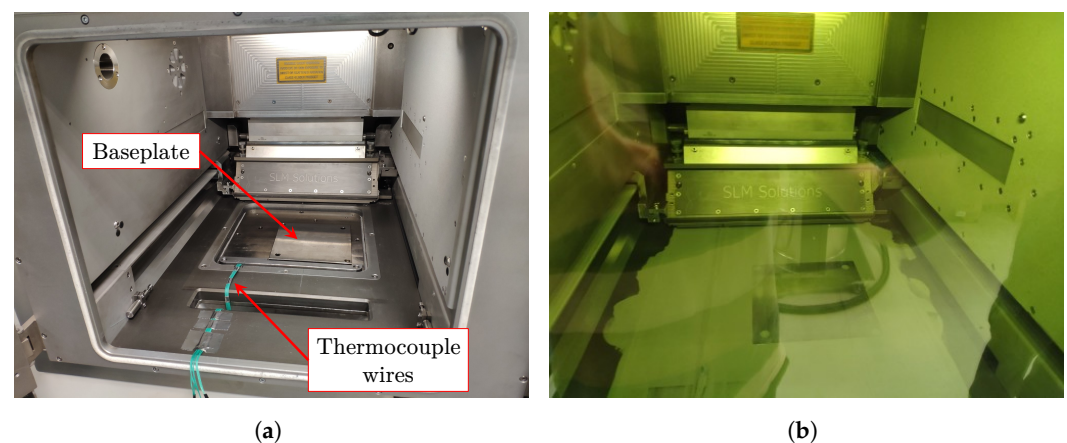


Figure 10. Experimental setup illustrating (a) the installation of the wired baseplate within the build chamber, highlighting the routing of wires through the main door and (b) the initial setup before starting the printing process.

4. Numerical Model Implementation

This section details the implementation of the multi-scale modelling approach described in the previous section to achieve the objectives of this paper.

The FE software used in this study is Finite Element Method Using Sub-grid Scales (FEMUSS). It is a cutting-edge computational framework developed at the International Center for Numerical Methods in Engineering (CIMNE) [26]. FEMUSS provides a powerful and flexible platform for high-fidelity numerical simulations. Its combination of AMR, thermo-mechanical coupling, and high-performance computing capabilities makes it ideally suited for addressing complex multi-physics problems in research and engineering. FEMUSS has been adapted to give support to different technologies in AM process, such as the ISM.

All modules implemented in FEMUSS can interact in an optimised manner in order to provide fast and accurate numerical simulations based on the Finite Element Method (FEM).

4.1. High-Fidelity Local Model

In what follows, a full description of the construction of the local model is presented.

4.1.1. Geometry and Mesh

The local model, a submodel of the bridge, was defined as shown in Figure 11. This submodel is located in correspondence with thermocouple TC-01, allowing the use of experimentally recorded temperatures for model calibration. Additionally, a portion of the baseplate was included in the submodel to accurately account for heat dissipation through the baseplate.

In AM, it is well known that the material often undergoes multiple cycles of melting and re-solidification across various layers. This continuous thermal cycling significantly affects the microstructure and mechanical properties of the fabricated components. The melt-pool, and consequently the heat-affected zone (HAZ), can extend over several layers, being subjected to changes based on the specific process parameters and material used. Furthermore, applied boundary conditions and the substrate (if any) considered at the bottom part can influence the inherent strain field. Therefore, the dimensions and the minimum number of layers at the local model must be analysed to determine the quasi-steady-state printing conditions to produce a homogeneous region to define inherent strain values.

To address these considerations, the chosen size of the deposited material in this study was larger than typical meso-scale local models used in the literature. Specifically, the model accounted for 48 layers within a cubic deposited domain of 2.88 mm.

Regarding the FE mesh generation, an initial coarse FE mesh was defined, composed of 180 Q1P0 hexahedral elements and 1634 nodes. This mesh can account for gradients far from the deposited zone. The deposition zone was automatically refined using uniform adaptive mesh refinement cycles to achieve an element size equal to the layer thickness (see Figure 12). This process results in a final mesh with 116,100 elements and 178,021 nodes. Mesh coarsening was not allowed to ensure that inherent strains were computed at the final stage without perturbations due to mesh coarsening.

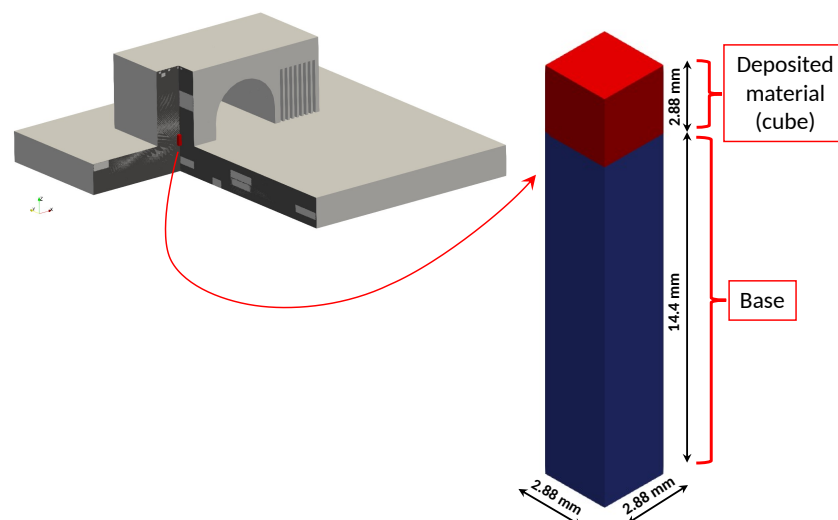


Figure 11. Local model definition. Geometry and dimensions.

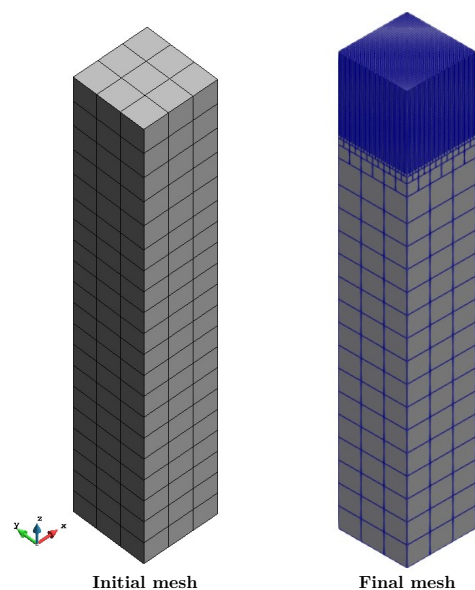


Figure 12. Local model mesh evolution.

4.1.2. Thermo-Mechanical Analysis

The thermo-mechanical model was defined following the procedure outlined in Section 2.1. The time of the simulation required to print the cube was 1142 s, including both exposure and recoating times considered in the simulation as deposition and cooling stages. After the deposition process, a final cooling stage was considered.

Time discretization was selected taking as reference the critical time increment, which was calculated as a function of the hatching process parameters. Using Equation (11), it can be found that the critical time increment is $\Delta t_{\text{crit}}^{\text{LI}} = 0.1951 \mu\text{s}$. This corresponds to a deposition length of $\Delta l_{\text{crit}}^{\text{LI}} = 1.77 \text{ mm}$, which exceeds half the side length of the deposited cube. Such a deposition length would position the cube boundaries too close to the melt-pool, potentially violating the assumptions made by Irwin et al. [28] in deriving the critical time increment. Therefore, after several preliminary trials, it was concluded that a deposition length of $\Delta l = 0.36 \text{ mm}$ ($\Delta t = 0.33 \mu\text{s}$) in each time step following the scanning sequence defined in the G-code file provides a more suitable balance between computational efficiency and accuracy.

The G-code used in the simulation was generated by incorporating the original scanning path file (as provided to the machine) along with the actual processing times. As shown in Figure 7, there are significant deviations between the actual laser exposure and recoating times compared to the nominal values. To account for these variations, manufacturing logs were utilised. These logs capture changes due to acceleration, deceleration, and other manufacturing strategies such as skywriting, which cause the actual laser speed to differ from the nominal value. Additionally, the recorded recoating times were incorporated to account for the cooling between layer deposition stages.

4.1.3. Initial and Boundary Conditions

Heat Transfer Analysis

The lateral boundary surfaces were considered adiabatic because of the low thermal conductivity of loose powder and assuming that heat is primarily extracted by heat conduction of the baseplate. Heat loss from top surface was incorporated into the convection and radiation model, with an equivalent heat loss coefficient defined as of $h_{\text{equ}} = 18 \text{ W}/(\text{m}^2 \text{ } ^\circ\text{C})$ (see Section 2.1.1). The environment temperature was set to $50 \text{ } ^\circ\text{C}$, representing the average temperature of the building chamber during the printing process. The initial temperature

of the baseplate domain was set to 200 °C. During the simulation, the bottom surface was maintained at this temperature due to the preheating temperature control activated in the printing machine. This temperature was held constant until the final cool-down stage, decreasing exponentially until reaching ambient temperature.

Mechanical Analysis

It is well known that mechanical boundary conditions are prone to affect the inherent strain distribution. To analyse their sensitivity, two different boundary conditions were defined:

- *BCFree*: all outer surfaces of the baseplate are constrained, while the lateral surfaces of the deposited material are free to move.
- *BCNotFree*: all outer surfaces of the baseplate are constrained. Additionally, the YZ plane surfaces (see Figure 13) of the deposited material are constrained from moving in the X direction, and the XZ plane surfaces of the deposited material are constrained from moving in the Y direction.

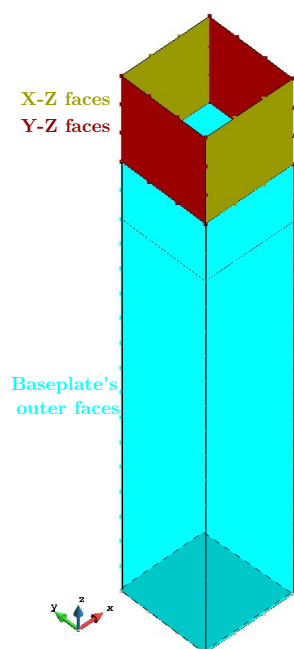


Figure 13. Faces where boundary conditions were defined.

4.1.4. Material Properties

The temperature-dependent material properties of the Ti-6Al-4V alloy were defined based on the literature [31]. This source provides averaged data from multiple references and includes additional experimental tests, offering a reliable initial guess for these properties. This comprehensive dataset ensures accurate and reliable material behaviour modelling under varying thermal conditions. Figure 14 shows all the temperature-dependent material properties used in the numerical models.

The effect of the powder was not considered in the heat transfer analysis (being considered almost adiabatic). The powder is only present on the top surface during the brief period when the laser scans and melts it. Consequently, its effect is negligible and can be accounted for by the convection coefficient applied to the top surface.

Regarding the relaxation temperature, it is strongly related to Ti-6Al-4V material behaviour at high temperatures, being established at 690 °C, based on the literature and previous works [32].

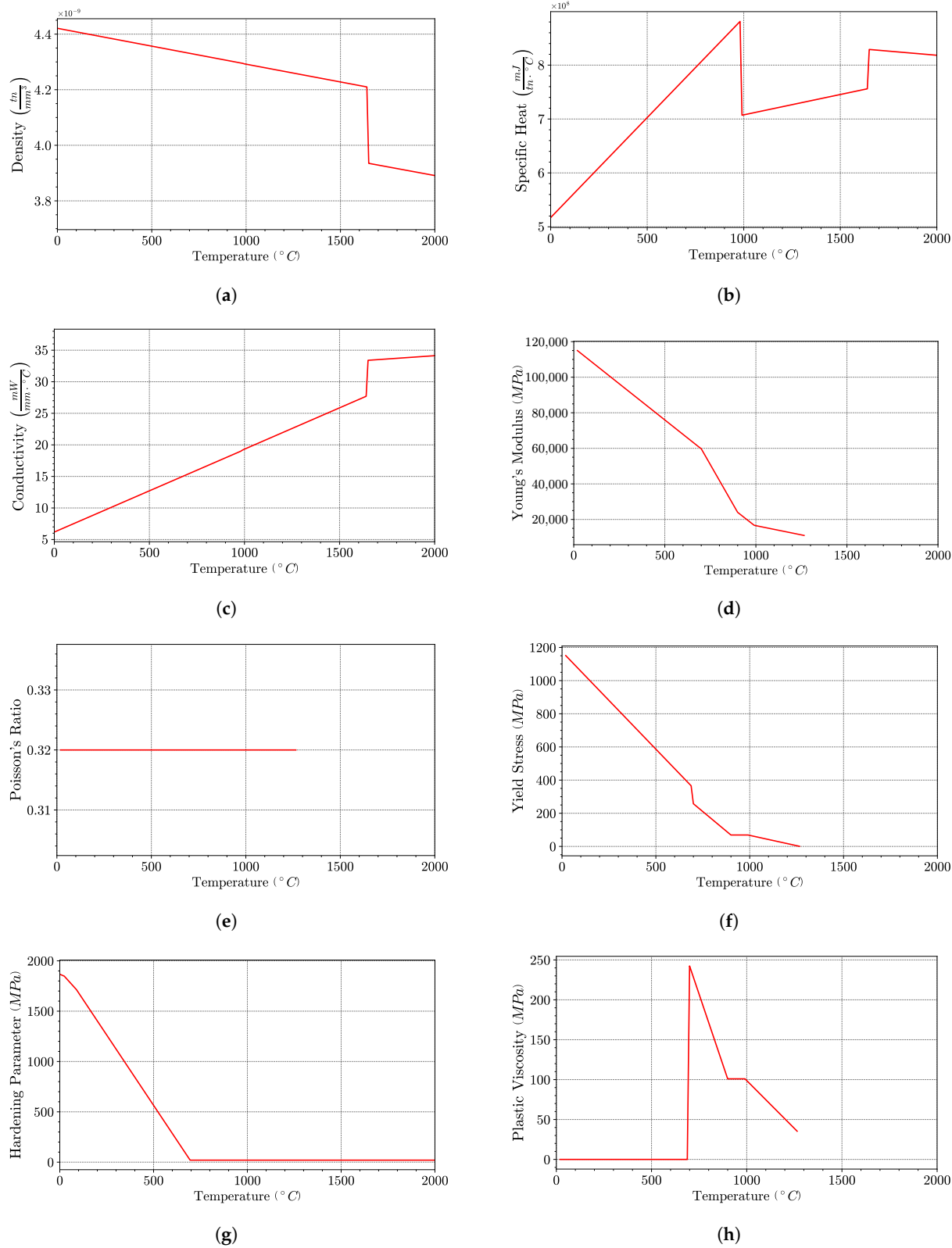


Figure 14. Cont.

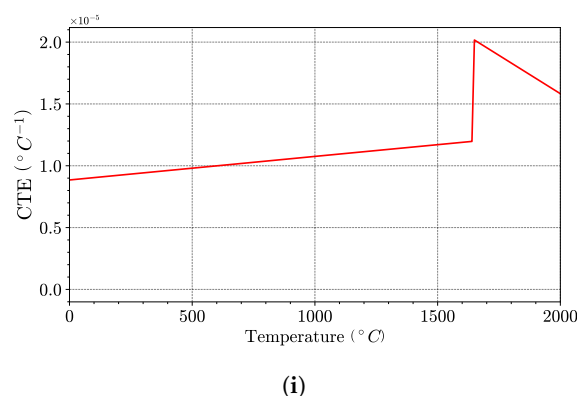


Figure 14. Temperature-dependent thermo-mechanical properties of Ti-6Al-4V material: (a) Density, (b) specific heat, (c) thermal conductivity, (d) Young's modulus, (e) Poisson's ratio, (f) yield stress, (g) isotropic linear hardening parameter, (h) plastic viscosity, and (i) thermal expansion coefficient.

4.2. Global Model

The global model acts as a validation checkpoint for the inherent strains calculated from both local and representative subdomain models. In this case, the inherent strain method described in Section 2.3 was applied to the geometry of the SBA actuator, ensuring the practical applicability of the approach. This step not only verifies the accuracy in the assessment of inherent strains but also demonstrates the effectiveness of the method in a real-world context.

4.2.1. Geometry and Mesh

The geometry of the SBA actuator (see Figure 5) allows for printing without any support structure in the given orientation. Although it appears to be a rectilinear tube with two fins, its axis is not perpendicular to the baseplate. Additionally, it contains many internal holes and attachment zones, which complicate automatic conformal meshing with hexahedral elements. Therefore, given the complexity of the geometry, an FE mesh was automatically generated using the layer-wise AMR algorithm [26], employing Q1P0 hexahedral elements. Before generating the mesh, specific element size requirements were established based on the geometry discretization accuracy and the layer height used in the ISM. In this case, a layer height of $h_{layer} = 1$ mm was considered. The target for the finest mesh size was set at 0.5 mm while a maximum element size of 2 mm was set for use where possible after coarsening.

In terms of AMR parameters, these requirements were translated into a maximum refinement level (Lev_{max}) of 10, a minimum refinement level (Lev_{min}) of 8, and a refinement height (h_{ref}) of 1 mm. An appropriate initial bounding box was defined for the geometry, which enables the feature that successively generated FE are equilateral. Within this bounding box, AMR is applied throughout the simulation. A snapshot of the generated mesh at the final activation step is presented in Figure 15.

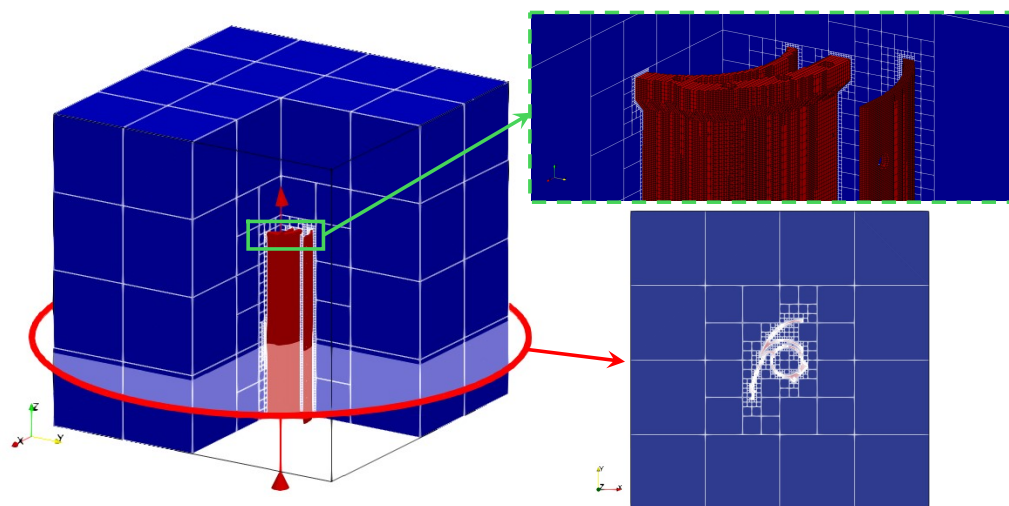


Figure 15. SBA mesh embedded in the initially defined bounding box mesh at the final layer activation step.

4.2.2. Boundary Conditions

The baseplate was excluded from the analysis domain. It was considered sufficiently stiff and was replaced by fixed Dirichlet boundary conditions during the ISM simulation.

4.2.3. Material Properties

The Ti-6Al-4V material properties used in the global analysis are the same as those employed in the local analysis (see Figure 14) but for the global model, only ambient temperature conditions and a linear elastic material model were considered. This ensures consistency between the local and global models while accounting for the different conditions and assumptions at the macro-scale.

5. Results and Discussion

This section presents the results of the inherent strain tensor calculation based on a high-fidelity thermo-mechanical local model. First, the results of the calibration are detailed. Then, the calculated inherent strain tensor is presented and compared to the one derived in previous work calculated using an empirical method [18]. Next, the inherent strain tensor is applied to a real component using the inherent strain methodology. The predicted distortions are then compared to experimental measurements and the results are discussed to validate the accuracy of the model.

Throughout this work, strain is plotted as a dimensionless quantity. Axis labels for strain reflect this convention.

5.1. Calibration of the Local High-Fidelity Model

The high-fidelity local model is based on the CWM approach, where a heat input model replaces the detailed physics of the melt-pool. Therefore, calibrating the parameters that define this heat distribution model is essential. The most sensitive parameter of the model is the heat absorption coefficient, which controls the power input into the model.

