Evaluation of a thermomechanical model for prediction of residual stress during laser powder bed fusion of Ti-6Al-4V

R.K. Ganeriwala^{a,*}, M. Strantza^b, W.E. King^a, B. Clausen^b, T.Q. Phan^c, L.E. Levine^c, D.W. Brown^b, N.E. Hodge^a

^aLawrence Livermore National Laboratory, 7000 East Ave, Livermore, CA 94550, USA
 ^bLos Alamos National Laboratory, Los Alamos, NM 87545, USA
 ^cNational Institute of Standards and Technology, 100 Bureau Dr, Gaithersburg, MD 20899, USA

Abstract

The build-up of residual stress in a part during laser powder bed fusion provides a significant limitation to the adoption of this process. These residuals stresses may cause a part to fail during a build or fall outside the specified tolerances after fabrication. In the present work a thermomechanical model is used to simulate the build process and calculate the residual stress state for Ti-6Al-4V specimens built with continuous and island scan strategies. A layer agglomeration, or lumping, approach is used to speed up the computations. A material model is developed to naturally capture the strain-rate dependence and annealing behavior of Ti-6Al-4V at elevated temperatures. Results from the thermomechanical simulations showed good agreement with synchrotron X-ray diffraction measurements used to determine the residual elastic strains in these parts. However, the experimental measurements showed higher residual strains for the specimen built with an island scan strategy; a trend not fully captured by the simulations. Parameter studies were performed to fully understand the advantages and limitations of the current simulation methodology. Reasons for both the computational and experimental findings are discussed.

Keywords: additive manufacturing; residual stress; thermomechanical modeling; Ti-6Al-4V; laser powder bed fusion

1. Introduction

The number of metal parts produced via laser powder bed fusion (L-PBF) additive manufacturing (AM) is rapidly growing. This process provides significant benefits over traditional manufacturing processes, including significantly reduced time between design and manufacture of parts, and the creation of parts with more geometric complexity than has previously been possible. However, due to the large thermal gradients and cooling rates inherent to the process, parts produced via L-PBF often contain high levels of residual stress and experience significant distortion. This may cause parts to fail during or after the build and/or fall outside of acceptable dimensional tolerances. In order for components produced via L-PBF to be used in

^{*}Corresponding author

Email address: ganeriwala1@llnl.gov (R.K. Ganeriwala)

mission-critical applications, a high degree of confidence is required in their quality. An essential piece of

- such qualification is the ability to accurately know the stress state within a part. Experimental techniques to measure the stress within a part built via L-PBF certainly play an important role here. However, since experimental measurement of the entire stress state is often not possible, having a validated model capable of reliably predicting these stresses is extremely valuable. Such a model can then be used to optimize process parameters and control the build process.
- As the physics governing L-PBF is quite complex, involving a wide range of time (from µs for laser-powder interaction phenomena to hours/days for a full part build) and length scales (layer size on the order of tens of µm to whole part dimensions up to tens of cm), having one model to accurately capture all aspects of the process is currently not practical. As such, models at different scales are being developed. For example, powder scale models [1] can accurately capture physics phenomena associated with smaller length scales, such as melt pool flow, spattering, denudation, and evaporative recoil pressure. However, such models are currently not capable of simulating the deposition of multiple layers due to computational expense.

Macroscale models, typically Lagrangian finite element codes, have shown the capability of modeling multiple layers at a time in order to predict residual stress and part distortion. In these models, complex physics phenomena such as melt pool flow and powder dynamics are typically neglected. However, even with these assumptions (and operating in a parallelized high performance computing environment), it is still not possible to simulate the entire process over an "engineering" configuration in a tractable amount of time. Thus, different strategies to speed up the computations, while retaining an acceptable level of accuracy, have emerged. To date, these strategies can broadly be categorized as follows:

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simulation of the full part.

1. Inherent strain based approaches, where a strain field from either (a) calibration experiments or (b) a full thermomechanical simulation at the process scale, is mapped layer-by-layer on to a macroscale

- 2. Agglomeration (or lumping) approaches, where many physical process layers are lumped into one larger computational layer and the full thermomechanical system of equations is solved.
- The inherent strain method was first proposed by Ueda et al. [2] for welding process modeling and later used for rapid prediction of welding distortions [3]. This is the basis for many commercial codes as it offers rapid prediction of part distortions since only the mechanical system, typically solely linear elastic, is solved on the macroscale part [4]. The basic idea behind this technique is that the thermal history, and hence subsequent plastic strain field, is constant for any point in a given part. This plastic strain field can be determined from either experimental calibration, or a process-scale simulation where enough layers are
- ⁴⁰ simulated over a small domain until the strain field of the bottom layers reaches a steady-state value. The calibrated/computed plastic (or inherent) strain field is then applied as an initial condition over a full layer on a macroscale simulation of the full part. After application of the plastic strains, a (typically) linear-elastic solver computes the required displacements and new equilibrium state of the part. Subsequently the next layer is added, again given an initial plastic strain field. This is repeated until the full part is built. The

- Imitations of the traditional inherent strain method [5] likely result from its inability to account for heating up of the part during the build and the fact that various geometries, such as thin walls or overhangs, will experience a different thermal history and thus have different plastic strain fields. Some commercial codes claim to account for such effects, though most of these methods have not been published in peer-reviewed journals.
- In Keller and Ploshikhin [6], a microscale thermal-only heat source model was calibrated and then applied to a mesoscale thermomechanical, elastoplastic simulation at the scale of an individual layer. The resultant inherent strain field was mapped to a macroscale mechanical model to predict distortions. The effect of varying scan patterns was taken into account by rotating the inherent strain tensor from the mesoscale model when applying it to a macroscopic layer. Desmaison et al. [7] looked at the effect of lumping
- ⁵⁵ multiple physical layers into one larger computational layer during the macroscale mechanical portion of the simulation. They found more accurate distortion results for a cantilever beam when the number of layers used in the macroscale model was as close to the physical value as possible. To keep simulation times reasonable, a re-meshing strategy was employed such that coarser elements could be used away from the free surface. Li et al. [8] developed a temperature-thread and a stress-thread method for fast residual stress
- and distortion predictions. In the temperature-thread approach, a mesoscale thermal history was mapped on to a thermomechanical macroscale model of the part. The stress-thread method involved mapping the residual stress field from a thermomechanical mesoscale model on to a macroscale mechanical analysis of the part. Both methods produced similar distortion curvature but the researchers found the temperature-thread method produced a slightly better match with experimental displacement measurements. Liang et al. [9]
 proposed a modified inherent strain method for rapid distortion predictions, which could later be used in topology optimization of AM structures. To date, all published inherent strain based approaches the authors
 - are aware of only offer validation through distortion comparisons.

