A Multiscale Thermomechanical Metal Additive Manufacturing Simulation and the Impact of Geometry on Residual Stress and Distortion

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A MULTISCALE THERMOMECHANICAL METAL ADDITIVE MANUFACTURING SIMULATION AND THE IMPACT OF GEOMETRY ON RESIDUAL STRESS AND DISTORTION

by

Luis Fernando Silva Velasco

A thesis submitted to the Graduate College in partial fulfillment of the requirements for the degree of Master of Science in Engineering (Mechanical) Mechanical and Aerospace Engineering Western Michigan University June 2020

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A MULTISCALE THERMOMECHANICAL METAL ADDITIVE MANUFACTURING SIMULATION AND THE IMPACT OF GEOMETRY ON RESIDUAL STRESS AND DISTORTION

Luis Fernando Silva Velasco, M.S.
Western Michigan University, 2020

Metal additive manufacturing is an enabling technology for the rapid prototyping and manufacturing of geometrically complex parts that would otherwise be difficult or impossible to manufacture. However, the manufacturing process can produce undesired residual stresses and distortions. The first part of the work describes the implementation of a multiscale, thermo-mechanical simulation modeling the metal powder bed fusion additive manufacturing process. NASA’s Micromechanics Analysis Code was is to incorporate the microscale effects of an evolving material porosity on the predicted macroscale residual fields. The simulation shows that modeling an evolving material porosity, as the material transitions from a metal powder to a solid, significantly affects the magnitude of the residual stresses and distortions, compared to a constant porosity model. The second part of this work uses the developed simulations to assess the effects of geometrical features. A linear regression shows that there is a correlation between the residual fields and the geometry. This suggests that it may be feasible to predictably influence the residual fields by modifying the geometry. This work is part of a larger work aimed at optimizing the geometry to minimize the residual stresses and distortions.
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-Luis Fernando Silva Velasco
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LIST OF ABBREVIATIONS

\( \varepsilon \) = sintered porosity, strain
\( \varepsilon_0 \) = initial porosity
\( \varepsilon_{\text{min}} \) = minimum achievable porosity
\( K \) = densification coefficient
\( \kappa \) = sintering coefficient
\( V_f \) = volume fraction
\( s \) = laser beam penetration depth
\( \eta \) = laser power transmission efficiency
\( r_0 \) = laser beam radius
\( v \) = laser linear speed
\( l, w \) = length and width of the laser scan area
\( \psi \) = specific energy input
\( P \) = nominal laser power
\( S_{xx} \) = stress in xx-direction
\( S_y, S_n \) = yield stress, stress at plastic strain n
\( \sigma, \sigma \) = stress tensor, stress tensor Vioglot representation
\( H \) = strain hardening term
\( U_i \) = displacement in the i-direction
\( \varepsilon^* \) = inherent strain
LIST OF ABBREVIATIONS – CONTINUED

\(v\) = Poisson’s ratio
\(E\) = modulus of elasticity
\(Q\) = heat per unit volume
\(q_b\) = heat flux at a boundary
\(c\) = specific heat capacity
\(\rho\) = mass density
\(k\) = thermal conductivity
\(h\) = convective heat transfer coefficient
\(\sigma\) = Stefan-Boltzmann constant
\(C\) = specific heat capacity
\(\alpha\) = coefficient of thermal expansion
\(T\) = Temperature

\(B\) = deformation matrix
\(D\) = constitutive matrix
\(N\) = shape function matrix
\(\kappa\) = thermal conductivity matrix
\(K\) = stiffness matrix
\(\tau\) = out of plane thickness, shear stress
LIST OF ACRONYMS

AM – Additive Manufacturing
DED – Direct Energy Deposition
DOF – Degree of Freedom
EBM – Electron Beam Melting
FDM – Fused Deposition Modeling
FE – Finite Element
GMC – Generalized Method of Cells
HIP – Hot Isostatic Pressing
ICME – Integrated Computational Materials Engineering
ISM – Inherent Strain Method
MAC – Micromechanics Analysis Code
NASA – National Aeronautics and Space Administration
PBF – Powder Bed Fusion
RS – Residual stress
RUC – Repeating Unit Cell
SIMP – Solid Isotropic Material with Penalization
SLS – Selective Laser Sintering
SLM – Selective Laser Melting
TGM – Temperature gradient mechanism
CHAPTER 1

INTRODUCTION

1.1 Motivation

Advancements in metal additive manufacturing (AM) have made it a viable solution for the rapid prototyping and manufacturing of geometrically complex parts. These complex parts can be difficult or impossible to manufacture with conventional subtractive manufacturing. However, additive manufacturing can be accompanied by large residual stresses. These stresses can lead to premature failure due to crack promotion or otherwise weaken the overall structure [1]. Also, the part deformation that occurs in conjunction with the residual stresses may cause unacceptable dimensional deviations. Although several post-treatment processes exist to mitigate these negative outcomes, the permanent deformation caused by plastic strain is not easily reversed.

1.2 Technical Problem

The prediction and reduction of these residual fields is desirable. Although residual stresses and plastic deformations occur at the local scale, it may be possible to mitigate the negative effects of additive manufacturing by modifying the macroscopic geometry. The larger project aims to produce an optimized geometry to minimize the residual fields, without adversely affecting the final application. Since, commonly, AM parts are already geometrically optimized for its final application, a multi-objective technique is required. This requires an objective function that
accounts for the manufacturing process, not just the final application of the part. The geometrical optimization is a component of the larger project and is outside the scope of this thesis work.

The first step in achieving the overall goal is to obtain a computational model of the manufacturing process. The model will be used to evaluate the residual fields at a given design point (geometry), required for an optimization scheme. Simulation of the additive manufacturing process is intrinsically difficult since the domain of interest occurs at the nano and micro scale, while the structures being simulated are in the macroscale domain. Thus, a multiscale solution is adequate. Also, the manufacturing process involves multiple physics, with the melting requiring thermo-fluid-dynamics, the material deposition and microstructural evolution requiring methods accounting for phase transformations, and resolution of the stress-strain fields requiring conventional mechanics at the macroscale. In addition, due to the addition of thin layers of material, the manufacturing process can be composed of thousands of steps each with different and moving boundary conditions, requiring a substantial number of time steps during the simulation. Due to these difficulties, many techniques have been used in the literature that drastically reduce the size of the problem by making several assumptions, such as the thermomechanical method where melt pool dynamics are not considered, and the inherent strain method, where the dynamic heat transfer physics are not considered.
1.3 Technical Goals

The first goal of this work is to simulate the metal powder bed fusion additive manufacturing process. As a sub-goal, the micromechanics of the simulation can be considered using the available tools from NASA. This can be used to study the effect of the micromechanics on the thermomechanical simulation. Specifically, the material’s evolving porosity (the air to solid volume fraction), changing from powder to solid, was chosen as the microscale variable of interest. In addition, this work lays the foundation to analyze other microscale effects on the macroscale. The inclusion of the micromechanics and its effects on the macroscale mechanics during the simulation of the manufacturing process is a step towards the implementation of an Integrated Computational Materials Engineering (ICME) method on metal additive manufacturing. Work in ICME aims to use computer simulations to design and engineer not only the final products but also their constitutive materials. This requires multiscale methods to simulate the evolving material properties during manufacturing. This first goal is achieved in Chapter 3 - An Evolving Porosity.

The second goal of this work is to examine the effects of geometry on the simulated residual stress and deformations acquired during manufacturing. This will assess the feasibility of the long-term goal of obtaining a geometry optimized for its manufacturing process. This feasibility study requires the tools developed in completing the first goal. This goal of assessing geometric effects is achieved and discussed in Chapter 4 - Geometry Effects with Inherent Strain and also in Chapter 5 - Geometry Effects with Thermomechanical FE.
CHAPTER 2
BACKGROUND AND LITERATURE REVIEW

2.1 Metal Additive Manufacturing

2.1.1 Process

Metal additive manufacturing processes include powder bed fusion (PBF) and direct energy deposition (DED) processes. Powder bed fusion processes include selective laser melting (SLM), and electron beam melting (EBM). These use a high-powered energy source (a laser or electron beam) to selectively melt or sinter sections of metal powder into a solid, a layer at a time [2]. A recoating mechanism ensures that a uniform layer of powder is added to the powder bed at each layer. An inert gas environment is used to contain the powder bed in a laser-based process, while electron beam melting uses a vacuum. Figure 2.1 shows an overall schematic of the powder bed fusion laser process.

The powder layers are relatively thin compared to the part size, typically 30-50μm for lasers, around 100μm for electron beams [2], thus requiring potentially thousands of layers to build up the geometry. Also, the powder bed fusion process will re-melt the underlying layer as the topmost layer is being melted. Direct energy deposition methods, in contrast to powder bed fusion, feed the material onto the part as it is being melted. The feedstock material is a metal powder or wire. Direct energy deposition methods typically have faster print times at the sacrifice of lower dimensional accuracy [2].
However, these manufacturing processes can suffer from significant residual stresses, stresses that may lead to unacceptable part distortion, and that can promote cracks, adversely affecting the life of the part [3]. Large distortions may also cause damage to the recoater system in PBF processes. Residual stresses arise primarily due to the large temperature gradients during the process. The temperature gradient mechanism (TGM) model reasons that the thermal expansion during heating induces stresses, since its displacement is constrained by the surrounding cooler material [4]. During the expansion, plastic strains may develop due to the loading. After the beam has passed over the material the shrinking material that is now cooling generates compressive stresses on its surroundings and tensile stresses on itself. The residual stresses remain since the material has been plasticly deformed. However, in practice, the complicated thermal history produces complex stress distributions [4]. The field strongly depends on all the factors affecting the temperature history, such as beam...
path, and dwell time. Figure 2.2 shows a simplified overview of the temperature gradient mechanism.

![Figure 2.2 - Simplified residual stress formation mechanism](image)

During the mechanical loading of the material, large changes in stress occur, characterized by three phases. Phase one has large temperature changes, phase two has large stress changes (tensile to compressive) and phase three results in the steady-state residual stress after creep relaxation [5]. Three types of residual stresses exist on three different scales: macroscale, microscale, and nanoscale [4]. However, micro- and nanoscale stresses have limited effects on the overall mechanical properties [4]. Microscale stresses arise from anisotropic effects of the material, while nanoscale stresses arise from coherency and dislocations [4]. Experimental data shows that typically compressive stresses arise towards the center of the part, while tensile stresses form at the outer surfaces of the material [6]. It is these tensile stresses that are detrimental to the fatigue life of the part.

Mercelis et al. [2] have shown that the residual stresses in metal additive manufacturing methods such as selective laser sintering (SLS) and selective laser melting (SLM) are significant, predicting stresses as high as 700 MPa in Inconel 718.
Li et al. in Ref. [4] cite residual stresses that are 50% to 60% above the materials yield strength. They also found that the manufacturing process parameters such as the beam size, power, and scanning speed affect the magnitude of the produced residual stresses, thus in-process methods exist to reduce these residual stresses.

In-process stress mitigation methods include closed-loop feedback control (controlling the heat source, aiming to homogenize the temperature distribution), thermal gradient control (preheating the ambient to reduce thermal gradients), scanning strategy control and mechanical control (laser shock peening) [4]. A scanning strategy in a chessboard pattern has been shown to cause less distortion than other scanning strategies [4].

