

A review of Computational Modelling of Additive Layer Manufacturing – multi-scale and multi-physics

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Abstract This paper presents a review of the state-of-the-art in computational modelling of the Additive Layer Manufacturing (ALM) process, with a description and examples of models being developed at Swansea University, and a comparison to efforts from other commercial and academic organisations.

As a process, ALM is strongly based on computational control and the production of net-shape parts, computational modelling is being used to understand and improve the process, as well as to create new and optimised functionality of components.

Modelling efforts range from discrete element models of powder flow, to micro-and macro-scale models of the laser melt-pool, coupled thermal-structural models to predict residual stress, and automated optimisation methods for the development of new components. Modelling can also be used at a microstructural level for the prediction of the bulk properties.

In all instances, the modelling is used with the purpose of increasing understanding to address known problems of the ALM process. Thus, as examples, residual stresses arise in metallic parts due to the requirement of building each layer from a base-plate with supports, and modelling can help reduce and optimise the support layout to produce as-built parts with minimal residual stress for maximum strength and minimum distortion. Understanding the heat transfer at the level of the melt-pool helps to reduce porosity and gas entrainment, as well as control the local heating rates which affect the formation of balling, which has been linked to surface roughness and also to porosity.

If one looks at the evolution of computational models for casting as an indication of the way in which computation of modelling of ALM could be going, one of the long-term, but most highly coveted achievements would be a full process model, which allows the integration of micro- and macro-models of the process, with life-time component property prediction and the capability of simulating design and manufacturing iterations for a final component with optimised functionality.

1 Introduction

Additive layer manufacturing (ALM) encompasses a variety of different techniques combining laser and Electron Beam Melting (EBM) with a powder bed, Wire and Arc Additive Manufacturing (WAAM), Selective Laser Sintering (SLS), Laser-engineered Net Shaping (LENS) and Direct Laser Deposition (DLD), as well as processes which are specific to plastics, such as Laminated Object Manufacturing (LOM) or Stereolithography Apparatus (SLA). An in-depth comparison and historic

evolution of these systems is given in the Wohler report 2012, [1], and a recent description by the same authors of industry trends can be found in [2].

A common background of these techniques is that they are, as a manufacturing process, undergoing a rapid evolution from a welding-based or rapid prototyping background into manufacturing processes in their own right, suited to low-volume production of components over a wide range of applications in the aerospace, automotive and medical sectors.

As a whole, ALM technologies are hailed as an interruptive or step-change technology opening up the freedom of design space by being able to go almost directly from Computer Aided Designs (CAD) to net-shape finished product, at the touch of a button. With sufficient penetration, this type of technology could have a significant impact on both the environment and on sustainable manufacturing, with large reductions in material wastage, more intricate, highly integrated components with optimised improvements (e.g. light weight, improved heat transfer characteristics). From the perspective of increased competitiveness, ALM offers lower cost components, more rapid product development and flexibility for the companies.

However, there are many challenges to be overcome to increase the acceptance by industry. These range from business considerations (e.g. limited build speed and sizes) to technical or inherent differences in the process from industry standards, which manifest themselves in the as-built material properties. When compared with subtractive processes (machining, forging, forming), and in common with other net-shape processes (casting, moulding, powder compaction), there are process parameters which lead to porosity at various scales, these in turn affect strength and life properties of the components, but they can be controlled. Other aspects which are of concern to end-users are surface roughness, minimisation of residual stresses and anisotropic elasticity properties, which are related to build directions.

Computational modelling has a relatively important role to play in addressing these challenges, when compared with its role in other manufacturing processes. Firstly, the digital nature of the process combined with the high flexibility or freedom of design immediately places the onus on a virtual development of the design. This means that operators and industry almost expect a seamless and rapid development of the link between the preliminary CAD design stage and a final optimised part, which is optimal from both the process as well as a functional perspective. Comparing this requirement with the historical development since the 1980s of full through-process modelling of casting, [3, 4, 5, 6], would suggest that this is another area of ALM which needs cautious expectations management.

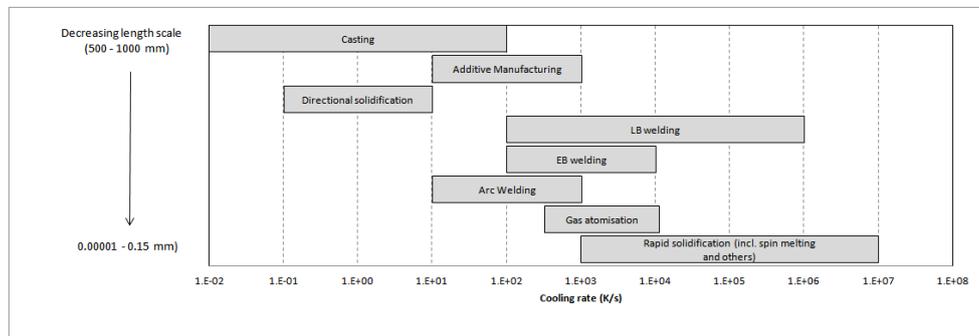


Figure 1 - Cooling rates for various solidification based processes, based on data from Elmer et al,[7], and Hofmeister et al, [8].