In this study, the calibration was performed using the experimental temperature history recorded by the TC-01 thermocouple (see its location in Figure 9). The calibration process involved minimising the error between the experimental and numerical temperature curves, using a combination of iterative methods and error minimisation techniques. This heat absorption coefficient was set to 0.55, which is consistent with values reported in similar studies [21]. Figure 16 presents both the experimental and numerical temperature curves at TC-01. The experimental curve exhibits an oscillatory pattern with several peaks

and troughs, especially at the beginning. This oscillation is attributed to the proximity of the thermocouple to the melt-pool during the deposition of the initial layers. As the melt-pool moves further away, the oscillations diminish.

Comparing the computed temperature curve with the experimental signal reveals a discrepancy in the early stages of the deposition, particularly in the peak temperature values. These differences can be attributed to the limited response time of the thermocouples, which were unable to capture the maximum temperature values accurately. Additionally, the discrepancy may be partly due to challenges in precisely identifying the thermocouple's exact measurement location. However, beyond this initial stage, the agreement between the predicted and measured temperatures is consistent and synchronised.

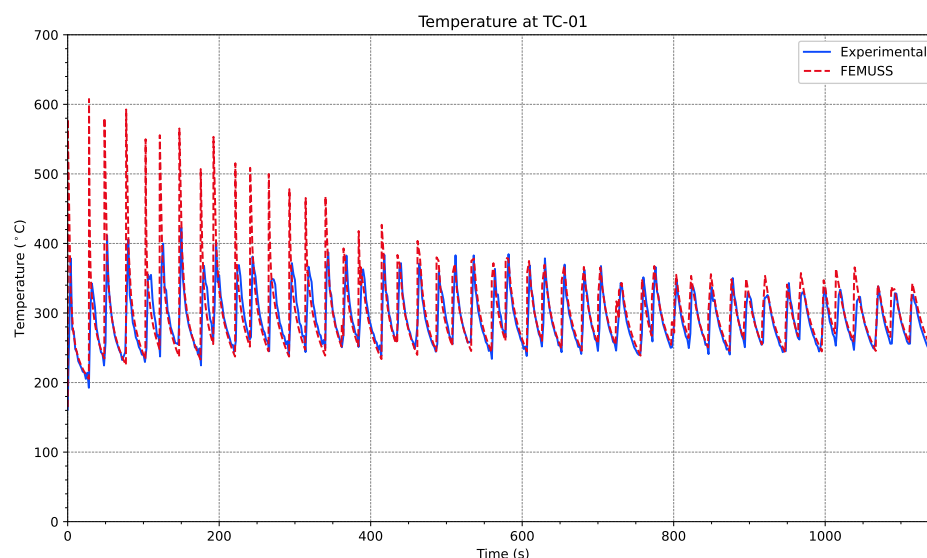


Figure 16. Comparison of simulated and experimentally measured temperature history at TC-1.

5.2. Inherent Strain Assessment

This section presents and discusses the inherent strains calculated using the procedure defined in Section 2.2. The computed results are analysed and their implications for the overall modelling approach are examined.

5.2.1. Definition of the Control Volumes

The inherent strain evaluation in the local model was conducted by applying Equations (12) and (13) to the control volume defined as a cube in the middle of the deposition. Five different sizes were chosen to assess the homogeneity of the calculated strains and their sensitivity to the chosen volume. The defined control volumes are illustrated in Figure 17. The smallest cube size is 4 layers high, whereas the largest cube corresponds to the height of the entire deposited volume (48 layers). This approach allows for a comprehensive assessment of the inherent strains and provides valuable insights into the layer thickness that can be used in real parts when applying the ISM for distortion prediction.

The smallest control volume was defined based on the number of layers affected by the heat source during the scanning sequence. In particular, the maximum penetration of the melt-pool and HAZ was analysed to assess its impact on the plastic strain value and, consequently, the inherent strain tensor. Figure 18 shows the evolution of equivalent plastic strain (PEEQ) at the centroid of the domain. As shown, plastic strain begins to develop when the material is first deposited ($t \approx 560$ s). It continues to evolve as subsequent layers are added, stabilising only after four additional layers are deposited ($t \approx 610$ s). Beyond this point, the plastic strain remains constant. Therefore, the minimum control

volume size required for inherent strain calculation corresponds to the height of these four deposited layers.

The inherent strain tensor was calculated at the end of the cool-down stage, in accordance with the simplified modelling approach used in the macro-scale model.

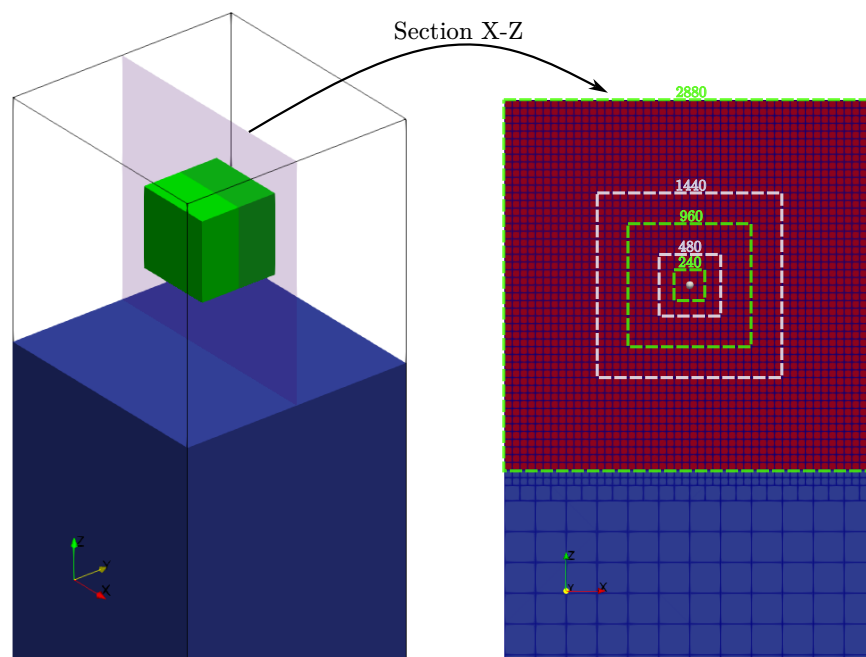


Figure 17. Defined control volumes at the centroid of the local model. All dimensions in μm .

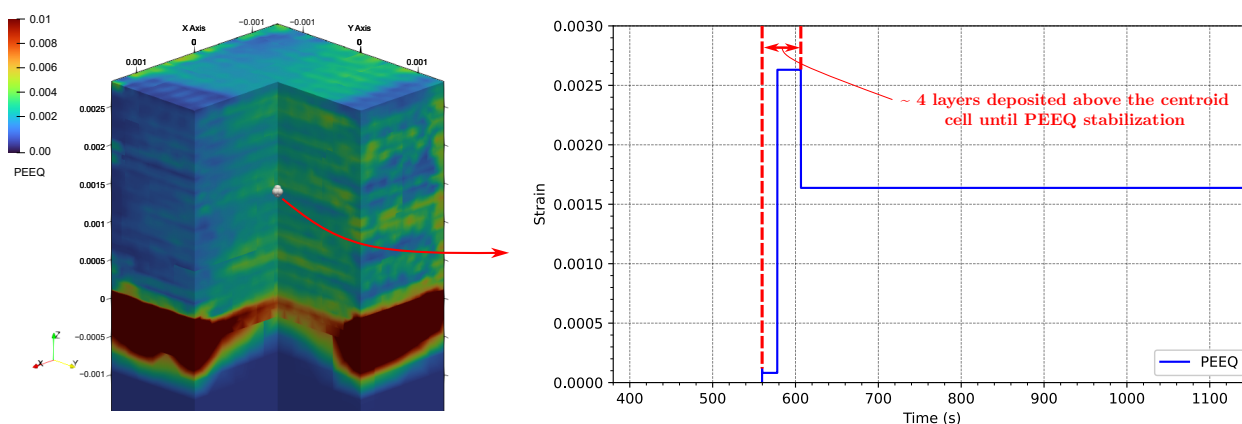


Figure 18. Evolution of PEEQ at a cell near the centroid of the deposited material.

5.2.2. Boundary Conditions and Control Volume Sensitivity

Two different mechanical boundary conditions were applied on the lateral surfaces of the deposited material to assess their effects on the inherent strain tensor (see Section 4.1.3). The influence of these boundary conditions can vary depending on the size of the control volume. Therefore, to provide a comprehensive understanding, a sensitivity analysis was performed considering both the boundary conditions and control volume sizes.

The inherent strain tensor components and their corresponding invariants for various control volume sizes, under both boundary conditions, are depicted in Figure 19 and Figure 20, respectively. In addition to the component-level analysis, the use of invariants provides a complementary method for this assessment. Invariant I_1 describes the dilatation behaviour (volume change), while I_2 accounts for distortions (change in shape). The contour plots of these invariants are plotted in Figure 21.

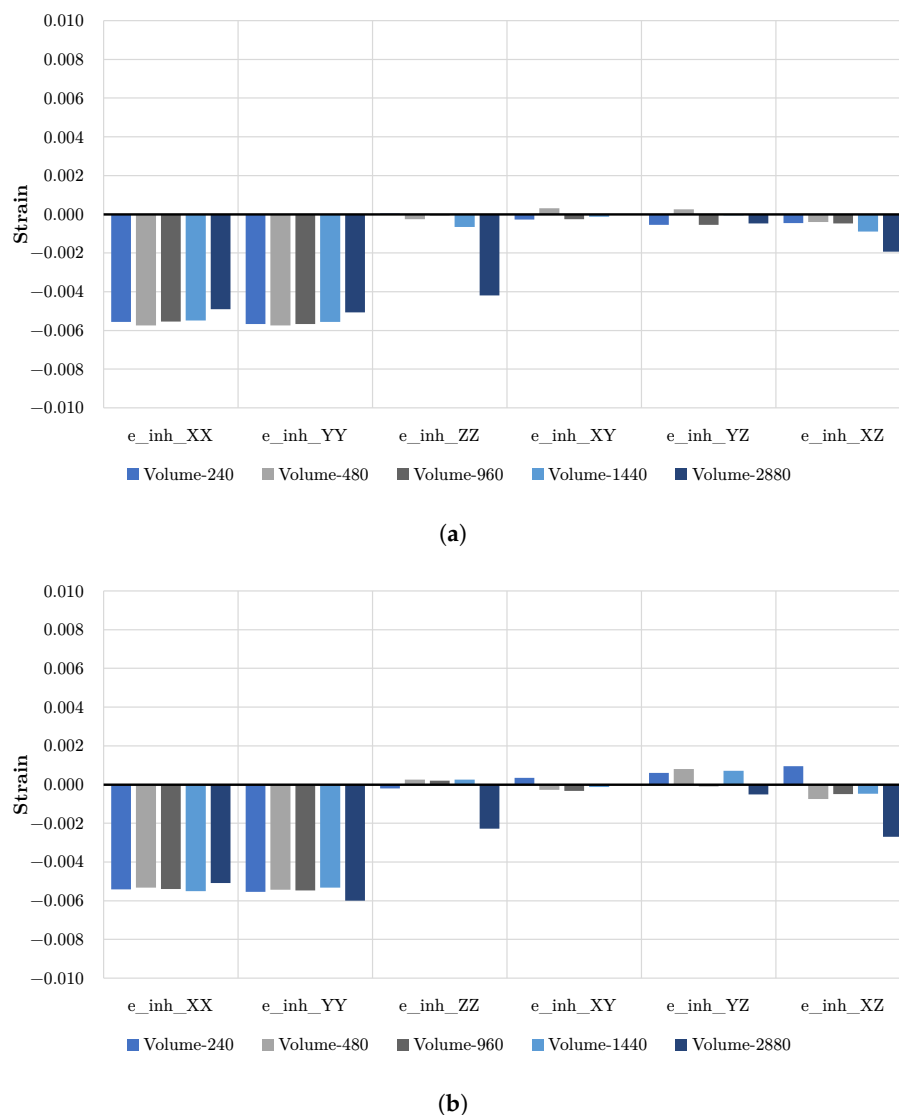


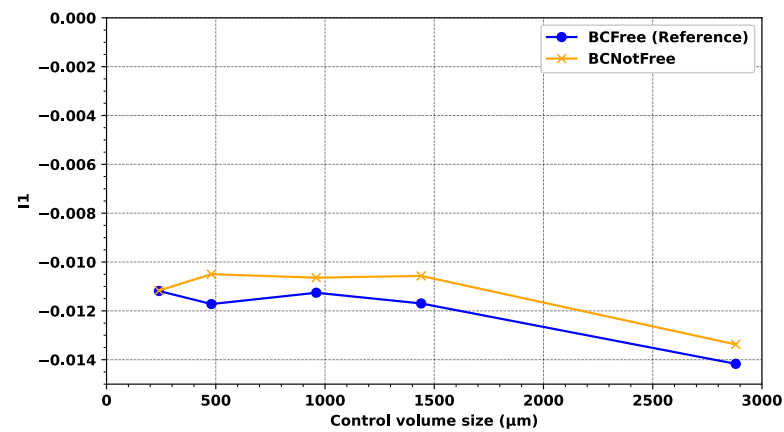
Figure 19. Inherent strain tensor components under different boundary conditions and control volume sizes: (a) BCFree boundary conditions and (b) BCNotFree boundary conditions.

For control volumes ranging from 240 to 1440 μm , the boundary conditions do not significantly influence the tensor components, indicating minimal sensitivity to the applied constraints within this range. Note that both I_1 and I_2 remain nearly constant.

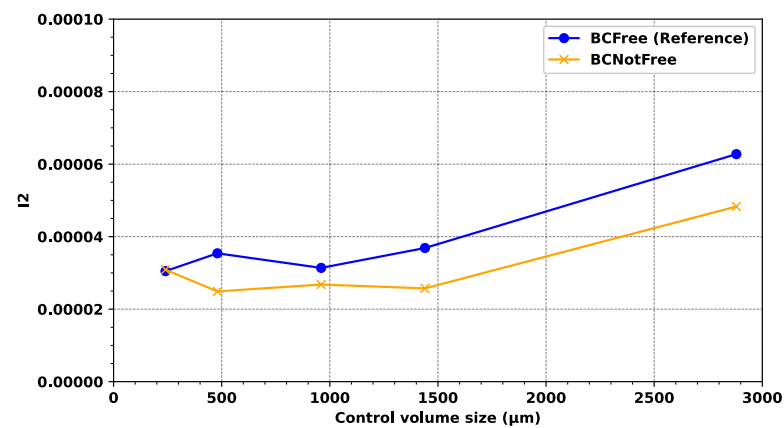
Additionally, it is significant that the XX and YY components dominate the strain tensor, exhibiting nearly identical values, which suggests isotropic behaviour in the XY plane. This may be attributed to the scanning strategy employed during deposition.

However, for the largest control volume, the boundary effects become more pronounced, particularly affecting the ZZ and XZ components of the inherent strain tensor. This sensitivity to boundary effects is further illustrated in the contour plots shown in Figure 21, where localised variations in these components are noticeable.

Therefore, this minimal sensitivity to the size for all control volumes, except the largest one, suggests that there is a maximum control volume size that is not affected by boundary effects. Although there is not enough resolution to precisely define this threshold, the analysis indicates that this critical size likely corresponds to approximately half of the total volume of deposited material.

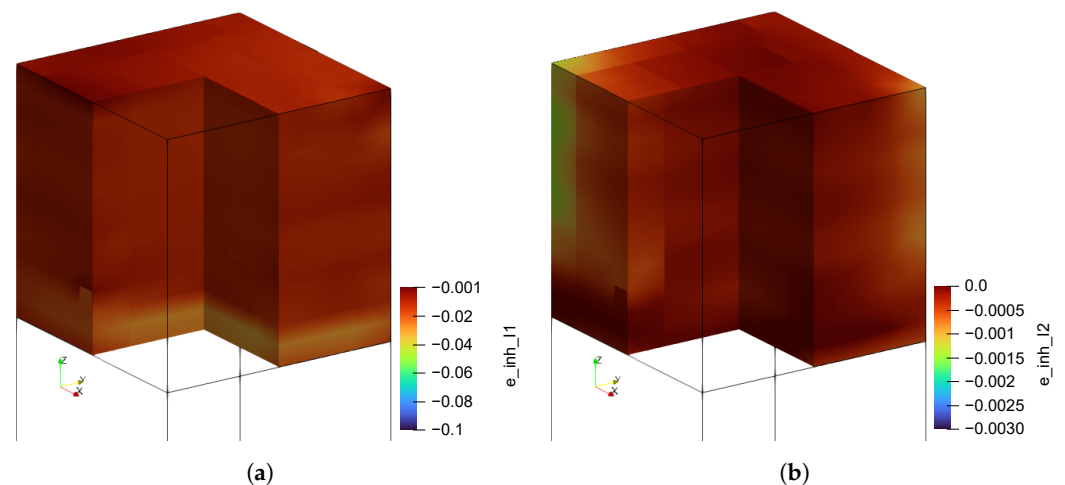


(a)



(b)

Figure 20. Inherent strain tensor invariants under different boundary conditions and control volume sizes: (a) variation in I_1 of the inherent strain tensor with respect to control volume size for both boundary conditions and (b) variation in I_2 of the inherent strain tensor with respect to control volume size for both boundary conditions.



(a)

(b)

Figure 21. Inherent strain tensor invariants contour plots at the end of the simulation: (a) contour plot of I_1 and (b) contour plot of I_2 .

Similarly, the smallest valid control volume for inherent strain computation was determined to be 240 μm (equivalent to four deposited layers). This size was found to be optimal for minimising the local model size needed for inherent strain calculation. In this specific case, the minimum control volume size aligns with the depth of the melt-pool

and HAZ. However, for other scanning strategies, additional layers may be necessary to achieve building strain homogenisation.

5.2.3. Optimised Local Model for Efficient Inherent Strain Calculation

Earlier analysis of volume and boundary condition effects suggests that the local model for the calculation of the inherent strain tensor can be optimised to reduce computational cost while maintaining accuracy. This optimisation involves minimising the local model size without compromising the reliability of the results. The following criteria must be met to ensure the model's efficiency:

- The control volume should not be smaller than 240 μm , which corresponds to the equivalent of four deposited layers.
- A minimum of four deposited layers must be present above the control volume so as to avoid plastic strain modifications.
- Enough spacing should be kept between the control volume and the lateral surfaces and the baseplate to prevent the influence of boundary effects.

The geometry of the local model that satisfies these requirements is depicted in Figure 22. A visual comparison between the initial and the optimised models is provided in Figure 23. By maintaining the same element size as in the initially proposed local model, the number of elements is reduced significantly, lowering the computational cost by 89% while preserving accuracy.

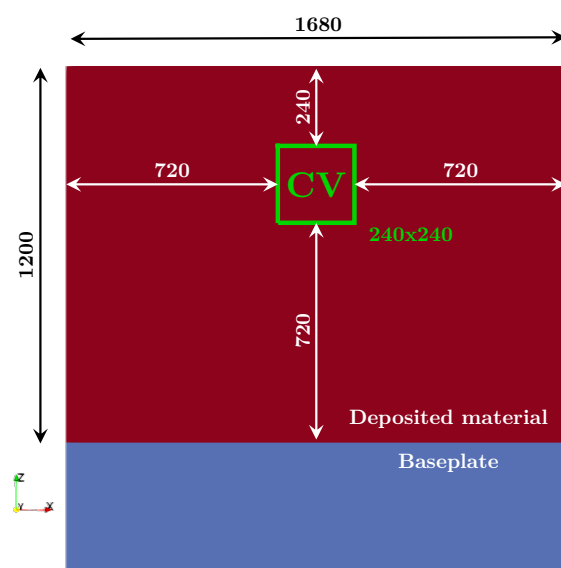


Figure 22. The 2D geometrical details of the optimised local model (units: μm).

A tensor component analysis and comparison with the initial local model were conducted (see Figure 24) to validate that the optimised model dimensions are sufficient for accurately calculating the inherent strain tensor. A 240 μm control volume was selected in both models for this comparison. The results confirm that the optimised local model can compute the inherent strain tensor with the same accuracy as the original model, while significantly reducing computational cost.

Additionally, the tensor was recalculated using a larger control volume of 480 μm . In this case, the tensor components—particularly the ZZ and off-diagonal components—became distorted, indicating the influence of boundary effects. Thus, the new local model size is determined to be optimal.