The other broad category of part-scale simulation techniques involves solving the coupled thermomechanical problem over the whole part, but often using a layer agglomeration/lumping strategy to speed up calculations. In this strategy, many physical layers are lumped into a larger computational layer to keep the total degrees of freedom and number of layers in the problem tractable. In Zaeh et al. [10], 1 mm layers were activated and heated all at once, a ratio of 20 process layers per computational layer. A similar approach is used in An et al. [11], where each agglomerated layer is heated simultaneously for the total amount of time it would take to physically scan over the equivalent number of process layers. Li et al. [12] looked at the

- ⁷⁵ effect of number of computational layers on the residual stress and distortion predictions for an L-shaped and bridge-shaped specimens, respectively. The previous work by Hodge et al. [13] used 1 mm computational layers to simulate a 316L SS part. A computationally enlarged (or agglomerated) laser heat source was used and scanned over each computational layer as would be done in the physical process. For all of these agglomeration approaches, validation was provided via neutron diffraction residual stress measurements, in
- ⁸⁰ addition to distortion comparisons.

In general, full thermomechanical simulations of an entire part (even when employing an agglomeration/lumping approach) require more computational expense than the inherent strain based approaches, but typically offer a more accurate prediction of the residual stress field. This is likely because the thermomechanical approach can at least partially account for the effect of part geometry on thermal history and due to the use of an elastoplastic material model throughout the simulations. The modeling approach in this paper builds off the previous work by Hodge et al. [13, 14].

2. Process Modeling

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A fully coupled thermomechanical model of the process was implemented within the multiphysics code Diablo [15] developed at Lawrence Livermore National Laboratory. Diablo is an implicit Lagrangian finite element code that uses distributed memory parallelism. Typical runs employ between 32 to 256 CPUs, though Diablo has been shown to scale well up to thousands of processors. The fully coupled thermomechanical process is solved via a staggered, operator splitting approach using linear hex elements. Time integration is performed via the Newmark method [16] for the mechanical system and via a generalized alpha approach [17] for the thermal system. The active sub-problems are solved successively within each time step and iterated over until they simultaneously converge.

The full process is modeled via the element activation technique where a new layer of "powder" elements are turned on at the time associated with the beginning of a new layer. A volumetric heat source (representing the laser) moves over the layer of elements according to the set scan path. As the elements are heated over the melt temperature, they are assigned material properties meant to represent those of the liquid material, provided that enough energy has been input to allow for phase change. These elements are then given bulk material properties upon cooling back below the melt temperature. After the laser has scanned over a layer and a specified amount of cooling time has passed, meant to mimic the actual process time, a new layer of elements are turned on. This process is repeated until the entire part is built. At the end of the simulation, elements connecting the part to the baseplate may be deactivated. This is meant to mimic the wire electrical discharge machining (EDM) process used to detach the part from the baseplate. This section goes into more detail regarding the specific thermal and mechanical models used, as well as the agglomeration methodology used to speed up the simulation.

2.1. Thermal Problem Description

The thermal problem is governed via the balance of energy,

$$\rho c_p \dot{T} = -\nabla_x \cdot \mathbf{q} + r, \text{ in } \Omega, \tag{1a}$$

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$$T(\mathbf{x}_T, t) = \bar{T}, \text{ on } \mathbf{x}_T \in \Gamma_T,$$
 (1b)

$$q(\mathbf{x}_q, t) = \bar{\mathbf{q}} \cdot \mathbf{n}, \text{ on } \mathbf{x}_q \in \Gamma_q, \tag{1c}$$

$$T(\mathbf{x},0) = T_0, \text{ on } \Omega \bigcup \partial \Omega, \tag{1d}$$

where ρ is density, c_p denotes the constant pressure specific heat, T represents temperature, **q** is the heat flux, and r represents external heat sources (the laser in this case) within the domain Ω . Γ_T is the portion

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of the boundary, $\partial\Omega$, with prescribed Dirichlet boundary conditions and Γ_q is the portion of the boundary with prescribed Neumann boundary conditions. The position in the current configuration is denoted by **x** and the operator $\nabla_x \cdot (\cdot)$ refers to the divergence of (\cdot) with respect to the current configuration. The heat flux is calculated via standard Fourier conduction,

$$\mathbf{q} = -\mathbf{k}\nabla_x T,\tag{2}$$

with **k** being the second order tensor of thermal conductivities and $\nabla_x(\cdot)$ referring to the gradient operator in the current configuration. The thermal conductivity is reduced to a single scalar value in the present simulation with the assumption of isotropy in the material.

The energy required for phase change from solid to liquid (and vice versa) is taken into account by solving the Stefan-Neumann phase change equations,

$$T(\mathbf{x}_p, t) = T_p, \text{ on } \mathbf{x}_p \in \Gamma_p,$$
(3a)

$$(\mathbf{k}_1 \nabla_x T_1 - \mathbf{k}_2 \nabla_x T_2) \cdot \mathbf{n} = \mathcal{L}\rho \frac{\partial \mathbf{x}_p}{\partial t} \cdot \mathbf{n}, \text{ on } \mathbf{x}_p \in \Gamma_p,$$
(3b)

where the surface internal to the body along which phase change is occurring is denoted by Γ_p . The subscripts $(\cdot)_1$ and $(\cdot)_2$ represent the phases on opposite sides of the phase interface, \mathcal{L} is the latent heat of phase change, and **n** is the unit normal vector to the surface Γ_p .

The energy input from the laser is modeled as a uniformly distributed volumetric heat source,

$$r = a \frac{P}{\pi R^2 d},\tag{4}$$

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with P indicating laser power, R denoting the specified beam radius, d the agglomerated powder layer depth, and a the material absorptivity. Modeling the beam as a uniformly distributed volumetric heat source is an assumption made to improve performance of the code (i.e. lower computational cost). Such an assumption is warranted in this case since the true profile of the beam is lost when agglomerating layers and beam size. Note that other commonly used approaches were also implemented and tested in Diablo, including the double ellipsoid model of Goldak [18] and the Gusarov model [19] wherein a Gaussian-like beam decreases in volumetric power exponentially with depth according to the Beer-Lambert law. Only a minimal difference in the ensuing stress/strain field was noticed when using these other beam types at the agglomerated scale.

Other heat transfer mechanisms, including radiation from the build surface to the environ-*Remark:* ment, convection to the flowing argon gas in the chamber, heat loss due to evaporation, and conduction to the surrounding powder have been neglected in the present simulation. The capability to include these

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additional boundary conditions is present in Diablo, but we neglected them to improve computation speed. For a small problem, such as the bridges simulated in this paper, it would not be computationally prohibitive to include these extra physics; however, for larger problems some of these highly non-linear boundary conditions (particularly heat loss due to evaporation) have been found to significantly slow convergence. For completeness, the simulations in this work were additionally run with the presence of all these additional

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heat transfer mechanisms. The ensuing stress/strain field was virtually identical (within 2 to 3%) to the results presented in this manuscript, indicating that they may be safely neglected in this case. For geometries with large overhangs or increasing cross-sectional areas, it is certainly necessary to include the presence of these additional physics, or else the part temperature will be over-predicted.