Another interesting aspect of ALM, from the perspective of computational modelling, is based on the manufacturing length scales. In a casting process, the local cooling rates are determined on a macroscale, thus directly linked to the size of the casting together with any thermal process control, such as mould pre-heating/cooling or feeder locations. Defects such as micro and macro shrinkage porosity and gas porosity across the length scales are often controlled to a certain extent through the manipulation of the filling, feeder locations and mould thickness – all of which are in range of centimetres. Simulation of the filling and solidification of a casting incorporating all of the heat transfer, fluid flow and solidification phenomena that conspire together to produce a final as-cast structure is an ambitious multi-scale numerical problem.

In comparison to casting, the manufacturing length scales of powder ALM processes are much smaller (0.1mm to 0.2mm) and closely related to the size of the melt pool, and solidification cooling rates are much higher, see Figure 1. Thus, in a multi-scale simulation, the linking across the length scales in which has always been quite difficult in casting simulations could be more achievable, and ultimately lead to the fabrication of components with designed microstructures.

There are a number of key areas which are being looked at using computational modelling, namely:

- 1) Thermal modelling of melting and solidification
- 2) Residual stress modelling
- 3) Topological and shape optimisation of components

2 Thermal modelling of powder melting and solidification

This is the fundamental modelling of the process during the application of the laser to a powder bed, the understanding from these models is helping to understand and control the levels of porosity as well as the formation of the microstructures giving an insight into the resulting material properties, from elastic anisotropy to tensile strength. The thermal history of a particular part is also the starting point for the residual stress analysis.

The majority of work which has been undertaken in thermal modelling either starts from a Fourier-equation thermal basis, or from a fluid-flow Navier-Stokes basis. In both cases, the length scale considered (μm , mm , cm) and the variation of physics involved means there is significant overlap between the various research groups.

Modelling is typically undertaken using analytical solutions, or numerical solutions using self-developed codes which are typically finite element, volume or finite difference based, or use commercial codes (ANSYS, FLUENT/CFX, ABAQUS).

The multiple physics which needs to be captured by a comprehensive model should include:

- 1) Melting and solidification
- 2) Free-surface re-construction, which will give an indication of residual porosity and might include compensation of shrinkage effects during solidification
- 3) Multiple phases liquid, gas and solid
- 4) Forced and natural convection of gas (argon) – this can be done by either conjugating the gas convective, advective or conductive heat transfer, or through heat transfer coefficient boundary conditions.
- 5) Laser beam as an energy source (either indirectly as moving thermal boundary condition or directly by radiative modelling).
- 6) Temperature dependent properties (thermal conductivity, density, specific heat capacity of solid and powder, radiative properties (absorption, reflectivity and emissivity), introducing significant non-linearity into the solution.
- 7) Temperature dependent surface tension of liquid metal in contact with powder, this property is typically approximated as data for specific alloys is difficult to obtain. However, it is an important property which determines to which extent the melt-pool flows are dominated by Marangoni convection, and the levels of capillary infiltration of the melt-pool into the powder-bed.
- 8) Alloy phase changes also can be incorporated which might identify regions of specific phases or even evaporative properties of alloys, this type of modelling might incorporate effects on the sub-micron level.

2.1 Macro-scale thermal modelling (mm to cm)

This is by-far the most common length scales at which modelling of the thermal characteristics of ALM is undertaken. Often based on previous work in welding during the late 1990s early 2000s, it is now routinely done for EBM, LENS, SLM. The Solid Freeform Fabrication Symposium has been run in Austin, Texas, USA since 1991, and publications in this symposium tend to be at the leading edge of AM developments, with researchers publishing similar work in journals a year or two later. From the proceedings, the progressive developments of models can be seen from the early 1990s with a sintering-basis, with empirical- and simple Fourier based sub-models, [9, 10, 11] to more complex 1-D models which integrate residual stresses [12], and 3-D thermal models, e.g. by Flach et al, [13], mainly for plastic material based processes (e.g. LOM, SLA).

Some preliminary 1-D and 2-D thermal-residual stress modelling work with a laser welding basis is used as an indicator of the application of the modelling to metal powder-based systems by Klingbeil et al, [14].