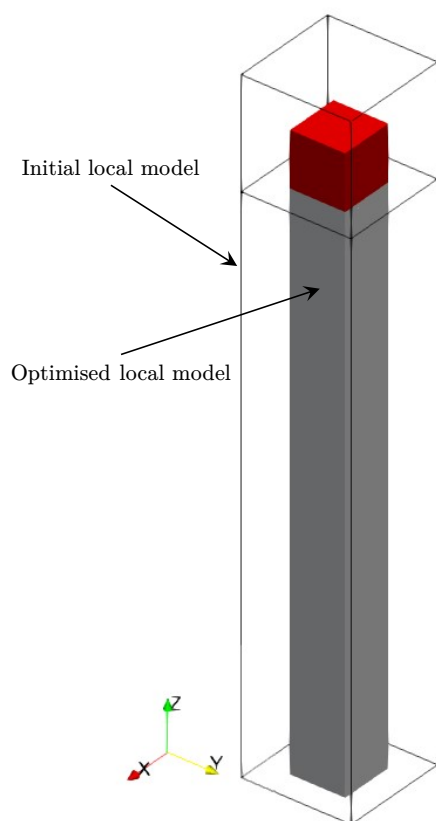


Figure 23. Comparison of initial and optimised local models.

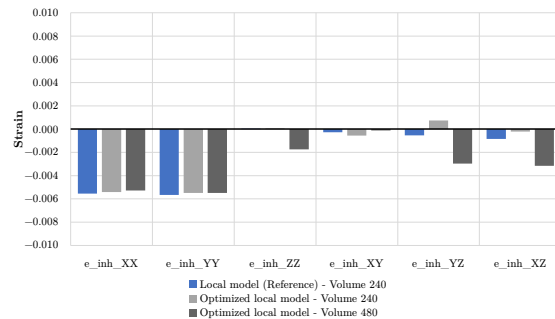


Figure 24. Comparison of inherent strain tensor components between initial and size optimised local models.

5.2.4. Contribution of Each Strain Component of the Inherent Strain

According to Equation (12), the inherent strain tensor is the sum of thermal, plastic, and activation strain tensors, where the thermal component is the primary driving factor. Figure 25a shows the contribution of each component for each component of the tensor using the 960 μm control volume. Frobenius' norm was employed to more clearly assess the contributions. Plastic and activation strain tensors' contributions were compared to the thermal strain tensor. These contributions are visualised in Figure 25b. The results indicate that the activation strain significantly impacts the inherent strain tensor, contributing nearly half of the value of the thermal strain, while the plastic strain contributes approximately 12%, which is less than initially expected. This lower contribution highlights that plastic strain is not the predominant factor to compute the inherent strain tensor. Thus, plastic strain modelling might be less critical than expected.

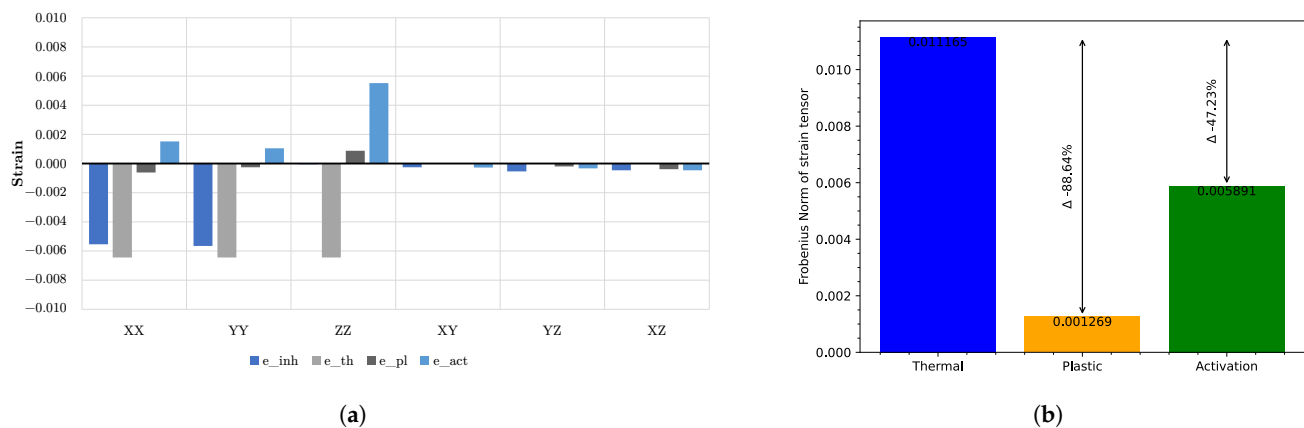


Figure 25. Inherent strain tensor components relevance in the 960 μm control volume cube: (a) components of the inherent strain tensor and (b) comparison of Frobenius' norm, using thermal strain as the reference.

5.2.5. Simplification of Inherent Strain Tensor Components

The inherent strain tensor component analysis carried out earlier suggests that the inherent strain tensor can be approximated as an isotropic strain tensor in the XY plane due to the homogenisation effect caused by the used scanning strategy and the summation of different layers.

To validate this approximation, the impact of neglecting off-diagonal components and the ZZ component was assessed by recalculating the Frobenius norm and strain invariants for the inherent strain tensor without these components. The results for the 960 μm control volume are shown in Figure 26. The comparison reveals no appreciable difference between the full tensor and the simplified tensor that excludes the off-diagonal and ZZ components. Consequently, the inherent strain tensor computed from the local high-fidelity model can be simplified as follows in Voigt notation:

$$\tilde{\epsilon}^{inh} = -0.0056 \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (14)$$

Furthermore, the inherent strain tensor derived from the calibrated local model was compared to the one obtained using an empirical method in a previous study [18]. Although the tensors are not directly comparable due to differences in the PBF-LB machines and process parameters used, both methods produced tensors with the same shape, i.e., an isotropic strain tensor in the XY plane.

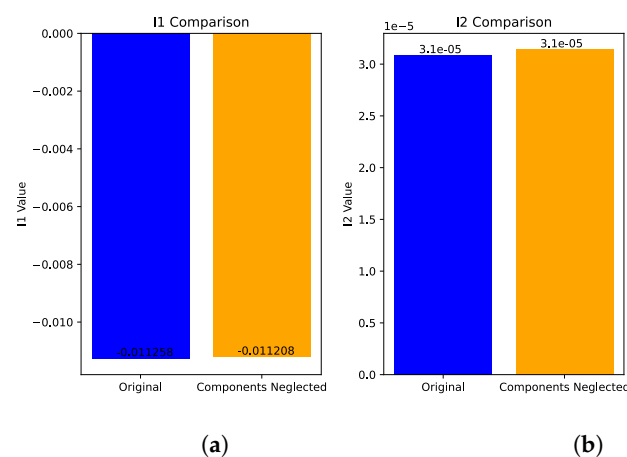


Figure 26. Effect of neglecting off-diagonal and ZZ components on the inherent strain tensor. The left plot (a) shows the comparison of the I_1 invariant. The right plot (b) presents the same comparison for the I_2 invariant.

5.3. Validation of Inherent Strains in the Global Model

Firstly, the effect of neglecting off-diagonal and ZZ components was further validated using the SBA industrial part. To this end, three different inherent strain tensors were applied: the full tensor, the tensor with only diagonal components, and the simplified tensor as proposed in Equation (14). The comparison of the displacement fields resulting from all three variants is shown in Figure 27. As can be observed, the differences between these displacement fields are negligible, indicating that the simplification of neglecting off-diagonal and ZZ components of the inherent strain tensor is valid, even when applied to complex industrial components.

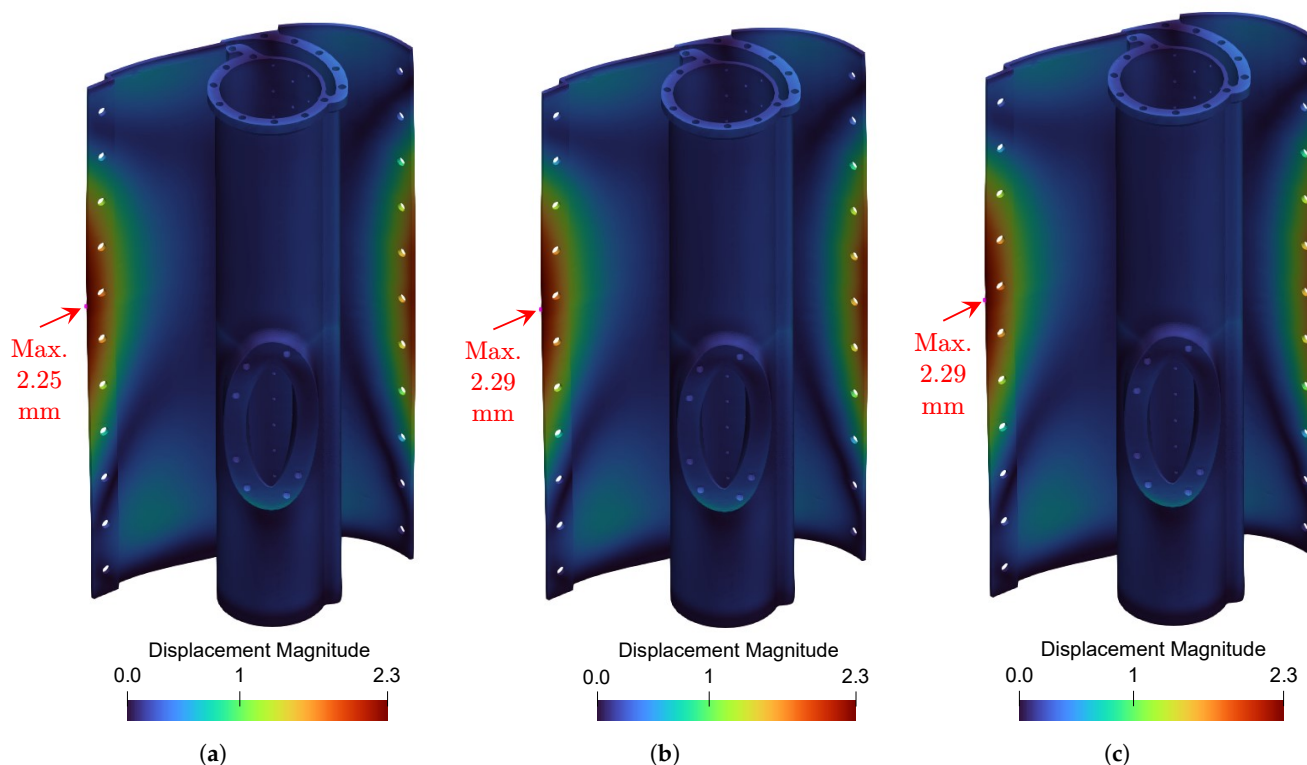


Figure 27. Displacement magnitude (mm) contour field in the SBA for different inherent strain tensors to assess the effect of neglecting off-diagonal and ZZ components: (a) Full tensor, (b) only diagonal components, and (c) isotropic tensor in the XY plane.

Then, the computed final deformed geometry was compared with the experimentally measured geometrical deviations. To this end, a geometrical deviation contour plot was generated from calculated displacement field and compared with experimentally measured deviations.

The comparison shown in Figures 28 and 29 demonstrates a good correlation between numerical predictions and experimental measurements. Although there are minor discrepancies, these can be attributed to several factors such as the inherent simplifications of the classical ISM as well as the specific boundary conditions used in the simulations. However, the results obtained are consistent with the expected accuracy of the ISM [33].

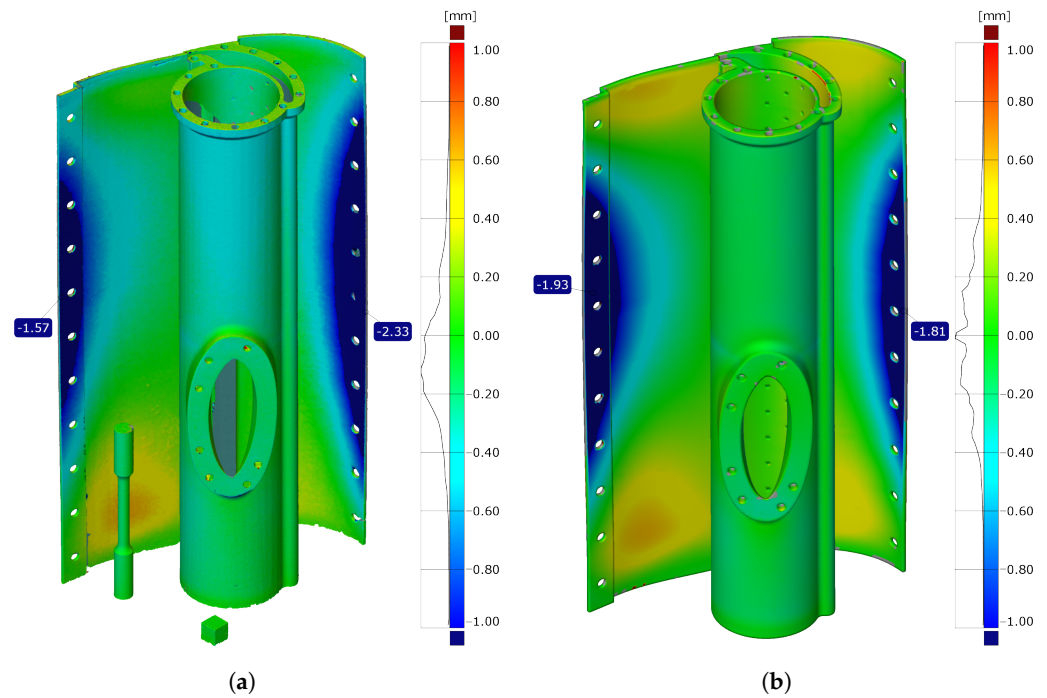


Figure 28. Front view of the deviation contour plot of the SBA: (a) experimental result and (b) numerical result.

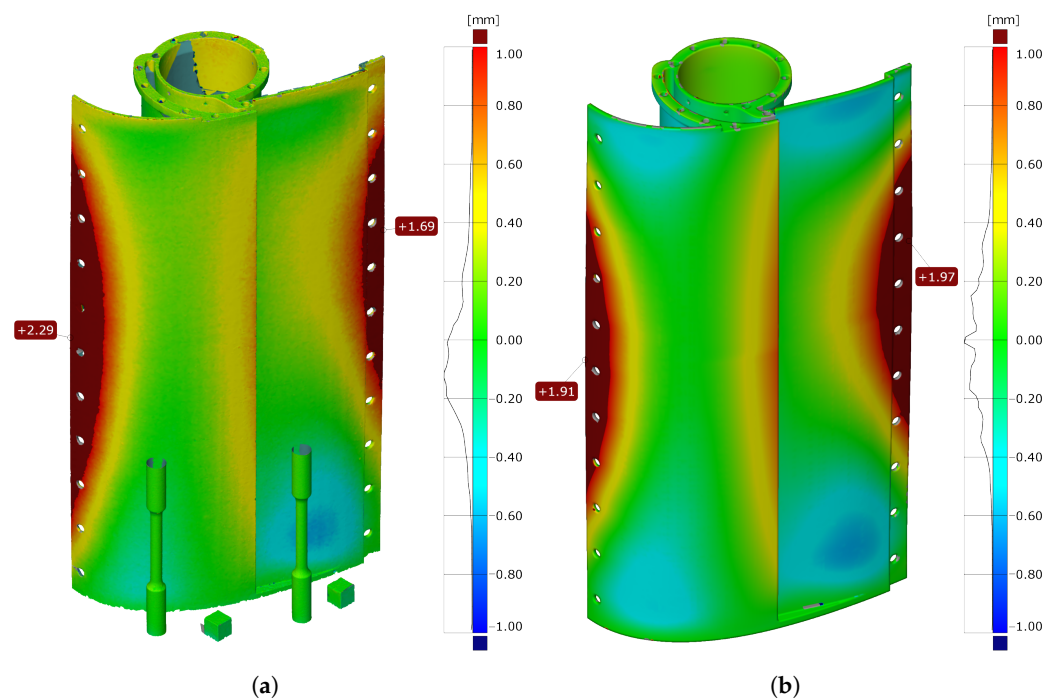


Figure 29. Back view of the deviation contour plot of the SBA: (a) experimental results and (b) numerical results.

6. Conclusions

This study presents a multi-scale modelling approach for calculating inherent strains in the PBF-LB process. The primary focus was to enhance the accuracy and effectiveness of the local models used to compute the inherent strains.

This high-fidelity model demonstrates its capability to produce reliable inherent strain tensors to be applied at the macro-scale level using an inherent strain methodology. The validity of the proposed approach is further supported by comparisons with previous

calculations obtained through empirical methodologies, highlighting its robustness and potential for practical application in additive manufacturing.

The key findings and implications of this study are summarised as follows:

- **High-fidelity model calibration:** The high-fidelity local model is calibrated using experimental temperature data to successfully predict temperature histories and inherent strain tensors. The calibrated model provides a robust tool for further analysis.
- **Inherent strain computation:** The computed inherent strain tensor is defined in terms of thermal, plastic, and activation strains. The results indicate that activation strains significantly contribute to the inherent strain tensor, emphasising the importance of the building strategy, thus being the scanning strategy a key factor of the PBF-LB process. Plastic strain, while relevant, was found to have a smaller impact than initially expected, allowing for further simplifications.
- **Control volume sensitivity:** The sensitivity analysis revealed that the size of the control volume plays a critical role determining the inherent strain tensor. A minimum control volume size of approximately four deposited layers was identified as optimal in the proposed local model, minimising the influence of boundary conditions.
- **Optimised local model:** An optimised local model was developed, achieving a significant 89% reduction in computational cost compared to the original local model, without compromising the accuracy of inherent strain calculations.
- **Simplified inherent strain tensor:** This study demonstrated that the inherent strain tensor could be approximated as an isotropic strain tensor in the XY plane, with negligible off-diagonal and ZZ components. This simplification did not significantly affect the accuracy of the results, validating its use in practical applications.
- **Validation with real components:** The inherent strain tensor derived from the high-fidelity local model was applied to the SBA actuator geometry. The predicted distortions were in good agreement with experimental measurements, despite minor discrepancies. This validation confirmed the practical applicability and accuracy of the proposed multi-scale modelling approach.
- **Comparison with empirical methods:** The calculated inherent strain tensor was consistent with the one obtained empirically as derived in previous studies.

While this study focuses on the methodology for numerically calculating inherent strains, future work could extend this approach to varying process parameters such as laser power, scanning strategy, and layer thickness, while keeping the geometry constant. This would further validate the robustness and applicability of the methodology under different manufacturing conditions. Additionally, exploring the application of this method to other materials would be valuable to assess its generalisability.

Author Contributions: Conceptualisation, I.S. and M.C.; data curation, I.S.; formal analysis, I.S.; investigation, I.S.; resources, M.C. and M.S.S.; methodology, I.S.; software, I.S., M.A.C. and C.A.M.; validation, I.S.; writing—original draft, I.S.; writing—review & editing, I.S., M.C., M.S.S., M.A.C. and C.A.M.; supervision, M.C. and M.S.S.; project administration, M.C. and M.S.S.; funding acquisition, M.S.S. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: The data that support the findings of this study are available from the corresponding author upon reasonable request.

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ENHANCED INHERENT STRAIN METHOD

7.1 Introduction

This chapter presents the third article in this thesis series. While the first and second articles focus on determining the inherent strain tensor (via experimental calibration and high-fidelity meso-scale local models, respectively) the work presented here advances the inherent strain method itself. Conventional [ISMs](#) assume a constant inherent strain upon deposition, neglecting the transient thermal effects that occur during the [PBF-LBs](#) process. However, non-uniform geometries and/or complex scanning strategies generate a dynamically evolving thermal field that influences the material behaviour.

The Enhanced Inherent Strain Method ([EISM](#)) proposed in this article integrates macro-scale temperature history into the inherent strain framework by introducing a temperature-dependent correction term to the precomputed inherent strain tensor. This modification enables a more physically realistic representation of the deformation mechanisms by capturing the effects of geometry and boundary conditions on thermal behaviour. Consequently, the model refines the prediction of distortions and residual stresses. Building upon the inherent strain calculations established in the previous articles, this work represents a step forward in improving the accuracy and reliability of inherent strain-based simulations.

7.2 Scientific contribution

This work extends the inherent strain methodology beyond the assumption of a constant strain tensor by incorporating part-scale temperature history into the framework. Unlike conventional [ISMs](#), which rely on a static inherent strain tensor, the proposed approach introduces a dynamic correction factor that accounts for the evolution of thermal fields during the [PBF-LB](#) process. This enhancement bridges the gap between simplified inherent strain-based models and high-fidelity thermo-mechanical simulations.

Furthermore, this study examines the impact of mesh refinement and adaptive layer lumping strategies on prediction accuracy. The findings indicate that capturing abrupt stiffness variations, such as shrink lines, is critical for numerical stability

and precision. The proposed methodology is validated on two Ti-6Al-4V geometries, demonstrating improved agreement between numerical predictions and experimental measurements. By enhancing the predictive capability of the inherent strain framework while preserving computational efficiency, this approach enables more accurate simulations suitable for industrial applications.