In addition, AM parts show a columnar microstructure in the build direction in nickel-based superalloys, titanium alloys, and stainless steels [4]. This alludes to the anisotropic mechanical properties seen in parts [7]. Thus, it is worthwhile to investigate the effects of the microstructure and anisotropy on the residual fields.

2.1.2 Post-Treatments

After manufacturing, heat treatment processes such as hot isostatic pressing (HIP) have significant benefits to the mechanical characteristics of a part. During HIPping parts are subjected to high temperatures and high pressures (1120 - 1240 °C, 100 - 165 MPa) for several hours (3 - 4 hr.) in an inert environment [8]. This treatment can significantly reduce the residual stresses, reduce the internal porosity and defects, and decrease the anisotropy of the material’s properties [8]. Shiomi et al. in
Ref. [9] showed that the HIPing of an metal additively manufactured beam specimen reduced the residual stresses up to 70%. In addition, HIPing of an SLM produced part can significantly increase its fatigue characteristics, due to the internal closing of pores, with further improvements when the surface of the part is conditioned (i.e. polished or machined) [10]. Other mechanical post-processing such as hard turning, shot peening, and grinding can generate potentially advantageous compressive stresses on the surface and subsurface [4]. Also, post-treatments can dramatically reduce the dislocation density, signifying a reduction of microscale residual stresses. Although post-processing can remove elastic deformations acquired during manufacturing, they cannot easily remove plastic strains/deformations. Thus, additional processing is required such as milling (subtracting) material into the desired shape/dimension. Processing that increases the manufacturing costs.

2.1.3 Experimental Measurements

Several experimental methods exist to measure residual stresses depending on the scale of the stress [11]. Mechanical methods rely on relaxing the residual stress in the part with a machining procedure. The deformation after the machining operation then is used to calculate the residual stress before the operation [11]. These methods are used to measure macroscale stresses (those that vary continuously over large scales). In the curvature method, the stressed part is sectioned into narrow strips (to avoid multiaxial stresses) and the deformation/curvature of the part after the stress relief is measured, with strain gauges for example. The stress can then be
calculated from the material properties [11]. The hole drilling technique is typically an inexpensive method to obtain an approximate measurement. Here, the stresses can be inferred from measurements of a rosette of strain gauges [11] after drilling a hole.

Similarly, a method often used in the literature [12] is to additively manufacture a cantilever beam. Removing this part from its substrate will cause the beam to deform. The amount of deformation can then be measured. The stress required to obtain that deformation can then be calculated (theoretically or experimentally).

Diffraction techniques use the measured interplanar spacing to calculate the elastic strain [11] and thus the stress. Note that this requires a stress-free interplanar spacing as a reference. X-ray diffraction has a penetration in the order of micrometers (thus limited to surface measurements) while electron diffraction can only be used with very thin samples [11]. Other methods also exist, such as ultrasonics, where the change in the speed of sound in the material can be used to calculate the average stress along the wave path [11].

2.2 AM Finite Element Simulation

The AM process has been simulated in the literature using several methods. These include thermomechanical simulations with the finite element method (FEM), thermo-fluid simulations with the finite volume method, inherent strain methods with FE methods, microscale lattice Boltzmann methods, phase-field modeling, and
microscale hybrid methods [3]. This work is concerned with the thermomechanical finite element method.

The temperature distribution of a moving point heat source can be approximated analytically by the Rosenthal solution [13]. The solution for a thick plate is shown in Eq. (2.2.1), where \( T_0 \) is the ambient temperature, \( P \) is the heat power absorbed into the material, \( v \) is the heat source velocity in the positive x-direction, and \( \alpha, k \) are the materials thermal diffusivity and conductivity respectively. However, the solution does not account for nonlinearities such as melt pool dynamics. Also, this analytical solution assumes constant material properties and neglects any latent heat. These shortcomings necessitate numerical solutions over the analytical solution in Eq. (2.2.1). In numerical simulations of the process, simulations that do not include temperature-dependent material properties usually lead to inaccurate results [3].

\[
2\pi T^* = \frac{1}{R^*} \exp\left(-\left(x^* + R^*\right)^2/2\right)
\]

\[
T^* = \frac{\alpha k}{P U} (T - T_0)
\]

\[
x^* = \frac{xv}{\alpha}, \quad y^* = \frac{yv}{\alpha}, \quad z^* = \frac{zv}{\alpha}
\]

\[
R^* = \sqrt{x^*^2 + y^*^2 + z^*^2}
\]

A major disadvantage with FE methods is that with large models, especially with nonlinearities included, are computationally costly. In addition, the thermomechanical finite element method does not lend itself to easily include other physics in the simulation such as melt pool thermo-fluid dynamics [3], and metal evaporation [14]. Neglecting these physics can lead to inaccurate results when simulating large scale models [3] since the temperature distribution and gradients
are the driving force in deformation and residual stresses. However, the fluid dynamics in FEM have been considered, approximating these physics by adjusting the thermal properties [15]. Thermo-fluid dynamics models have been conducted [16] (using an electron beam as the heat source) that includes fluid viscous effects, and phase transformations. Bauereiß et al. [17] used lattice Boltzmann method which included capillary and wetting effects to simulate the melt pool dynamics to predict defects.

2.2.1 The Thermomechanical FE Method

An uncoupled thermomechanical simulation is a two-step simulation, where first a transient thermal field is solved. The temperature distribution is then used in a quasi-static mechanical simulation as the loading. A quasi-static mechanical solution is used since the wave propagation speed of a mechanical transient problem for typical materials is orders of magnitude higher than the wave propagation speed of a thermal transient problem. Thus, it is assumed that the mechanical problem is in a quasi-steady state relative to the transient thermal problem.

For completeness, a condensed overview of the derivation of the thermal finite element method is shown here. For details, the reader is referred to Cook [18]. The governing differential equation for the two-dimensional heat transfer problem is shown in Eq. (2.2.2), where \( \tau \) is the out of plane thickness; the three dimensional version is similar. Note that in this document, vectors are denoted by an underline
while matrices are denoted by boldface typeset. Also note the following notation, 

\( (\cdot)_{x} = \frac{\partial(\cdot)}{\partial x} \).

\[
\frac{\partial}{\partial x} \left( \tau k_{x} T_{x} + \tau k_{y} T_{y} \right) + \frac{\partial}{\partial y} \left( \tau k_{y} T_{y} + \tau k_{z} T_{z} \right) + 2h(T_{w} - T) + \tau Q = c \rho \tau \dot{T} \tag{2.2.2}
\]

\[
\hat{\partial} = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix}; \quad T_{x} = \begin{bmatrix} T_{x} \\ T_{y} \\ T_{z} \end{bmatrix}; \quad \mu = \begin{bmatrix} l \\ m \\ n \end{bmatrix} \tag{2.2.3}
\]

Using the definitions shown in Eq. (2.2.3), where \( l, m, n \) are the direction cosines, the general three-dimensional governing differential equation can be succinctly written as shown in Eq. (2.2.4), where \( \mathbf{k} \) is a matrix of thermal conductivity (in the global coordinate system) and \( Q \) represents heat generation rate. Essential (on temperature) and nonessential (on heat fluxes \( q_{b} \)) boundary conditions can then be applied on this equation. For the two-dimensional problem, the boundary heat flux due to convection is, \( q_{b} = h(T_{w} - T) \). The boundary heat flux due to radiation is \( q_{b} = \eta \sigma(T_{r}^{4} - T^{4}) \), where \( \eta \) is the absorption value, and \( \sigma \) is the Stefan-Boltzmann constant, note that \( T \) must be in absolute units.

\[
\hat{\partial}^{T} (\mathbf{k} \cdot T_{x}) + Q = c \rho \dot{T} \tag{2.2.4}
\]

\[
\sum q_{b} = \mu^{T} \cdot \mathbf{k} \cdot T_{x} \tag{2.2.5}
\]

The functional to be minimized for the 2D problem can then be written as shown in Eq. (2.2.5), adding the convective boundary condition that is normal to the 2D plane. Discretizing the domain using the finite element method as shown in Eqs.
(2.2.6), the functional can then be written as shown in Eq (2.2.8) for a single element, where definitions are as shown in Eqs. (2.2.7).

\[
\Pi = \int \frac{1}{2} (T_e^T \cdot \kappa \cdot T_e - QT + c \rho T^T) dV + \int \left( f_b + h T_e \cdot T - \frac{1}{2} h T^2 \right) dV \tag{2.2.5}
\]

\[
T = N \cdot T_e; \quad T_e = B \cdot T_e; \quad B = \partial \cdot N
\tag{2.2.6}
\]

\[
k = \int_{V} B_{th}^T \cdot \kappa \cdot B_{th} dV
\]

\[
h = \int_{S} h N^T N dS
\]

\[
c = \int_{V} c \rho N^T N dV
\tag{2.2.7}
\]

\[
r_B = \int_{S} f_b N^T dS
\]

\[
r_h = \int_{S} h T_e N^T dS
\]

\[
r_Q = \int_{V} Q N^T dV
\]

\[
\Pi_{elem} = T_e^T \cdot (K - h) \cdot T_e + T_e^T \cdot (c \cdot \dot{T_e} + r_q - r_Q - r_h)
\tag{2.2.8}
\]

After assembling into global matrices (denoted by capitals) and making the functional stationary \( \left( \frac{\delta \Pi}{\delta T} = 0 \right) \) leads to Eqs. (2.2.9) [18]. This equation can then be integrated through time numerically to obtain the solution. Note that the thermal problem does not have second-time derivatives on temperature.

\[
C \dot{T} + K_{th} T = R_{sh}
\]

\[
K_{th} = K + H
\tag{2.2.9}
\]

\[
R_{sh} = R_b + R_h + R_Q
\]

Once the temperature at a time step is found, it can be applied as a load to the static structural problem. Typically, the same mesh and element type that was used
for the thermal problem is used for the mechanical problem, thus temperatures are already known at the nodes. If a different mesh is used, the temperature can simply be interpolated onto the new mesh using the shape functions of each mesh. The temperature change (from a reference point) is used to compute the thermal strains from the given vector of thermal expansion coefficients, as shown in Eq. (2.2.10), dimensions of the vectors are shown for convenience.

\[ \varepsilon_{T,3x1} = \alpha_{3x1} \Delta T_{1x1} \]  

(2.2.10)

The loading caused by this initial thermal strain must be applied on the right-hand side of the static mechanical FE Eq. (2.2.11). This thermal force is computed from Eq. (2.2.12), where \( \mathbf{D} \) is the constitutive matrix. In post processing, the thermal strain is then subtracted from the computed mechanical strain to compute the stress, Eq.(2.2.13). This process ensures that when a temperature change is applied to an unrestricted structure, the structure will deform, yet no stress will be present and vice-versa, as expected.

\[
\mathbf{K} \cdot \mathbf{U} = \mathbf{F} 
\]

(2.2.11)

\[
\begin{array}{c}
\int_{\Omega,\Omega_1}\left( \mathbf{B}_{\text{stress,}\Omega_3} \right)^T \cdot \mathbf{D}_{3x3} \cdot \mathbf{\varepsilon}_{T,3x1} \, d\Omega \\
\end{array} 
\]

(2.2.12)

\[
\sigma_{3x1} = \mathbf{D}_{3x3} \cdot \left( \mathbf{\varepsilon}_{\text{mech}} - \mathbf{\varepsilon}_{T} \right)_{3x1} 
\]

(2.2.13)

The uncoupled thermomechanical method is a one-way method, that is the mechanical simulation does not influence the thermal simulation. In the coupled thermomechanical method, the thermal and mechanical problems are solved simultaneously, thus allowing for heat generation due to strains (such as plastic
strain) to be included in the thermal simulation. For the work presented in this thesis (described in Chapter 3 - An Evolving Porosity on page 27), the uncoupled method was used, assuming heat generation from plastic strain rates are negligible.