One of the original macro-based models on a ceramic powder melting process by Dai et al, [15], which was done using ANSYS FE with relatively large 2mm elements to predict thermal and residual stresses. The residual stress technique in ANSYS is the well-known element birth-and-death techniques described in more detail in section 3 of this paper. This year also saw the development of simple 1D finite volume models [16] for metal powders, to understand the relationships between laser beam diameters, laser power input and duration on melt depth and re-solidification time. Another paper that year by [17] presented a macro-model to DMLS using ESI's 2D and 3D Finite Element based model SYSWELD on a 0.4 cubic mm part that was analysed thermally and for residual stresses, using a parametric sensitivity analysis.

A 2D finite volume method treating metal powder as a continuum was used by Cheng et al, [18] and [19], to understand the penetration of re-melting upon existing layers below the sintered layer, as a function of laser scanning velocity.

In [20, 21, 22], Dai et al further develop their 3D ANSYS thermal model for ceramic powders, and obtain a good correlation to experimental temperatures obtained by pyrometer, and which are subsequently linked by post-mortem to microstructures and temperatures.

As a slight divergence from the powder-bed based system, blown powder deposition is modelled by [23] in 2D axis-symmetric, self-developed code to improve the design of coaxial nozzle design, in a manner very similar to gas atomisation models. Again another digression into blown powder methods, specifically LENS by Wang et al, [24] and DLD by Liou et al, [25], focuses on the comparison between modelling and experimental data with a good correlation. The work was generally inspired by the perceived lack of fundamental thermal verification data slowing the advancement of residual stress modelling and microstructural based property predictions.

Modelling of the Scanning Laser Epitaxy (SLE) process was done by Acharya et al [26] in 3D using ANSYS CFX, with a laser beam radius of 0.75mm, and 3.5 cubic mm melt zone thermal maps were used with a Columnar Equiaxed Transition (CET) model to understand the dendritic growth mechanisms, and predict the underlying solidification microstructure. From this study, it was shown that omission of Marangoni convection would increase the melt pool dimension by up to 10%, with a critical knock-on effect on the prediction of microstructural boundaries between Columnar Equiaxed Transition (CET) to Oriented to Misoriented Transitions (OMT).

A model of the selective laser sintering of nylon powder was presented by Diller et al, [27], in which the commercial code ANSYS FLUENT was used with a number of advanced physical modelling attributes, as well as comparing to thermal imaging data, with a moderately-good thermal correlation. The intention of this work was to use modelling output as a guide for a programmable heater control in the machine.

An interesting study coupling 3D FEM software ABAQUS and a design of experiments is undertaken by Cheng et al, [28], on the Electron Beam Melting process using the metal powder Ti-6Al-4V. Although the correlation of the measured and simulated temperatures was poor, the approach holds significant promise for the development of a process envelope for quality control.

A good review of previous modelling efforts generally is given by Zeng et al, [29], themselves also including their own 3D ANSYS-based thermal macro-model. They conclude that whilst a large amount of development has taken place in thermal modelling, further work is needed in analytical/parametric control-side algorithms. This review also concludes that further work is required at the smaller length scales, i.e. the micro- and meso-length scales, which is the subject of the next section.

2.2 Micro- to meso-scale thermal modelling (μm to mm)

The computational modelling at this length scale tends to primarily incorporate the full thermo-fluid dynamics of the melt pool with a free-surface, which may treat the powder as discrete particles or as a continuum. In terms of numerical solutions, this can be done using self-developed finite element, volume or difference schemes or commercial codes such as ANSYS FLUENT/CFX.

A more recent development is the application of the Lattice-Boltzmann method to laser powder-bed AM modelling. Whilst LB method has not had the commercial development in computational fluid dynamics that has been seen in finite element, volume and difference based packages, it actually has a number of advantages over these more traditional approaches. The first is that it is “meshless”, so does not require complex mesh, or grid based software to be able to handle complex geometries. It has a relatively simple implementation, and adding more transport equations does not necessarily make the codes more complicated. It is highly parallelisable, and by nature time-dependent, so transient problems are handled naturally. On the other hand, the LB methods also suffer from a number of problems. The definition of boundary conditions can be complicated, often posed in non-dimensional units, have a less physical basis than those used in traditional methods. Also, there can be loss of continuity during the solution. Furthermore, the discrete nature of the underlying grid means that surfaces tend to be of a discrete nature, and prone to step errors as with the finite difference method.

One of the first applications of LB to laser-based powder bed was by Attar et al, [30, 31, 32], and more recently by Markl et al, [33], all focussing primarily on the Electron Beam Melting process, however, the principles of the method are equally applicable to lasers based systems with appropriate consideration of the heat flux distribution and penetration into the powder.

In addition to the standard questions being asked from modelling, such as what are the peak temperatures and melt-pool dimensions, some other questions which can be specifically posed to the micro-models are:

- 1) Can they predict the occurrence and reasons for existence of the various types of porosity?

