

An Indian-Australian research partnership

Project Title: **Machine learning accelerated finite element squared multiscale solvers for additive manufacturing simulations**

Project Number **IMURA0952**

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Research Clusters:

Research Themes:

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The research problem

There has been significant research in additive manufacturing (AM) as a viable and efficient manufacturing technique for metallic systems. This is primarily due to its relatively lower costs and faster processing times. Furthermore, one of the most promising benefits of AM is the goal-oriented design of new materials, since it provides a tremendous flexibility in the definition of the microstructure through the tuning of process parameters. However, to move from prototypes and demonstration 3D models to real industrial use, one must certify the quality of the outcomes. Certification is based on extensive experimental testing. It is both expensive and time-consuming, lowering the AM potentials. Virtual certification through advanced simulation tools linking the AM process with the component performance are required to eventually unlock the full potential of this technique.

A deep knowledge of the microstructure of the material being generated is required to link process and performance. However, due to the inherent variability in microstructure and properties of the AM materials, process-structure-property relationships have not been established systematically for these materials. Furthermore, due to the extreme heating and cooling rates involved, predicting these properties from models/simulations remains a challenge. Another challenge with modelling these processes is due to the fact that change in state of the material occurs from liquid to solid and involves further phase changes as the material reaches its final state. Due to the said state and phase changes, residual stresses develop in the material, which are detrimental to its subsequent mechanical properties. However, the numerical approximation of these multiscale phenomena is unaffordable, usually involving a finite element microscale solver per Gauss point in the full scale finite element model.

Project aims

The long-term objective of this research collaboration is to provide an advanced scientific computing framework able to produce high-fidelity simulations linking process and performance in a time scale compatible with the desired time-to-market of AM products. It involves the design of a multiscale physics-based thermo-mechanical finite element modelling framework that combines (1) a macro-scale thermo-mechanical solver for the process simulation that will provide the thermal history and residual stresses; (2) an accurate description of the melt pool region and its surrounding heat affected zone; (3) a phase-field solver that will use such information to predict the micro-structure morphology of the metal; (4) a crystal plasticity solver using this morphology to provide the mechanical response of the material; (5) a finite-element-squared solver that combines a macro-scale mechanical solver with the crystal plasticity model to take into account the micro-structure morphology at the performance simulation of the AM component; (6) deep neural network approximation of the micro-scale solver in order to make simulations computationally feasible. Fig. 1 illustrates the ultimate multiscale solver that we want to develop. Currently, Prof. Badia and his team, in collaboration with Prof. Davies (at Monash), have already developed and validated thermal solvers for the thermal simulation of the process (part (1)). They also have developed solid mechanics macroscopic solvers (i.e., part of (4)). The accurate simulation of the so-called heat affected zone is the objective of a PhD thesis being carried out by Mr. Eric Neiva under the supervision of Prof. Badia.

This thesis will focus on ingredients (2)-(5), i.e., phase field and crystal plasticity models, which represent the micro-scale part of the final AM solver, the finite element-squared model and the deep neural network-based acceleration. This part will benefit from the expertise of Prof. Patra in the modelling and discretization of these phenomena. For addressing these issues, the proposed modelling framework will have the following features:

1. Crystal plasticity constitutive equations for modelling the deformation behaviour under the influence of the said residual stresses and also the post-processing mechanical properties. Deformation in these metallic systems is mediated via dislocations and crystallographic deformation mechanisms needed to be accounted for to accurately capture the orientation-dependent microstructure evolution and mechanical properties. Since one of the main limitations of AM objects is the poor properties under fatigue, we will use models that will accurately predict this behaviour.
2. We will consider PF models to determine the solidification microstructure, e.g., by using the Cahn-Hilliard model. Residual stresses will be incorporated through the introduction of elastic strain energy and plastic dissipation in the solid phases. Another essential aspect to be considered in the certification of AM is the effect of microporosity on fatigue. Microporosity appears when the solid fraction in the mushy zone increases and the liquid is not able to flow freely to compensate shrinkage. In this sense, we want to consider multiphase-field models with a pore phase, taking into account pore-liquid interface curvature to include pinching effects. To reduce complexity, binary alloys will be used in first stages, e.g., Ni-Nb as a simplified representation of Inconel. With regard to numerics, unfitted spline-based spaces are perfectly suited for PF, which involves fourth-order derivatives, thus requiring C^1 -continuity. The already available adaptive octree meshes will be essential to efficiently capture interfaces. The PF model microstructure will be parameterized with respect to grain size distribution, grain shape (elongated vs equiaxed) distribution, grain orientation distribution (texture), porosity, and residual stress distribution. These parameters will be used to determine synthetic microstructures, representative of PF microstructures, through statistical distributions, which will be used by CP models.
3. Model validation: Model predictions of both the microstructure evolution and mechanical properties will be validated with relevant data available in the open literature. Specifically, microstructure characterization data of AM grain morphologies will be used to validate the phase field predictions, and post-build mechanical property data will be used to validate the crystal plasticity predictions.