7.3 Summary and conclusions

The enhanced inherent strain method proposed in this work accounts for the influence of part-scale thermal history on strain accumulation in the PBF-LB process. By introducing a temperature-dependent correction to the inherent strain tensor, the model captures transient thermal effects, refining its predictive accuracy for distortions and residual stresses.

Experimental validation on a non-symmetric bridge and a SBA confirms that incorporating temperature history significantly improves prediction accuracy, reducing systematic errors observed in conventional ISMs. A sensitivity analysis further highlights the necessity of adapting layer lumping strategies based on geometry-dependent stiffness variations to maintain numerical stability. Although the additional thermal analysis increases computational time, the improved prediction fidelity justifies the extra cost, making the method viable for industrial process optimisation.

This work complements the inherent strain tensor calibration methodologies presented in previous chapters, representing an important step toward a more reliable and computationally efficient modelling framework for PBF-LB.

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Article

Integrating Temperature History into Inherent Strain Methodology for Improved Distortion Prediction in Laser Powder Bed Fusion

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Abstract: Powder bed fusion–laser beam (PBF-LB) additive manufacturing enables the production of intricate, lightweight metal components aligned with Industry 4.0 and sustainable principles. However, residual stresses and distortions challenge the dimensional accuracy and reliability of parts. Inherent strain methods (ISMs) provide a computationally efficient approach to predicting these issues but often overlook transient thermal histories, limiting their accuracy. This paper introduces an enhanced inherent strain method (EISM) for PBF-LB, integrating macro-scale temperature histories into the inherent strain framework. By incorporating temperature-dependent adjustments to the precomputed inherent strain tensor, EISM improves the prediction of residual stresses and distortions, addressing the limitations of the original ISM. Validation was conducted on two Ti-6Al-4V geometries—a non-symmetric bridge and a complex structure (steady blowing actuator)—through comparisons with experimental measurements of temperature, distortion, and residual stress. Results demonstrate improved accuracy, particularly in capturing localized thermal and mechanical effects. Sensitivity analyses emphasize the need for adaptive layer lumping and mesh refinement in regions with abrupt stiffness changes, such as shrink lines. While EISM slightly increases computational cost, it remains feasible for industrial-scale applications. This work bridges the gap between simplified inherent strain models and high-fidelity simulations, offering a robust tool for simulation-driven optimisation.

Keywords: additive manufacturing; inherent strain; distortion; thermo-mechanical model; finite element modelling; macro-scale; powder bed fusion; Ti-6Al-4V



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1. Introduction

Powder Bed Fusion-Laser Beam (PBF-LB) has emerged as a transformative technology in metal Additive Manufacturing (AM), offering the unique ability to fabricate highly complex and optimised components directly from digital designs. PBF-LB aligns with the principles of Industry 4.0, providing industries such as the aerospace, defense, automotive, and healthcare sectors with tools to create lightweight, high-performance components

while minimizing material waste and production time [1,2]. The technology's ability to support topology-optimised designs and intricate geometries has made it a key driver of innovation across these sectors [3]. PBF-LB also offers notable environmental advantages. The process is inherently material efficient, using only the necessary amount of metal powder for fabrication, with excess material often being recyclable [4,5]. These factors collectively support sustainable manufacturing principles, aligning with global efforts to minimize the environmental impact of industrial processes.

Despite its transformative potential, PBF-LB faces persistent residual stresses and distortions challenges. These issues arise from the rapid thermal cycles, steep temperature gradients, and complex phase transformations that are intrinsic to the layer-by-layer deposition process [6,7]. They can not only compromise the dimensional accuracy and structural integrity of manufactured components but also pose barriers to the widespread adoption of PBF-LB in high-value industrial applications. Addressing these challenges requires robust predictive tools capable of capturing the multi-physics nature of the process, including thermal, mechanical, and metallurgical interactions.

Physics-based numerical simulations have become indispensable for understanding the complex phenomena underlying the PBF-LB process and for guiding process parameter optimisation. These techniques enable detailed analysis of thermal, mechanical, and metallurgical interactions that govern the quality and performance of manufactured components [8]. Among these methods, the Inherent Strain Method (ISM) has emerged as a computationally efficient alternative for predicting residual stresses and distortions in PBF-LB. Originally developed for welding processes [9], ISM was adapted for additive manufacturing due to its ability to approximate complex thermo-mechanical interactions using predefined strain fields. This simplification allows ISM to achieve significant reductions in computational cost, making it attractive for industrial-scale problems, where computational resources are often a limiting factor. Studies by Mohammadtaheri et al. [10] and Bayat et al. [11] highlight the widespread adoption of ISM in PBF-LB modelling, particularly in predicting distortions and optimising process parameters. Additionally, these studies highlight the successful integration of ISM into commercial software platforms, boosting its use in industrial applications.

Surrogate modelling has recently become an interesting tool to accelerate the simulation process even further [12]. Indeed, it has been used in combination with inherent strain numerical models to generate the required datasets for training, ultimately resulting in almost instantaneous predictors that can be successfully applied even in design optimisation [13]. Improving inherent strain-based modelling methodologies not only enhances predictive accuracy but also improves the quality of datasets used to train surrogate models, thereby advancing their reliability for PBF-LB applications.

The ISM, in its original and most widely adopted form, provides a simplified yet practical approach to modelling the residual stresses and deformations that arise during metal AM. Its implementation is thoroughly documented in the literature [9,14,15]. Broadly speaking, the methodology involves a sequence of mechanical, linear elastic simulation steps combined with a prescribed activation strategy. Typically, the simulation proceeds layer-by-layer, and at each simulation step, a new layer is activated, and the inherent strain is applied. Multiple layers are often lumped and activated simultaneously, thereby reducing the number of incremental steps as well as the total number of elements, which ultimately decreases the overall computational cost. The inherent strain tensor can be experimentally calibrated by measuring distortions in test coupons [15] or can be derived from high-fidelity thermo-mechanical simulations at the meso-scale [16].

Over time, refinements in ISM have emerged to improve accuracy in residual stress and deformation predictions [17–19]. These advancements primarily focus on refining the methods used to derive inherent strains from local thermo-mechanical models.

The original ISM assumes that each deposited layer inherits a constant inherent strain state, neglecting spatial and temporal variations in the thermal field. While this assumption enables large computational savings, it may oversimplify the process physics, particularly in parts featuring non-uniform geometries or complex scanning strategies where steep thermal gradients may occur. Consequently, conventional ISM frameworks might struggle to predict residual stresses and distortions accurately in certain scenarios [20]. Addressing these shortcomings is crucial for advancing the fidelity and reliability of ISM in PBF-LB applications.

Recent efforts have begun to address this limitation by including local thermal histories into the ISM [19,21]. For instance, Pourabdollah et al. [22] introduced a variant of the ISM tailored for Electron beam powder bed fusion (PBF-EB), which accounts for both compressive plastic strains adjacent to the melt pool and thermal strains associated with the evolving macroscale thermal field during fabrication. Although PBF-LB differs from PBF-EB in some aspects, the underlying challenges of representing localized temperature gradients and their influence on residual stresses remain comparable. This insight motivates extending thermal-history-informed ISM variants to the PBF-LB context.

In this paper, we present an Enhanced Inherent Strain Method (EISM) for PBF-LB, which integrates part-scale temperature evolution into the original ISM. Unlike high-fidelity thermo-mechanical analysis, this approach computes only the average temperature field evolution, which is largely influenced by the part geometry and boundary conditions. While the starting point of the EISM remains a precomputed inherent strain tensor (including thermal, plastic, and other strain components) as in ISM, this is further adjusted based on the computed part-scale temperature history. This adaptation provides a more physically realistic representation of the deformation mechanisms by accounting for the geometry- and boundary-condition-induced effects on thermal behaviour.

The findings of this study are particularly relevant to engineers, researchers, and industrial practitioners working to optimise PBF-LB processes. Engineers and researchers can leverage the proposed modelling advancements to refine process parameters for specific geometries and boundary conditions, thereby reducing distortions and residual stresses. Industrial practitioners can integrate these methodologies into simulation-driven design workflows to predict and mitigate manufacturing defects. Furthermore, these improvements in inherent strain-based modelling enhance the quality of training datasets for surrogate models, ultimately contributing to more efficient and accurate design optimisation.

In summary, this work aims to enhance the accuracy and practicality of the ISM for PBF-LB by integrating part-scale thermal histories into the framework, resulting in an EISM. The specific objectives are to

- Develop the EISM: incorporate thermal history effects to improve the physical accuracy of residual stress and distortion predictions.
- Validate predictive accuracy: compare EISM and ISM results with experimental data for parts with complex thermal gradients.
- Assess computational efficiency: evaluate and compare the computational cost and performance of ISM and EISM.

The remainder of this paper is organized as follows:

- Modelling Approach (Section 2) details the enhanced inherent strain modelling approach, including how macro-scale thermal histories are integrated into the original ISM framework.

- Experimental Campaign for Calibration and Validation (Section 3) describes the experimental campaign, including the tested geometries, materials, process parameters, and measurement techniques used for calibration and validation.
- Numerical Implementation (Section 4) presents the numerical implementation of the EISM in the selected testing geometries, including mesh generation, boundary conditions, and computational settings.
- Results and Discussion (Section 5) compares EISM and ISM predictions with experimental data, discussing the effects of mesh size, layer lumping, and computational efficiency.
- Conclusions (Section 6) summarizes the key findings and outlines future research directions.

By addressing these objectives, this study advances the predictive accuracy and applicability of simulation-based process optimisation in PBF-LB.

2. Modelling Approach

The EISM is a sequentially coupled layer-by-layer thermo-mechanical analysis method. A general overview of the methodology is illustrated in Figure 1. The following subsections detail the key considerations and the overall solution procedure.

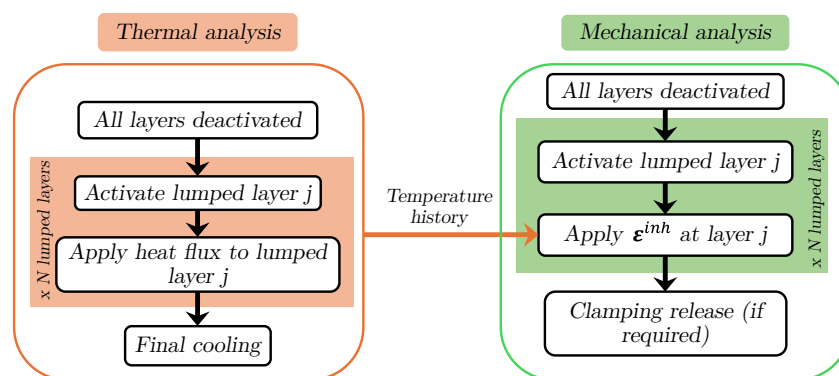


Figure 1. Overview of the EISM methodology, showing the sequential coupling between thermal and mechanical analyses.

2.1. Thermal Analysis

The layer-by-layer macro-scale thermal model follows the approach outlined in previous studies [23]. In this work, it is used to calculate the average temperature field evolution of the printed domain before the subsequent layer is deposited.

The heat transfer within the domain is governed by the transient heat conduction equation:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \dot{Q} \quad (1)$$

where ρ is the material density, c_p is the specific heat capacity, T is the temperature, t is time, k is the thermal conductivity, and $\dot{Q}$ represents heat rate generation per unit volume, including heat input from the laser or other energy sources.

To reduce computational time, several layers can be lumped together, and a time-averaged volumetric heat source, $\dot{Q}$, is applied to the entire volume of the lumped layers during an equivalent time step. The time step for the j -th lumped layer is computed as

$$\Delta t_j = \sum_{i=n \cdot (j-1) + 1}^{n \cdot j} (t_i^{laser} + t_i^{recoater}) \quad (2)$$

where i is the layer counter, n is the number of layers in each lump, and t_i^{laser} and $t_i^{recoater}$ correspond to the laser exposure and recoating times for layer i , respectively.

The time-averaged heat source is computed within the FEM framework by modelling the moving heat source as a “concentrated moving heat source” [24,25]. Using this approach, the energy input to the system is determined based on the scanning sequence. During each time step, the algorithm identifies all elements intersected by the laser and applies the corresponding heat flux to these elements. This method accounts for different scanning patterns and process parameters for each layer, offering the flexibility needed to accurately simulate diverse additive manufacturing process conditions.

Heat losses at the boundaries are modelled via convection and radiation.

- **Convection:** $q = h(T - T_\infty)$, where h is the heat transfer coefficient, and T_∞ is the ambient temperature.
- **Radiation:** $q = \epsilon\sigma(T^4 - T_\infty^4)$, where ϵ is the emissivity, and σ is the Stefan–Boltzmann constant.

2.2. Mechanical Analysis

The mechanical equilibrium is described by the quasi-static balance of momentum equation:

$$\nabla \cdot \sigma + \mathbf{b} = 0 \quad (3)$$

where σ is the Cauchy stress tensor and $\mathbf{b}$ represents body forces per unit volume.

The constitutive relationship of the material is

$$\sigma = \mathbf{C} : \epsilon^e \quad (4)$$

where $\mathbf{C}$ is the fourth-order constitutive tensor, and ϵ^e is the elastic strain tensor.

Under the assumptions of small strain theory, the elastic strain tensor can be computed as

$$\epsilon^e = \epsilon^{total} - \epsilon^{inh} \quad (5)$$

where $\epsilon^{total} = \nabla^s(\mathbf{u})$ is the total strain tensor, and ϵ^{inh} is the inherent strain tensor.

2.3. EISM Considerations

The inherent strain tensor includes all non-elastic strain components. It is defined as

$$\epsilon^{inh} = \epsilon^{total} - \epsilon^e = \epsilon^{th} + \epsilon^{pl} + \epsilon^{act} \quad (6)$$

where ϵ^{th} is the thermal strain tensor, ϵ^{pl} is the plastic strain tensor, and ϵ^{act} is the activation strain tensor.

ϵ^{inh} can be obtained through either meso-scale thermo-mechanical simulations or experimental calibration [15,16]. This precomputed inherent strain tensor will hereafter be denoted as $\epsilon^{inh,0}$ and is subsequently used as input data in methodologies based on inherent strain theory.

In the original ISM, ϵ^{inh} is assumed to be constant for each material point and is applied at the moment of material deposition:

$$\epsilon^{inh} = \epsilon^{inh,0} \quad (7)$$

The EISM enhances the original approach by incorporating temperature dependence. The scope is to make ϵ^{inh} both temperature and time dependent, using the average temperature of the deposited domain. Consequently, $\epsilon^{inh,0}$ is enhanced with the thermal

strain history calculated in the layer-by-layer macro-scale thermal analysis (as detailed in Section 2.1). Thus, the inherent strain ϵ^{inh} applied in EISM is expressed as

$$\epsilon^{inh} = \epsilon^{inh,0} + \Delta\epsilon^{th} \quad (8)$$

The layer lumping strategy should be applied carefully, as plastic strain typically stabilizes only after several layers have been deposited, as demonstrated in [16]. Since the objective is to enhance $\epsilon^{inh,0}$ while preserving the plastic and activation components unchanged, the minimum number of layers to be considered in the calculations must be carefully determined.

The thermal strain depends on the thermal field and is computed as

$$\epsilon^{th} = [\alpha(T) \cdot (T - T_{ref}) - \alpha(T_0) \cdot (T_0 - T_{ref})]I \quad (9)$$

where T is the current temperature, $\alpha(T)$ is the temperature-dependent secant thermal expansion coefficient, T_{ref} is the reference temperature for the expansion coefficient, and T_0 is the initial temperature of the material at the start of the simulation.

Note that $\epsilon^{inh,0}$ typically accounts for the total thermal deformation during the cooling procedure. Thus, for $T = T_{ref}$, the deformation reaches its maximum value:

$$\epsilon^{th,0} = [-\alpha(T_0) \cdot (T_0 - T_{ref})]I \quad (10)$$

However, the thermal analysis provides the temperature field of the component just before the deposition of the next (lumped) layer. The temperature distribution is generally non-uniform in space, depending on the specific scanning pattern, geometry, and boundary conditions. Therefore, the actual thermal deformation is recovered by EISM by including the missing contribution $\Delta\epsilon^{th}$, defined as

$$\Delta\epsilon^{th} = [\alpha(T) \cdot (T - T_{ref})]I \quad (11)$$

Thus, the ϵ^{inh} applied in EISM is

$$\epsilon^{inh} = \epsilon^{inh,0} + [\alpha(T) \cdot (T - T_{ref})]I \quad (12)$$

where T is the current temperature at the component.

It is important to note that at the end of the process, when all material points reach the reference temperature, $\Delta\epsilon^{th}$ reduces to zero, and the applied ϵ^{inh} aligns with that of the ISM.

Additionally, in EISM, material properties are considered temperature-dependent, marking another distinction from the original ISM. This temperature dependence leads to different behaviour of the deposited material as the process progresses.

2.4. Material Deposition Modelling

The material deposition approach employed in both the heat transfer and mechanical analyses is the birth–death element technique. In this approach, a new layer of elements is activated at each time step.

The activation strategy is carefully designed to address the behaviour of inactive elements that share nodes with active ones. In the heat transfer analysis, it is ensured that the temperature at the integration points of these inactive elements remains equal to the initial temperature specified at the nodes. This guarantees a smooth thermal transition and prevents unrealistic temperature gradients during activation.

Similarly, in the mechanical analysis, initial deformations may occur in inactive elements due to the displacement of shared nodes with active elements. To counteract this, activation strains are applied as described in [25,26]. These strains compensate for the deformations, ensuring that the newly activated elements are in a stress-free configuration upon activation. This approach maintains consistency in the mechanical response and avoids introducing spurious residual stresses into the model.

3. Experimental Campaign for Calibration and Validation

The experimental campaign described in this section was conducted to provide the necessary data for the calibration and validation of numerical models used in inherent strain modelling. The experiments aim to capture critical thermal and mechanical behaviours during the manufacturing process, enabling a more accurate prediction of distortions and residual stresses. A detailed description of the experimental setup and results for the majority of the work is available in [16]. For completeness, a summary of the earlier work is provided here, along with details of additional distortion and residual stress measurements conducted for this study.

Two geometries, both manufactured using the Ti-6Al-4V alloy on an SLM 280 HL machine, were investigated:

- The **non-symmetric bridge** geometry (Figure 2), chosen for its simplicity, allowed for an analysis of local temperature, distortion, and residual stress. It was manufactured on a baseplate with dimensions of $150 \times 150 \times 24 \text{ mm}^3$.
- The **Steady Blowing Actuator (SBA)** (Figure 3), representing a complex industrial application, was ideal for studying distortions in larger, more complex designs. It was manufactured on a baseplate with dimensions of $160 \times 160 \times 30 \text{ mm}^3$.

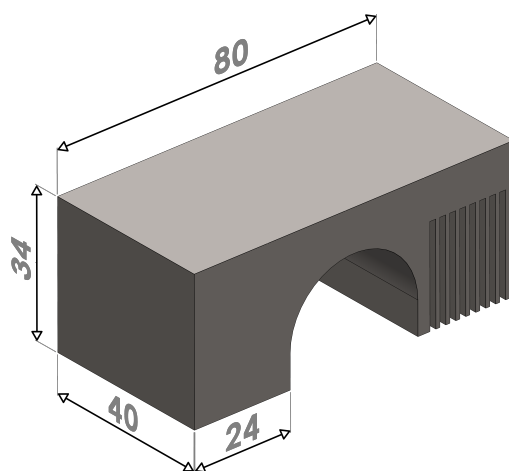


Figure 2. CAD model of the non-symmetric bridge geometry (units: mm).

Key process parameters were carefully optimised to ensure high-quality part fabrication, as detailed in [16]. To account for real process variations, laser exposure and recoating times were monitored (Figure 4). These measurements revealed significant deviations from theoretical values, which, if neglected, could have a substantial impact on the accuracy of the predicted temperature history.