- 2) Can there be porosity based upon internal or external gasses, hollow particles already existing within the metal powder, or inter-particulate void gas?
- 3) At high laser energy input with larger melt-pools taking longer to solidify, is there a potential for shrinkage to create porosity or voids, which are not necessarily filled with gas? Can keyholing take place, as is known to happen in welding applications?
- 4) What are the dominant melt-pool mechanisms of mass transfer: temperature dependent surface tension (Marangoni convection), temperature dependent density (thermal convection), and thermo-capillary forces?
- 5) Can argon be entrained by convection into the melt-pool, and remain trapped during solidification?
- 6) Can micro-models be used to predict the resulting microstructures, including phases and orientations?
- 7) Is there any significant evaporative loss of elements by vaporization from within the composition of alloys?

3 Residual stress prediction

As it is necessary to have a thermal history of a built part in order to predict the residual stresses, a few of the publications mentioned in the previous section are also relevant to this section, namely Jiang et al, [34] and Dai et al [15]. One of the original macro-based models on a ceramic powder melting process by Dai et al, [15], was done using ANSYS FE and relatively large 2mm elements to predict thermal and residual stresses using the element birth-and-death techniques, which was also done for Selective Laser Sintering by Ibraheem et al, [35].

More recent work on parts built by SLM of powder metals has been done by Zaeh et al, [36], including a validation using Neutron diffractometry, and concludes that their models were adequate but could be improved by looking at more layers.

Generally, 2D and 3D finite element based simulations seem to be the preferred route, particularly 3D models for fidelity, but they come with a large overhead in computational model development and speed, particularly if the goal is to look at large real components. To this extent, similar limitations of the FE techniques have been found by Ding et al who are looking at Wire and Arc Layer Manufacturing [37], for particularly large components of the order of 0.5m. These researchers have managed an 80% reduction (60 hours) in computational time by replacing the transient thermal distributions with a steady state one, without any loss of accuracy in the residual stress predictions.

For powder-based AM systems, Mercelis et al, [38] have also been looking for alternative, faster and simpler empirical methods based on experimental data.

3.1 Multi-scale modelling (from μm to cm)

This section describes areas of thermo-physical modelling of AM which are considered to be at the cutting edge of developments, particularly in predicting thermal and residual stress distributions in AM parts using multi-scale modelling, i.e. joining it all together.

A successful implementation of multi-scale modelling would involve having multiple or adaptive discretisations, see Zhang et al, [39] – at the level of the melt-pool, a fine mesh/grid would solve for all the detail (including Marangoni recirculation and free-surface), and capture the laser thermal flux distribution with high fidelity. A coarser discretisation or background grid then acts to distribute the temperature through diffusion on the scale of the component and build chamber.

Recent publications by Pal et al, [40], describe meshing and solution strategies (e.g. based on eigenmodel solvers) being applied specifically to Additive Manufacturing processes in a way which is tens of times faster than the more-generic commercial packages. The ultimate goal of this work is to develop in-situ physical modelling which can run along-side thermal imaging control systems to optimise the build.

Keller et al, [41], described the multi-scale approach adopted within AIRBUS's Integrative Simulation and Engineering of Materials and Processes division (ISEMP), which includes a simplification of the layer descriptions and adaptive time stepping, but at the same time a stronger connection to the complete component through the machine-based sliced CAD. The group have three interconnected models, which they call the powder model (μm), the hatching model (mm) and the layer model (cm).

4 Case Studies

4.1 Case study 1 – Macro-modelling of the melt pool with Marangoni convection

In an excellent book by Gladush et al, [42], there is an entire chapter dedicated to mechanisms of laser processing of metal surfaces and specifically a section dedicated to selective laser melting. They make reference to previous publications by Gusarov et al, [43, 44, 45] that attribute the Marangoni or temperature-dependent surface tension variations to the onset of the Rayleigh instabilities which cause the melt-pool to break up, or “ball”.

Some preliminary sub-modelling has been done by the authors using FLUENT to isolate the importance of the Marangoni based convection as shown in Figure 2, where a 10mm wide laser beam is pointed at a 5mm metal substrate to induce a melt pool. The material properties used are given in Table 1. A time step of 0.01s was used for a total simulation time of 0.6s. The model is a 2D cross-section cut through the melt-pool with the beam pointing downwards and traveling into the paper.

It is important to stress that no gravity or buoyancy-based thermal convection was enabled, so that the re-circulation in the melt-pool is purely driven by temperature-dependent surface tension forces.