To resolve the continuously changing geometry, element “birth and death” (activation and deactivation), “quiet” elements, and a combination of these two methods are used in the literature [19]. For the element birth and death technique, in the first step of the simulation, all the elements are deactivated, that is they are not included in the solution (more specifically in \( \mathbf{K} \mathbf{U} = \mathbf{F} \)). Element layers are then activated in subsequent steps, as the heat source is passed over the elements, until a fully completed part. The advantage of this method is that the model has a relatively small number of degrees of freedom (DOF) at the start and more DOF are added as the simulation progresses. The quiet element technique is similar; however, all of the elements are included in the solution, and elements that are yet to be included in the solid geometry are assigned material properties several orders of magnitude smaller than the solid material properties. Nonzero material properties are assigned to avoid numerical difficulties. The hybrid method is a combination of these two methods. In this method, a whole layer of elements is activated (included in the solution) while elements, where the laser has not yet passed over, are assigned powder or weak material properties. This hybrid method is used for this work.

As described in Section 2 - Metal Additive Manufacturing on page 4, a typical layer thickness during manufacturing is in the order of 30 - 100 μm. In addition, the laser diameter is also in the order of 100 μm. Very high thermal gradients result from
a small laser diameter [14]. It is impracticable to have a mesh density that is fine enough to resolve these features when a full-scale model is being simulated. Thus, it is typical to cluster many printed layers into a single layer (a super-layer) of elements during the FE simulation [20], along with an element density on the printing plane that does not capture such high thermal gradients. Typically during a simulation at the macroscale (part sized), the laser diameter is set to a value much larger than reality [21]. The lumping of printed layers onto a single or a couple of element layers can be justified by considering that the laser path is typically rotated at every printed layer, thus the effect of the detailed laser raster pattern is averaged out over several layers [20]. Also, ref. [22] studied the effect of lumping many printed layers into an equivalent super-layer of elements. Results show that the lumping can drastically reduce the number of DOF in the models with a small accuracy penalty, comparing simulation to experimental results. However, the size of the equivalent layer (i.e. the number of printed layers in the element layer) should not be done arbitrarily, as the error increases as more printed layers are lumped [22].

In simulating the additive manufacturing process, nonlinearities in both thermal and mechanical problems exist, mainly nonlinearities in the heat input (the heat input is a function of time) for the thermal problem, plasticity in the mechanical problem (residual stresses arise due to plasticity) and temperature and time-dependent material properties in both problems. Thus, an iterative solution is required for both problems. If the mechanical solver requires a smaller time step (to obtain a smoother load input for convergence), the thermal problem must be solved
again at that new time step. Thus, the time step size is typically limited by the mechanical problem. It is evident that the thermomechanical method requires considerable computational power to simulate the entire manufacturing process, especially for large models.

To mitigate these computational inefficiencies, other methods have been utilized in the literature. These methods include mesh coarsening, where the current topmost layer uses a high-density mesh used to resolve the solution in the heat-affected zone, while a coarse mesh is used in areas far from the zone [21]. Thus, it is possible that growing the geometry (from the addition of material) does not lead to more nodes in the finite element problem. Since the heat-affected zone is moving with respect to time as new layers of material are deposited, the model must be re-meshed. The solution is interpolated at every mesh change to a master fine mesh for postprocessing.

Other methods to reduce the problem size to allow the simulation of large models include the equivalent scanning method [3]. The equivalent scanning method applies a representative surface heat flux to a target volume or to an entire layer at a time [3], instead of modeling the laser path at every time step in the thermomechanical simulation. Another method used is the inherent strain method (ISM).
2.2.2 The Inherent Strain Method

The inherent strain method (ISM) drastically reduces the problem size by avoiding the thermal simulation, and directly applying any irreversible strains as an initial strain in the mechanical problem. Temperature-dependent properties are not needed since properties at room temperature are used [3]. These inherent strains include the residual plastic, creep, and phase transformation strains produced by the thermal loading and unloading. ISM relies on the assumption that small patches of material all experience a similar thermo-mechanical history, thus no need to model a moving heat source, as the irreversible strain produced by the heat source is directly applied to the mechanical problem [3]. This assumption is reasonable considering that the laser scanning pattern is repetitive. The inherent strain method was initially conceived for the computation of welding mechanics. The metal AM process is in a sense a continuous welding process, hence the application of the inherent strain method on the additive manufacturing process. Eq. (2.2.14) provides the definition of inherent strain [22]. Since the inherent strain is applied to the static mechanical simulation, the part has had enough time to cool, thus thermal strains are neglected. Furthermore, strains due to phase transformations and creep are typically neglected, thus the inherent strain is approximately only the plastic strain [22].

\[
\varepsilon^* = \varepsilon_{total} - \varepsilon_{elastic} \\
= \varepsilon_{plastic} + \varepsilon_{thermal} + \varepsilon_{phase} + \varepsilon_{creep} \tag{2.2.14}
\]

However, the assumption that this strain is the same everywhere is not accurate for the AM process as it is for its original intended usage, a welding process
[22]. The strain produced is dependent on the boundary conditions and thermal boundaries, which are changing in AM, thus this method may be inaccurate for complex parts, or parts for which the inherent strain applied has not been calibrated. In addition, the method assumes the same strain for all the layers, however, in AM, the inherent strain from the layers above could change the plastic strain of the layers below. It has also been shown [12] that this inherent strain is highly dependent on laser scanning pattern and orientation. Liang et al. [22] states that the inherent strains decrease sharply near the ends of the layers due to differences in the thermal and mechanical boundary conditions.

Eq. (2.2.15) shows how this strain is applied to the static FE mechanical problem, noting that this equation is equivalent to Eq. (2.2.12). That is the inherent strain is treated as an initial strain (equivalent to an initial thermal strain). Eq. (2.2.16) through Eq. (2.2.19) show how the mechanical problem conventionally solved in the finite element method.

In addition, since the laser pattern is rotated at every printed layer, it is usually assumed that the inherent strains in the print plane are equal (i.e. $\varepsilon_{xx}^* = \varepsilon_{yy}^*$). This is assumed since the lumped element layer represents many printed layers, thus the in-plane strains are averaged out, since the laser scan pattern is rotated at every layer.

$$ f = \int_{\Omega} B^T D \varepsilon^* dV $$ \hspace{1cm} (2.2.15)

$$ u = K^{-1} f $$ \hspace{1cm} (2.2.16)
\[ \varepsilon_{\text{tot}} = Bu \]  
\[ \varepsilon_{\text{mech}} = \varepsilon_{\text{tot}} - \varepsilon^* \]  
\[ \sigma = D\varepsilon_{\text{mech}} \]

During the simulation, like the thermomechanical method, element activation and deactivation is used to activate a layer of elements representing several AM layers. Then the inherent strain is applied to the whole layer of elements at a time [22]. This in addition to avoiding the thermal simulation aids in the computational time.

The specific inherent strain is either experimentally determined or found with a high-fidelity thermomechanical FEM simulation on a small representative volume. Only normal components of the inherent strain tensor are considered as these are the dominant strains [12]. This inherent strain can be experimentally obtained [12] by simply applying an estimated strain onto a model using this method to predict a distortion on a part. This part can then be manufactured, and the distortion measured. The simulation can then be iterated with a different inherent strain until the model agrees with the experimental measurements. A root-finding numerical algorithm can be used to iterate through the simulation.

It has been shown that the laser path (and thus the temperature distribution) affects the effective inherent strain [12]. A major disadvantage of the inherent strain method is that calibration of the applied inherent strain may lead to accurate results for one geometry; however, it may predict inaccurate results with other geometries [3].
2.2.3 Incremental Plasticity

For completeness, a summary of incremental plasticity is given here, since it is plasticity that is responsible for the accumulation of residual stresses in part after the loading has been removed. This section is a review of reference [23]. The analogous rheological model commonly used to illustrate the concepts of plasticity is given in Figure 2.3.

Figure 2.3 - Plastic rheological analogy

The yield criterion provides a threshold for the onset of plasticity for a given loading and internal material parameters (history-dependent). The yield criterion is shown in Eq. (2.2.20), where $\sigma$ represents the stress tensor, and $\alpha$ are internal state parameters. Positive values for this function are inadmissible, values less than zero represent an elastic state, while a state at the boundary ($f = 0$) represents a plastic state of stress. With a perfectly plastic model (no hardening) the stresses in the stress tensor must be redistributed around the yield surface (represented by $f = 0$) if the loading is to be plastic.

$$f(\sigma, \alpha) \leq 0 \quad (2.2.20)$$

Typically, the von Mises criterion is used as the yield criteria. Using this the yield criteria can be written as shown in Eq. (2.2.21). Note that the yield stress $\sigma_0(\alpha)$ is not a constant, as it is loading history dependent due to material hardening. Since
any stress state where the yield function is greater than zero is not possible, this implies that any loading/unloading (i.e. a stress increment \(d\sigma\)) must stay on the surface, implying \(df \leq 0\), named the consistency equation, where a \(df < 0\) represents an unloading condition. For a perfectly plastic material (no hardening), this can be written as in Eq. (2.2.22), where \(\nabla f\) is defined as \(\nabla f^T = \begin{bmatrix} \frac{\delta f}{\delta \sigma_{xx}} & \cdots & \frac{\delta f}{\delta \tau_{xz}} \end{bmatrix}\).

\[
f(\sigma, \alpha) = \sigma_y(\sigma) - \sigma_0(\alpha)
\]

\[
\sigma_y = \sqrt{\frac{1}{2}(\sigma_x - \sigma_y)^2 + \frac{1}{2}(\sigma_y - \sigma_z)^2 + \frac{1}{2}(\sigma_z - \sigma_x)^2 + 3\tau_{xy}^2 + 3\tau_{yz}^2 + 3\tau_{zx}^2}
\]

\[
= \sqrt{\tau_{12}^2 + \tau_{13}^2 + \tau_{23}^2} = \sqrt{J_2}
\]

\[
df = \nabla f^T \cdot d\sigma \leq 0
\]

The increment in plasticity is assumed to be decomposed of an increment inelastic strain and an increment in plastic strain as shown in Eq. (2.2.23). An increase in plastic strain is then assumed to be normal to the gradient of the yield function (the associative rule) as shown in Eq. (2.2.24).

\[
d\varepsilon = d\varepsilon_e + d\varepsilon_p
\]

\[
d\varepsilon_p = d\lambda \cdot \nabla f
\]

Then the incremental stress-strain relationship is written as in Eq. (2.2.25).

