Interlinking multiphysics and multiscale simulations with topology optimization in additive manufacturing processes

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Summary Even though process simulation for 3D printing have progressed substantially over the past decade and across multiple length-scale, the major issue is about how to link these simulations and then perhaps to combine these interlinked holistic models with topology optimization techniques for getting an improved design. Here the solution is the use of multi-scaling laws which are; homogenization, material multi-scaling and finally, process multi-scaling. The first two multi-scaling techniques allow for extracting macroscopic properties of an entire part based on the data generated by process simulations at lower dimensions, namely micro- and deposition-scale models while process multi-scaling methods enable fast and robust computation of a real-size sample and such models can be improved by involving the material multi-scaling calculations into them. Finally, this holistic model can be incorporated into the topology optimization calculations for a far better design of a part with ultimate no sign of a process-induced defect, under the flag of physics-aware topology optimization.

MANUSCRIPT

Additive manufacturing (AM) or 3D printing has proved itself as a superior manufacturing method in the 21st century when it comes to flexibility and production of complex designs. AM is envisioned to be one of the main pillars of the 4th industrial revolution. An important sub-branch of AM, metal AM, has also shown its strengths and capabilities in various industries such as aerospace, medical, energy, injection moulding, etc. There are many factors that make AM a unique process and one of which, the most notable one, is AM's unmatched freedom in manufacturing complex geometries. For instance, in the injection moulding industry, sophisticated cooling channels cannot be manufactured by means of conventional subtractive-based production methods, especially when it comes to drilling helical channels embedded in a metallic block. While, AM and metal AM (MAM) specifically allow for producing such complex geometries.

Apart from the mentioned engineering mindset-based solutions, MAM has opened a new paradigm allowing for advanced computational design methods to be integrated within the manufacturing loop. Topology optimization (TO) is one of the most successful computational design methods that predicts the part geometry based on a number of input parameters or optimization objectives. Examples can be for instance optimal heat sinks for minimizing an underlying electronic chip's temperature [1], a flow mixer in the laminar domain [2], a mechanical bracket with maximal stiffness at a minimum mass, etc. TO'ed components are, however, extremely difficult to process using conventional production methods and again, only AM or MAM can realize such advanced geometries.

After listing number of pros of AM/MAM processes, it is worth noting that there are several difficulties associated with manufacturing parts using these processes. AM and in specific MAM have a very narrow and limited process window that makes it very cumbersome to identify the proper set of process parameters just be the sole use of experimental investigations. Therefore, advanced numerical simulations have been considered as a powerful add-on that can reduce the number of trial-and-error attempts in experimentation substantially. As the defects or anomalies in MAM parts cover a wide variety, it asks for several types of numerical simulations to model these defects to unravel the main causation mechanisms thereafter.

Figure 1 shows an overview of the defect types typically observed in MAM components and one can accordingly categorize these defects into three distinct categories of micro-scale, deposition-scale and part-scale. In micro-scale models, the aim is to predict the growth and formation of micron-size instances such as dendrites or grains. There are several modelling methods that allow for simulation of dendrites and grains, one can for instance point out to the Monte-Carlo Pox (MC) method, cellular automata (CA) method and finally the perhaps the most complicated one, the phase field (PF) model. On a higher length-scale there is the deposition-scale models and similarly to the micro-scale models, they also have several sub-categories and branches. Deposition-scale models are primarily divided into three classes of; powder-gas dynamics models where the focus in only on the interaction between the powder particles and the gas phase, melt pool dynamics models that focus on simulating relevant physical phenomena in the vicinity of the deposition site and finally, fully coupled models where the two aforementioned sub-categories are combined. Melt pool dynamics models constitute the largest fraction of deposition-scale models and have several types depending on the physics involved and the level of complexity e.g. flat surface models, large surface deformation model, etc [3].

As these models are quite computationally heavy, running such a simulation on an entire part is impossible while maintaining a sufficient mesh resolution to be able to resolve the laser beam. In this situation, part-scale simulations are a remedy [4].