2.2. Mechanical Problem Description and Material Model

The mechanical problem is governed by the balances of mass and linear momentum,

$$\dot{\rho} = \rho \nabla_x \cdot \mathbf{v}, \text{ in } \Omega, \tag{5a}$$

$$\rho(\mathbf{x}, 0) = \rho_0, \text{ on } \Omega \bigcup \partial \Omega, \tag{5b}$$

$$\rho \ddot{\mathbf{u}} = \nabla_x \cdot \boldsymbol{\sigma} + \rho \mathbf{f_b}, \text{ in } \Omega, \tag{6a}$$

$$\mathbf{u} = \bar{\mathbf{u}}(\mathbf{x}_u, t), \text{ on } \mathbf{x}_u \in \Gamma_u, \tag{6b}$$

$$\mathbf{t} = \bar{\mathbf{t}}(\mathbf{x}_t, t), \text{ on } \mathbf{x}_t \in \Gamma_t, \tag{6c}$$

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0, \text{ on } \Omega \bigcup \partial \Omega, \tag{6d}$$

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$$\mathbf{v}(\mathbf{x},0) = \mathbf{v}_0, \text{ on } \Omega \bigcup \partial \Omega, \tag{6e}$$

where \mathbf{v} is velocity, \mathbf{u} denotes displacement, $\boldsymbol{\sigma}$ denotes the Cauchy stress tensor, and $\mathbf{f}_{\mathbf{b}}$ represents any body forces ($\mathbf{f}_{\mathbf{b}} = \mathbf{0}$ in this simulation). The boundary conditions are represented by Equations 6b and 6c where Γ_u is the portion of the boundary with prescribed displacements and Γ_t the surface with prescribed tractions $(\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n}).$

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The flow strength of Ti-6Al-4V exhibits a significant strain rate dependence at elevated temperatures [20, 21]. However, many researchers use a strain rate independent model when calculating stress, presumably

for ease of implementation and to reduce computation time. Such models are not able to directly capture annealing behavior, or stress and plastic strain relaxation at elevated temperatures, and often require prescription of a tuned "stress free" temperature, with no physical significance, to best match experimental results [22]. Stress and strain relaxation behavior can be captured naturally through viscoplastic models

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results [22]. Stress and strain relaxation behavior can be captured naturally through viscoplastic models based on dislocation motion, dislocation density, and microstructure evolution [21, 23, 24]; however, such models are more computationally expensive, often contain a large number of parameters which must be fit to data, and would be hard to carry over to other materials without extensive testing.

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A material model able to capture strain rate effects and annealing behavior, but with a minimal number of physically relevant constitutive parameters, was implemented following an approach similar to that used by Goldak [25, 26] in computational welding mechanics. This approach combines three different classes of material models depending on temperature, and is designed to best represent the behavior of metals within each of the associated temperature ranges. It can be summarized as follows:

- 1. Strain rate independent plasticity for $T < 0.5T_m$,
- 2. Viscoplasticity (strain rate dependent plasticity) for $0.5T_m \leq T < 0.8T_m$,
 - 3. Maxwell-type viscoelasticity for $T \ge 0.8T_m$.

In the above descriptions, T_m is the melting temperature of the material in an absolute temperature scale (i.e., Kelvin) and T is the temperature at a given point. With this approach, different material behavior can be represented at every point in the domain, depending on temperature. This produces no problems with convergence, provided stress continuity is maintained when transitioning between temperature intervals. A more thorough description of each model, and how stress continuity is maintained during transitions, is provided next. Note that the temperature ranges specified above are only approximate and may vary based upon material behavior.

2.2.1. Rate independent material model

A finite deformation, rate independent material model was implemented based on the work of Simo [27, 28, 29]. This is an isotropic hyperelastic model involving a multiplicative decomposition of the deformation gradient into its elastic, F_e, and plastic, F_p, components,

$$\mathbf{F} = \mathbf{F}_{\mathbf{e}} \mathbf{F}_{\mathbf{p}}.\tag{7}$$

This decomposition is critical as it allows for easily coupling to the viscoplastic and viscoelastic material models, as the elastic portion of the calculations remain the same throughout. The stress is broken up into its volumetric and deviatoric components, which are calculated separately,

$$\boldsymbol{\sigma} = -p\mathbf{1} + \boldsymbol{\sigma}',\tag{8}$$

where p is the hydrostatic pressure or the volumetric portion of the stress, σ' is the deviatoric portion of the stress tensor, and 1 is the 2nd order identity tensor. Incorporating thermal strains, the hydrostatic pressure

is given as [29],

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$$p = -\frac{\partial U(J)}{\partial J} - \frac{\partial M(T,J)}{\partial J},$$
(9a)

$$U(J) = \frac{1}{2}\kappa \left(\frac{1}{2}(J^2 - 1) - \ln(J)\right),$$
(9b)

$$M(T,J) = -3\alpha(T - T_{ref})\frac{\partial U}{\partial J},$$
(9c)

where κ is the bulk modulus of the material, $J = det(\mathbf{F})$, and α is the linear secant coefficient of thermal expansion (CTE). U(J) is the volumetric portion of the strain energy density function and M(T, J) contains the contributions due to thermal expansion.

The deviatoric stress is broken into its elastic portion, $\sigma'_{\mathbf{e}}$, and the plastic corrector, σ'_{p} ,

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma}'_{\boldsymbol{e}} + \boldsymbol{\sigma}'_{\boldsymbol{p}}.\tag{10}$$

The stress is updated in an incremental manner, with complete details regarding the update procedure and numerical implementation provided in [28]. Linear isotropic hardening, based on the effective plastic strain, determines the yield surface,

$$\sigma_y = \sigma_o + H_{iso}\epsilon_p,\tag{11}$$

where σ_y is the flow stress, σ_o is the initial yield stress, H_{iso} is the isotropic hardening coefficient, and ϵ_p is the effective plastic strain (as defined in [28]). All material properties are assumed to be temperature dependent.