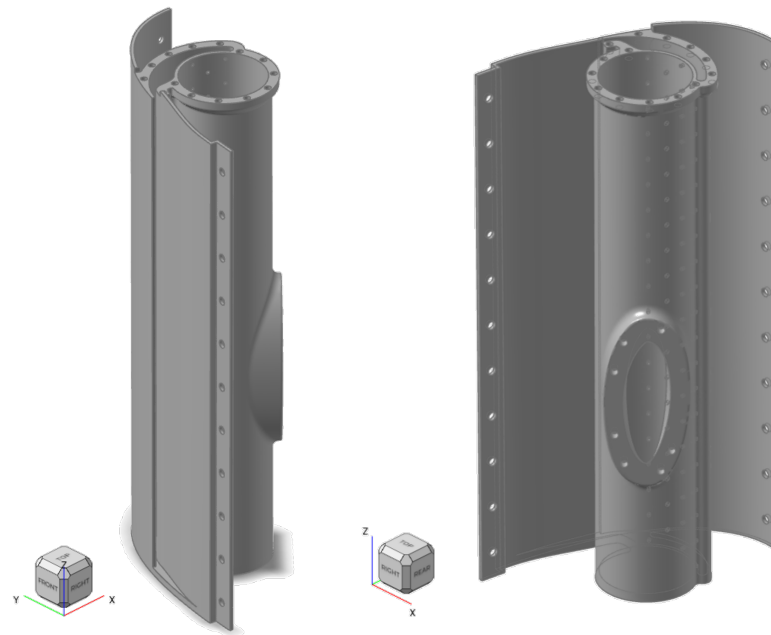
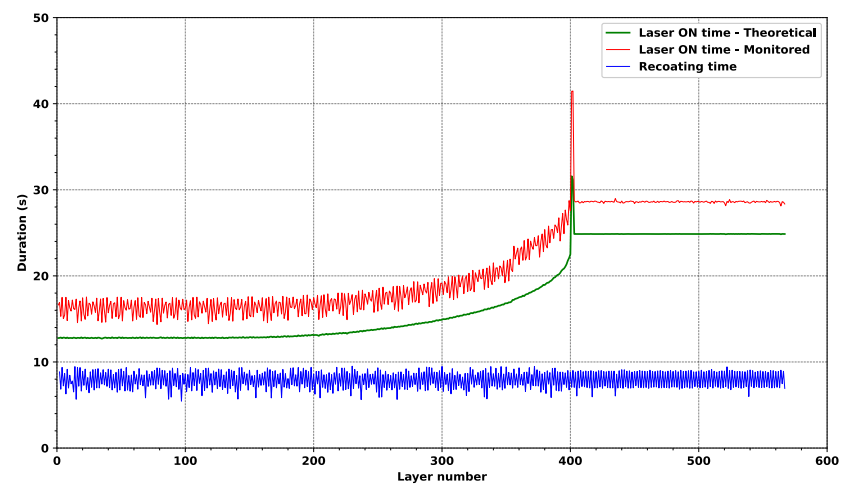
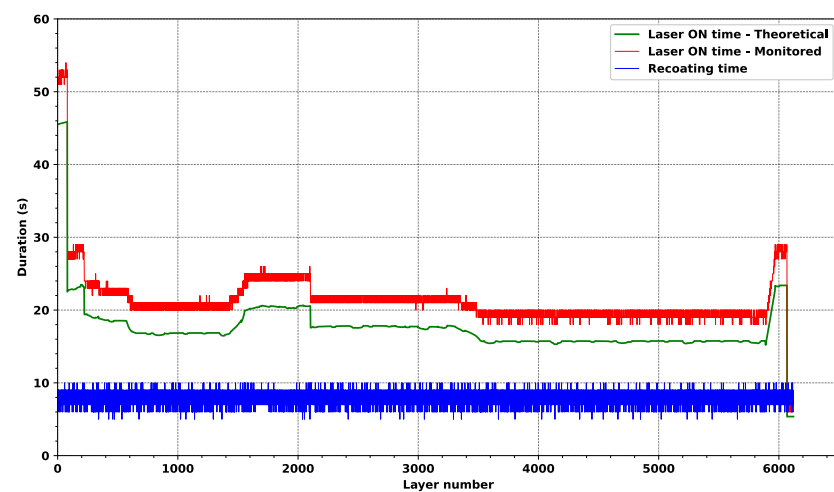


Figure 3. CAD model of the SBA actuator geometry. Bounding box dimensions: $101 \times 137 \times 306$ (mm³).



(a)



(b)

Figure 4. Laser exposure and recoating time data: (a) non-symmetric bridge and (b) SBA actuator.

Temperature measurements were conducted at six specific locations of the bridge using K-type thermocouples embedded in the baseplate (Figure 5). These measurements provided critical data for validating the macro-scale thermal models.

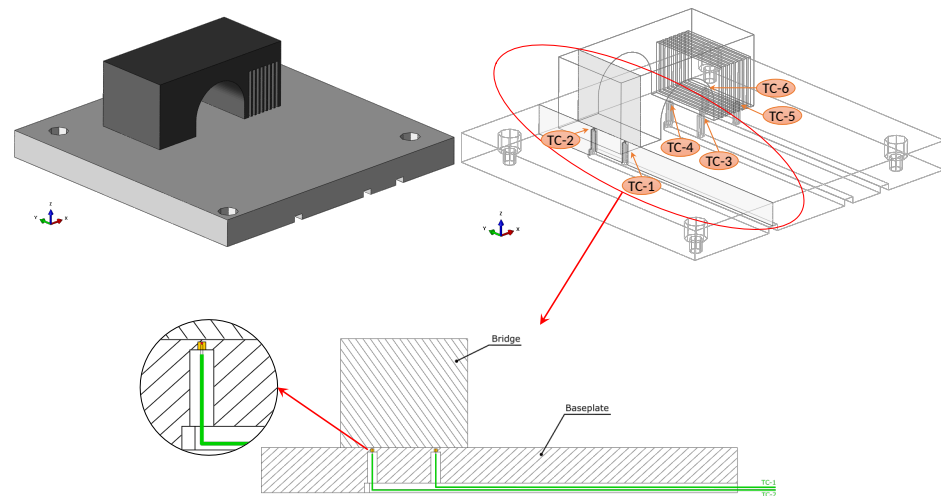


Figure 5. Schematic of thermocouple (TC) locations within the baseplate. Each thermocouple is labelled as TC-x, indicating its specific position. The detail view provides a detailed representation of the thermocouple arrangement, highlighting their placement within machined blind holes to measure temperatures as close as possible to the top surface of the baseplate.

Distortion measurements were performed for both geometries. For the non-symmetric bridge, distortion was measured after printing along the front path depicted in Figure 6, without applying any stress relaxation treatment. Subsequently, the bridge was partially cut from the baseplate using wire Electrical Discharge Machining (wEDM) to release part of the residual stress. After cutting, the deflection of the top surface was measured along the top path shown in Figure 6. Figure 7 illustrates the state of the bridge before and after cutting. For the SBA geometry, the entire manufactured part was scanned with a 3D scanner to capture its deformed shape. This information was subsequently used to perform a detailed deviation analysis.

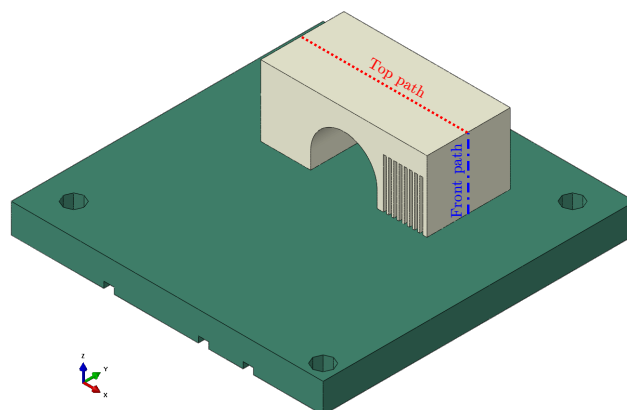


Figure 6. Schematic showing front and top paths where distortion measurements were taken for the non-symmetric bridge.

In addition, residual stress measurements were performed on the bridge using the incremental hole drilling technique, employing an MTS-3000 RS measurement machine and following the ASTM E837-13a standard. Measurements were taken at three points on different surfaces, as shown in Figure 8. This technique involved creating blind holes and measuring strain relief with a high-precision CEA-062UL-120 strain gauge, providing valuable insights into the distribution of residual stresses.

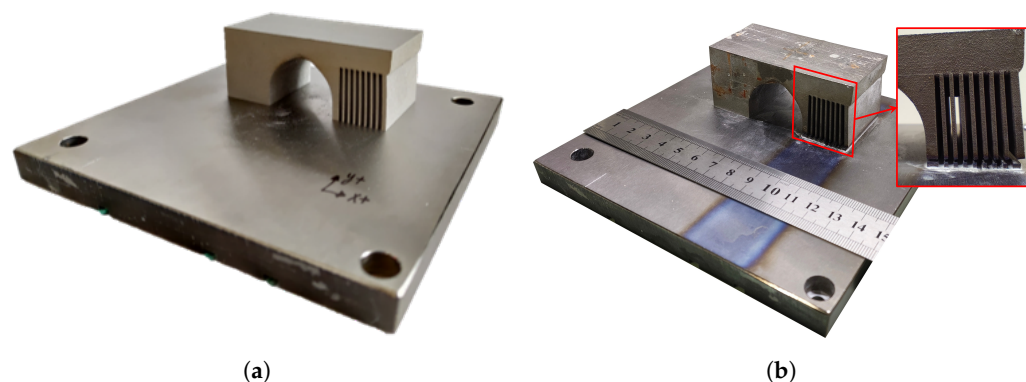


Figure 7. State of the bridge geometry before and after partial cutting to release residual stress: (a) state of the bridge before the cut and (b) state of the bridge after the cut. The detailed view highlights the cut zone, where the bridge was partially released from the baseplate.

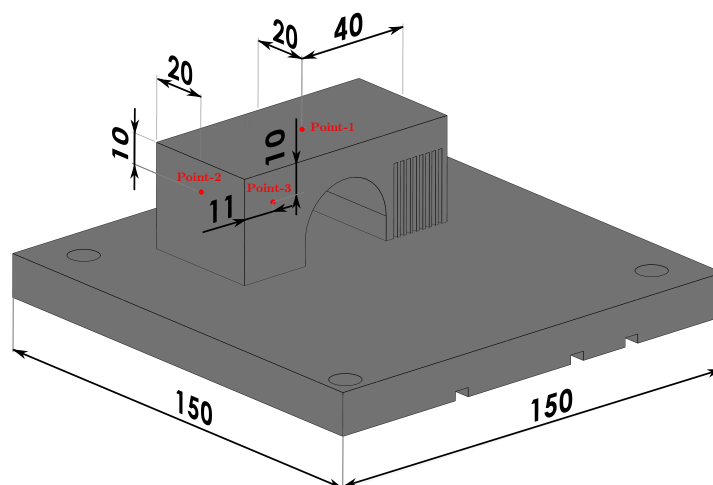


Figure 8. Locations of the three measurement points for residual stress analysis on the non-symmetric bridge.

4. Numerical Implementation

This section outlines the numerical implementation of the EISM modelling approach for both geometries described in Section 3.

The Finite Element (FE) software employed for the simulations was ABAQUS. This software provides general-purpose finite element simulation capabilities as well as specialized tools for simulating additive manufacturing processes, which incorporate machine-specific information and process parameters.

All simulations were conducted using parallel computing with the linear iterative solver of ABAQUS/Standard, utilizing 24 CPUs (Intel Xeon E5-2690v3) and 192 GB of RAM.

4.1. Material Properties

The material properties of the Ti-6Al-4V alloy were defined based on the literature [27]. Temperature-dependent material properties and a linear elastic material model were considered (see Figure A1) to ensure consistency between the local models used for inherent strain computation [16] and the part-scale models analysed in this paper.

It is essential to acknowledge the influence of material property dispersion on the physical properties of elements produced using PBF-LB. Anisotropy in mechanical properties, induced by factors such as scanning strategy, layer thickness, and build orientation, can significantly affect performance. To address these factors to some extent, the reliable source [27] was used, where material properties were obtained by averaging data from

multiple references. Additionally, in-house experiments conducted by Ganeriwala et al. provided further insights to partially account for material property dispersion. However, the modelling scale and physics considered in these methodologies do not allow to predict texture or anisotropy.

The precomputed inherent strain tensor, $\epsilon^{inh,0}$, used in this study was directly adopted from [16]. In Voigt notation, the tensor is expressed as

$$\tilde{\epsilon}^{inh} = -0.0056 \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (13)$$

4.2. Geometrical Model and FE Mesh

Figures 9 and 10 show the 3D geometrical domain and the corresponding FE global meshes for the non-symmetric bridge and the SBA, respectively. The baseplate was included in both models to account for the heat sink effect it induces during the simulation. Non-coincident meshes were employed for the printed parts and the baseplates, connected using a “Tie” constraint to ensure continuity in both temperature and displacements.

To analyze the effect of mesh size on simulation accuracy, two different meshes were defined for the non-symmetric bridge (see Figure 11), consistent with the lumping strategy. In the first mesh, the characteristic element size is approximately 0.24 mm. This element size was selected based on the findings of a previous study described in [16], which concluded that a minimum lumping size of four layers is required to achieve plastic strain stabilization. This mesh ensures that at least one element exists per lumped layer, maintaining numerical accuracy. In the second mesh, a characteristic element size of 0.96 mm was used, allowing for a minimum lumping of 16 layers. This coarser mesh provides a comparative basis to evaluate computational efficiency versus accuracy.

For the SBA, a conformal unstructured hexahedral mesh was generated using a sculpting technique. This approach ensured compatibility with the complex geometry while maintaining high-quality mesh elements.

The total number of elements and nodes for both models are summarized in Tables 1 and 2, respectively.

In both the heat transfer and mechanical analyses, identical meshes were used, differing only in element types. For the heat transfer analysis, DC3D8 elements were utilized, while C3D8R elements were employed for the mechanical analysis.

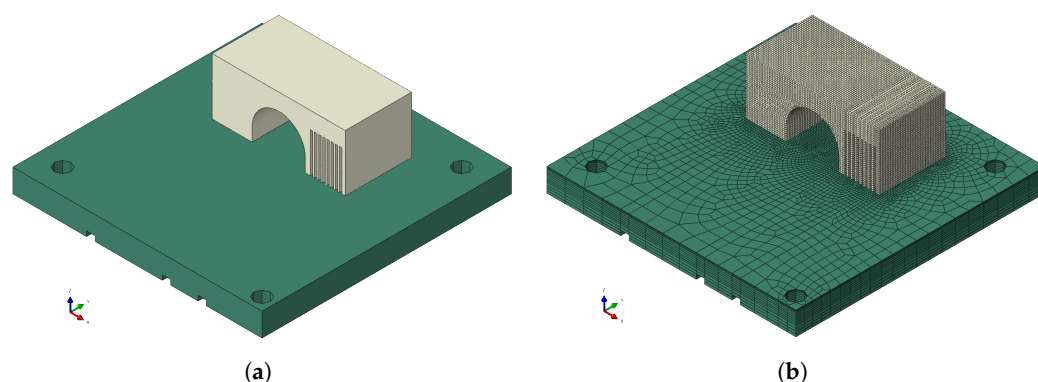


Figure 9. Geometrical model and FE mesh of the non-symmetric bridge, including the baseplate: (a) geometrical model and (b) 3D FE mesh.

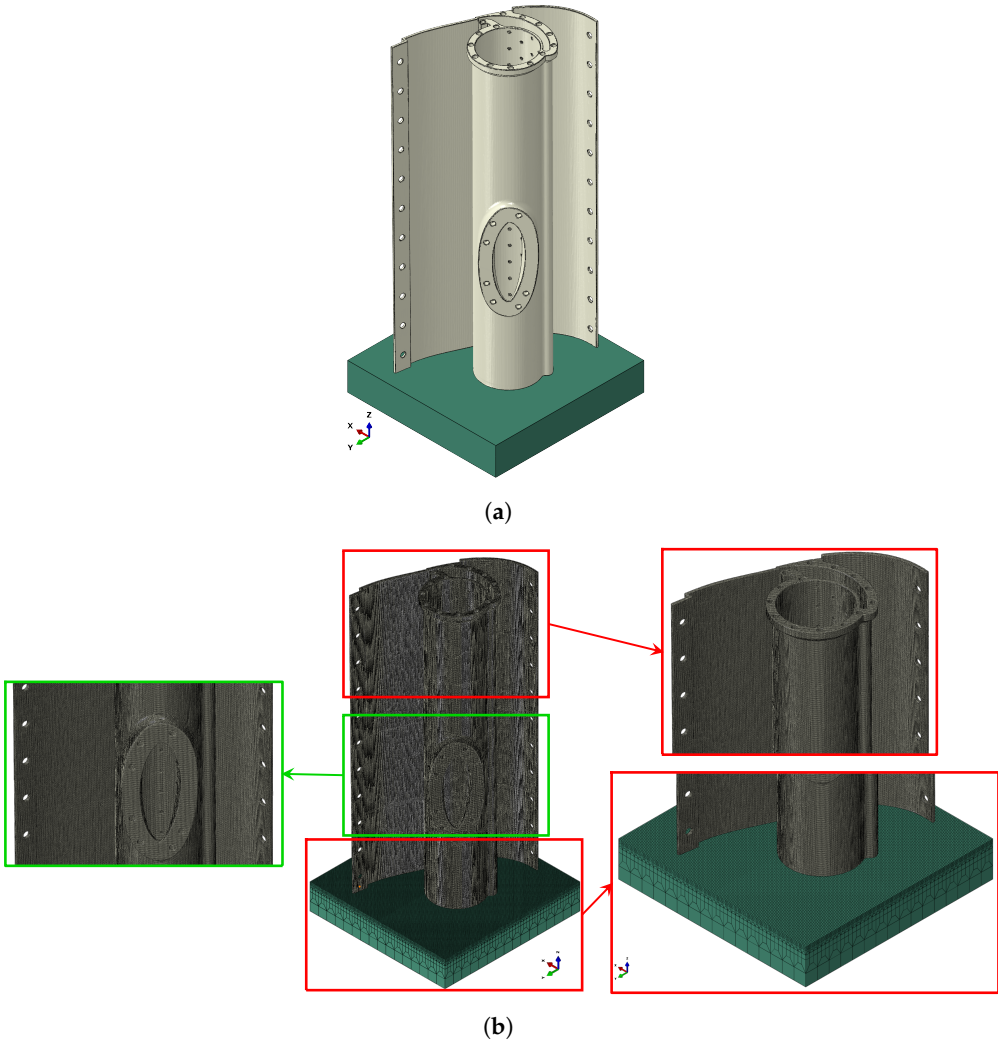


Figure 10. Geometrical model and FE mesh of the SBA with the baseplate: (a) geometrical model and (b) 3D FE mesh.

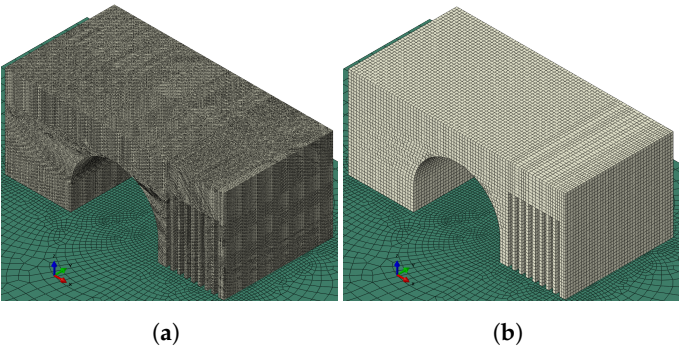


Figure 11. Comparison of non-symmetric bridge meshes with different characteristic element sizes: (a) fine mesh with a characteristic element size of 0.24 mm and (b) coarser mesh with a characteristic element size of 0.96 mm.

Table 1. Summary of the non-symmetric bridge model meshes.

Part Name	Number of Elements	Number of Nodes
Baseplate	90,202	98,499
Bridge 0.24 mm	4,912,640	5,156,025
Bridge 0.96 mm	73,400	88,150

Table 2. Summary of the SBA model mesh.

Part Name	Number of Elements	Number of Nodes
Baseplate	98,048	110,216
SBA	3,952,927	4,646,774

4.3. Initial and Boundary Conditions

4.3.1. Thermal Analysis

The baseplate preheating was incorporated into the model by assigning an initial temperature of 200 °C to the baseplate, along with a temperature boundary condition applied to its bottom surface to maintain this temperature during the printing stage. In the subsequent cool-down stage, the temperature was decreased exponentially until it reached ambient temperature.

Heat loss from the top surface was modelled using an equivalent heat loss coefficient of $h_{equ} = 18 \text{ W}/(\text{m}^2\text{K})$, consistent with the value used in [16]. The environment temperature was set to 50 °C, representing the average temperature of the building chamber during the printing process.

Heat loss to the surrounding powder was also modelled using the same convective heat transfer coefficient applied to the top surface of the part. For the non-symmetrical bridge, a preliminary sensitivity analysis revealed that heat loss to the surrounding powder had minimal impact on the results. This can be attributed to the relatively low temperatures observed in the macro-scale heat transfer analysis compared to those obtained in high-fidelity simulations, as well as the small height of the part, which enables efficient heat extraction primarily through conduction to the baseplate. In contrast, for the SBA, heat evacuation to the surrounding powder becomes significant due to the greater height of the part. As the deposited layer moves further away from the baseplate, the efficiency of heat conduction through the baseplate diminishes, making heat loss to the surrounding powder more critical.