\[
d\sigma = D^{ep} \cdot d\varepsilon
\]

\[
= D \cdot (d\varepsilon - d\varepsilon_p)
\]

\[
= D \cdot d\varepsilon - \lambda \cdot d\varepsilon_p
\]

\[
= D \cdot d\varepsilon - D \cdot d\lambda \cdot \nabla f
\]
Substituting Eq. (2.2.25) into the consistency equation and solving for \(d\lambda\) gives Eq. (2.2.26).

\[
d\lambda = \frac{\nabla f^T \cdot D \cdot d\varepsilon}{\nabla f^T \cdot D \cdot Vf}
\] (2.2.26)

Then substituting back into the incremental stress-strain relationship Eq. (2.2.24) and solving for \(D^{ep}\) gives Eq. (2.2.27), noting that \(D\) is a square matrix.

\[
D^{ep} = D - \frac{D \cdot \nabla f \cdot \nabla f^T \cdot D}{\nabla f^T \cdot D \cdot Vf}
\] (2.2.27)

To include hardening effects, a uniaxial stress-strain curve (piecewise linear) is used to calculate a hardening term \(H\). Since the stress-strain curve (typically obtained experimentally) is locally linear the hardening term can be calculated as shown in Eq. (2.2.28). Note, \(E_1\) and \(E_2\) are the slopes of the curve at two different points.

\[
ds_{\sigma} = E_2 d\varepsilon_{eq}
\]

\[
= E_2 \left( \frac{d\sigma}{E_1} + d\varepsilon_{p,eq} \right)
\]

\[
= \frac{E_2}{1 - E_2/E_1} \cdot d\varepsilon_{p,eq}
\]

\[
H = \frac{E_2}{1 - E_2/E_1}
\] (2.2.28)

For isotropic hardening the yield surface grows equally in all directions in the principle stress space, this implies \(\frac{d\sigma}{d\varepsilon_{p,eq}} = \frac{d\sigma_0}{d\varepsilon_{p,eq}} = H\). Thus, \(\sigma_0(\varepsilon_{p,eq}) = \int H \cdot d\varepsilon_{p,eq}\), and again \(H\) can easily be calculated from the stress-strain curve as shown in Eq. (2.2.28).
Thus, $\sigma_0(\alpha) = \sigma_0(\varepsilon_{p,eq})$, where the equivalent plastic strain is found similarly to the von Mises stress formulation. This also implies that $d\varepsilon_{p,eq} = d\lambda$ from the solution of $d\lambda$ in Eq. (2.2.26). Then the consistency equation can then be written as Eq. (2.2.29), where the second half assumes isotropic hardening. Thus, the incremental plasticity constitutive matrix is shown in Eq. (2.2.30) found using a similar derivation as above. Note that Eq. (2.2.30) is nonlinear, thus requires an iterative numerical algorithm to solve, typically a modified version of Newton-Raphson is used. Return algorithms are also used to ensure that the yield criterion is always satisfied (i.e. $f \leq 0$) when solving the equations numerically. In the finite element method, the tangent stiffness matrix is defined similarly as its linear version ($K = \int_\Omega B^T \cdot D \cdot B d\Omega$) however, with $D$ replaced by $D^{ep}$.

$$\frac{\delta f}{\delta \sigma} d\sigma - \frac{\delta \sigma_0}{\delta \alpha} d\alpha = \frac{\delta f}{\delta \sigma} d\sigma - H d\varepsilon_{p,eq} = 0$$

(2.2.29)

$$D^{ep}(\varepsilon_{p,eq}) = D - \frac{D \cdot \nabla f \cdot \nabla^T f \cdot D}{H + \nabla^T f \cdot D \cdot \nabla f}$$

(2.2.30)

### 2.3 The Generalized Method of Cells

This work makes use of NASA’s Micromechanics Analysis Code MAC) which implements the generalized method of Cells (GMC) MAC/GMC. A brief review is included here for background. The generalized method of cells uses a Repeating Unit Cell (RUC) to represent the microstructural domain of heterogeneous material [24]. This section provides a brief description of GMC as described in Aboudi [24]. Each repeating unit cell then contains sub-cells that are representative of distinct phases
or distinct materials in a composite, in this case, neighboring metal particles and trapped air in the metal powder during the sintering process. This is shown in Figure 2.4. The material properties and dimensions of each sub-cell can then be used to compute the effective homogenized macroscopic response (stress/strain, thermal/mechanical material properties) of the repeating unit cell [24]. These effective material properties are used as the constitutive model in the FE simulation, effectively cascading the microstructural response onto the macroscale.

The method of cells assumes the displacement of every subcell (denoted by \(\alpha, \beta, \gamma\)) is linear. For a doubly periodic subcell, this can be written as shown in Eq. (2.3.1). Note that the origin of the \(\tilde{x}_i\) frame is at the center of each subcell. This equation introduces several micro-variables \(\phi^{(\beta\gamma)}_i, \psi^{(\beta\gamma)}_i\) for every subcell. These can be solved for by enforcing continuous displacements at every subcell interface and with adjacent unit cells. This is done in an average sense, that is as shown in Eq. (2.3.2). The subcell strains and stresses can then be found from elastic theory. The
cell’s homogenized stress and strain is then the volume-averaged of every subcell. Note that the total strain (and therefor the stress) is constant in every subcell. Then subcell traction continuity is also enforced at the interfaces. This gives sufficient equations to solve for all the micro-variables, thus the subcell’s constitutive relationship can be found. Using the volume average strains the RUC’s homogenized constitutive relationship can be found as shown in Eq. (2.3.3), where \( b_{ij} \) is found from the micro-variables (by solving a system of equations) and the subcell’s geometry. An overbar represents an averaged quantity. Also, for a given macroscopic state, the state of all the subcells can be found using a localization matrix. For more details, the interested reader is referred to [24].

\[
\begin{align*}
\mathbf{b}^{(\rho \gamma)} & = \mathbf{w}^{(\rho \gamma)}(x) + \bar{\Phi}_i^{(\rho \gamma)} + \bar{\Psi}_i^{(\rho \gamma)}, \quad i = 1, 2, 3 \\
\int_{-\frac{L}{2}}^{\frac{L}{2}} \left( u_i^{(1\gamma)} \bigg|_{\frac{x_1}{2}}^{\frac{x_1}{2}} - u_i^{(2\gamma)} \bigg|_{\frac{x_1}{2}}^{\frac{x_1}{2}} \right) = 0 \\
\begin{bmatrix}
\bar{\sigma}_{11} \\
\bar{\sigma}_{22} \\
\bar{\sigma}_{33}
\end{bmatrix} & = \begin{bmatrix}
b_{11} & b_{21} & b_{31} \\
b_{12} & b_{22} & b_{32} \\
b_{13} & b_{23} & b_{33}
\end{bmatrix} \cdot \begin{bmatrix}
\bar{\varepsilon}_{11}
\end{bmatrix} \\
& & (2.3.3)
\end{align*}
\]

The generalized method of cells can incorporate the complex multi-scaled nonlinear material analysis and account for the coupling between thermal, strain, plasticity, and multi-phase effects. The generalized method of cells has the advantage that it can capture the phenomena more natively at the microscale, as opposed to other microstructural to macrostructural estimates, such as the Voigt approximation or the Reuss approximation [24, p. 105].
CHAPTER 3
AN EVOLVING POROSITY IN METAL SLS

This chapter describes the work conducted by Silva et al. in source [25]. This chapter investigates the effect of modeling the evolving material properties based on the predicted porosity in-tandem with the conventional time-dependent thermomechanical AM simulation. The goal of this chapter is not to present validated results, but to show that material evolution (specifically porosity) can have a significant effect on the large-scale residual stresses and distortions.

A regression model from source [14] was used to predict the material porosity from the applied laser characteristics, laser diameter, power, and velocity. The porosity is then used as input to predict the homogenized macroscale material properties. Properties of Inconel 625 were used as the pristine material properties. To aid in computational speed, these material properties were precomputed for a range of volume fractions (porosity) and a range of temperatures, using NASA's Micromechanics Analysis Code with the Generalized Method of Cells (MAC-GMC). This is used to compute the elastic modulus, Poisson’s ratio, thermal conductivity, specific heat capacity, coefficient of thermal expansion, and the plastic stress-strain response (pointwise incremental plasticity).

As a comparison, the simulation was conducted with material porosity kept at a constant, simulating a homogeneous material. A comparison with a homogenous model and the evolving model shows that the evolving porous model predicts larger distortions with greater residual stresses.
3.1 Implementation

3.1.1 Thermomechanical Set-up

Details of the thermomechanical method are given in Section 2.2 AM Finite Element Simulation on page 9. The nonlinearity from the temperature-dependent material properties, the temperature-dependent plasticity model, radiation effects in the thermal model, and the changing materials from powder to solid require an iterative solution at every time step. Modeling of liquid phases, the latent heat of a solid to liquid phase change, and any creep effects are neglected. The open-source FE software CalculiX was used to perform the simulations. Access to the source code permitted a highly configurable simulation.

External thermal loading was accomplished through a user-defined subroutine in CalculiX. This allows for controlled laser properties such as its path, intensity, and applied heat flux distribution. It has been shown that the laser scanning pattern influences the residual stresses of the final part [26]. Thus, the open-source 3D slicer software, Slic3r, was used to generate g-code describing the laser path of the part. The laser path produced by Slic3r is intended for a fused deposition modeling (FDM) 3D printing process. However, it was deemed the path produced was appropriate for the intent of this application since the software is highly configurable and can be set-up with various laser scanning strategies.

A script was written to parse the g-code. It estimates the time required to perform each g-code operation from the laser speed. The script then interpolates the position of the laser at regular time intervals to populate a tabulated file. This file
was then read by the user-defined subroutine (DFLUX) during the runtime in CalciX.

The user subroutine reads the file and applies a Gaussian distributed volumetric heat flux $Q$ as computed by Eq. (3.1.1) from Ref. [27] to the corresponding integration points, at the current simulation time, simulating the laser energy input [28]. Note that, the expression $\pi(1 - \exp(K_z s))$ is a unitless constant in this model at approximately -59.959. The variables $x$ and $y$ are the distances from the beam’s center in the respective directions to the integration point, and $z$ is the distance from the top surface to the integration point. The laser center is moved in steps, as described by the tabulated file. The file must be only read once on the first call to the subroutine. This was implemented using the SAVE keyword in Fortran to keep the tabulated data in memory between subroutine calls.

$$Q(x, y, z) = \frac{k K_z \eta P}{\pi (1 - \exp(K_z s))} \exp(-kr^2 - K_z z)$$

$$r^2 = x^2 + y^2$$

$$K_z = 3/s$$

$$k = 3/r_0^2$$

Element activation simulates the addition of material deposited at every layer. A deactivated element is not computed as part of the solver pass. This method is described in Section 2.2 - AM Finite Element Simulation on page 9. Each layer of elements represents several layers of the AM process, as the thickness of an FE element is substantially larger than the thickness of a powder layer. The element thickness for this work was chosen at 1 mm for ease of computation and proof of concept. Justification of this approximation is discussed in Section 2.2 - AM Finite
Element Simulation on page 9. A new layer of elements is added after the laser has finished passing through the previous layer. During the activation, since the layer below the newly added elements has already been strained, an artificial strain is added to the newly activated elements. This ensures that the newly added, yet deformed element is stress-free.