205 2.2.2. Viscoplastic material model

Strain rate dependent effects are captured through the enabling of viscoplasticity parameters as a function of temperature. A Perzyna (overstress) type approach [30] is employed such that,

$$\dot{\epsilon}_p = \left(\frac{\phi}{\eta}\right)^{\zeta},\tag{12a}$$

$$\phi = \tilde{\sigma} - \sigma_y. \tag{12b}$$

Here ϕ represents the Von Mises yield function and $\tilde{\sigma}$ is the effective Von Mises stress, given as $\tilde{\sigma} = \sqrt{\frac{3}{2}\sigma' : \sigma'}$. This formulation works out to be a non-linear hardening law where the following yield function is observed,

$$\phi - \eta \left(\dot{\epsilon}_p\right)^{1/\zeta} = 0. \tag{13}$$

This viscoplastic model is activated by the temperature dependent viscosity coefficient, η , and exponent, ζ . The exact viscoplastic stress state is solved for via Newton iterations during the plastic correction phase. Upon inspection of Equation 13, it is clear that as $\eta \to 0$ the rate independent model is recovered. Thus merely ramping up the viscosity parameters as a function of temperature allows for a smooth transition of stress between the rate independent and viscoplastic models.

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Note that there are an abundance of potential viscoplasticity models developed for AM or welding purposes (for example, see [21, 23, 31, 32]) that could have been implemented in this study; however, many of these models contain a large number of parameters, typically associated with the physics behind dislocation motion, which require extensive testing to determine. Additionally, these models may require a large number of intermediate calculations, increasing overall computational expense and potentially increasing the number

of iterations required to reach a converged solution within a time step. The current model was chosen for its 220 minimal impact on computational expense and relative simplicity in determining the appropriate viscosity parameters, while still effectively capturing the macroscopic rate dependent behavior in the temperatures and strain rates of interest. Other viscoplasticity models, incorporating a more accurate representation of the underlying physics, could potentially be used here if necessary.

2.2.3. Viscoelastic material model 225

A Maxwell-type viscoelastic model is used to model complete stress relaxation when $T \ge 0.8T_m$ based on the hyperelastic, finite deformation algorithm from Simo and Hughes [33]. Maxwell viscoelasticity can be modeled as a spring (elastic term) and linear dashpot (viscous damping) acting in series.

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The elastic portions of the stress tensor are calculated in an identical manner to that in the rate independent and viscoplastic material models. Viscosity effects are introduced solely on the deviatoric portion of the stress tensor. A relaxation function, q(t), is introduced,

$$g(t) = \gamma_{\infty} + \sum_{i=1}^{N} \gamma_i e^{-t/\tau_i}.$$
(14)

In the case of a Maxwell fluid with only a single spring-dashpot system connected in serial ($N = 1, \gamma_{\infty} =$ 0, $\gamma_1 = 1$), this relaxation function reduces to,

$$g(t) = e^{-t/\tau}$$
. (15)

The relaxation time, τ , is defined as,

$$\tau = \frac{\sqrt{2}\eta}{3\mu},\tag{16}$$

where μ is the shear modulus. With this formulation of the relaxation time, the viscosity coefficient η works 235 out to be the same as that used in the viscoplastic model if $\sigma_y = 0$ and $\zeta = 1$, allowing for stress continuity when transitioning between the viscoplastic and viscoelastic models. It is important to mention that η should be interpreted as the thermally activated viscosity due to dislocation motion, as opposed to the liquid viscosity.

Equation 8 can now be modified to incorporate viscous effects on the deviatoric stress contributions, 240

$$\boldsymbol{\sigma} = -p\mathbf{1} + \int_{-\infty}^{t} g(t-s) \frac{d}{ds} \boldsymbol{\sigma}' ds.$$
(17)

The volumetric stress contribution is the same as that from the rate independent model. Similar viscous effects can be applied to the volumetric portion as well, though that is not pursued in the current model. A detailed solution algorithm for the viscoelastic model, along with calculation of consistent tangent moduli for linearization, is presented in [33].

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Finally, it is important to note that the effective plastic strain parameter present in the rate independent and viscoplastic models, has no role in this viscoelastic formulation. However, it is necessary to prescribe some sort of evolution law for this internal variable upon return to the plasticity models. As metals generally enter a "mushy zone" around $0.8T_m$ [26], it is assumed that enough dislocation motion happens at this temperature such that any accumulated work hardening due to plastic strains is lost. Thus the plastic strain is reset (i.e. $\epsilon_p = 0$) when entering the viscoelastic model.

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2.3. Material Parameter Determination and Evaluation against Experimental Measurements

Temperature dependent material parameters for Ti-6Al-4V were determined by averaging data from multiple sources [20, 34, 35, 36, 37, 38, 39]. Recognizing the fact that material properties for additively manufactured components sometimes differ significantly from wrought material properties, often exhibiting an increased yield strength but decreased ductility, in-house measurements were performed on Ti-6Al-4V 255 tensile specimens built via L-PBF to determine room temperature mechanical properties [40]. The complete set of thermomechanical material properties used are listed in Tables 1 and 2 as a function of temperature. The effects of microstructure on material properties are not directly considered in this model, outside of the temperature dependent material properties.

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To evaluate the material model, single element tests were performed to compare the predicted stressstrain response with experimental measurements, provided in [20], for Ti-6Al-4V at varying temperatures and strain rates. This comparison is shown in Figure 1. According to the model formulation, rate independent plasticity is used for the 20 °C and 200 °C comparisons, while the viscoplastic model was used at 700 °C and 900 °C. Due to the viscosity parameters used, namely leaving the viscosity exponent $\zeta = 1$, the simulation

results collapse to essentially the same value at 0.01/s and 0.001/s at 700 °C and 900 °C. This approximation 265 is justified by the experimental data as close agreement is generally observed between the measurements and the model.

Remark 1: The material properties used for this model were averaged from multiple sources and thus are not completely identical to those that would be indicated if calibrated solely from the data in [20].

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Remark 2: A valid question may be related to whether this model is calibrated over the proper strain rates. To this end, it is possible to get a quick estimate of the strain rates present during the L-PBF process. Typically cooling rates on the order of 10^6 °C/s are observed around the melt pool [41, 42]. As the CTE



Figure 1: Comparison between experimental and simulation stress-strain response for Ti-6Al-4V at varying temperatures and strain rates, showing how strain rate effects become more significant at higher temperatures (experimental results from [20]). Simulation predictions are the curves with open-circle markers.

of Ti-6Al-4V is on the order of 10^{-5} , this would indicate a maximum strain rate of 10/s. However, as stress does not form as the material is near or above melting, it is reasonable to assume that the relevant strain rates for model calibration are 1/s or below for L-PBF of Ti-6Al-4V. Numerical simulations confirm this at the temperatures shown in Figure 1.