4.3.2. Mechanical Analysis

The thermal history obtained from the heat transfer analysis was used to compute the thermal strains for the structural analysis. The initial temperature for the baseplate was consistent with the value used in the heat transfer analysis, while the temperature of the building chamber was assigned as the initial temperature for the deposited material.

Moreover, the bottom surface of the baseplate was fixed in all directions to simulate the clamping effect typically achieved with bolts during the manufacturing process.

4.4. EISM Analysis Characteristics

The simulation consisted of two stages in both the heat transfer and mechanical analyses: printing and cooling. For the non-symmetric bridge, an additional third stage was included in the mechanical analysis to simulate the partial removal of supports. This stage enabled the evaluation of distortions resulting from the partial release of residual stresses due to support removal, complementing the analysis of distortions generated in the as-built state (i.e., after cooling in the second stage).

The computation of the time-averaged heat flux, as described in Section 2.1, relies on the actual scanning strategy provided in an event-series format [24]. To convert the original machine file into this format, Python scripting was employed, utilizing built-in libraries for data parsing and manipulation. During this conversion, experimentally monitored laser exposure and recoating times (illustrated in Figure 4) were incorporated to ensure the accuracy of the simulation input. Additionally, the heat absorption coefficient, calibrated in [16], was included in the calculation.

The time incrementation for the simulation was calculated automatically based on Equation (2), considering the defined layer lumping strategy. For the non-symmetric bridge, two layer lumping options ($n = 4$ and $n = 16$) were defined to perform a sensitivity analysis. The first lumping option, corresponding to an equivalent layer thickness of 0.24 mm, represents the minimum possible thickness that satisfies the requirements of the precomputed inherent strain tensor. The second lumping option, with a thickness of 0.96 mm, is four times greater and represents the maximum allowable layer thickness for achieving mesh convergence when using one element per layer thickness.

5. Results and Discussion

This section presents the results of applying the EISM to the two geometries described in Section 3.

In both cases, the numerical results are compared with experimental data and the original ISM methodology. This comparative analysis aims to provide a thorough evaluation of the EISM approach by integrating insights from experimental benchmarks and existing modelling techniques.

Additionally, for the non-symmetric bridge, an extended analysis was conducted to examine the effects of layer lumping and element size on simulation accuracy and computational efficiency.

5.1. Non-Symmetric Bridge

The combination of two different meshes (0.24 mm and 0.96 mm), two lumping options ($n = 4$ and $n = 16$ layers), and two methodologies (ISM and EISM) results in the analysis cases summarized in Table 3.

Table 3. Summary of analysis cases for the non-symmetric bridge.

Case	Name	Lumping	Element Characteristic Size (mm)	Methodology
#1	lump-4_mesh-024_ISM	4	0.24	ISM
#2	lump-16_mesh-024_ISM	16	0.24	ISM
#3	lump-16_mesh-096_ISM	16	0.96	ISM
#4	lump-4_mesh-024_EISM	4	0.24	EISM
#5	lump-16_mesh-024_EISM	16	0.24	EISM
#6	lump-16_mesh-096_EISM	16	0.96	EISM

5.1.1. Temperature Evolution

According to Table 3, three heat transfer analyses were conducted for cases #4 to #6. In all instances, the temperature evolution at the six thermocouple positions was plotted (Figure 12). The numerical curves for all cases are nearly identical, indicating that neither the studied lumping strategies nor the mesh sizes significantly affect the thermal behaviour at these points.

When compared to the experimental curves, the macro-level heat transfer analysis is unable to capture the detailed local thermal history at the thermocouples (as expected). However, it effectively captures the average temperature evolution throughout the manufacturing process. Beyond the initial transient period, the agreement between the simulated and measured temperatures is acceptable, with the simulated results closely synchronized with the reference signal.

Different contour-fill plots of the temperature were plotted to evaluate further the impact of layer lumping and mesh size on the temperature output (Figure 13). Minor differences are observed in the bridging zone, a typical hot spot region caused by the overhanging effect. As expected, the smallest lumping case produces slightly higher peak

temperatures. However, these differences are negligible and do not significantly impact the EISM predictions.

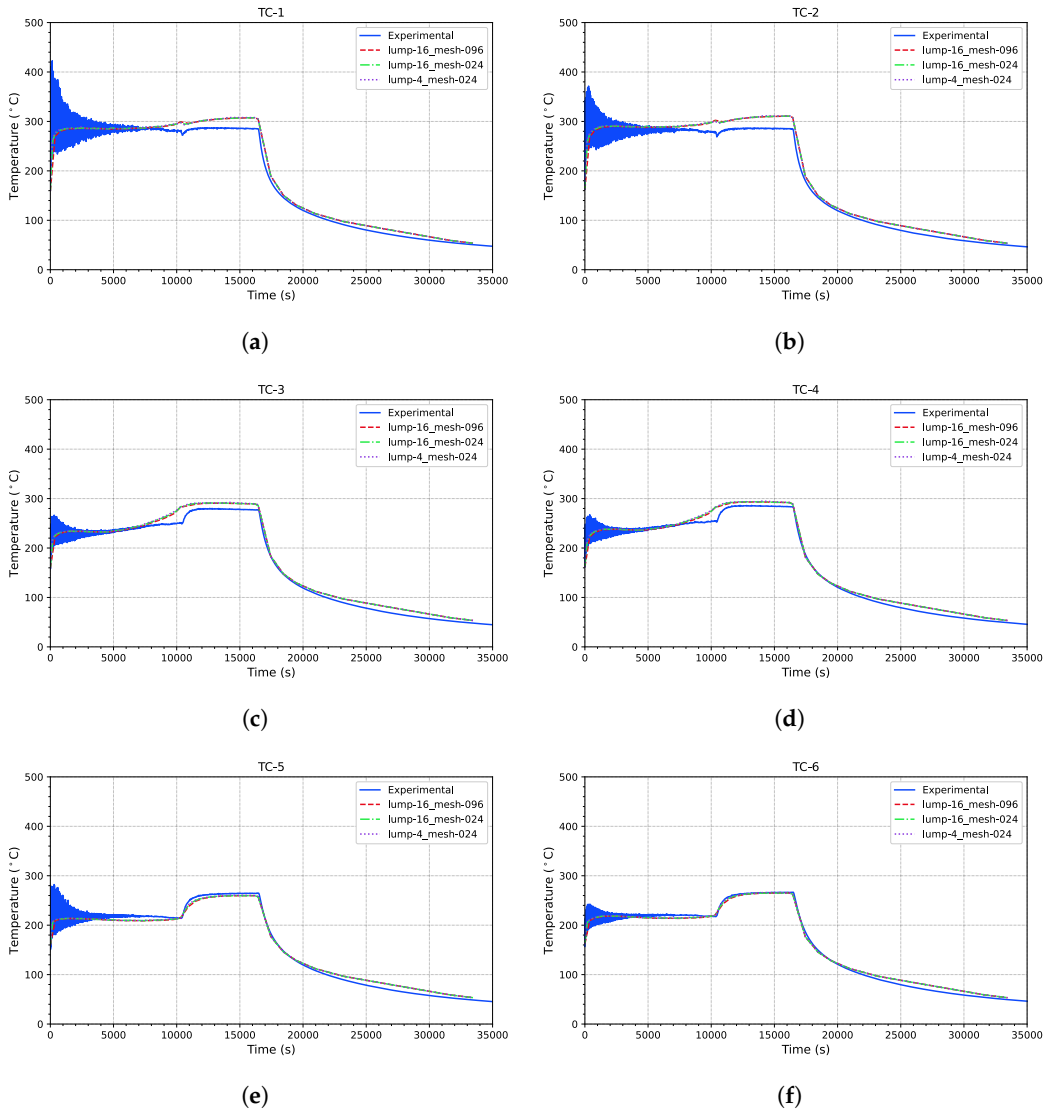


Figure 12. Comparison between numerically predicted and experimentally recorded temperature histories at the thermocouple locations: (a) TC-1, (b) TC-2, (c) TC-3, (d) TC-4, (e) TC-5, and (f) TC-6.

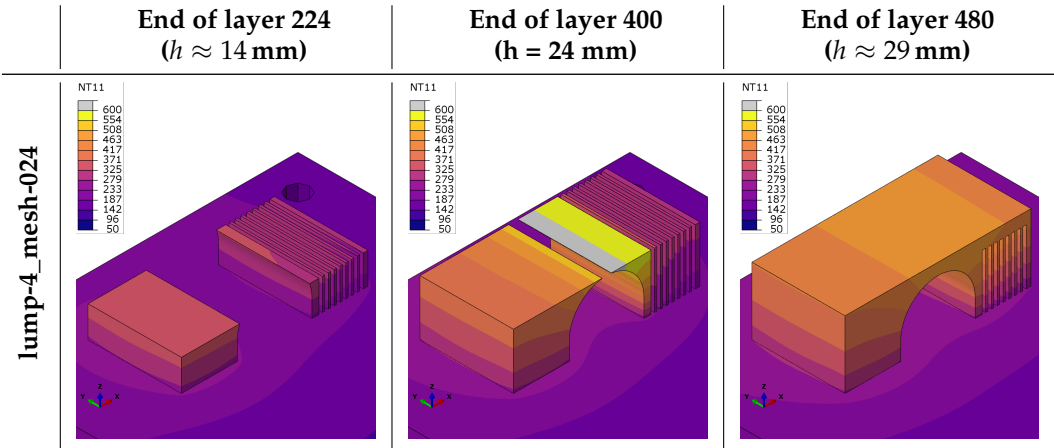


Figure 13. Cont.

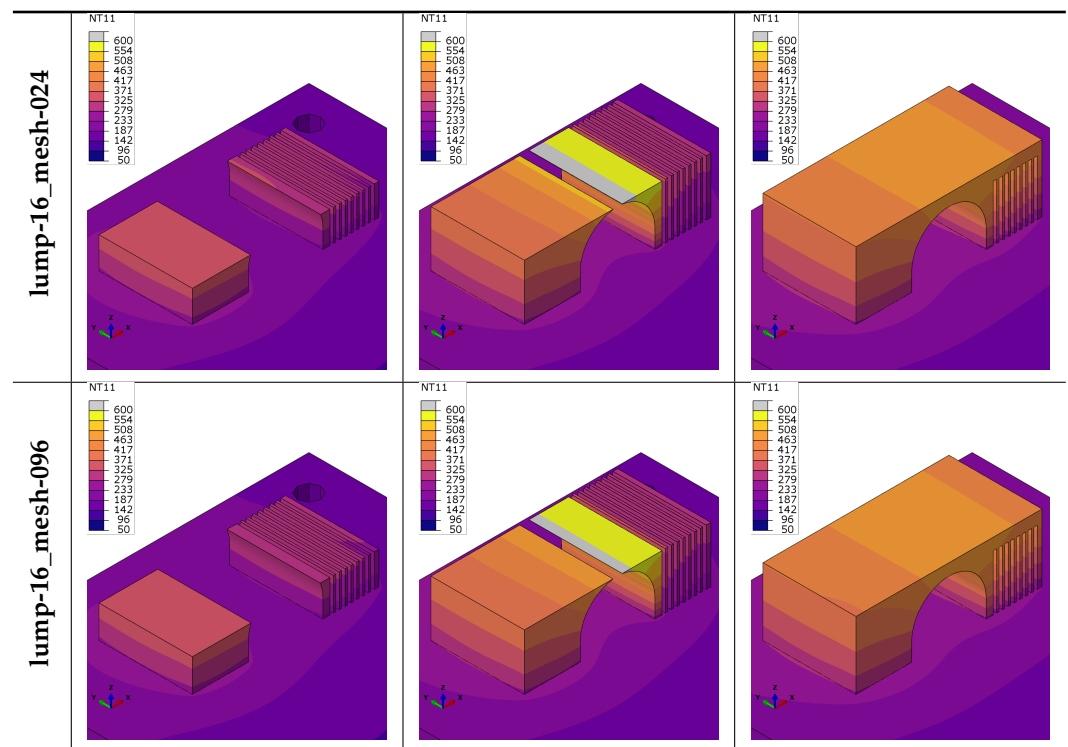


Figure 13. Evolution of the temperature field of the non-symmetric bridge during the deposition process.

5.1.2. Distortion

The distortion prediction of the non-symmetrical bridge was evaluated based on the deflection curves along the paths illustrated in Figure 6. The longitudinal distortion was analyzed along the front path prior to the partial removal of supports. Conversely, the vertical distortion of the top surface was assessed along the top path after the supports were removed.

The deflection along the top path provides an indirect means of evaluating the residual stress state of the bridge, particularly the residual stress in the top parallelepiped section. As shown in Figure 14, regardless of the layer lumping strategy, element size, or analysis methodology employed, all cases accurately predict the distortion curve measured experimentally. This indicates that the overall residual stress state at the end of the printing process is well captured by the simulations.

In contrast, the longitudinal deflection exhibits a different behaviour. This deflection represents the distortions that occur during the printing process and is assessed in the as-built state, after the entire domain has cooled. As seen in the experimental deflection curve in Figure 15, the curve consists of two distinct curvatures. The lower curvature corresponds to the rightmost support, while the upper curvature corresponds to the top blocky part of the bridge.

The analysis cases summarized in Table 3 reveal varying distortion behaviours based on modelling aspects. To evaluate the numerical results, two key metrics were computed to quantify the prediction quality of the numerical models relative to the experimental reference curve: the Mean Absolute Percentage Error (MAPE) and the Percent Bias (PBIAS). These metrics, detailed in Table 4, provide insights into the accuracy and bias of the models.

When analysing the effect of the modelling methodology, the ISM-based cases (#1–#3) fail to accurately predict the longitudinal deflection curve. High MAPE values (ranging from 50.87% to 56.63%) and significant negative PBIAS (up to −56.64%) indicate large prediction errors and a consistent underestimation of deflection. While ISM can capture the top path deflection, it fails to accurately predict the front path behaviour.

In contrast, the EISM-based cases (#4–#6) demonstrate improved prediction accuracy. The MAPE values are significantly lower, with the best-performing case (#4, lump-4_mesh-024_EISM) achieving a MAPE of 10.85% and a near-zero PBIAS (0.01%). All EISM cases successfully predict the upper profile of the front path deflection. For the lower profile, however, accurate predictions are achieved only when a four-layer lumping strategy is employed.

This explains why cases with a larger lumping size (#5 and #6) exhibit higher MAPE values (approximately 16%) and moderate negative PBIAS (around -9%). These results can be attributed to a singularity effect caused by an abrupt change in stiffness within the structure. Specifically, the rightmost support begins to deflect when layers corresponding to the top blocky part are deposited. During the initial layers, the shrinkage generated by the newly deposited material is counteracted by a progressive increase in stiffness. This phenomenon highlights the importance of using a small lumping size during these initial layers, as it directly affects the curvature of the support leg. This effect often manifests as well-known shrink lines.

Consequently, a small layer lumping size is not necessary for the entire part. Instead, using a smaller lumping size just in the initial layers of the top blocky section would be sufficient to capture the deflection of the support leg reliably.

Interestingly, the variation in mesh size has minimal impact on the distortion curve for a given lumping strategy (see Figure 15b). This finding suggests that employing a one-element-per-layer-thickness strategy is sufficient for accurate predictions, reducing computational complexity without sacrificing accuracy.

Overall, the EISM methodology shows significant improvement over the ISM methodology. In the best case (#4), EISM achieves a 79% reduction in MAPE compared to the best ISM case (#1), where MAPE is reduced from 50.87% to 10.85%. Similarly, EISM improves the PBIAS from -47.47% (#1) to near zero (0.01%, #4), eliminating the systematic underestimation observed in the ISM results. These improvements highlight the enhanced ability of EISM to accurately capture both the location and magnitude of distortions in the bridge structure.

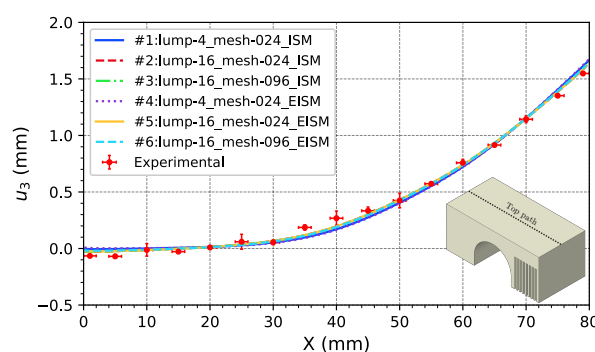


Figure 14. Top path distortion comparison between numerical and experimental data.

Table 4. Summary of MAPE and PBIAS metrics for the front path distortion curves in numerical analysis cases presented in Table 3.

Case	Name	MAPE (%)	PBIAS (%)
#1	lump-4_mesh-024_ISM	50.87	-47.47
#2	lump-16_mesh-024_ISM	56.63	-56.64
#3	lump-16_mesh-096_ISM	56.15	-56.21
#4	lump-4_mesh-024_EISM	10.85	0.01
#5	lump-16_mesh-024_EISM	16.04	-8.95
#6	lump-16_mesh-096_EISM	15.96	-9.09

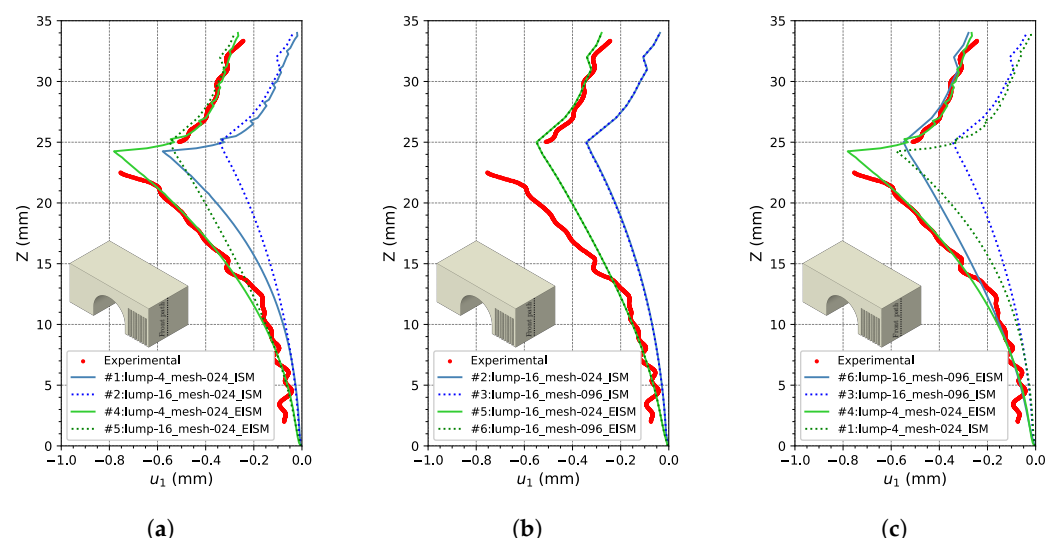


Figure 15. Front path distortion for the non-symmetric bridge, illustrating the influence of (a) layer lumping, (b) mesh size, and (c) methodology.

5.1.3. Residual Stress

The von Mises stresses at the points defined in Figure 16 were compared with the experimentally obtained values (see Figure 16a). A depth of 0.6 mm was chosen for the comparison to avoid superficial elements and to ensure direct comparison with stress values computed at integration points, without averaging effects.

The numerical cases #1 and #4 were used for the comparison (Figure 16b). Both simulations show good agreement with the hole drilling data, except at point 3, where experimental uncertainties are likely due to near-surface measurements exceeding 70% of the yield stress (ASTM E387-13a).

Overall, the simplified modelling methodologies provide reasonable approximations of the residual stress state, even if not explicitly designed for high-fidelity stress predictions.

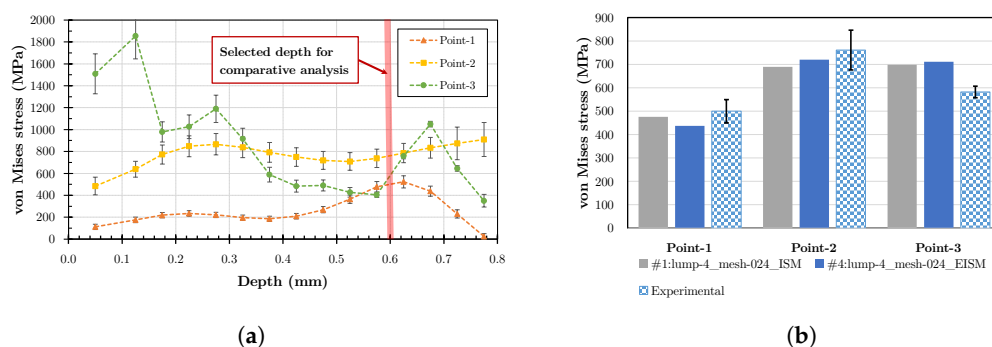


Figure 16. von Mises residual stress measurements and comparison at three points. (a) Experimentally measured evolution through the depth and (b) comparison with numerical results.