Another python script performs the sectioning of a predetermined FE mesh into sets of element layers during preprocessing. After reading the input mesh file, the script categorizes each element into a layer and then appends the element list to the input file. Since the categorizing of the elements is not dependent on previous steps, the script was coded to execute in parallel. This was accomplished by splitting the elements into partitions and then categorizing each partition of elements on an independent thread. Finally, the categorized elements from each thread are merged into a master list to be written to the output file. In the input deck, the *STEP card was used in with the *MODEL CHANGE card to perform the addition of the layers, in CalculiX. Thus, the input deck is read once, while the laser information and material data (discussed in the next section) are read at every iteration. Figure 3.1 shows the overall flowchart of the implementation.
At a given time step, each layer of elements contains sintered and powdered material. The distinction is made by the material properties of the integration point. A layer is initialized with powered material properties. During runtime sintered material properties are assigned once the laser has passed over the integration point. This is the hybrid method as discussed in Section 2.2 - AM Finite Element Simulation on page 9.

The mechanical simulation uses incremental pointwise plasticity as the material constitutive law, assuming isotropic hardening. Here, creep effects were neglected. This was implemented within a user material subroutine by a call to the incremental plasticity subroutine native to CalculiX. The plastic material properties used along with the rest of the material properties are discussed in the next section.
3.1.2 Porosity and Material Properties

Internal, solution-dependent state variables are used to track the physical state of the material microstructure. Solution-dependent state variables in CalculiX exist for each integration point in the model. Thus, a single element can have different material properties at each of the integration points in a simulation. One solution-dependent state variable is used to store the currently predicted porosity of the material and another to differentiate powder from a sintered material. For visualization purposes, a third was used to store the current elastic modulus of the material.

CalculiX sources were modified to allow for a thermal and structural user material capable of altering material properties as determined by interpolating the material properties in a lookup table. A predetermined table of material properties (discussed in the next section) were tabulated the material constitutive relationship (elastic modulus, Poisson's ratio, and plastic strain/stress pairs), thermal conductivity, specific heat, and thermal expansion coefficients as a function of temperature, material state (powder or solid) and volume fraction of air to solid (porosity) of the sintered material. How this precomputed table was populated is discussed shortly. This was accomplished by modifying the “materialdata_me.f” and “materialdata_th.f” subroutines in CalculiX to accept material properties from a third Fortran subroutine. This subroutine read the properties from the tabulated file and perform a 2D interpolation of the table (once for temperature and again for porosity). If the temperature or porosity being requested is out of bounds from the
values specified in the table, the closest temperature or porosity in the table is used (no extrapolations).

The evolution of the porosity of the sintered material $\varepsilon$ is predicted during runtime from Eq. (3.1.2) obtained from Ref. [14], where $\varepsilon_0$ is the initial porosity of the powder (assumed here to be 0.3), and $\varepsilon_{\text{min}}$ is the minimum attainable porosity (assumed here to be 0.0001). The assumptions for the initial and minimum values of porosity are preliminary, used to establish the method. In the future, these properties will be measured. Note that, the densification coefficient $K$ is a function of powder diameter, distribution, and material properties. Here, it was assumed to be constant at $18.97 \text{ mm}^3/\text{kJ}$, as a preliminary value from Ref. [14].

The specific energy input $\psi$ is calculated using the laser power $P_z$, laser linear velocity $v$, and the laser beam area, characterized by $l$ and $w$, as shown in Eq. (3.1.4). Here, the product $lw$ is taken as $\pi r_0^2$. The volume fraction $V_f$ of the sintered material is taken as $V_f = 1 - \varepsilon$ that is $V_f = 1$ represents 100% solid and $V_f = 0$ represents 100% air. The laser penetration was assumed to exponentially decay into the material as shown in Eq. (3.1.5) [29], $K_z$ is as defined in Eq. (3.1.1). It was also assumed that the estimated porosity $\varepsilon$ for an already sintered layer (the layers below the topmost layer) can be used as the initial porosity $\varepsilon_0$ in Eq. (3.1.3) for subsequent passes of the laser, at each time step. Thus, the porosity of all the layers in the model change during the simulation.

$$\ln(1 - D) = -K\psi$$

(3.1.2)
\[ D = \frac{\varepsilon - \varepsilon_0}{\varepsilon_{\text{min}} - \varepsilon_0} \]  \hspace{1cm} (3.1.3)

\[ \psi = \frac{P}{vlw} \]  \hspace{1cm} (3.1.4)

\[ P_z = \eta P \exp(-K_z z) \]  \hspace{1cm} (3.1.5)

Figure 3.2 shows a simplified illustration of the evolving porosity as the laser passes over the powder for the SLS process. Note that Eq. (3.1.2) is the empirical approximation to the solution to the underlying differential equation (3.1.6), where \( \kappa \) (kappa) is the sintering rate constant. The sintering rate constant is a function of the laser specific energy input \( \psi \). Note that Eq. (3.1.2) predicts the final porosity after a laser pass (no dependence on time), while Eq. (3.1.6) is time-dependent. Both equations have been shown to be a reasonable representation to model the real porosity evolution [14].

![Figure 3.2 - Changing porosity](image)

\[ \dot{\varepsilon} = -\kappa \varepsilon \]  \hspace{1cm} (3.1.6)

The macroscopic homogenized material properties were precomputed using NASA’s Micromechanical Analysis Code – Generalized Method of Cells (MAC-GMC). A triply periodic open-cell RUC was chosen for the representative arrangement of the partially sintered material, as shown in Figure 3.3. In the figure, a dark blue rectangular subcell represents a solid material, and a translucent blue represents air.
Note that this RUC is assumed to be isotropic, thus no need to store any anisotropic material properties.

GMC calculates the material properties in an average sense [24]. That is, the stress carried by the RUC in a direction is evenly carried across the subcells. Stress concentrations due to corners are not resolved. Thus, a spherical microstructure would effectively be represented as a rectangular cuboid subcell in GMC.

![Triply periodic open-cell RUC](image)

Figure 3.3 - Triply periodic open-cell RUC

Properties of solid Inconel 625 were used for the solid material, tabulated in Table 3.1. The mechanical properties of air (voids due to porosity) were estimated as 7 orders of magnitude smaller than the mechanical properties of the solid material. The computed sintered material properties are plotted in Figure 3.4 with respect to temperature. The figure shows that the yield strength and the stress for a given plastic strain decrease as the volume fraction decreases. A similar decrease in those properties can be seen as the temperature increases. All the material properties computed by MAC-GMC are tabulated in Table A.1 in the appendix.
Table 3.1 - Solid Inconel 625 properties used as a function of temperature

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>20</th>
<th>200</th>
<th>400</th>
<th>700</th>
<th>900</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ GPa</td>
<td>204</td>
<td>193</td>
<td>181</td>
<td>161</td>
<td>145</td>
</tr>
<tr>
<td>$v$</td>
<td>0.312</td>
<td>0.303</td>
<td>0.301</td>
<td>0.309</td>
<td>0.284</td>
</tr>
<tr>
<td>$\rho$ kg/m$^3$</td>
<td>2700</td>
<td>2700</td>
<td>2700</td>
<td>2700</td>
<td>2700</td>
</tr>
<tr>
<td>$k$ W/m°C</td>
<td>9.8</td>
<td>12.5</td>
<td>15.3</td>
<td>19.8</td>
<td>23.3</td>
</tr>
<tr>
<td>$c$ J/kg°C</td>
<td>410</td>
<td>456</td>
<td>511</td>
<td>600</td>
<td>630</td>
</tr>
<tr>
<td>$a = \frac{1}{c}$</td>
<td>12.6E-6</td>
<td>13.1E-6</td>
<td>13.6E-6</td>
<td>15.0E-6</td>
<td>1.60E-05</td>
</tr>
<tr>
<td>$S_1$ MPa</td>
<td>618</td>
<td>610</td>
<td>491</td>
<td>501</td>
<td>195</td>
</tr>
<tr>
<td>$S_2$ MPa</td>
<td>727</td>
<td>736</td>
<td>574</td>
<td>689</td>
<td>190</td>
</tr>
<tr>
<td>$S_3$ MPa</td>
<td>803</td>
<td>876</td>
<td>625</td>
<td>721</td>
<td>167</td>
</tr>
<tr>
<td>$S_4$ MPa</td>
<td>0.036</td>
<td>0.0782</td>
<td>0.0670</td>
<td>0.1024</td>
<td>0.0535</td>
</tr>
<tr>
<td>$S_5$ MPa</td>
<td>0.092</td>
<td>0.2469</td>
<td>0.1139</td>
<td>0.1584</td>
<td>0.2225</td>
</tr>
<tr>
<td>$S_6$ MPa</td>
<td>0.204</td>
<td>0.3030</td>
<td>0.2387</td>
<td>0.4685</td>
<td>0.4908</td>
</tr>
</tbody>
</table>

Figure 3.4 - Sintered material homogenized macroscopic stress-strain curve

---

1 Note: The density values used in Table 3.1 are erroneous and do not represent the density of solid Inconel 625. Density of Inconel 625 is approximately 8440 kg/m$^3$. However, the density would only directly affect the thermal solution from a higher thermal mass, leading to lower peak temperatures for a given laser power. In addition, the material would cool more slowly once the laser has passed over. If a greater laser power is given to reach melt temperatures, the thermal gradient ahead of the laser is expected to change only slightly, yet the gradient behind the laser should reduce (due to a slower cooling). This likely will produce lower residual stress values.
The powdered material properties were set equal to the sintered material properties, except for the modulus of elasticity, at a given temperature and volume fraction. The modulus was estimated to be an order of magnitude smaller than that of the sintered material for a given volume fraction at room temperature. As the temperature of the powder increases, the modulus of the powder was set to linearly increase, until 700 °C, at which the modulus of the powder was made the same to that of the sintered material, at a given volume fraction. This was done to avoid strong C1 discontinuities in material properties and to avoid the strain-softening of the solid Inconel at high strains and temperatures, aiding in numerical convergence. It was assumed that this slow change in powder material properties to sintered material modulus would not adversely affect the results since the spatial gradient of temperature is extremely high near the laser. Thus, the temperature of the powder material is close to room temperature a small distance away from the laser, and at room temperature, the powder material has a low modulus. These powder material estimates are preliminary and used to establish the methodology. In the future, these properties can be measured and the sensitivity of the results to these properties investigated. Figure 3.5 shows how this modulus changes with temperature and volume fraction. The solid line represents the linear interpolation used during runtime for temperatures not tabulated.
3.2 Results

3.2.1 Boundary Conditions

The geometry used, along with the bed and mesh is shown in Figure 3.6. It is customary in the literature that the cartesian coordinate system is oriented such that the positive z-direction is the build direction. The dimensions of the printed part are 12 mm by 12 mm by 3 mm, while the bed is 9 mm by 1.5 mm by 18 mm. The mesh used linear 8-noded hexahedral elements. The bottom of the bed was set to a constant temperature of 70 °C, with no displacements. The elements in the mesh were approximately 1mm on each side. This allowed the heat flux from the laser beam (with a characteristic radius of 2.5 mm) to be applied to several integration points during a time step. The layer thickness was taken as 1mm; thus, one element was used through the thickness of a layer.