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2.4. Agglomeration Approach

The agglomeration strategy was based off the previous work by Hodge et al. [13]. The five process parameters included in this method are: (1) powder layer depth, (2) laser spot size, (3) laser power, (4) laser scan speed, and (5) total layer time. To speed up the computations, the powder layer depth and beam 280 diameter were scaled up to 0.5 mm and 1 mm (0.5 mm radius), respectively in the computational domain. An entire layer of elements is activated simultaneously at the time associated with switching layers. The physical scan path was then followed using these agglomerated layers and beam size. The scan speed was held fixed to the physical process value but the laser power was increased to ensure complete phase change for this much larger beam and agglomerated powder layer depth. The obvious method for choosing how much

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to increase the laser power is to use the value which would conserve the total energy input into the domain. However, doing this leads to overheating since many of the energy loss mechanisms present in the physical problem are not taken into account, most notably the heat loss due to evaporation and due to radiation (see previous discussion regarding the implementation of these Neumann boundary conditions). Also note that

T(K)	$ ho \; \left({kg} / {m^3} ight)$	$c_p \left(J/kg - K \right)$	$k \left(W / m - K \right)$	$\alpha \left(10^{-6} / K \right)$
273	4421	517	6.18	8.85
1254	4295	881	19.0	10.72
1264	4293	707	19.2	10.74
1913	4210	756	27.7	11.97
1923	3935	829	33.4	20.17
3550	3731	779	36.8	0.0

Table 1: Thermal properties of Ti-6Al-4V as a function of temperature (density, specific heat, thermal conductivity, and linear CTE). 1264 K is the β -transus temperature, 1923 K is the melting temperature, and 3550 K is the vaporization temperature. All values are linearly interpolated between points and held constant outside the range of this table.

T(K)	E (GPa)	$\sigma_y \ (MPa)$	$H_{iso} (MPa)$	$\eta~(MPa)$
293	115	1151	1828	0.0
961	60.7	365.8	0.0	0.0
973	59.8	257.6	0.0	242.4
1173	24.0	69.0	0.0	101.0
1264	16.7	69.0	0.0	101.0
1538	11.0	0.0	0.0	35.35

Table 2: Mechanical properties of Ti-6Al-4V as a function of temperature (Young's modulus, yield stress, isotropic hardening coefficient, and viscosity coefficient). 1538 K is the viscoelastic start temperature. All values are linearly interpolated between points and held constant outside the range of this table.

	Physical Process	Agglomerated Value
Powder layer depth	$30 \ \mu m$	$0.5 \mathrm{~mm}$
Laser beam diameter	54 μm	$1 \mathrm{mm}$
Laser power	100 W	10,000 W
Laser scan speed	$600 \ mm/s$	$600 \ mm/s$
Average time per layer	$17 \ s$	$283 \ s$

Table 3: Physical process and agglomerated computational parameters

the uniform volumetric heat input used has a different heating profile as compared to the actual process beam, which typically has a Gaussian profile. Thus, the agglomerated beam power was numerically tuned to be the minimum value which allowed for complete melting of the initially powder material. Finally, the total inter-layer time (accounting for time required to re-coat) was scaled from the physical process value by the ratio of the agglomerated powder layer depth to the physical powder layer depth, such that the total part build time was kept constant. Agglomerated and physical process parameter values are given in Table 3.

3. Problem Description and Process Parameters

Four different Ti-6Al-4V bridge specimens were built using different scan strategies, as illustrated in Figure 2. The dimensions of these bridges are shown in Figure 3. The scan strategies used are as follows:

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1. A1: continuous, serpentine scan, with orientation rotated from 0° (parallel to x-axis) to 90° (parallel to y-axis) between layers

- 2. A2: continuous, serpentine scan, with orientation rotated from -45° to $+45^{\circ}$ between layers
- 3. B1: island scan (2.5 mm x 2.5 mm) with rotating 0° to 90° scans between islands and layers
- 4. B2: island scan (2.5 mm x 2.5 mm) with rotating -45° to +45° scans between islands and layers
- The parts were built on a Concept Laser M2 machine¹ without support structures. Each specimen was built on a Ti-6Al-4V hybrid build plate, which was bolted to the larger machine baseplate. Four of these hybrid build plates, one for each specimen, could fit in the machine at a time. No contour scans were performed and there was a 1 mm x - y shift in island location between layers. The islands were scanned in a random sequence each layer, as generated via the machine software. The hatch spacing between laser passes was 105 µm.

¹Certain commercial entities, equipment, or materials may be identified in this document to describe an experimental procedure or concept adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, Los Alamos National Laboratory, or Lawrence Livermore National Laboratory, nor is it intended to imply that the entities, materials, or equipment are necessarily the best available for the purpose.



Figure 2: Scan strategy illustration with 2.5 mm x 2.5 mm islands for the case of B1 and B2 scans.



Figure 3: Bridge dimensions (all units in mm)

Property	Scale factor
Specific heat, c_p	0.5
Thermal conductivity, \boldsymbol{k}	0.01
Young's modulus, ${\cal E}$	0.1
Yield stress, σ_y	0.1

Table 4: Scale factors relating properties of powder to fully consolidated (bulk) material. All other properties are considered the same for both cases.

In the model, layers get added as initially powder material, which is assigned reduced material properties compared with fully consolidated material. The liquid phase is represented by the change in material properties above the melting temperature. Upon cooling back below the melt temperature, those formerly powder elements are given bulk material properties, on an element-by-element basis. The scale factors associated with powder versus bulk material properties are listed in Table 4. All remaining material/process parameters are provided in Table 5.

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Dirichlet displacement and temperature boundary conditions are applied on the baseplate. The boundary and prescribed initial conditions can be summarized as follows:

$$\mathbf{u} \cdot \mathbf{n} = 0, \text{ on } \mathbf{x}_u \in \Gamma_u, \tag{18a}$$

$$T = 303 \ K, \ \text{on} \ \mathbf{x}_T \in \Gamma_T, \tag{18b}$$

$$T(\mathbf{x}, t = 0) = 303 \ K, \ \text{on} \ \Omega \bigcup \partial \Omega, \tag{19a}$$

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$$\mathbf{u}(\mathbf{x}, t=0) = \mathbf{0}, \text{ on } \Omega \bigcup \partial \Omega, \tag{19b}$$

$$\mathbf{v}(\mathbf{x}, t=0) = \mathbf{0}, \text{ on } \Omega \bigcup \partial \Omega.$$
(19c)

The boundary Γ_u is prescribed as all sides and the bottom surface of the baseplate, while Γ_T is prescribed as solely the bottom of the baseplate (see depiction in Figure 4). The initial temperature and activation temperature of each layer is set at 303 K and initial displacement set to **0**. To save computation time, only a portion of the baseplate was modeled, extending 10 mm from each edge of the bridge in x and y, and with a z-height of 10 mm. A voxel mesh was used to represent the bridge geometry while maintaining the constraint of a 0.5 mm computational layer height.