5.1.4. Computational Efficiency

To provide a comprehensive evaluation of the proposed methodologies, the computational time for each analysis case was recorded and compared. For the comparison, cases #1, #3, #4, and #6 were selected.

Case #4 was identified as the best-performing case providing the most accurate predictions. However, to establish reference data for computational costs, cases involving the ISM methodology and the 16-layer lumping option (which produces satisfactory results except for the singularity observed at the support leg) were also included.

Table 5 summarizes the total CPU time for the selected cases. The results demonstrate that the choice of layer lumping is critical: regardless of the methodology employed, the computational cost increases by approximately 40 times when using smaller lumping sizes.

Regarding the choice of methodology, applying the EISM approximately doubles the computational time required for the ISM due to the need to solve the heat transfer problem alongside the mechanical analysis.

In this context, adaptive layer lumping emerges as a promising option for capturing stiffness changes that occur during the printing process. These stiffness changes can be efficiently identified through pure geometric analysis, as demonstrated in [28]. Furthermore, since smaller layer lumping requires finer mesh resolutions, mesh adaptivity techniques could also be employed to effectively account for this phenomenon.

Table 5. Comparison of computational time for representative bridge analysis cases.

Case	Name	Total CPU Time (h)		
		Thermal	Mechanical	Total
#1	Lump-4_Mesh-0.24_ISM	-	5.64	5.64
#3	Lump-16_Mesh-0.96_ISM	-	0.15	0.15
#4	Lump-4_Mesh-0.24_EISM	5.45	7.19	12.64
#6	Lump-16_Mesh-0.96_EISM	0.13	0.17	0.30

5.2. SBA

For the SBA, a 16-layer lumping option was selected, resulting in approximately one element per layer thickness. This choice was driven by the large size of the analysis domain and the resulting trade-off in resolution. Under these conditions, it was acknowledged that capturing local distortion magnitudes at shrink-lines with high fidelity might not be feasible. Consequently, two numerical cases were analysed, as summarized in Table 6.

Table 6. Summary of analysis cases for the SBA.

Case Name	Lumping	Element Characteristic Size (mm)	Methodology
SBA_ISM	16	0.96	ISM
SBA_EISM	16	0.96	EISM

5.2.1. Temperature Evolution

To evaluate the overall behaviour of the part concerning temperature evolution, various instants of the temperature field were plotted, similar to the approach used for the bridge case. In this analysis, relevant time instants were selected to represent different stages of the process, highlighting critical aspects such as hot spots, the effect of part height, and heat dissipation through the surrounding powder (Figure 17).

In this case, the temperature control established at the platform level of the machine loses its effectiveness as the height of the part increases. This is because the greater height reduces the efficiency of heat transfer by conduction, making it more challenging to maintain uniform temperature throughout the part.

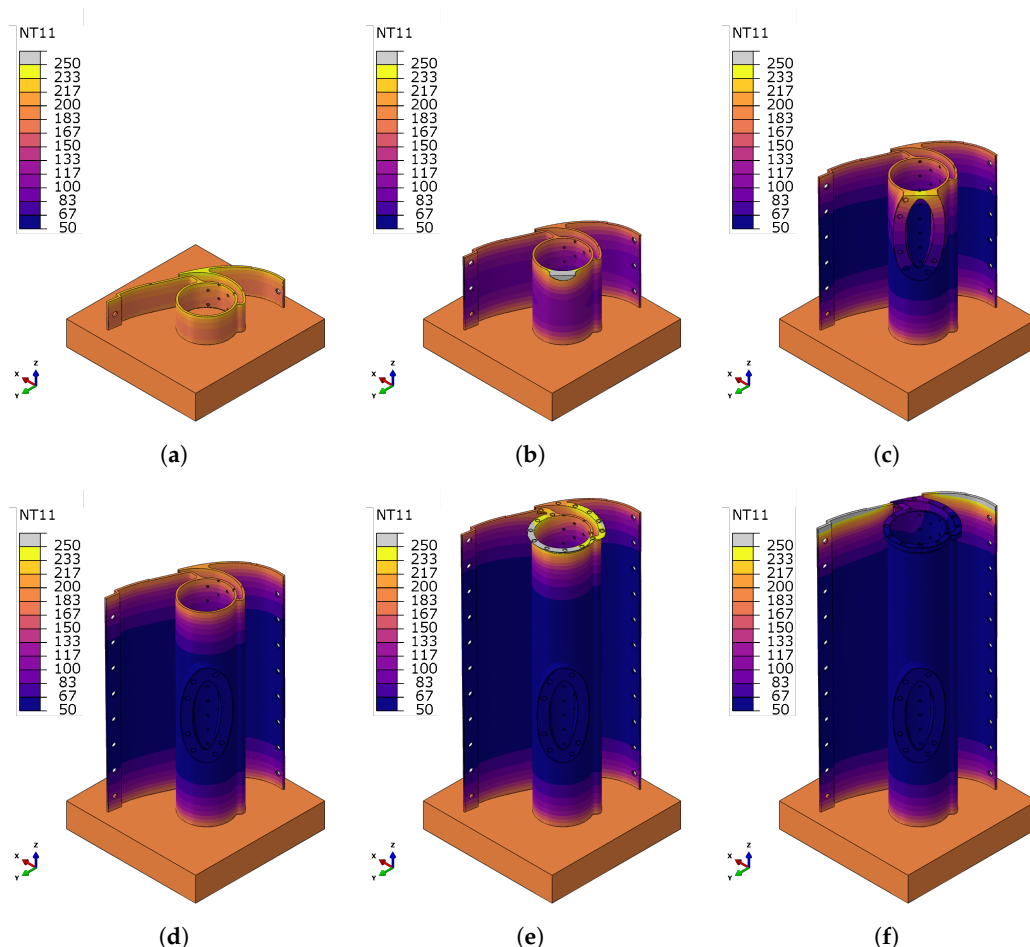


Figure 17. Temperature contour plots of the SBA actuator at different printing stages: (a) $h \approx 30$ mm, (b) $h \approx 78$ mm, (c) $h \approx 164$ mm, (d) $h \approx 230$ mm, (e) $h \approx 298$ mm, and (f) $h \approx 305$ mm.

5.2.2. Inherent Strain Evolution

Assessing the evolution of the actually applied inherent strain is crucial to better understand the differences between the ISM and EISM methodologies.

The applied inherent strain at any time is expressed in Equation (12).

To this end, 10 points were selected along the height of the SBA, and the evolution of ϵ_{xx}^{inh} was plotted for both methodologies (see Figure 18a,b).

In the ISM, the full precomputed inherent strain tensor, $\epsilon^{inh,0}$, is applied instantaneously upon the activation of each layer, assuming a uniform strain distribution throughout the layer. Conversely, in the EISM, the inherent strain evolves dynamically during the simulation, governed by the temperature history of each point. This evolution is illustrated in Figure 18b for Point 1, as described by Equation (8). The total applied inherent strain at the end of the simulation satisfies $\epsilon^{inh} = \epsilon^{inh,0}$, but the intermediate evolution of ϵ^{inh} is temperature-dependent.

For points near the baseplate, a significant portion of $\epsilon^{inh,0}$ is applied predominantly toward the end of the printing process. This is due to prolonged thermal cycles resulting from temperature control in the platform during deposition. In contrast, points near the final layers experience an inherent strain that approaches $\epsilon^{inh,0}$ almost instantaneously upon layer activation, closely resembling the behaviour observed in the original ISM.

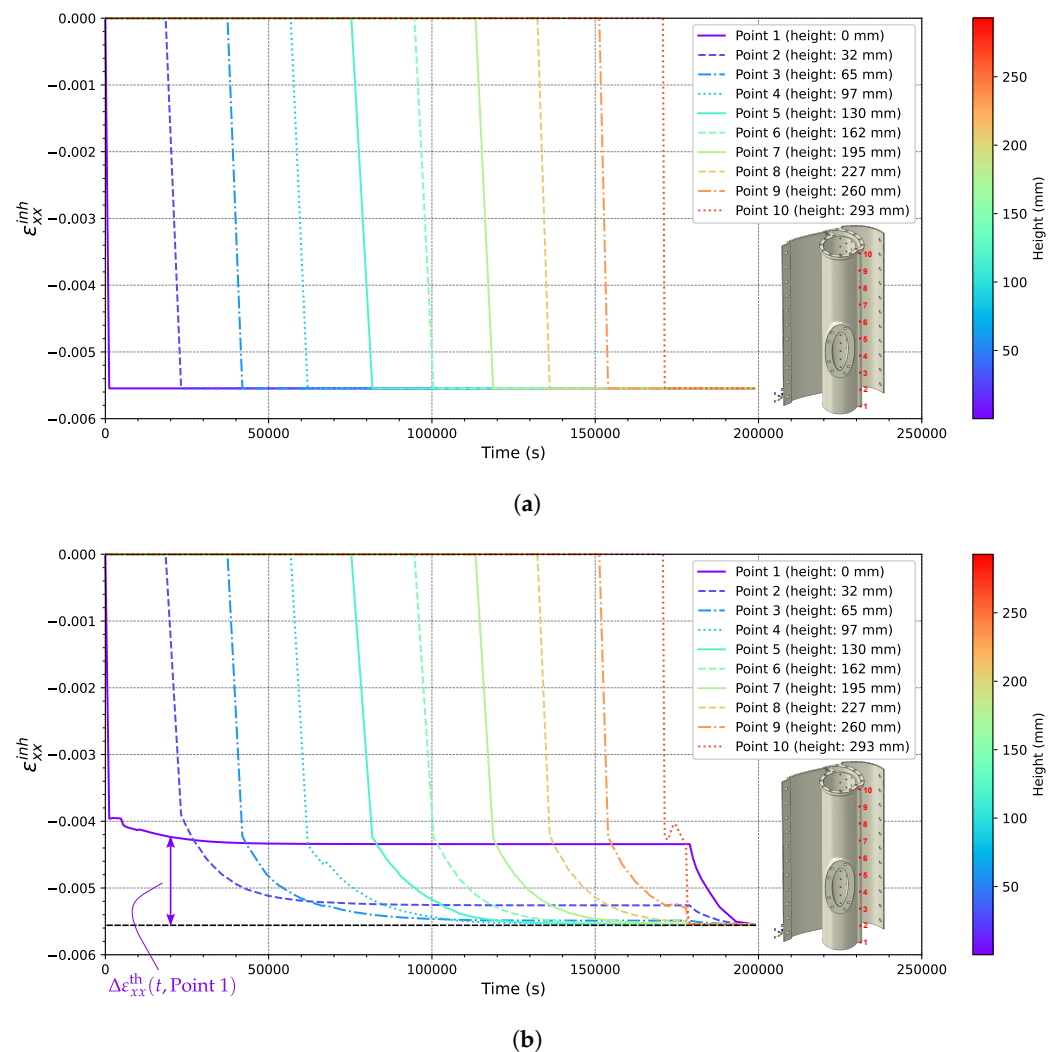


Figure 18. Evolution of ϵ_{xx}^{inh} at different points along the height of the SBA part: (a) ISM methodology and (b) EISM methodology.

5.2.3. Distortion

Geometric deviations were calculated by comparing the computed final deformed geometries obtained using both methodologies with the nominal geometry of the SBA. Additionally, geometric deviations were calculated for the experimentally measured deformed shape relative to the nominal geometry. All these deviation contour plots are shown in Figure 19.

When comparing the different deviation contour plots, it can be observed that the ISM method qualitatively captures the overall distortion behaviour of the part; however, some discrepancies are evident. For instance, the locations of the maximum and minimum deviations are not accurately predicted, with these deviations appearing on the opposite wing of the part.

Conversely, the EISM method successfully predicts both the location and magnitude of the deviations. Furthermore, discrepancies in the top section of the part are significantly reduced when using the EISM, demonstrating its superior accuracy in capturing distortion.

A more rigorous way to assess the accuracy of numerical models involves calculating geometric deviations using the experimentally measured deformed shape as a reference. This approach generates deviation contour plots, as represented in Figure 20. If a numerical model were perfectly accurate, no deviations would be observed. The evaluation of numer-

ical models’ prediction accuracy was performed using the metrics of average deviation and its sigma, with the corresponding values summarized in Table 7.

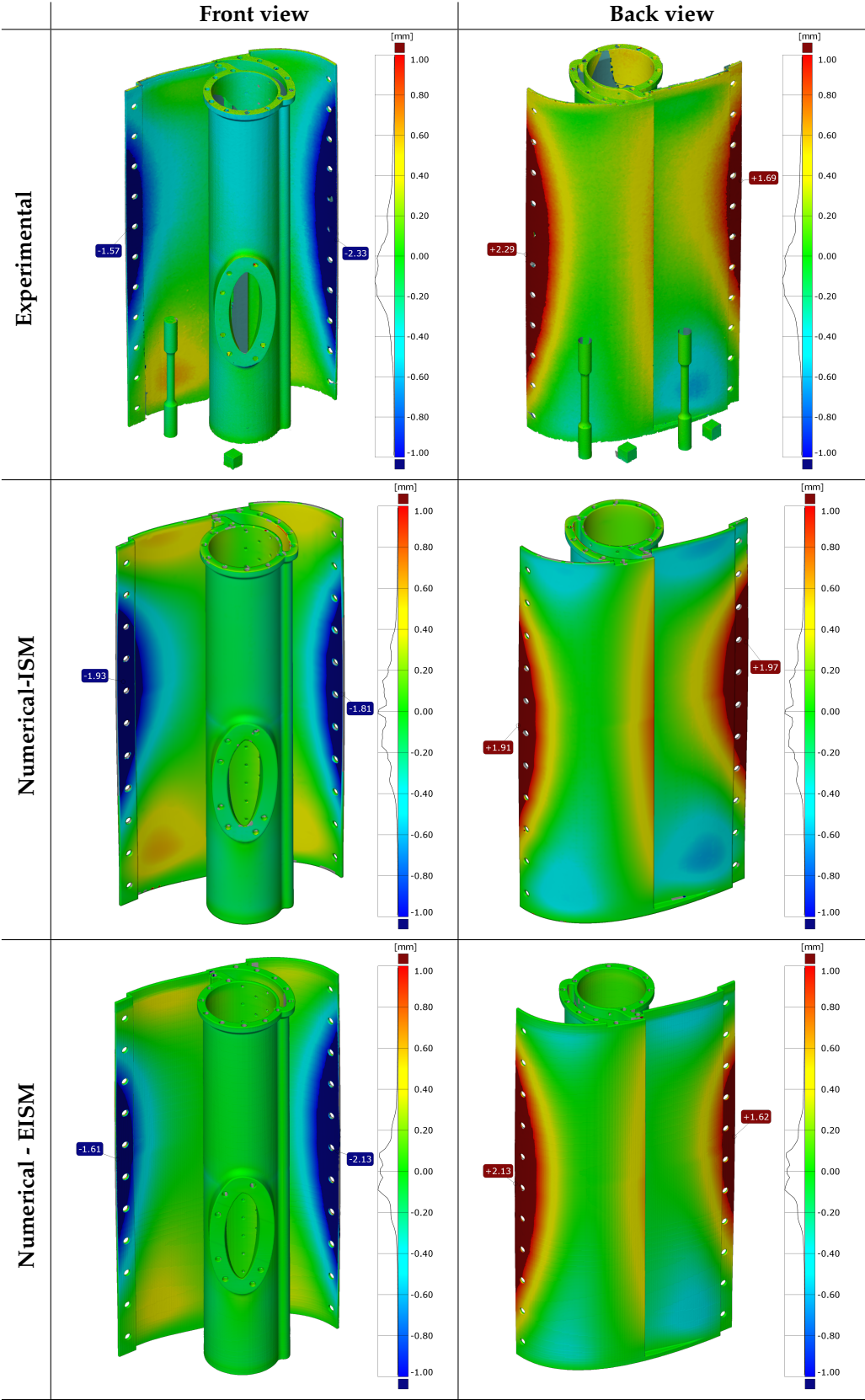


Figure 19. Deviation contour plots of the SBA, calculated relative to the nominal geometry. Results are shown for experimental data (top row), numerical-ISM (middle row), and numerical-EISM (bottom row), with front and back views.

The results show that the EISM method (SBA_EISM) achieves an average deviation of 0.00 mm and a lower sigma value of 0.09 mm, indicating both high accuracy and consistency in predicting the experimentally observed deformation. In contrast, the ISM method (SBA_ISM) exhibits a slight bias, with an average deviation of -0.01 mm, and a higher sigma value of 0.15 mm, reflecting greater variability and less reliability in its predictions. Consequently, SBA_EISM demonstrates a 100% improvement in average deviation, effectively eliminating the bias observed in SBA_ISM, and achieves a 40% improvement in sigma, signifying greater consistency in predicting geometric deviations.

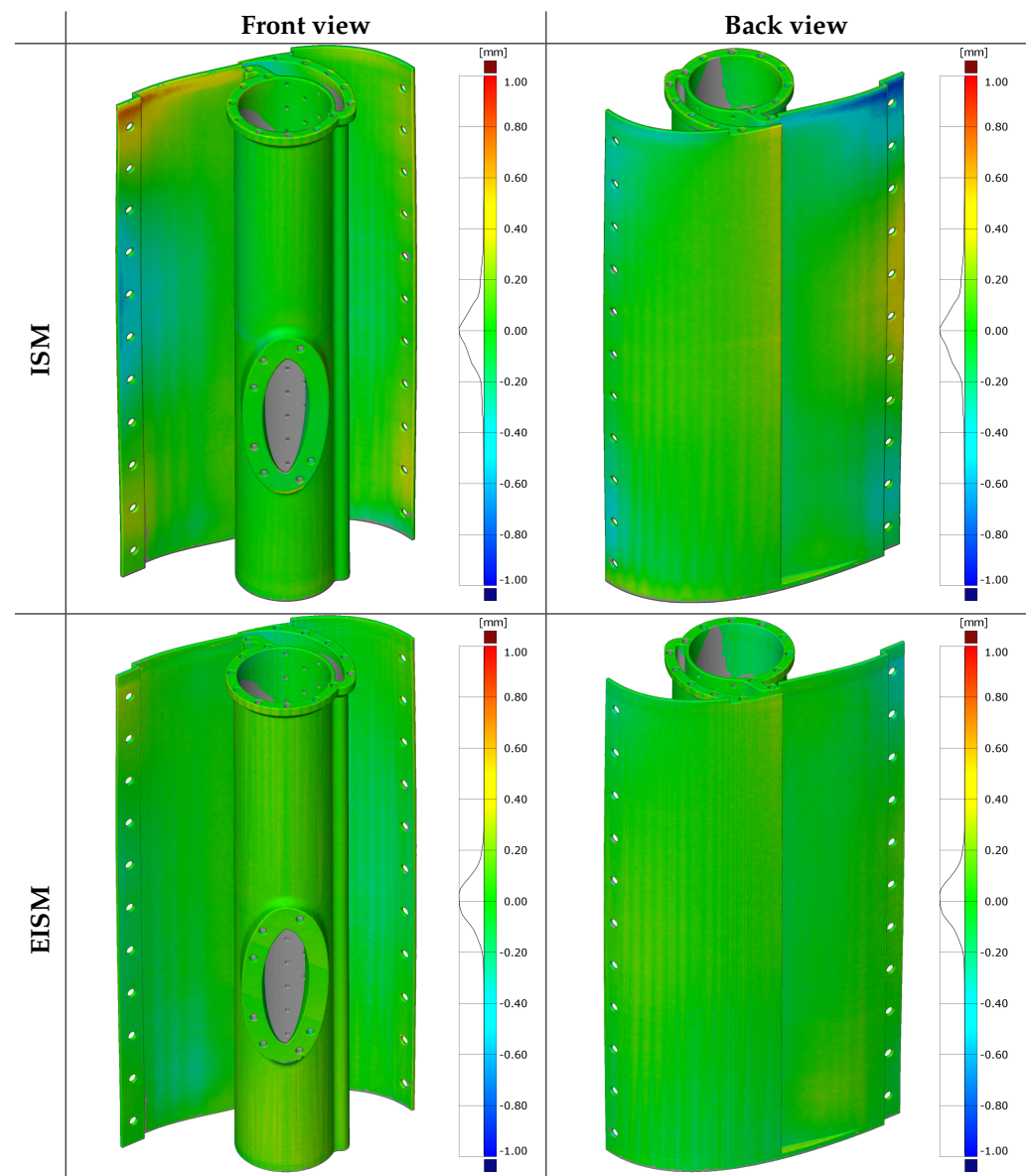


Figure 20. Deviation contour plots of the SBA, calculated relative to the experimentally measured deformed geometry. Results are shown for ISM (**top row**) and EISM (**bottom row**), with front and back views.