To avoid the computational cost of modeling the conductive heat flux into a physical region of excess powder, the heat carried away by the powder surrounding the part was modeled as an effective convective heat transfer boundary condition, to
avoid the computational cost of modeling the conductive heat flux into a physical region of excess powder. Here it was assumed that the unmodeled powder changed temperature from its maximum at the surface of the part to its steady-state, far-field temperature within 10 mm. This gives an effective convective heat transfer coefficient of $h_{\text{eff, powder}} = \frac{k}{L} = 362 \ \frac{W}{m^2K}$, with an estimated conductive coefficient of $k_{\text{powder}} = 3.62 \ \frac{W}{mk}$. The powder thermal conductive coefficient $k_{\text{powder}}$ was estimated from MAC-GMC with a volume fraction of 66%. A changing convective boundary condition was applied to the current topmost surface with a convection coefficient of $h_{\text{air}} = 100 \ \frac{W}{m^2K}$. A radiation boundary condition was also applied to the current topmost surface. The effective absorption for the radiation was assumed to be 50%. The ambient temperature of the air was assumed to be 70 °C, as well as the bed preheat temperature. The bed preheat temperature was also set to 70 °C. Figure 3.7 illustrates these boundary conditions.
Figure 3.6 - Geometry and mesh used, labeled points corresponding to Table 3.3

Figure 3.7 - Boundary conditions applied

Figure 3.8 shows the scanning pattern used. The laser path was discretized into time steps of 0.05 seconds for the FE simulation, as shown. The same path was used for all the layers. At a laser speed of 100 mm/s (as shown in Table 3.2), a layer was scanned in about 5 seconds. With a dwell time (time between layers) of 1 second
per layer, and 12 layers in the model the total simulated print time is 72 seconds. A dwell time of a second was enough to cool the part to ambient temperature in the simulation. Values used for the laser properties for Eq. (3.1.1) are listed in Table 3.2, adapted from Jayanath [21].

Table 3.2 - Laser parameters

<table>
<thead>
<tr>
<th>η</th>
<th>r₀ mm</th>
<th>s mm</th>
<th>P W</th>
<th>v mm/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.5</td>
<td>1</td>
<td>2.250</td>
<td>100</td>
</tr>
</tbody>
</table>

3.2.2 Evolving Porosity

Post-processing was accomplished with the open-source software ParaView. Figure 3.9 shows the results of the simulation at the midpoint of part completion. Figure 3.10 shows the results at the end process after cooling. Corresponding graphs are shown at the same scale.
c) Temperature, °C

d) $S_{yy}$, MPa

e) Porosity

f) $S_{zz}$, MPa

Figure 3.9 - Results at $t = 31.5s$, evolving porosity, no deformation shown
Figure 3.10 - Results at the end of print, $t = 72s$, deformation magnified by 20x, evolving porosity

Figure 3.11 shows the estimated porosity evolution at a specific node in the model. It shows that the predicted porosity decays from its initial value to its minimum value in approximately a second. The abrupt change in slope in the porosity vs. time plot corresponds with the position of the laser relative to the point in the material.

Figure 3.11 - Estimated porosity vs. time, at node point C

The stresses in Figure 3.9 and Figure 3.10 on page 42, subplots b, d, and f show that there are primarily compressive residual stresses on the outer surfaces while...
tensile towards the center. In addition, there are stress concentrations where the part meets the bed, as expected. Also, the residual stresses in the z-direction are the greatest compared to the other two orthogonal stresses.

The porosity plot in Figure 3.10 subplot e shows that there is still some porosity at the top surface. This could be due to the laser having passed over the top surface only once. The temperature plot in Figure 3.9 subplot c, shows that the temperature is greater inside the part than at the top surface. This temperature gradient may be explained by the convective and radiative boundary conditions on the surface combined with the volumetric heat flux. The temperature dependence of the elastic modulus can also be seen in Figure 3.9 subplot a.

The deformation in Figure 3.10, shows that the part swells at the center, with a small amount of deformation towards the top horizontal edges. This behavior also is seen during the simulation of the process, not just after part completion. Also, the top four corners of the part tend to point in the positive z-direction.

3.2.3 Constant Porosity

A second model with a constant porosity of 10% was simulated for comparison. All other parameters including the mesh were kept the same as the previous evolving porosity simulation. Corresponding graphs are shown at the same scale as the previous simulation. The material properties were taken as only dependent on temperature and material state (powder or sintered). Figure 3.12 and Figure 3.13 shows the results of this simulation.
Figure 3.12 - Results at $t = 31.5s$, constant porosity, no deformation shown
The elastic modulus plot in Figure 3.12 subplot a shows that compared to Figure 3.10 subplot a, the change in the material's modulus from sintered to powder is more severe. This can adversely impact numerical convergence.

Figure 3.12 and Figure 3.13 show a similar trend in residual stresses at the end of the simulation and similar temperatures during the printing of the part. However, comparing subplots f (stresses in the z-direction), the evolving material model tends to show greater stresses in magnitude. Table 3.3 shows a comparison of residual stresses and distortions, at surface points A and B labeled on the geometry used in Figure 3.6 on page 40. The table shows that the differences in the models can be significant and that the evolving porosity model does not always give greater residual stresses or distortions.
Table 3.3 - Residual stress and distortion comparison

<table>
<thead>
<tr>
<th></th>
<th>Point A</th>
<th></th>
<th>Point B</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Constant Porosity</td>
<td>Evolving Porosity</td>
<td>% increase in magnitude</td>
<td>Constant Porosity</td>
</tr>
<tr>
<td>$S_{xx}$ MPa</td>
<td>-77</td>
<td>-55</td>
<td>-29%</td>
<td>-450</td>
</tr>
<tr>
<td>$S_{yy}$ MPa</td>
<td>-60</td>
<td>-16</td>
<td>-73%</td>
<td>-11</td>
</tr>
<tr>
<td>$S_{zz}$ MPa</td>
<td>-210</td>
<td>-246</td>
<td>17%</td>
<td>-38</td>
</tr>
<tr>
<td>$U_{xx}$ mm</td>
<td>-.00894</td>
<td>-.016807</td>
<td>88%</td>
<td>.001025</td>
</tr>
<tr>
<td>$U_{yy}$ mm</td>
<td>.000809</td>
<td>.006235</td>
<td>671%</td>
<td>.000174</td>
</tr>
<tr>
<td>$U_{zz}$ mm</td>
<td>-.002287</td>
<td>-.013365</td>
<td>484%</td>
<td>.002095</td>
</tr>
</tbody>
</table>

3.3 Discussion and Conclusion

Figure 3.14 shows a comparison of the von Mises stress at the final print time, after cooldown. The figure shows that modeling an evolving porosity results in higher overall residual stresses with larger deformations. The models show a similar stress distribution trend, with an evolving model having slightly higher magnitudes. These observations can also be seen comparing subplots b, d, and f of Figure 3.10 and Figure 3.13. The equivalent plastic strain in the models is compared in Figure 3.15; again, it shows a similar distribution, with higher magnitudes. Both models used the same laser parameters, boundary conditions, and mesh.

Figure 3.14 - Von Mises stress, at t=72s, deformation magnified by 20x
The peak positive normal stress in the z-direction was calculated at 230 MPa for the evolving porosity model, while the constant porosity model showed a peak positive stress of 145 MPa. The evolving model had a peak displacement of 0.027 mm while the constant model had a peak displacement of 0.016 mm.

This increase in deformation and residual stresses is likely due to the regions with high porosity having to carry the same load (due to thermal strains and constraints by the surrounding material) yet with a lower microscopic cross-sectional area. This reduced cross-sectional area can be seen by comparing the microscopic architectures in Figure 3.3. The higher applied stresses may result in higher plastic strains, leading to higher residual stresses at part completion and higher part deformation.

These results show that including microscale phenomena, specifically the porosity, may lead to significant changes in the predicted macroscopic fields. Although including microscale phenomena adds more complexity (and slightly more computational time), this addition may lead to more accurate results. Thus, it may be important to model this and other microscale phenomena, such as grain
orientation. This work lays the foundation for including anisotropic thermal and mechanical material properties as well as the addition of material microstructure evolution and other microstructural effects.

Note that no experimental validation has been conducted on the presented work. This includes validation of the porosity model used in addition to the predictions made by the simulation. Furthermore, it is expected that the mesh used here is not able to resolve the fine details in the solution.

This work used the densification coefficient $\kappa$, coupled to a time-dependent thermal history, to yield an evolving volume fraction. The volume fraction is used with GMC to provide predictions of temperature and volume fraction dependent stress-strain and plasticity at the micro-scale. These material properties, used in a macro-scale finite element model, compute evolving volume fraction dependent residual stresses. In short, evolving volume fractions impact porosity and consequently impact the residual stresses and deformation.
CHAPTER 4

GEOMETRY EFFECTS WITH INHERENT STRAIN

Due to the limitations of the full thermomechanical method, the inherent strain method was used here to obtain results in a practicable time frame, at the cost of some approximations in the solution. Despite these approximations (as described in Section 2.2.2 - The Inherent Strain Method on page 18) the advantage of fast computational times may outweigh the disadvantages, making it possible to obtain the final residual stresses and distortions of relatively large structures. For simple models (such as the cantilever beam with supports) the inherent strain method has shown to produce satisfactory predictions comparing to experimental results [12]. Here the inherent strain method along with a dense mesh is used to study the effects of geometry on the overall distortion and stress on the parts, despite Bugatti et al. [3] suggesting that the ISM can lead to inaccurate results. Some of these geometries and associated ISM models are then compared against the full thermomechanical method not only for accuracy but for similar trends. Again, it is not the goal of this chapter to produce experimentally validated results.

4.1 Methodology and Implementation

The inherent strain applied was chosen as the volume-averaged plastic strain as computed with the thermomechanical model used in Chapter 3 - An Evolving Porosity. In addition, since each element layer represents many AM layers, it was assumed that the inherent strain was the same in the build plane (the x-y plane)
since, during manufacturing, the laser scan pattern is rotated at every layer to avoid the accumulation of stress [12]. Furthermore, since each AM layer is thin in the build-direction (the z-direction), it was assumed that the inherent strain in this direction was zero. Thus, the applied inherent strain for these models is: $\varepsilon^* = [\varepsilon_{xx} \; \varepsilon_{yy} \; \varepsilon_{zz} \; \varepsilon_{xy} \; \varepsilon_{xz} \; \varepsilon_{yz}]^T = [-0.004 \; -0.004 \; 0 \; 0 \; 0 \; 0]^T$. These values are approximately the same values as calibrated numerically and from experiments in Ref. [3]. Note that these strains are a strong function of processing parameters [3].

To implement this method with CalculiX, a few minor modifications to its source code were needed. This modification allowed the inherent strains to be applied at a set of elements. Unmodified, CalculiX only allows the specification of one initial strain at one integration point in one element at a time, impracticable for this application. Two steps in CalculiX were required to simulate and load the layer. This is because adding a set of elements (a layer) requires artificially adding strains to the newly added layer since the layer before is already strained, thus the new elements are deformed, yet with no stress. A second step then loads the whole layer at a time with the inherent strain. Section 2.2.2 - The Inherent Strain Method on page 18 reviews the method.