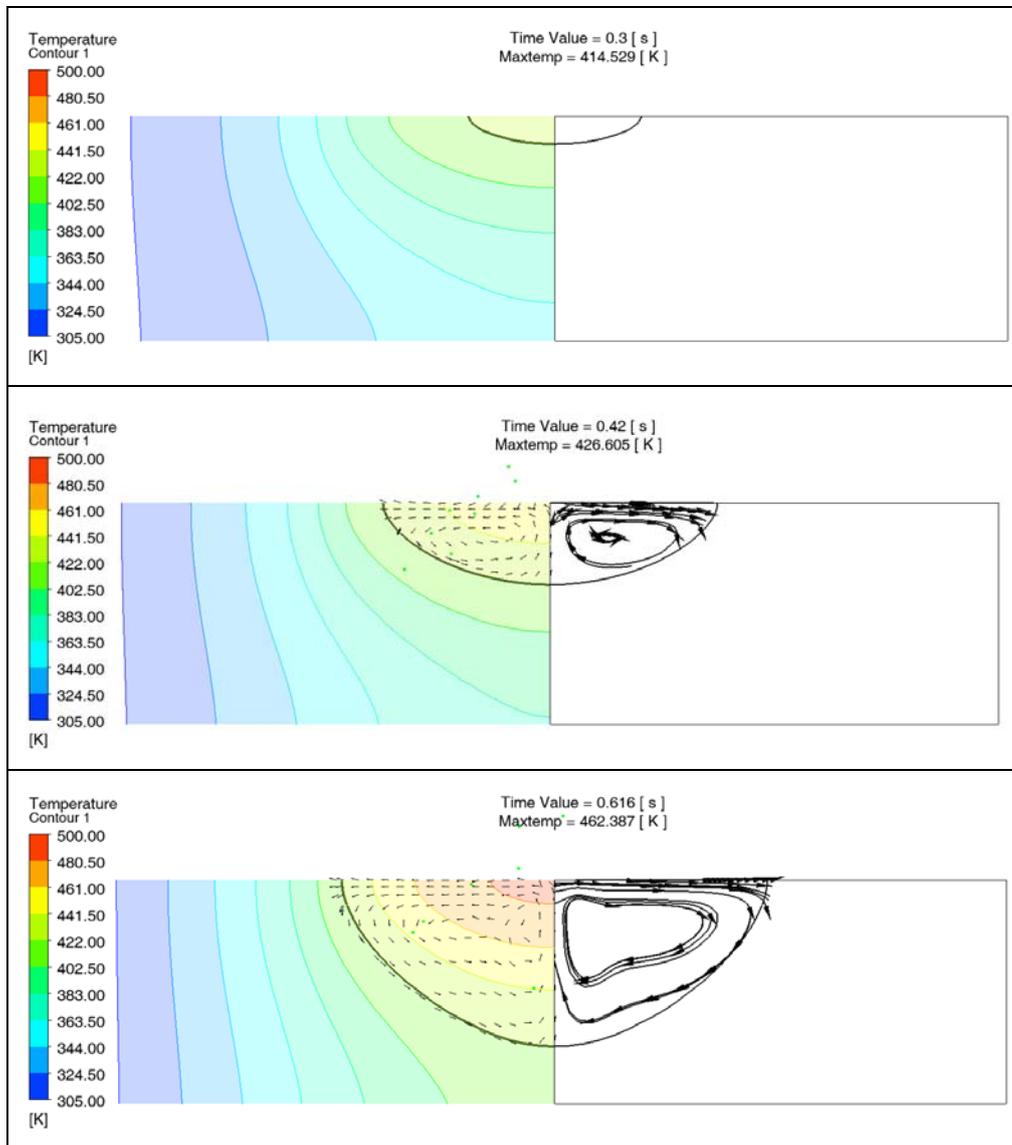


Figure 2 – 2D thermo-fluid modelling of the melt-pool at a macro-scale

As the laser is kept on, the size and temperatures of the melt-pool increases, and at about 14 degrees above the solidus temperature, the surface tension forces overcome the melt-pool viscous inertia to create a clock-wise recirculation zone.

Note, from the streamlines alone, it could be concluded that any low-mass or massless particles close to or emanating from the boundary of the melt pool would be entrained towards the centre of the melt pool.

4.2 Case Study 2 – FLUENT modelling of the powder melting at the micro-scale

An example of a micro-scale model being developed at Swansea University by the authors is shown Figure 3.

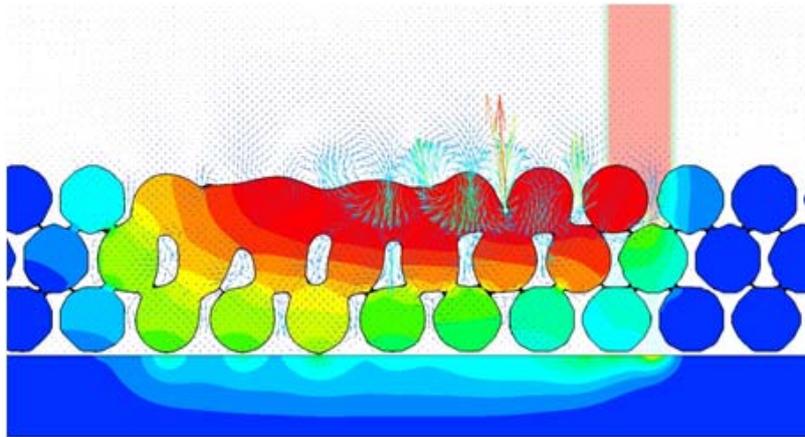


Figure 3 - Modelling using FLUENT of a metal powder melt pool

A 3-particle thick layer of closely packed mono-sized powder particles of 70 μ m diameter are melted by a pulsed 200W laser, with a 70 μ m focal diameter, as shown in Figure 4. This model comprises:

- 1) Melting and solidification – In FLUENT this is done using the Enthalpy-Porosity method of Voller et al, [46].
- 2) Free-surface re-construction, which will give an indication of residual porosity and might include compensation of shrinkage effects during solidification – In FLUENT, there are various ways to model the interface between phases, but only one of them, the VOF method works with melting and solidification.
- 3) Multiple phases liquid, gas and solid – In FLUENT, for a single metal material melting under a single gas shield, there needs to be three phases, all termed “liquid phases”, one representing the Argon, one the melt pool and the other the un-melted material. The solid phase is given a high value of viscosity and a cell-level source term resistance to make advection negligible.
- 4) Forced and natural convection of gas (argon) – this can be done by either conjugating the gas convective, advective or conductive heat transfer, or through heat transfer coefficient boundary conditions. In the above example, boundary conditions consist of Walls, Mass-Flow-in, Outflow. Above the powder layer, the right hand side boundary has a mass-flow-in, where a small 0.01 kg/s flow of argon is introduced, and allowed to exit via a outflow boundary condition on the left hand side boundary. The bottom boundary of the base plate can either be given a very high heat transfer coefficient (1000 W/m²K) or the temperature is fixed to ambient (300K), to simulate the very rapid cooling.

- 5) Laser beam as an energy source (either indirectly as moving thermal boundary condition or directly by radiative modelling). In the case above, the laser has been modelled using a moving source term along the top boundary, with the Discrete Ordinate radiative heat transfer model. This had to be programmed into FLUENT using User Defined Functions (UDFs).
- 6) Temperature dependent properties (thermal conductivity, density, specific heat capacity of solid and powder, radiative properties such as absorption, reflectivity and emissivity), introduce significant non-linearity into the solution. The material properties used for the simulation are given in Table 1, and it should be noted that the properties were not selected from a real alloy, but given a low melting point and wide freezing range to avoid long computational times in these preliminary simulations.
- 7) Temperature dependent surface tension of liquid metal in contact with powder, this property is typically approximated as data for specific alloys is difficult to obtain. However, it is an important property which determines to which extent the melt-pool flows are dominated by Marangoni convection, and the levels of capillary infiltration of the melt-pool into the powder-bed.
- 8) Alloy phase changes also can be incorporated which might identify regions of specific phases or even evaporative properties of alloys, this type of modelling might incorporate effects on the sub-micron level.