Property	Value
Effective absorptivity, a	0.3
Latent heat of melting, \mathcal{L}_m	$299.6 \ ^{kJ}\!/_{kg}$
Melting temperature, T_m	1923 K
Poisson's ratio, ν	0.32
Viscosity exponent, ζ	1.0
Initial temperature, T_0	303 K

Table 5: Remaining material/process parameters



Figure 4: Schematic depiction of boundary conditions for this problem

4. Experimental Strain Measurements

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Synchrotron X-ray diffraction was used as a tool to determine the residual strain state within the specimens. Energy dispersive diffraction was performed at the Cornell High Energy Synchrotron Source (CHESS) using the A2 Beamline, which utilized a polychromatix X-ray beam with effective spectrum from 50 keV to 150 keV. By measuring the diffracted photon energy at a fixed measured diffraction angle, the lattice spacings of the specimens could be determined. Comparing the measured lattice spacings to those measured from a stress-free sample extracted from the specimens allowed for the elastic strains to be calculated. The

- diffraction volume was a rhomboidal-shape with dimensions 0.2 mm x 1.5 mm x 0.2 mm, where the long 335 dimension is along the incident beam direction. X-ray diffraction measurements were performed at many locations across the middle cross-sectional plane of the bridge. This allowed for contour maps of the three orthogonal strain components (ϵ_{xx} , ϵ_{yy} , and ϵ_{zz}) to be produced along this cross-section, the plane located at y = 2.5 mm if the bottom-left corner of the bridge (indicated by the red dot in Figure 4) has location (0, (0, 0). Full details regarding the X-ray diffraction measurements and strain determination methodology are
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5. Results and Discussion

provided in Strantza et al. [43].

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Using results from the simulations, we can get an idea of the stress state throughout the part, supplementing the X-ray diffraction measurements which were only completed for a single cross-section. The build direction stress (σ_{zz}) for the bridge simulated using the continuous scan strategy with 0° to 90° rotation between layers is shown in Figure 5. Notice how the interior of the bridge is in compression, which is balanced by tensile stresses on the exterior surfaces. These results are in line with those typically seen in L-PBF builds (see, for example [44]).

5.1. Comparison between experimental and model results

To evaluate the model, a comparison between the simulated elastic strains and measured lattice strains was performed. In the following sections, we just refer to them as strains for simplicity and to not disrupt the flow of the paper.

For consistency with the experiments, the simulation results were integrated over the same diffraction volume as the measurements, although the effect of this integration on the simulation results was minor.

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It should also be mentioned that other than the computational tuning used to determine the minimum power necessary for complete phase change of the agglomerated powder layer, no other tuning of the initial simulation parameters was performed in producing these results.

A comparison of results between the measured and simulated strains is shown in Figures 6 and 7 for the continuous scan strategy with 0° to 90° rotation between layers and island scan strategy with 0° to 90° rotation between islands, respectively. The results are shown both before and after the left leg of the bridge 360 is cut off the baseplate via wire EDM. These plots show the strains along a cross section in the center of



Figure 5: Simulated build-direction stress, σ_{zz} (MPa) before EDM, shown for the continuous 0°/90° scan strategy

the bridge (the plane y = 2.5 mm) as the strains were only measured along this plane. The outer edges of the bridge (approximately 0.25 mm for the x and z strains and 0.5 mm for the y strains) were unable to be experimentally measured and are thus excluded from both the simulation and experimental plots. Good qualitative agreement is observed between the simulated strains and those measured via X-ray diffraction in these figures. Quantitative line-out comparisons are provided Figure 8. Only a comparison between the continuous $0^{\circ}/90^{\circ}$ and island $0^{\circ}/90^{\circ}$ samples are shown here as these two scan strategies produced the largest difference in measured residual strains; and thus represent the most interesting scan strategies to compare against the model. A comparison between this model and experimental measurements for the continuous scan with $\pm 45^{\circ}$ degree rotation between layers was presented in [43]. Complete data regarding the measurements and experimental results from all four scan strategies will be presented in a companion publication.

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From the post-EDM results shown in Figures 6(b) and 7(b), a significant amount of strain/stress relaxation can be seen on the leg cut from the baseplate, most prominently visible for the build direction (z)strains. A more modest change in the x-strains is also noticed as the bridge deflects upwards and goes from tension to a more compressive state along the lengthwise direction. Very little change in strains is noticed in the y-direction, as should be expected since very little movement occurs along this axis. These trends are observed in the experimental measurements as well as the simulations, validating the assumption that the EDM process can be modeled by simply deactivating the relevant baseplate elements.

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From the diffraction measurements before EDM, it can be seen that the simulations tend to over-predict the build direction strains a bit near the part boundaries and interface with the baseplate. One reason for this may be explained by the constant temperature, Dirichlet boundary condition applied to the bottom of the computational baseplate. In reality the baseplate is known to heat up as parts are built [45]; however, accurate temperature measurements of the baseplate were unavailable for these builds and the authors wanted



Figure 6: Comparison between measured and simulated strains (units of microstrains) (a) before and (b) after the left leg of the bridge is cut off the baseplate via EDM for the continuous $0^{\circ}/90^{\circ}$ scan strategy. Results are from a cross section taken along the center of the bridge.



Figure 7: Comparison between measured and simulated strains (units of microstrains) (a) before and (b) after the left leg of the bridge is cut off the baseplate via EDM for the island $0^{\circ}/90^{\circ}$ scan strategy. Results are from a cross section taken along the center of the bridge.

to avoid a "fitting" approach where model parameters (specifically, baseplate temperature in this case) are

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tuned to better match measurements. The rigid mechanical boundary condition, applied to the bottom of the computational baseplate, may also have been a bit too restrictive in this scenario, as the bridges were built on smaller hybrid baseplates placed on top of the full machine baseplate. These hybrid baseplates may have exhibited a small amount of flex as the part was being built, which would not be allowed with the specified boundary condition. Other error sources can be attributed to the material properties, effective absorptivity, and layer and beam agglomeration method used. When scaling up the computational layers, the precise cooling rates and thermal history of each point in the part are not conserved.

Finally, while the experiments actually showed a modest increase in strains for the island scan cases as compared to continuous scans, the simulations were very similar for all cases. To illustrate this difference quantitatively, line-out comparisons of the strains were taken along the height for the middle of the left bridge leg at x = 3.75 mm and along the length near the top of the bridge at z = 7.75 mm. The results for both the simulations and experimental measurements are shown in Figure 8. Note that the error bars present in this figure are associated with the uncertainty in the diffraction peak fitting; these do not account for the complete experimental uncertainty.

In Figure 8(a), the biggest difference between scan strategies can be noticed in the line-out for the build direction, or z-strain component. Notice how the measured z-strains are greater in magnitude for the island scan, especially near the bottom of the part. However, the simulation results are extremely similar in both cases. In Figure 8(b) it is observed that the magnitude of the longitudinal (or x-direction) strains are quite noticeably greater for the island scans. In this case, the simulations correctly predict this trend, but underestimate the magnitude of the difference. The reason the simulation results are unable to correctly capture all the scan strategy effects is again believed to lie in the agglomeration/lumping methodology used. By using 0.5 mm layers and a 0.5 mm beam radius, the localized scan strategy information becomes effectively lost. More discussion on the presence of higher stresses for the island scan cases is given in Section 5.3.