### 4.2 Geometry and Validation

A cube 10 mm to a side with a blind hole 5 mm deep was chosen as the geometry due to its simplicity and likelihood of demonstrating significant residual stresses. The diameter of the hole was varied from 0 mm (no hole) to 8 mm, producing nine
specimens. Quadratic 20-noded brick elements with a global size of 0.5 mm on a side were used. Figure 4.1 shows the mesh used for the geometry with a 6 mm diameter hole. The bottom nodes were constrained with no displacements (surface denoted by dashed lines in the figure). The inherent strain was applied at every layer, each layer being 0.5 mm thick (one quadratic element thick).

![Figure 4.1 - Geometry of 10 mm cube, Ø 5 mm, 5 mm blind hole](image)

For stress distribution validation predicted by the inherent strain model, a coarsely meshed thermomechanical model was simulated. Material properties of Inconel 625 at room temperature and fully dense were used for the inherent strain model. The geometry and boundary conditions in Figure 4.1 were used for the inherent strain model. Similar boundary conditions and laser scan pattern as in Chapter 3 were used for the thermomechanical model.

Figure 4.2 shows the von Mises stress at the mid-cross-section of the part. Note that all three plots have the same deformation magnification, but the right plot (thermomechanical simulation) has a different scale on stress. The figure shows similar (although not exact) deformations between the two methods, with similar overall trends in stress distribution. A major difference in deformation being the thin
walls surrounding the hole. The inherent strain method predicts wrapping here while the thermomechanical method does not. The thermomechanical method used also predicts smaller stress magnitudes. In addition, the inherent strain method shows a smoother contour of stress compared to the thermomechanical model. This, however, is likely explained by the coarse mesh used for the thermomechanical model. The inherent strain method also produced overall tensile stress at the outer surfaces, while compressive stresses towards the center of the part, as expected from a literature review. Despite these differences, the distribution of stress and displacement are similar between the two models. Thus, it is assumed that the inherent strain model is capable of producing accurate trends in stress distribution and deformation with respect to the geometry.

![Figure 4.2 - Inherent Strain and thermomechanical comparison, 8 mm diameter, deformation magnified 20x](image)
This inherent strain was then applied to a finely meshed (≈ 0.5 mm cube linear hexahedral elements) supported cantilever 100 mm long, 3 mm thick, 10 mm wide beam model. Material properties of room temperature Inconel 625 used. Supports are 10 mm long (in the z-direction). Stress and deformation are shown in Figure 4.3. The tip displacement is at 4.7 mm. Buchbinder et al. [30] obtain tip displacements in the range 1 – 8 mm for a 50 mm long and 0.5 – 5 mm thick beam specimens made from ALSi10Mg aluminum alloy. Different tip displacements were obtained due to different preheat temperatures. Liang et al. [22] obtained a displacement of 0.58 mm with a 76.6 mm long beam made from Inconel 718. Clearly, the tip displacement is highly dependent on processing parameters (and material), thus such a comparison may not be adequate. However, the overall shape, order of magnitude of deformation, and stress distribution agree with the literature [31]. A calibration with experimental testing is needed to obtain more accurate results.
4.3 Results

The hole diameter of the nine specimens are shown in Table 4.1 along with the volume-averaged von Mises stress (i.e. $S_{avg,vm} = \frac{1}{V} \int S_{vm} dV$). Volume averaged quantities were chosen for comparison since each specimen has different volumes. Plots showing the von Mises stress distribution is shown in Figure 4.4. All plots are shown at the same scale.

**Table 4.1 - Inherent strain, geometrical feature results**

<table>
<thead>
<tr>
<th>Hole diameter (mm)</th>
<th>Volume (mm$^3$)</th>
<th>Max displacement (mm)</th>
<th>Max von Mises (MPa)</th>
<th>Volume averaged von Mises (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 (no hole)</td>
<td>1000</td>
<td>0.081734</td>
<td>768.83</td>
<td>452.59</td>
</tr>
<tr>
<td>1</td>
<td>996.14</td>
<td>0.081363</td>
<td>773.39</td>
<td>454.05</td>
</tr>
<tr>
<td>2</td>
<td>984.35</td>
<td>0.08041</td>
<td>783.29</td>
<td>455.51</td>
</tr>
<tr>
<td>3</td>
<td>964.78</td>
<td>0.078917</td>
<td>793.19</td>
<td>456.21</td>
</tr>
<tr>
<td>4</td>
<td>937.27</td>
<td>0.076971</td>
<td>800.11</td>
<td>451.98</td>
</tr>
<tr>
<td>5</td>
<td>901.98</td>
<td>0.074356</td>
<td>801.15</td>
<td>443.58</td>
</tr>
<tr>
<td>6</td>
<td>858.83</td>
<td>0.071471</td>
<td>798.48</td>
<td>436.18</td>
</tr>
<tr>
<td>7</td>
<td>807.70</td>
<td>0.068305</td>
<td>797.39</td>
<td>430.85</td>
</tr>
<tr>
<td>8</td>
<td>748.8</td>
<td>0.065311</td>
<td>799.81</td>
<td>429.65</td>
</tr>
</tbody>
</table>
Figure 4.4 - Von Mises stress, various hole diameters, deformation magnified 20x
The plots in Figure 4.4 show that the hole acts to reduce the stress near the bottom surface of the hole. This is presumably due to the traction free surface at the bottom of the hole. Figure 4.5 shows how the output results (volume-averaged von Mises stress, maximum von Mises stress, and maximum displacement) vary as a function of the diameter. Note that the vertical axes do not start at zero. As shown in plots a and b, of Figure 4.4, the stress distribution around the small-diameter hole is relatively unaffected by the presence of the hole. This may explain the initial increase in the averaged stress in Figure 4.5, as the average stress would increase due to the absence of material (small stress not present due to the absent material that would otherwise decrease the average). The maximum stress observed occurred at the bottom where the clamped boundary condition was applied, as expected.

The maximum displacement occurred at the four outer vertical edges of the cube for all the specimens. It may be reasoned that the maximum displacement decreases as the diameter increases due to the negative inherent strain applied in equal magnitudes in the $x$ and $y$ direction at a whole layer, thus contracting the
circular walls inward. This is different from the thermomechanical model where the load is applied only where the laser is currently located.

### 4.4 Discussion and Conclusion

The results presented in Figure 4.5 show that the diameter of the blind hole affects the volume-averaged von Mises stress as well as the maximum displacement and stress. Note that maximum stress can be dependent on stress concentrations which are in turn dependent on geometry. However, the corner radii of all the corresponding corners in the model are kept constant, at an ideal 90 degrees. It is also important to note that these results may be skewed due to boundary effects, as the hole approaches the edge of the specimen with larger diameters. These results support the hypothesis that the macroscale geometry influences the residual fields.
CHAPTER 5

GEOMETRY EFFECTS WITH THERMOMECHANICAL FEA

To further assess the effects of geometry on the solution, a slightly more complex geometry was investigated using the thermomechanical model developed in Chapter 3. Investigating more geometrical variables may prove beneficial to evaluate the geometry effects. Using the thermomechanical model would also make possible to circumvent some of the disadvantages of the inherent strain method (discussed in Section 2.2.2 - The Inherent Strain Method). This required a few modifications to the implementation used in Chapter 3 since significant numerical convergence problems were encountered when applying the developed model to larger geometries.

5.1 Methodology and Implementation

Modifications to the thermomechanical model include incorporating a viscoplasticity material constitutive model. Viscoplasticity aids in numerical convergence by allowing the stress state to exceed the yield surface, this being a less restrictive constraint for the solver. This is possible since the material response is time-dependent, thus the response (stress) of the material is higher at higher strain rates. In contrast, incremental plasticity requires the stress state to lay on the yield surface when yielding (steady-state). Implementing this material model in CalculiX with the user subroutines described in Chapter 3 simply required calling the built-in viscoplasticity model. The viscoplasticity model used is the power creep law as shown in Eq. (5.1.1), where $A, n, m$ are temperature dependent material properties, $\sigma$ is von
Mises stress and $\dot{\varepsilon}$ is the steady state strain rate, such that the total strain is $\varepsilon_{total} = \varepsilon_{elastic} + \varepsilon_{inelastic} + \dot{\varepsilon} t$.

$$\dot{\varepsilon} = A\sigma^n t^m$$ (5.1.1)

A limitation with the implementation is that constant viscoplasticity material properties where used. Typically, the viscous properties of materials are highly temperature dependent. However, it may be reasoned that since the temperature quickly increases (within milliseconds in the models) from room temperature to melting temperature and back to room temperature (within approximately a second in the simulations), and because strains near melting temperatures have less impact on stress than those at lower temperatures, viscoplasticity properties at high temperature may not be as important as those at lower temperatures. Having no available method to validate the temperature-dependent viscoelastic material properties in the subject material, it is assumed that these coefficients are constant.

Another modification to the implementation described in Chapter 3 includes using the porosity model shown in Eq. (3.1.6) (repeated below in Eq. (5.1.2) for reading convenience). Note that $\dot{\varepsilon}$ in Eq. (5.1.2) refers to porosity rate opposed to strain rate in Eq. (5.1.1). The differential was solved numerically in the DFLUX subroutine in CalculiX using forward Euler, since $\kappa$ is a function of the laser specific power. Regression coefficients from Ref. [14] where used.

$$\dot{\varepsilon} = -\kappa \varepsilon$$ (5.1.2)

A final major modification included the ability to apply a different laser pattern at every layer. This is necessary if the cross-sectional geometry changes at every
layer. This was accomplished by storing laser position in a 3D table for look-up at runtime.

Linear 8-node hexahedral elements were used with approximately 1 mm in the x-direction and y-direction dimensions while 0.5 mm was used in the z-direction. This was done to add two layers of elements at every additional AM simulated layer while keeping the thickness of the AM layer at 1 mm. This is different from what was done in Chapter 3, where only one layer of elements was added at a time. Preliminary mesh convergence studies (not presented in this document) showed that adding two layers of elements at a time provided more refined results that were similar to the literature [32].

As a preliminary validation, a cantilevered beam geometry was simulated. Figure 5.1 shows the deformation and stress of the specimen before (translucent) and after removing it from its base (relieving some stress). The deformation shown is consistent with the literature. The tip displacement for this 100 mm long and 3 mm thick beam is 0.52 mm. Again comparing to Liang et al. in reference [22], 0.58 mm was measured experimentally from a 76.6 mm long beam (thickness dimension not given). Note that this displacement is also highly dependent on processing parameters (laser scan pattern, preheat temperature, etc.). Thus, this comparison might not be adequate, but it shows that the simulation has a reasonable solution.

![Figure 5.1 - Preliminary cantilevered beam simulation](image)
5.2 Results

A nozzle-shaped geometry with three geometric parameters to be varied was chosen to represent a small aerospace structure, shown in Figure 5.2. This geometry is simple enough to model with few parameters yet complicated enough to produce interesting results that can be experimentally validated in later work.

Latin hypercube sampling (LHS) was used to obtain a distribution of the geometric parameters within the design space while utilizing only a modest number of finite element runs. Latin hypercube sampling has the advantage that it can lead to faster converged results with fewer sample points compared to the Monte Carlo method [33]. This is done by dividing the normal cumulative function into $n$ ranges and sampling each range, where $n$ is the number of desired trials/experiments. Then for a given variable, it is assigned one of the $n$ ranges for every trial, unique at every trial. The value of that variable is then obtained from the inverse cumulative function using the value from its assigned range. This assignment of a range to a variable can be random or it can be optimized to maximize the Euclidean distance between each
of the trials in the sample space. This was done here using libraries in the R programming environment.