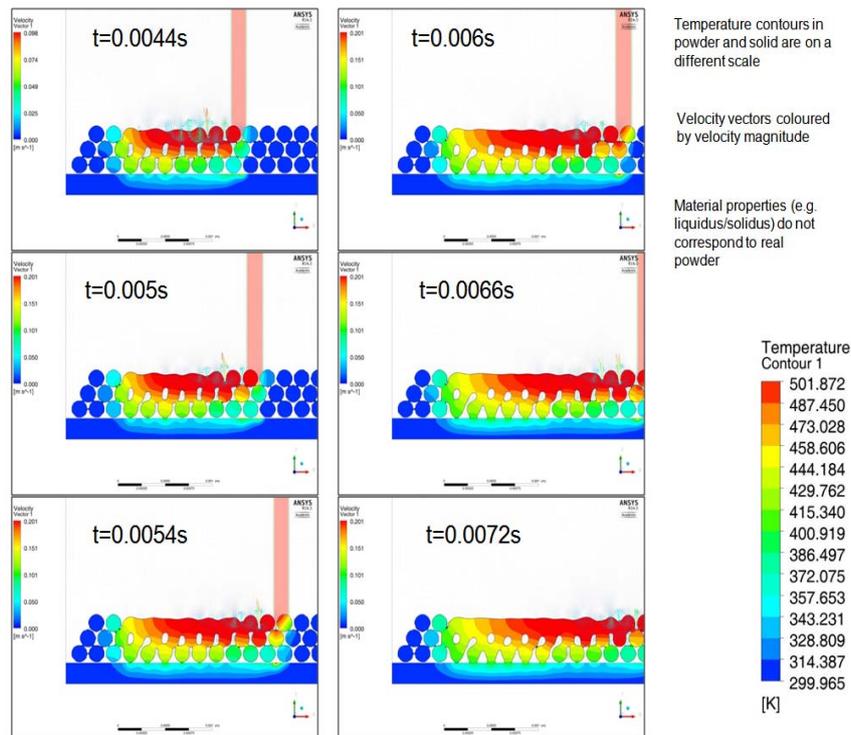


Figure 4 – Micro-scale modelling using FLUENT

Table 1 – Materials property requirements for simulations

| Property | Material/phase | Value | Units |
|------------------------|--------------------|-----------|-------------------|
| Density | Argon | 1.6228 | kg/m ³ |
| | Liquid metal | 4000 | kg/m ³ |
| | Solid | 7900 | kg/m ³ |
| Thermal conductivity | Argon | 0.0158 | W/m-K |
| | Liquid metal | 30 | W/m-K |
| | Solid | 30 | W/m-K |
| Specific heat capacity | Argon | 520.64 | J/kg-K |
| | Liquid metal | 680 | J/kg-K |
| | Solid | 680 | J/kg-K |
| Liquidus | Solid/Liquid metal | 500 | K |
| Solidus | Solid/Liquid metal | 400 | K |
| Latent heat | Solid/Liquid metal | 10000 | J/kg |
| Viscosity | Argon | 2.125e-05 | kg/m-s |
| | Liquid metal | 0.01 | kg/m-s |
| Surface tension | Argon/liquid metal | | N/m |
| | Liquid metal/solid | | N/m |
| | Argon/solid | | N/m |
| Absorption coefficient | Argon | | 1/m |
| | Liquid metal | 1000 | 1/m |
| | Solid | | 1/m |
| Scattering coefficient | All | 0.5 | 1/m |
| Refractive index | All | 0.1 | |

4.3 Case Study 3

Based on the algorithms developed by Attar et al, the authors have developed a stand-alone 3D Lattice-Boltzmann code in FORTRAN, results of which are shown in Figure 5, on a 100x100x200 element domain for 316L steel powder, laser power 200W, mean particle size 50 μm , layer thickness 100 μm , element size 5 μm , constant surface tension 1.65 N/m.

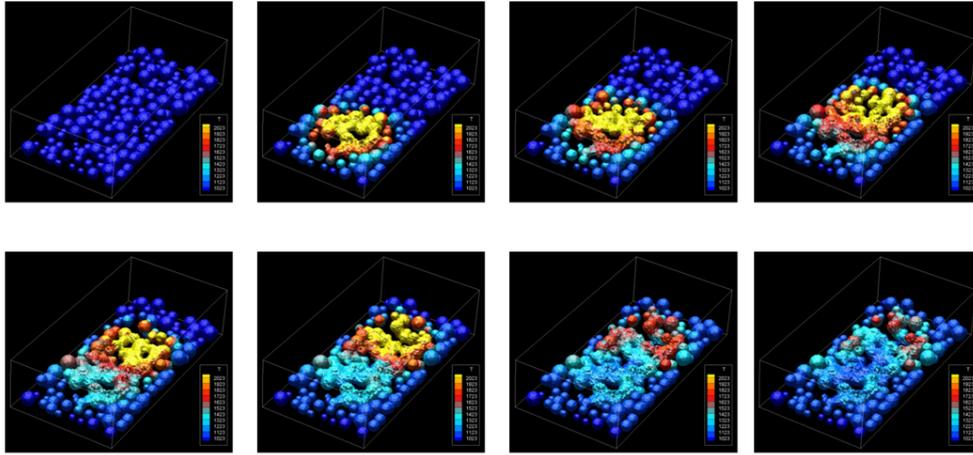


Figure 5 – 3D Lattice-Boltzmann simulation of a 316L stainless-steel metal powder being melted by a 200W laser

A 2D version of the code has been used to investigate the effect of laser settings on the predicted porosity of the final build. Figure 6 shows a graph of predicted density versus line energy, where line energy is calculated as laser energy divided by the velocity of the laser beam. The model is currently able to capture the increasing density with increasing line energy as observed in practice. However, at a certain point it is often observed that a maximum density is obtained in experiments and further increases in line energy lead to a small decrease in density. One possible explanation for this involves the role of Marangoni forces in and their tendency to retain gas bubbles within the weld pool (Figure 2).