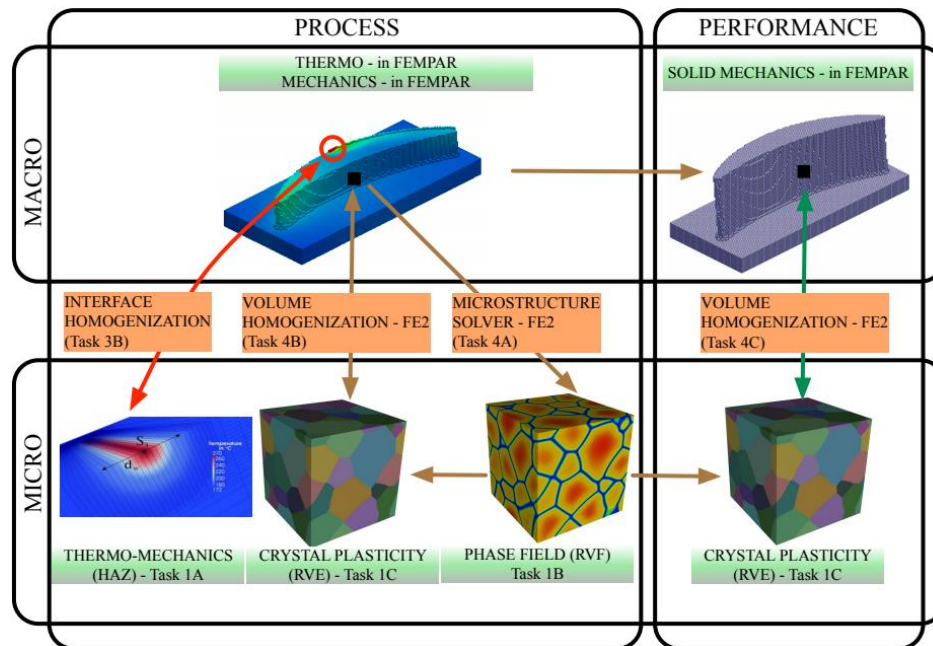


Illustration 1: Towards a multiscale finite element framework that links process and performance. This thesis covers the PHASE FIELD solver and its interaction with the CRYSTAL PLASTICITY model (tasks 1B and 1C in the figure).

Expected outcomes

The novelty of this proposed research lies in that a unified framework for modelling both the processing and mechanical properties will be developed for the first time. The modelling framework can be used to predict the process-structure-property correlations in AM materials and guide relevant experiments and manufacturing processes.

How will the project address the Goals of the above Themes?

The project addresses the “Advanced Computational Engineering, Simulation, and Manufacture”. As stated above, its expected outcome is to develop unprecedented computational tools for additive manufacturing simulations.

Potential RPC members from IITB and Monash

Prof. Chris Davis (expert in Additive Manufacturing, Monash, chris.davies@monash.edu)
 Prof. K. Narasimhan (expert in forming simulations of metals, IITB, nara@iitb.ac.in)
 Prof. P.J. Guruprasad (expert in finite element method and crystal plasticity, IITB, pjguru@aero.iitb.ac.in)

Capabilities and Degrees Required

An ideal candidate should have a Bachelors and/or Masters degree in Materials Science/ Mechanical/ Aerospace Engineering/ Mathematics/ Physics. Experience in at least two of the following three criteria is desired:

- Background in mechanics of materials;
- Expertise in numerical methods for PDEs (finite element methods);
- Expertise in programming (Julia, Python, C, C++, Fortran, etc)

Potential Collaborators

Jerome Droniou (expert in numerical methods for PDEs, jerome.droniou@monash.edu)

Chris Davies (expert in Additive Manufacturing, chris.davies@monash.edu)

Ricardo Ruiz-Baier (expert in numerical methods for PDEs)

Indradev Samajdar (expert in thermomechanical processing and microstructure characterization, indra@iitb.ac.in)

Select up to **(4)** keywords from the Academy's approved keyword list (**available at <http://www.iitbmonash.org/becoming-a-research-supervisor/>**) relating to this project to make it easier for the students to apply.

Computational Fluid Dynamics and Mechanics; Computer Simulation; Modelling and Simulation; Maths