Thirty sample points were chosen; specimens whose solution converged (24 of the 30) are shown in Figure 5.3 and Table 5.1 on page 64. A representative mesh used along with its laser 3D scan pattern is shown in Figure 5.4. The laser pattern is rotated by approximately 90 degrees at every layer. Similar boundary conditions to that of Chapter 3 were used.
Table 5.1 - Sampled LHS inputs

<table>
<thead>
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<th>Specimen</th>
<th>Thickness (mm)</th>
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<th>Length (mm)</th>
</tr>
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<td>16</td>
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<td>14</td>
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<td>8.308</td>
<td>20</td>
</tr>
<tr>
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<td>7.736</td>
<td>8</td>
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<tr>
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<tr>
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<td>8.516</td>
<td>10</td>
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</table>

Figure 5.3 - Sampled LHS inputs

Figure 5.4 - Representative mesh and laser scan pattern, specimen #1

Figure 5.5 shows a representative von Mises stress plot (same specimen shown in Figure 5.4) before and after the clamped boundary conditions at the bottom are removed. Removing these boundary conditions simulated the part being cut off from the building bed. The intended undeformed geometry is also shown in the background for reference. Similarly, Figure 5.6 on page 66 shows the same plot at the mid-cross-
Section. Parallel camera projection was used for these figures for comparison with the original geometry.

Figure 5.5 - Representative von Mises stress plots, before (left) and after (right) stress relieving, deformation magnified by 100x, specimen #1
As shown in the previous figures, the deformation of the part significantly increases while its stress decreases after the part is removed from its clamped
conditions, as expected. The figures also show that this deformation after removing is greatest near the bottom. This is likely due to the clamped condition giving rise to higher plastic strain since the material is being constrained. Figure 5.5 that there are point-like areas of higher von Mises stress throughout the part, especially towards the top. This is likely due to the scanning pattern used. Figure 5.7 shows that as expected the solution produced tensile stresses towards the outer surfaces (especially at the inner surface) while compressive towards the center.

Figure 5.8 shows 3D scatter plots of the results obtained for all the specimens, before removing the clamped boundary conditions. The radius and thickness are shown in the $x$ and $y$ axes, while the length is shown by color and by the size of the points in the plots. The variables chosen of interests are the maximum von Mises stress, maximum diametrical displacement (change of the nozzle diameter), the volume-averaged magnitude of displacement, and the volume-averaged von Mises stress. The maximum von Mises plot (upper left) shows a correlation between this and the radius of the part. Likewise, a correlation can be seen between the volume-averaged displacement and the radius of the part (lower left). Other correlations are difficult to visually observe but can be inferred from the regressions of the output variables relative to the input variables.
Figure 5.8 - Solution at the end of print, before removing from bed

Figure 5.9 shows the results after removing the clamped boundary conditions. In addition to the two correlations observed previously (max stress and average displacement), the figure shows a positive linear correlation with the maximum diametrical displacement (upper right plot) and radius. This maximum displacement (shrinkage of the diameter) occurs at the base of the part where the clamped boundary condition is applied. This correlation is expected, as a larger initial distance (diameter in this case) will produce a larger end displacement (diameter change), assuming a constant strain.
A linear and quadratic regression was performed on the results to quantify the above observations, using the R programming environment. Partial results of the linear regression are shown in Table 5.2, with the full table and quadratic regression results in the appendix. P-values less than 5% are accepted as indicating statistically significant correlation coefficients whereas the coefficients themselves indicate the magnitude of the impact of the independent variable. The observations described from the plots are corroborated by the coefficients and p-values.
Table 5.2 - Linear regression results; partial table; MPa - mm units

<table>
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<th>Dependent Variable</th>
<th>Independent Variable</th>
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<th>After Stress Relief</th>
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<td></td>
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<td>Coefficient</td>
<td>Pr(&gt;</td>
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<td><strong>Max ( S_{\text{vm}} )</strong></td>
<td>(Intercept)</td>
<td>1228.1</td>
<td>2.03E-09</td>
</tr>
<tr>
<td></td>
<td>Thickness</td>
<td>-44.3</td>
<td>0.009931</td>
</tr>
<tr>
<td></td>
<td>Radius</td>
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<td>0.000208</td>
</tr>
<tr>
<td></td>
<td>Length</td>
<td>1.29</td>
<td>0.702959</td>
</tr>
<tr>
<td></td>
<td>R-squared</td>
<td>63.28%</td>
<td>45.99%</td>
</tr>
<tr>
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<td>P-value</td>
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<td>0.005572</td>
</tr>
<tr>
<td><strong>Max. ( U_{\text{dia}} )</strong></td>
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<td>4.55E-01</td>
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<tr>
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</tr>
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<td>68.97%</td>
</tr>
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<td>P-value</td>
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<tr>
<td><strong>Avg. ( S_{\text{vm}} )</strong></td>
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<td>P-value</td>
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<tr>
<td><strong>Avg. ( U_{\text{mag}} )</strong></td>
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<tr>
<td></td>
<td>R-squared</td>
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<td>77.36%</td>
</tr>
<tr>
<td></td>
<td>P-value</td>
<td>0.3033</td>
<td>1.04E-06</td>
</tr>
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</table>
Figure 5.10 - Quadratic regression fitted plots, before stress release

Figure 5.10 and Figure 5.11 show the fitted curves for quadratic regression. Regression statistics are tabulated in the appendix (Table A.4). Again, the size of the points corresponds to the length geometric parameter. As expected, a quadratic regression provides higher $R^2$ values, as the regression can capture some non-linearity in the effects of the design space on the output variables.
Figure 5.11 - Quadratic regression fitted plot, after stress release
5.3 Discussion and Conclusion

All the $R^2$ values in Table 5.2 show are less than 80% for the linear regression, indicating that the regression is not perfect, hinting that there are: 1) factors beyond geometry that impact the output variables 2) some unidentified noise in the simulation results or 3) that linear and second-order regressions do not capture the nature of the non-linearity between inputs and outputs. Even though each simulation is completely deterministic from its given inputs, the approximations required by the thermomechanical FE simulations (coarse mesh, oversized laser diameter, oversized element layers, etc.) in combination with the additional assumptions and approximations made in the implementation (laser pattern, boundary conditions, etc.) may lead to fictitious noise in the results. These assumptions and approximations are discussed in Section 2.2.1 - The Thermomechanical FE Method, in Section 3 - Implementation, and in Section 3.2.1 - Boundary Conditions. In addition, the simulation results may be sensitive to other simulation parameters not tested such as thermal boundary conditions, maximum temperature laser scan pattern, porosity model, etc.

Figure 5.12 shows the predicted porosity for a representative specimen. It shows that the part is not completely dense. Likely, this is not realistic. This is a drawback of using a coarse laser scanning pattern (shown in Figure 5.4 on page 64), required by the larger laser diameter compared to what is physically used in AM. The areas of high porosity in Figure 5.12 correspond to areas where the laser diameter and scan pattern did not provide adequate coverage. Note the scan pattern is based on a path development tool used for fused deposition modeling rather than selective
laser sintering. Hence it does not contain any overlap with respect to the assumed laser diameter. This may be a source of some of the noise seen in the stress plots (Figure 5.5, Figure 5.6, and Figure 5.7).

**Figure 5.12 - Representative porosity, no deformation shown, specimen #1**

In addition to the work presented here, CalculiX sources have been modified to perform a super-integration scheme in calculating the mass, stiffness, and force matrices/vectors. The thermomechanical simulation implemented here necessitates a laser diameter comparable to the size of the elements, or else the energy of the laser will not be accurately captured. This is due to high thermal gradients and a small number of integration points in Gaussian quadrature (2 points in every direction for a linear hexahedral element). Performing a super integration scheme would allow for smaller laser diameters to be used that are closer to the manufacturing parameters. This effectively mitigates mesh dependency with respect to the heat flux calculation. 5-point and 10-point integration schemes were implemented. Future work can
incorporate this integration scheme to better represent the manufacturing process, aiding in accuracy.

Nonetheless, the results indicate that there is a statistically significant dependence of the three varied dimensions (length, thickness, and radius) on the four chosen output variables (maximum diametric displacement, maximum von Mises stress, average von Mises stress, and average displacement). The sensitivity of the simulation results on the three geometrical parameters are shown by the regression coefficients in Table 5.2. Thus, it may be possible to influence the residual displacements and residual stresses by varying the overall geometry.
CHAPTER 6

CONCLUSION

Despite the tremendous advantages of metal additive manufacturing, the lack of predictable distortions limits the dimensional precision and lack of predictable residual stresses cause structural durability challenges that may require post-treatments to mitigate. Thus, improvements in the predictability of these fields before or during the manufacturing process are highly desired. This necessitates a computational simulation of the process to predict the residual fields. This work presents a multiscale thermomechanical simulation capable of capturing the microscale evolving porosity phenomena. The simulation showed that the inclusion of porosity evolution can have a significant effect on the predicted residual stress and residual deformations. Thus, it may be important to include this and other microscale phenomena into thermomechanical simulations of metal additive manufacturing. Although the inclusion of these microscale phenomena requires more computational power and increases the simulation complexity and number of properties required, it has the potential to obtain more accurate results. It also lays the foundation to incorporate other microscale phenomena such as anisotropy for the SLS process and melting, laser melt tracks, and layering effects for the SLM process as well.

A study on how the geometry affects the predicted residual fields is also presented, using the implemented computer simulation. The regression correlation between the geometry and the residual fields show that the geometry can indeed have
a predictable effect on the residual fields. This predictability is important to producing an optimized geometry in a larger study which is slated for future work.

It is important to note that a major limitation of this thesis is the absence of experimental validation. It is possible (and even probable) that there exist several discrepancies between the results presented here and experimentally measurable quantities since the various parameters in the models (such as the inherent strain applied, material properties, simulated laser parameters, laser scan pattern, etc.) have not been calibrated. However, it is not the intent of this work to produce validated results but to merely demonstrate trends and distributions. The conclusions described here should not change due to these discrepancies. Validation of the results is the subject of ongoing research.
REFERENCES


aluminum components using SLM,” RTejournal, pp. 1–16, 2011.


## APPENDIX

Table A.1 - Porous material properties, from MAC/GMC using Table 3.1

<table>
<thead>
<tr>
<th>Material</th>
<th>(T (°C))</th>
<th>(V_f)</th>
<th>(E) (MPa)</th>
<th>(v)</th>
<th>(\rho) (kg/m³)</th>
<th>(k) (W/m°C)</th>
<th>(C) (J/kg°C)</th>
<th>(\alpha) (1/°C)</th>
<th>(\sigma_y) (MPa)</th>
<th>(\varepsilon_{p,1})</th>
<th>(S_1) (MPa)</th>
<th>(\varepsilon_{p,2})</th>
<th>(S_2) (MPa)</th>
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<td>0.66</td>
<td>7,550</td>
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<td>270</td>
<td>1.26E-5</td>
<td>324</td>
<td>0.032</td>
<td>270</td>
<td>0.088</td>
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<td></td>
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<td>7,550</td>
<td>0.225</td>
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<td>1,780</td>
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<td>270</td>
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### Table A.3 - Linear regression results, Chapter 5, MPa - mm units

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