5.2. Model parameter studies

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To see the effects of (1) strategy used to scale up parameters from the physical scale to the agglomerated scale and (2) agglomerated layer height and beam size, the researchers performed a few parameter studies with the current model. The first study looked at changing the beam power and scan speed scaling strategy. While the approach used for the comparisons above was to hold the scan speed constant but increase the power such that complete phase change occurs for the agglomerated layer, one could easily envision other possible scaling methods. Three additional such techniques were tried:

1. Hold the power constant but slow down the scan speed, such that the total time spent scanning over an agglomerated layer is equal to the time that would be spent scanning over the equivalent volume at

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Figure 8: Line-out comparisons of simulated and measured strains for the continuous and island $0^{\circ}/90^{\circ}$ scan strategies along (a) x = 3.75 mm and (b) z = 7.75 mm

the physical process scale,

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$$v_a = v_p \frac{d_p R_p}{d_a R_a} = 1.94 \ ^{mm/s},\tag{20}$$

where v is scan speed, d is powder layer depth, R is beam radius, $(\cdot)_a$ denotes the agglomerated value of the specified property, and $(\cdot)_p$ denotes the physical process value.

2. Increase the power to produce complete phase change and additionally decrease the scan speed such that the total amount of time required to scan over an individual layer is kept constant,

$$v_a = v_p \frac{R_p}{R_a} = 32.4 \ mm/s.$$
⁽²¹⁾

- 3. Heat an entire agglomerated layer at once, applying heat over a 0.1 s interval (approximately the time a single point receives heat input from all adjacent passes of the laser each layer at the physical scale).
- In all cases, the total amount of time between layer start points is held fixed (see Table 3) by adjusting the interlayer time appropriately. In Figure 9, the strain results of these three alternate scaling strategies were compared against the baseline strategy (where scan speed is held constant, $v_a = v_p = 600 \text{ } mm/s$) and against the experimental strain measurements for the continuous 0°/90° scan scenario. The results in Figure 9 were produced by sampling points along a vertical line located at x = 3.75 mm, the center of the left leg of the bridge before EDM.
 - A few observations can be made from these plots. First, it can be seen that the baseline beam speed scaling strategy produces the closest match to the experimental results across all strains. The results from

using the slowest moving laser ($v_a = 1.94 \text{ mm/s}$) greatly under-predict the strains in the y and especially z-directions. This can be explained by the fact that the thermal gradients and cooling rates produced from

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moving the beam so slowly are significantly smaller than those in the physical process since there is much more time for conduction to occur as the beam is moving. The case of scaling the scan speed such that total scan time per layer is held fixed ($v_a = 32.4 \text{ mm/s}$) also under-predicts the z-direction strains, likely due to reducing the vertical thermal gradients and cooling rates as well. There is also an artificially large layer-tolayer variation, especially in the y-strains, with this scaling technique. Such variation is not as apparent for

- the case of $v_a = 1.94 \text{ mm/s}$ or the baseline case of $v_a = 600 \text{ mm/s}$. The reason such variation is not present in the former is likely due to conduction having enough time to even out the thermal gradients present from changing scan orientation, while in the latter there is not enough time for conduction to occur in a layer. which also minimizes the impacts of changing scan orientation on the x and y thermal gradients. Finally, it should be observed that heating the entire layer at once produced very similar results as the baseline case.
- This can be explained by the fact that there is very little time for in-plane conduction to occur during the 445 heating of a layer due to the high beam speed and agglomerated beam size. The beam scans over the entire layer before the previous passes have had a chance to cool significantly, explaining the similar results to those obtained from heating the entire layer simultaneously. However, heating the entire layer at once decreased computation time slightly over five hours to just one hour using 32 processors, an approximately five-fold decrease in run time for this geometry. 450

The second parameter study performed involved varying the agglomerated layer height along with the corresponding beam size. These comparisons were again made for the continuous $0^{\circ}/90^{\circ}$ scan strategy using a fixed computational scan speed of 600 mm/s. The baseline simulations used an agglomerated layer height and beam radius of 0.5 mm (for a computational-to-physical layer height ratio of 16.7). Comparisons were made against simulations using a computational layer height and beam radius of 1 mm (a layer height ratio of 33.3) and 0.25 mm (a layer height ratio of 8.3). The results of these simulations were compared against the measured strains along a line at x = 3.75 mm in Figure 10.

From these plots, several interesting trends are observed. All three layer height resolutions show similar

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results for the x and y strains, though there is a bit more layer-to-layer variation from alternating scan orientation present when using 1 mm layers. The similarity in x and y for all three layer heights is not surprising as the temperature gradients in these directions are more a function of scan strategy and part geometry than layer size. However, the z-direction strains show a clear trend of increasing as the layer height is refined. This can be explained by the heat input model, where volumetric heating is evenly applied over a single layer. As the layers decrease in thickness, this increases the z-direction temperature gradient. The measured z strains actually lie somewhere in between the 0.25 mm and 0.5 mm computational layer height results for the majority of the part (except at the very bottom of the bridge leg). This shows that the optimal layer height ratio lies somewhere between 8.3 and 16.7, at least for the current material, geometry, and agglomeration strategy. When using more refined layers, a more accurate representation of the heat



Figure 9: Effects of changing beam agglomeration strategy, shown for a line down the center of the left bridge leg (at x = 3.75 mm). The most accurate results were obtained with the baseline strategy where scan speed is equal the physical process value and power is increased to produce complete melting. Heating the entire layer at once also produced very similar results.



Figure 10: Effects of changing computational layer size and beam radius, shown for a line down the center of the left bridge leg (at x = 3.75 mm). The z-strains increased as the layer height gets refined, indicating the need for a more accurate heat input model once computational layer height gets closer to the physical process value.

input is necessary in order to produce the correct thermal gradients and subsequent stress/strain results. However, it is worth observing that the 0.25 mm simulations produced the most accurate results near the top surface for the x and y strains. The 1 mm and 0.5 mm results bend the opposite way of the experimental results at the uppermost point. This can likely be explained by the lack of thermal cycles experienced near the top surface for the coarser meshes, as contrasted with the physical process.

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Remark: Running simulations at finer layer heights greatly increased the computation time, such that it was not feasible to run at layers finer than 0.25 mm with the current simulation framework. For comparison, the baseline simulation at a 0.5 mm layer height required 5.25 hours using 32 processors (168 cpu-hrs), while the simulation with 0.25 mm layers required 50.8 hours using 144 processors (7,315 cpu-hrs), a 43-fold increase in cpu-hrs.

