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Editorial: Advances in computational modeling of additive manufacturing processes

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Editorial on the Research Topic

Advances in computational modeling of additive manufacturing processes

Metal additive manufacturing (AM) is an emerging technology enabling the manufacturing of highly complex geometries with location-specific properties. The multiphysics and multiscale nature of metal AM processes pose significant challenges for comprehensive process models of coupled physical phenomena occurring during and after fabrication. While novel experimental techniques, such as dynamic transmission electron microscope, *in situ* X-ray imaging and diffraction, and high-speed thermal imaging, have significantly advanced the understanding of the fundamental physics in AM, computational modeling has been playing an increasingly significant role in addressing the process-structure-property relationship with discovering the qualitative interactions of complex physics at different temporal and spatial scales. Advancement in computational models, ranging from macroscale models for thermal stress and materials properties, mesoscale models for powder spreading/deposition and melt pool dynamics, and microscale models for solidification microstructure and solid phase transformation, has been made in recent years. This Research Topic seeks contributions to developing effective process models for AM development and implementing models for AM materials development.

Computational efficiency has been one of the main roadblocks in using physics-based process models to study the entire history of the AM fabrication process. Three of the four articles in this Research Topic address how to effectively simulate the thermal history and residual stress in metal AM processes. The conventional method has been to mimic the laser movement with mesh activation, which requires fine mesh with small time steps. The computational cost is relatively high. Nain *et al.* firstly validated the classic Goldak's double

ellipsoid laser heat source model for the Directed Energy Deposition (DED) process by applying the conventional method using COMSOL™. The predicted thermal history at selective points in Stainless Steel 316L thin wall matched the experimental results with model calibration. To address the computational time, an elongated ellipsoid heat source model that averages the heat source over a given length of the laser track was implemented to replace the transient laser movement, where large time steps can be applied. Their numerical study suggested that by increasing the length of the ellipsoid heat source, computation time reduces exponentially, however, with growing computation errors. A parametric study indicated that with the right heat source length, the computational efficiency could increase up to ten times while keeping the relative temperature error below 10%. Moreover, a correction factor was introduced to reduce further the computation error, which was estimated as a function of the heat source length. This study confirmed that transient thermal history could be accurately modeled by introducing an effective heat source with additional corrections.

With a similar concept, Tangestani et al. independently developed a hybrid line heat model that integrates a 3D Gaussian distribution heat source over a defined time increment based on the laser movement for the laser powder bed fusion (LPBF) process. The Part I of the study validated the beam-scale model by comparing experimentally measured melt pool sizes of nickel-based superalloy RENÉ 65 under a wide range of process parameters. Compared with the beam scale model, the newly proposed hybrid line heat model exhibits lesser accuracy in predicting the melt pool geometries and the peak temperatures. However, the relative error for cooling rate and the nodal temperature after solidification was below 5%. An incremental step of twenty times the laser beam diameter was used to demonstrate the method. The hybrid line heat model was shown to be more than 1,500 times faster than the beam scale heat model. It is a significant computational gain in simulating the thermal history in the LPBF process. The computational efficiency of the thermal model allowed the prediction of the thermal history line by line via the laser scanning strategy. With the validated accuracy of nodal temperature history below solidus, the Part II of the study is to sequentially couple the thermal model with the ABAQUS™ mechanical model to study the residual stress in thin-wall structures in LPBF. The simulations of the beam-scale and hybrid line heat models consistently showed good agreements with the experimental X-Ray diffraction measured residual stresses. The average variations between the beam scale and hybrid line models were below 3% for all time increments in the stress tensor components. Thirty times speed up was measured for the mechanical model with the case of an incremental step of twenty times the laser beam diameter. Further, the dynamic mesh-coarsening algorithm improves the computational time by a factor of 3.3, allowing parallel computation of the thermal and mechanical solutions. Such developments in both thermal and mechanical modeling provide a path to accurately predict the

residual stress variation due to laser parameters and scanning strategies at the part scale.

Targeting the process and structure relationship, Sjöström et al. coupled a thermal model with a thermodynamics model to understand the as-built microstructures in LPBF. The thermal history of 18Ni300 maraging steel under different process parameters was simulated using the MSC simulation software Simufact Additive. A one-way coupling was then performed to extract the temperature information needed for the Thermo-Calc software package to predict the elemental micro-segregation, martensite start temperature, and martensite fraction. Although with limitations in addressing the detailed thermal history at the melt pool level, neglect of defects, and residual stress, the study demonstrated a powerful modeling tool to link process parameters, e.g., laser speed, laser power, heating efficiency, and baseplate temperature, to the as-built microstructure information during the printing of alloys in LPBF. Their study showed that a higher energy density that causes increased cooling rates could lead to a more significant degree of micro-segregation within the cellular solidification structure, which, in turn, leads to lower martensite start temperature and more retained austenite at the intercellular regions. The model's further development could enable the two-way coupling to accurately study the stress evolution and microstructure formation in LPBF.

The Research Topic of the original articles compiled in this Research Topic touches on the key challenges of computational modeling of AM processes. They offer exciting pathways to study detailed physics at different temporal and spatial scales with improved computational efficiency and data exchange across the scales.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

Conflict of interest

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