Table 7. Deviation metrics for numerical models compared to experimental measurement.

Case Name	Average Deviation (mm)	Sigma (mm)
SBA_ISM	-0.01	0.15
SBA_EISM	0.00	0.09

5.2.4. Computational Efficiency

Table 8 summarizes the total CPU time for the selected cases. Like in the bridge case, applying the EISM approximately doubles the computational time due to the need to solve the heat transfer problem alongside the mechanical analysis. Therefore, the accuracy requirement must be well justified. For example, when compensation strategies are to be applied, the EISM is preferable, as it provides refined predictions for predeformation.

Table 8. Comparison of computational time for SBA analysis cases.

Case Name	Total CPU Time (h)		Total
	Thermal	Mechanical	
SBA_ISM	-	12.35	12.35
SBA_EISM	8.69	14.19	22.88

6. Conclusions

This work introduced an Enhanced Inherent Strain Method (EISM) for Powder Bed Fusion-Laser Beam (PBF-LB) that incorporates macro-scale temperature histories into the inherent strain formulation. By selectively adjusting the thermal strain component of the precomputed inherent strain tensor according to the evolving thermal field, the EISM more accurately reflects local thermo-mechanical conditions, improving the prediction of distortions and residual stresses compared to the original Inherent Strain Method (ISM).

The methodology was validated against two distinct Ti-6Al-4V geometries: a non-symmetric bridge and a more complex Steady Blowing Actuator (SBA). Comparisons between numerical predictions and experimental measurements of temperature, distortion, and residual stress demonstrated that the EISM offers improved accuracy over the conventional ISM.

The EISM demonstrated notable improvements over the original ISM. For the non-symmetric bridge, Mean Absolute Percentage Error (MAPE) in distortion predictions decreased from 50.87% (ISM) to 10.85% (EISM), representing a 79% improvement. Additionally, EISM eliminated the systematic underestimation observed in ISM, reducing Percent Bias (PBIAS) from -47.47% to 0.01% . For the SBA, EISM reduced the sigma value of geometric deviations compared to experimental measurements from 0.15 mm (ISM) to 0.09 mm, a 40% improvement. EISM also accurately predicted the location and magnitude of maximum distortions, whereas ISM exhibited discrepancies.

A sensitivity analysis revealed that neither the mesh size nor the layer lumping strategy significantly affects the global temperature evolution. However, careful selection of layer lumping and mesh refinement is necessary for layers corresponding to geometry features that represent structural transitions (where abrupt stiffness changes occur, such as those associated with the formation of shrink lines).

Although the EISM approximately doubles computational time compared to the ISM due to the thermal analysis, the added cost remains moderate and justified when higher accuracy is needed. This balance is particularly valuable for industrial applications aiming to reduce trial-and-error procedures and increase confidence in simulation-driven decision-making.

In conclusion, the EISM framework represents a step forward in bridging the gap between simplified original inherent strain-based models and high-fidelity thermo-mechanical simulations.

Future efforts will focus on integrating adaptive mesh and layer lumping strategies as well as exploring automated methods to identify regions requiring finer resolution. Another promising research line could involve improving the thermal model to calculate

the temperature history needed in the EISM more efficiently, thereby reducing the computational cost. Such enhancements could further refine the balance between computational efficiency and predictive accuracy. Additionally, extending the EISM approach to other alloys, part geometries, and process parameters will broaden its applicability and increase its relevance in industrial practice.

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Appendix A

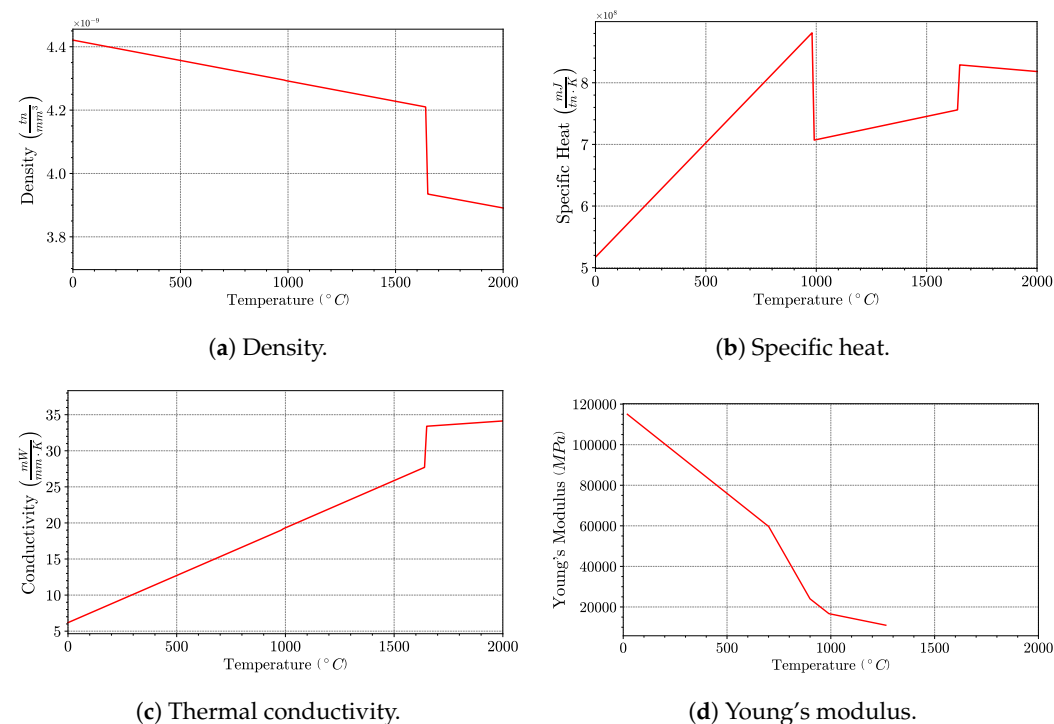


Figure A1. Cont.

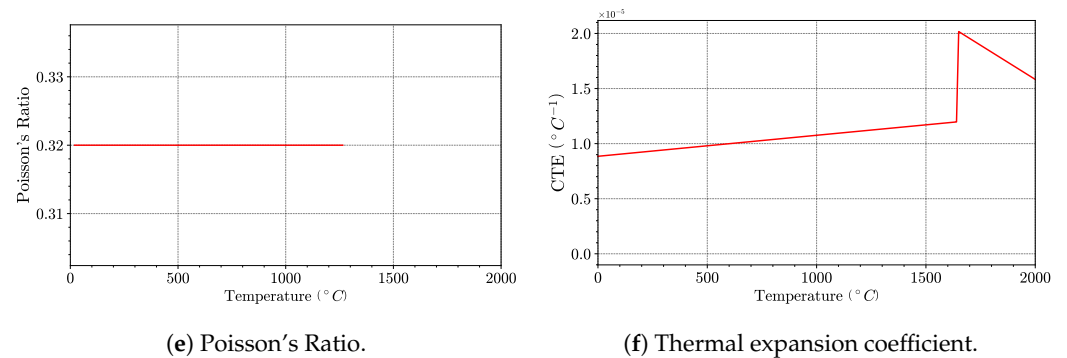


Figure A1. Temperature-dependent thermo-mechanical properties of Ti-6Al-4V material.

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CONCLUSIONS AND FUTURE WORK

This final chapter summarises the key findings of the research presented in this thesis, explicitly addressing the objectives outlined in the introduction. It presents the specific conclusions drawn from the research conducted in each paper integrated into this work and highlights the main contributions of the thesis. Furthermore, a critical reflection on the study's limitations is provided, followed by proposals for future research directions.

8.1 Overall summary of the research

The primary objective of this thesis was to **develop and validate an efficient numerical methodology for predicting distortions in Ti-6Al-4V components manufactured via the Powder Bed Fusion - Laser Beam (PBF-LB) process**. The research specifically focused on enhancing the Inherent Strain Method (**ISM**) to improve its accuracy and industrial applicability. To achieve this, the study integrated the following key developments:

- **An empirical (inverse) approach for inherent strain calculation was developed and validated (*Objective 1*)**, using twin-cantilever structures. Distortion measurements obtained after partial cutting confirmed the robustness and accuracy of the methodology for inherent strain extraction. The proposed approach provided reliable distortion predictions, making it well-suited for industrial applications.
- **A meso-scale thermo-mechanical approach was developed to accurately compute inherent strain tensors (*Objective 2*)**, offering a precise representation of the thermal and mechanical behaviours characteristic of the **PBF-LB** process. The model provided crucial insights into the complex interactions between process parameters and mechanical responses, demonstrating strong predictive capability at local scales. This enabled the reliable extraction of inherent strain tensors for seamless integration into macro-scale simulations.
- **The original **ISM** was refined into an Enhanced Inherent Strain Method (**EISM**)**, incorporating a dynamic correction factor that accounts for the evolution of thermal fields during the **PBF-LB** process. This enhancement significantly improved predictive accuracy and generalisation capabilities, effectively bridging

the gap between simplified inherent strain-based models and high-fidelity thermo-mechanical simulations.

- **Rigorous validation of the developed numerical methodologies was conducted (*Objective 4*)**, ensuring confidence in their predictive capabilities. An extensive experimental campaign involving three distinct geometries (twin-cantilever beams, a non-symmetric bridge, and a Steady Blowing Actuator (SBA)) provided temperature, distortion, and residual stress measurements for thorough model validation. The EISM and high-fidelity models exhibited strong agreement with experimental data in predicting distortions, confirming their accuracy and reliability.
- **Industrial validation of the EISM was successfully conducted (*Objective 5*)**, using the SBA as a case study. The results demonstrated the model's applicability in industrial settings, highlighting its potential to reduce trial-and-error iterations and improve additive manufacturing workflows.

8.2 Conclusions

The following subsections summarise the main conclusions drawn from this dissertation.

8.2.1 *Conclusions on the empirical methodology for determining inherent strains in PBF-LB (Paper 1)*

- An inverse calibration methodology based on twin-cantilever bending tests was successfully developed and validated. The measured spring-back after partial cutting (wEDM) was used to iteratively determine the *inherent strain* tensor under linear-elastic assumptions, enabling accurate calculation of inherent strains for distortion prediction.
- The calibrated inherent strain values, when applied within the ISM framework, yielded distortion predictions with errors below 10% relative to experimental measurements. This approach proves particularly effective for early-stage design processes in industrial applications.
- Distortion magnitude and distribution were significantly influenced by the scanning strategy and structural geometry. Longitudinal scanning produced the largest distortions, transverse scanning the smallest, and 45° and 90° rotating patterns exhibited intermediate distortion levels.
- The scanning strategy directly impacted the in-plane inherent strain tensor components. Rotating scanning patterns led to nearly isotropic in-plane inherent strains, simplifying numerical modelling. Additionally, the inherent strain tensor could be assumed as orthogonal in the studied cases; however, this assumption should be further examined for more complex geometries.

8.2.2 *Conclusions on the high-fidelity thermo-mechanical numerical model for inherent strain calculation (Paper 2)*

- A high-fidelity meso-scale thermo-mechanical model was developed as a numerical alternative to empirical calibration for inherent strain calculation. This model performed detailed transient simulations of multiple deposited layers, capturing the evolution of inherent strains throughout the [PBF-LB](#) process. The final strain fields were homogenised to compute the inherent strain tensor, which was subsequently used in part-scale [ISM](#)-based simulations.
- The computed inherent strain tensor was defined in terms of thermal, plastic, and activation strains. Results revealed that activation strains play a dominant role in defining the inherent strain tensor, highlighting the significant influence of scanning strategy in the [PBF-LB](#) process. While plastic strains contributed to overall deformation, their impact was found to be smaller than initially expected, allowing for potential model simplifications.
- A sensitivity analysis revealed that both the size and position of the control volume, which represents the subdomain where homogenised inherent strains are computed, play a critical role. Defining an optimal control volume while minimising the influence of boundary conditions led to the development of a refined version of the local model, achieving an 89% reduction in computational cost without compromising the accuracy of inherent strain calculations.
- The study confirmed that the inherent strain tensor could be effectively approximated as an isotropic tensor in the XY plane, with negligible off-diagonal and ZZ components. This finding aligns with the conclusions drawn from the empirical methodology for determining inherent strains, further reinforcing the validity of this assumption.
- The inherent strain tensor obtained from the high-fidelity local model was successfully validated against experimental results. Distortion predictions for the [SBA](#) actuator geometry showed strong agreement with measured deformations, demonstrating the practical applicability and reliability of the proposed multi-scale modelling approach.
- The inherent strain tensors derived from numerical simulations closely matched those obtained through empirical calibration, reinforcing the reliability of the physics-based numerical approach. This consistency highlights the potential of using numerical simulations to generate inherent strain databases, enabling broader industrial adoption of the [ISM](#) based methodologies.

8.2.3 *Conclusions on the development of the Enhanced Inherent Strain Method ([EISM](#)) (Paper 3)*

- This work introduced an Enhanced Inherent Strain Method ([EISM](#)) for Powder Bed Fusion - Laser Beam ([PBF-LB](#)) that integrates macro-scale thermal history into the inherent strain formulation. By dynamically adjusting the thermal

strain component of the precomputed inherent strain tensor according to the evolving thermal field, the method accounts for geometry- and boundary-condition-induced thermal gradients. This enhancement significantly improves the accuracy of distortion and residual stress predictions, making it particularly effective for complex geometries and scanning strategies.

- The **EISM** demonstrated superior accuracy compared to conventional **ISM** implementations, particularly for industrial-scale components where non-uniform heating effects are more pronounced. Validation against experimental results showed that for the non-symmetric bridge, the Mean Absolute Percentage Error (**MAPE**) in distortion predictions improved by 79% compared to the original **ISM**. Similarly, for the **SBA**, the standard deviation of geometric deviations was reduced by 40%. Additionally, the **EISM** accurately captured both the location and magnitude of maximum distortions, whereas the **ISM** exhibited discrepancies.
- A sensitivity analysis revealed that neither mesh size nor layer lumping significantly affects global temperature evolution. However, careful selection of layer lumping and mesh refinement is essential in regions with structural transitions (e.g., shrink-line formations or abrupt stiffness changes) to ensure numerical stability while maintaining computational efficiency.
- Despite the additional computational cost of a macroscopic thermal simulation, the **EISM** remains significantly more efficient than fully coupled thermo-mechanical models. Although it approximately doubles the computational time compared to the **ISM**, this trade-off is justified for applications requiring higher accuracy, particularly for reducing trial-and-error procedures in industrial settings.

8.3 Contributions of this research

This dissertation presents several original contributions to numerical modelling methodologies for distortion prediction in **PBF-LB** of Ti-6Al-4V components. These contributions align with the research objectives outlined in **Chapter 1** and can be summarised as follows:

- **Development of an empirical methodology for inherent strain calibration.** A robust *inverse engineering* method was proposed and validated, enabling the efficient determination of inherent strain tensors from a minimal set of test coupons and straightforward distortion measurements. This significantly enhances the robustness and ease of industrial implementation.
- **Establishment of a high-fidelity meso-scale framework for inherent strain calculation.** A local thermo-mechanical model was developed to capture the rapid heating-cooling cycles inherent to the **PBF-LB** process. By simulating multiple layers and homogenising local strain fields, the approach provided

inherent strain tensors highly consistent with experimental evidence, ensuring accurate part-scale distortion predictions.

- **Proposal and validation of an Enhanced Inherent Strain Method (EISM).** A temperature-dependent correction to the inherent strain tensor was introduced, bridging the gap between purely static ISM assumptions and real-time thermal effects. This novel approach significantly improved accuracy for geometrically complex parts while maintaining the computational efficiency.
- **Comprehensive experimental validation framework.** A rigorous validation campaign was conducted using three geometries of increasing complexity (twin-cantilever beams, a non-symmetric bridge, and a SBA). Distortion, temperature, and residual stress data were systematically collected, confirming the predictive accuracy and robustness of both high-fidelity and simplified numerical models.
- **Demonstration of industrial applicability on a complex component.** The EISM approach was applied to an aeronautical Steady Blowing Actuator (SBA), demonstrating its capability to handle large, intricate designs with acceptable computation times. This validation highlights the method's suitability for real-world additive manufacturing applications, facilitating broader industrial adoption of simulation-driven design strategies.

8.4 Limitations and discussion

Several assumptions and simplifications constrain the scope and accuracy of the present findings:

1. **Assumption of a uniform precomputed inherent strain tensor across the entire domain.** Both the original ISM and the EISM assume that, by the end of the simulation, the same inherent strain tensor is applied uniformly throughout the entire domain. While this assumption has been validated in many cases (demonstrating strong agreement between predictions and experiments) it may not hold for certain geometries or materials where other inelastic strain components (e.g., plastic, transformation-induced) play a more significant role. In such cases, the simplified methodology may require refinement to ensure broader applicability and accuracy.
2. **Sensitivity to layer lumping and mesh refinement.** While the macro-scale thermal analysis demonstrated robustness, layer lumping and mesh refinement require careful selection, particularly in regions with abrupt stiffness transitions (e.g., shrink-line formations). Insufficient refinement in these areas may lead to inaccuracies in local distortion predictions.
3. **Exclusion of support structures.** While support structures are frequently used in PBF-LB, this study explicitly excluded thin-walled and lattice supports (see Chapter 1). As a result, the direct applicability of the proposed methodology to geometries that heavily rely on intricate support structures or bridging features remains unverified.

4. **Assumption of isotropic material behaviour.** The models assume uniform, isotropic material properties, which simplifies calculations but may underestimate distortions and residual stresses in builds exhibiting strong crystallographic textures or directional grain growth.
5. **Experimental dataset limited to Ti-6Al-4V.** The methodology was developed and validated using Ti-6Al-4V, a widely used alloy in aerospace and biomedical applications. Its applicability to other metallic systems (e.g., Inconel, stainless steels, or aluminium alloys) requires further calibration or modifications to the high-fidelity local model.
6. **Computational cost constraints.** Despite the simplifications introduced, simulating large or geometrically complex parts remains computationally demanding. While alternative approaches, such as reduced-order modelling or physics-informed machine learning, could help mitigate these challenges, their integration was beyond the scope of this thesis. Future work should explore such techniques to enhance computational efficiency while maintaining predictive accuracy.

8.5 Recommendations for future work

Based on the outcomes, limitations, and insights gained in this research, the following future research directions are recommended:

- **Refinement of precomputed inherent strain distributions.** Future work should move beyond the assumption of a uniform precomputed inherent strain tensor by exploring spatially varying inherent strain distributions. Geometry-aware heuristics and region-based mapping could improve accuracy in complex geometries. However, achieving this refinement requires high-fidelity thermo-mechanical simulations to capture detailed distributions of plastic and activation strains.
- **Adaptive meshing and layer lumping strategies.** Future research should focus on integrating adaptive meshing and adaptive layer lumping strategies in ISM-based methodologies to enhance computational efficiency while maintaining accuracy. To this end, automated methods for identifying regions that require finer resolution (such as areas with abrupt stiffness changes, closely linked to defects like shrink-lines) should be explored. These advancements could further optimise the trade-off between computational cost and model fidelity.
- **Improvement of the thermal model.** Enhancing the efficiency of the macro-scale thermal model in the EISM framework could reduce computational costs while maintaining predictive accuracy. Faster temperature history calculations would improve the balance between computational efficiency and accuracy.
- **Extension to other materials and process conditions.** Adapting the inherent strain calculation methodologies and the EISM approach to different alloys, part

geometries, and processing parameters would increase their industrial relevance and broader applicability.

- **Support structure modelling and optimisation.** Incorporating support structure effects into inherent strain or [EISM](#)-based simulations would enable application to more complex geometries. Automated optimisation strategies could be explored to balance distortion minimisation with efficient support usage.
- **Integration of Machine Learning (ML) techniques.** Future research could explore Physics-Informed Machine Learning ([PIML](#)) and [ROM](#) to enhance distortion prediction in [PBF-LB](#). [PIML](#) can improve inherent strain computation by integrating physics constraints with data, while [ROM](#) techniques can enable faster and more scalable simulations. The development of real-time digital twins and uncertainty-aware [ML](#) models could further enhance prediction accuracy and enable adaptive compensation strategies for industrial applications.
- **Automated software integration for industrial use.** Embedding the [EISM](#) methodology into commercial [AM](#) software platforms could facilitate broader industrial adoption. Future developments should focus on user-friendly implementations, automated calibration workflows, and seamless integration with machine data to streamline the use of distortion prediction models in manufacturing environments.

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