5.3. Thermal studies of continuous and island scans

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Perhaps the most interesting observation from the experimental measurements is the presence of higher residual strains/stresses, especially near the part boundaries, when using island scan strategies. This at first

appears counter to the conventional wisdom of islands helping reduce residual stress, though a recent study by Ali et al. [46] also found increased residual stress when using island scans for Ti-6Al-4V. One possible reason that island scanning may produce higher residual stress than continuous scans is due to the extra mechanical constraints that may be imposed by island scans [47]. With continuous scan strategies, there is always a free surface bordered by unconsolidated powder where the material is free to expand/contract as necessary. However, this free surface is not always present during island scans. For example, consider the scenario where the laser scans over an island that is surrounded by neighboring islands which have already been scanned. In this scenario, there are solid boundaries on all sides of the island being scanned. This

creates extra mechanical constraints which would contribute to increased residual stress.

Figure 11(b) shows the norm of the thermal gradients. This is defined as,

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Another possible explanation for the observance of higher strains near the edges of the bridge may be attributed to the presence of "mini-islands" near the part boundaries. These mini-islands are a result of the 1 mm x - y island shift per layer and the necessity for the scan strategy to stay within part bounds. A simulation was set up to model the thermal effect these mini-islands may have near a part boundary. This simulation was run at the actual process scale using the physical process parameters (see Table 3). A 495 Gusarov-type beam [19] was used for this simulation to provide a more accurate heat source model (see [14] for full implementation details within Diablo). The temperature of a node located 3 mm above the baseplate and 0.5 mm from the edge of the part was tracked for three representative scenarios: a full island (2.5 mm x 2.5 mm), a half island (1.25 mm x 2.5 mm), and a continuous scan with 5 mm track length (as used in the continuous scan strategy at 90°). The results of this study are shown in Figure 11(a). The temperature 500 plot shows an increased cooling rate and lower "plateau" temperature for the half island case, which can be explained by less heat buildup from prior scans. The higher cooling rates can lead to higher thermal gradients and increased residual stress. Additionally, the lower plateau temperature can also lead increased stress due to an increased yield stress and hence ability for the material to store elastic strain energy.

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$$\|\nabla T\| = \sqrt{\left(\frac{\partial T}{\partial x}\right)^2 + \left(\frac{\partial T}{\partial y}\right)^2 + \left(\frac{\partial T}{\partial z}\right)^2},\tag{22}$$

where the partial derivates of temperature are evaluated using a central finite difference scheme. The thermal gradient norm starts at an increased value as the powder is initially at a slightly lower temperature than the recently consolidated material beneath it. This temperature equilibrates some causing the decrease in thermal gradient until heat from the laser reaches the tracked node, increasing the gradients. From this plot it is clearly observed that the half island case exhibits a higher thermal gradient after the laser has finished its pass and the part is slowly cooling down. This again can be attributed to less residual heat from previous

scans and would contribute to higher residual stress.

The notion of increased thermal gradients and lower interlayer temperatures leading to higher residual stress in Ti-6Al-4V is supported by the work of Denlinger et al. [48], which found that increasing dwell time between layers in a laser-based direct energy deposition process increased residual stress for Ti-6Al-4V



Figure 11: (a) Temperature history and (b) norm of the temperature gradient for a point located 0.5 mm from the part edge for a full island (2.5 x 2.5 mm), a half island (1.25 x 2.5 mm), and a continuous scan with 5 mm track length. The half island case exhibits an increased cooling rate and higher temperature gradient after the laser passes.

specimens. The results indicate that AM built Ti-6Al-4V contains less residual stress when it remains at elevated temperatures during the build process, likely due to smaller thermal gradients and the reduced yield stress of Ti-6Al-4V at higher temperatures.

Note that these temperature history results are shown when the laser is scanning over the layer above the tracked node, which is the last time the tracked node rises above the melt temperature. Additionally, 520 the thermal studies were performed on an isolated area surrounded by powder (i.e. assuming that the area surrounding the full or half islands had yet to be scanned). The continuous scan case was over a domain beginning 2.5 mm before the tracked node and 0.5 mm after it. Increasing the length of the domain scanned prior to the tracked node past this value did not yield any further differences in temperature history. Finally,

it is important to remark here that these are merely possible explanations of the increased strains found when 525 using island scans. Additionally, these findings are likely material and geometry dependent, and thus should not be viewed as a general observation. Further investigation is necessary before any definitive conclusions can be drawn.

6. Conclusions

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The current work presents a method for simulating the residual stress build up in Ti-6Al-4V parts produced via laser powder bed fusion. A material model was developed to naturally capture the strain rate dependence of Ti-6Al-4V and annealing behavior at elevated temperatures, without requiring the tuning of an unphysical stress-free temperature. Synchrotron X-ray diffraction measurements were performed on four bridge-shaped specimens produced with different scan strategies to determine the residual elastic strains present in those parts. Comparisons between the measured and simulated strains showed mostly good 535 qualitative and quantitative agreement, but additionally yielded interesting insights into some of the current model's limitations. Finally, thermal parameter studies at the physical process scale provided additional insight into the observed strain differences resulting from different scan strategies.

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The agreement between the measured and simulated strain results allows for confidence in using the simulation results to visualize the complete stress state throughout the part, supplementing the measurements which were only performed along a single cross-sectional plane. However, from these measurements it became apparent that the layer and beam size agglomeration techniques used in this work were unable to fully capture scan strategy effects. Recognizing this, simulations run by heating an entire agglomerated layer at once produced a significant decrease in computation time while producing very similar results to simulations

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that actually followed the physical scan pattern with an agglomerated beam. This suggests that it is not worth the extra computational effort to actually follow the laser beam path when using 0.5 mm or larger computational layers and beam size.

Another significant outcome of this work was the measured presence of higher residual strains, especially near part boundaries, for the bridges built using island scan strategies. Potential explanations could be due to the extra mechanical constraints present during island scanning and the presence of mini-islands at the 550 part edges, which are produced by the path generation software to stay within part bounds. Simulations at the physical process scale suggest that higher cooling rates and thermal gradients are seen within these mini-islands due to less prior heat buildup from previous scans. Though further investigation of this finding is necessary and these results should not be generalized beyond the current material and geometry at this point. 555

The authors are currently pursuing spatially and temporally adaptive techniques to allow for higher fidelity simulations to be run in tractable times. These higher fidelity simulations, combined with a more physical representation of the heat input, should be able to more accurately capture differences in scan strategy and other process parameters. This seems to be the direction industry is moving as well, as some of the commercial codes appear to be moving away from the quick, elastic-only inherent strain approach, and toward coupled thermomechanical elastoplastic simulations. Ultimately, the need still exists for a fast and accurate thermomechanical solver able to predict process parameter and scan strategy effects in minimal time, for any geometry, such that potential issues could be mitigated during the course of a build. The authors believe that properly formulated adaptivity in both space and time will be required to eventually meet this goal.

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