However, currently the gap in the literature is not on advancing these three modelling branches, namely the micro-, deposition- and part-scale independently or separately, but knowing how to link these models by means of proper multi-scaling approaches. There are three types of multi-scaling implementations: material multi-scaling (integrated computational materials engineering – ICME), homogenization and finally, process multi-scaling. The objective of the first two multi-scaling techniques is to extract macroscopic properties from a local and detailed micro- or meso-scale simulation, whereas the task of the process multi-scaling is to ease the computation of the process simulations at part-scale [5]. These process multi-scaling simulations could be updated based on material multi-scaling techniques while getting data from lower scale models (micro and deposition-scale) and then process multi-scaling can be subsequently used for running an updated TO simulation where the process constraints are accounted for. One instance of this entire holistic computational design is shown in **Figure 1** and one can notice the stark difference between using a conventional TO and the use of an updated TO or the so-called physics-aware TO with process constraints that takes information from an updated part-scale simulation.

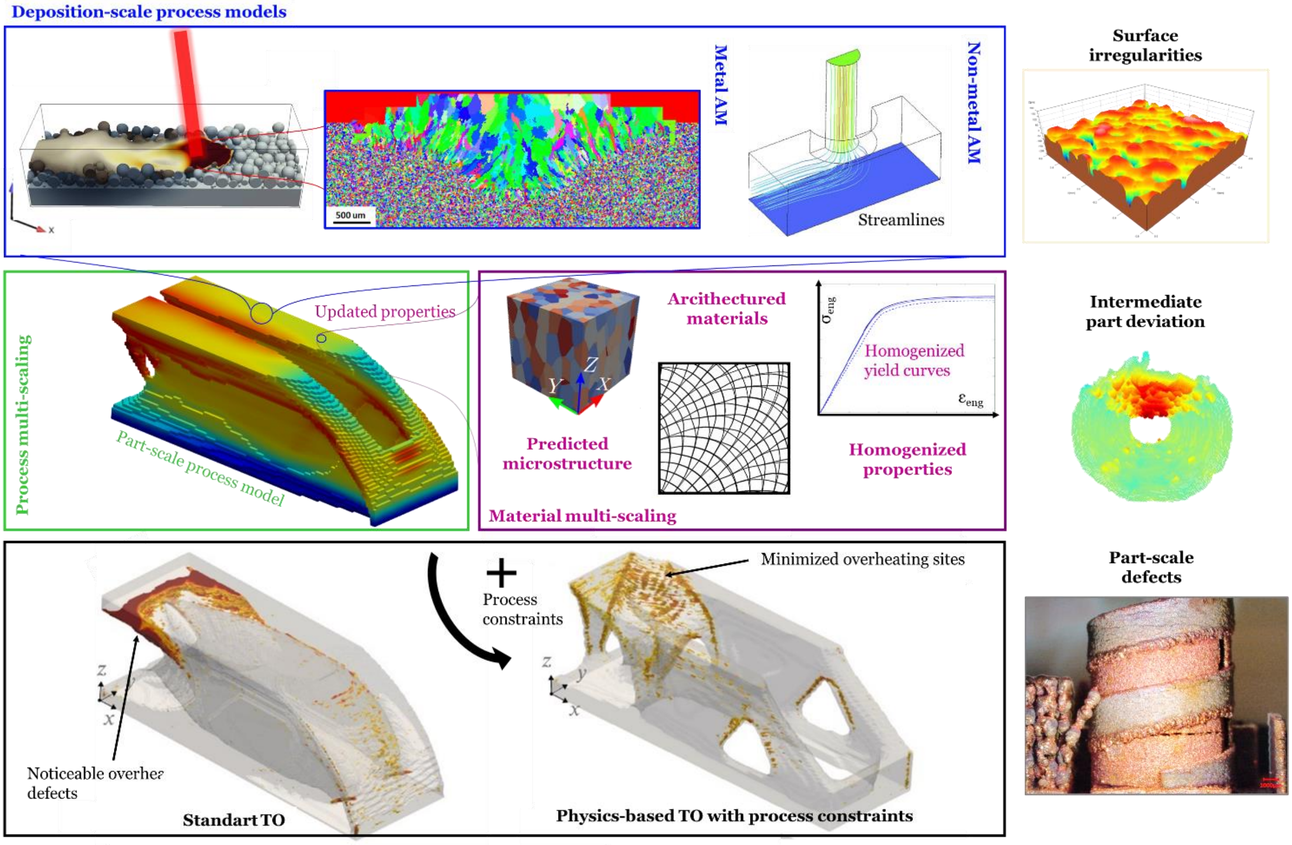

Figure 1: An overview of the holistic computational design for AM where lower-scale models such as micro and deposition-scale simulations are interlined within larger dimension models through multi-scaling techniques. Then part-scale models can be incorporated into TO for getting improved designs without process defect signatures as shown in the black box on the right hand side.

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