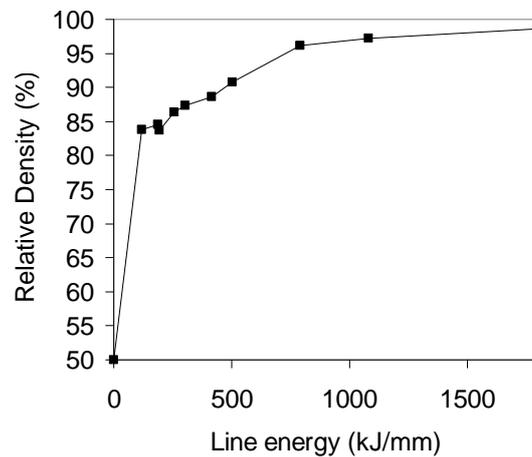


Figure 6 - Predicted densification curve for 316L from Lattice-Boltzmann simulations

Figure 7 shows two simulations for the same input parameters except the left hand figure has a temperature dependent surface tension (Marangoni convection) whereas the right hand figure has a constant surface tension (no Marangoni). An increase in melt pool size when Marangoni convection is present is evident. More work is required in this area to fully elucidate the effects of Marangoni convection on final porosity.

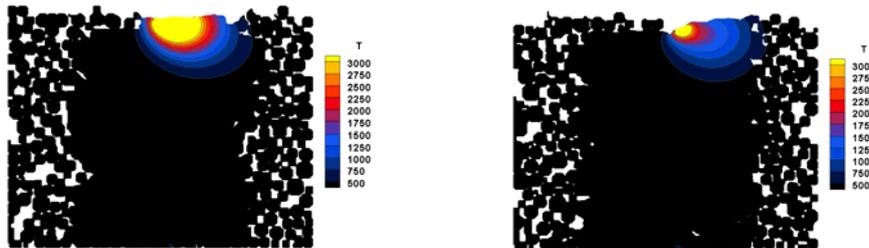


Figure 7 – Effect of including the Marangoni convection into the LBM simulations – note the increased size of the melt-pool

4.4 Case Study 4

This case study comprises work done at Swansea for the prediction of residual stress modelling using an ANSYS thermal-structural coupled analysis with element- and birth.

The Gaussian model for a heat source is adopted. The external heat flux q has been assumed to be a Gaussian heat flux as done by Roberts et al [47]:

$$q = \frac{2P}{\pi r_0^2} e^{-\frac{2r^2}{r_0^2}} \quad (1)$$

where P is the laser power, r_0 is the spot radius and r denotes the radial distance.

A 304mmx76mm rectangular plate has been considered. The plate is made of steel and is isolated at 22°C at the four edges, and fully clamped on the longer edges. A moving heat flux q with a power P is applied on the plate surface.

As the applied heat flux moves, this results in a variation of temperature on the plate. The transient temperature distribution will generate a variation of stress (residual stress generated by heat).

To determine residual stresses in the plate due to the material build up (ALM), a simulation procedure is developed based on a transient thermal analysis to determine the thermal behaviour of the plate, and a structural analysis to determine plate stress levels due to the plate thermal behaviour.

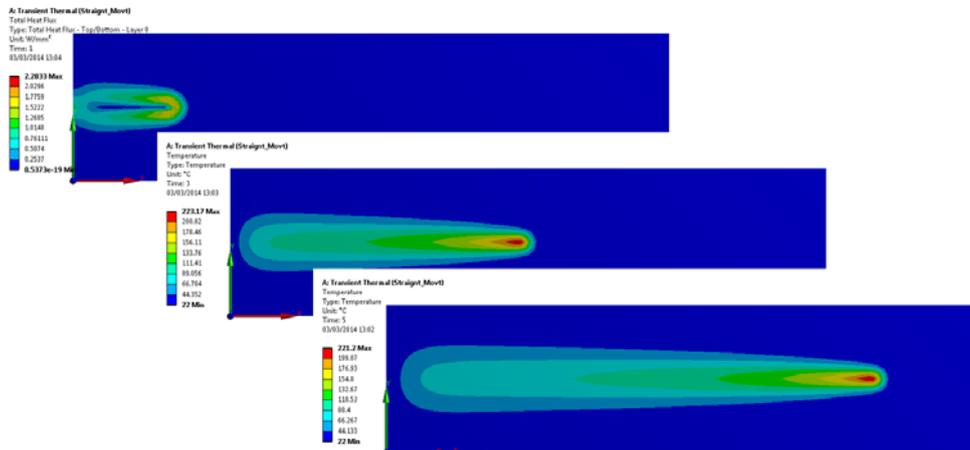


Figure 8 – Transient temperature at 1s, 3s and 5s (thermal analysis)

Two models are tested here, one is a true transient analysis that cycles in time (at each time-step level) between thermal and structural calculations: two-way thermal-structural interaction (TSI), whilst the second model transfers the final thermal data to the structural analysis to calculate stresses due to heat build-up in the plate: one-way thermal-structural interaction.

Findings, presented in Figure 8, Figure 9 and Figure 10, show that at the end of the build, residual stresses calculated without cycling procedure (1-way TSI) are underestimated (about 8%) in contrast to those obtained by the cycling scheme (2-way TSI).

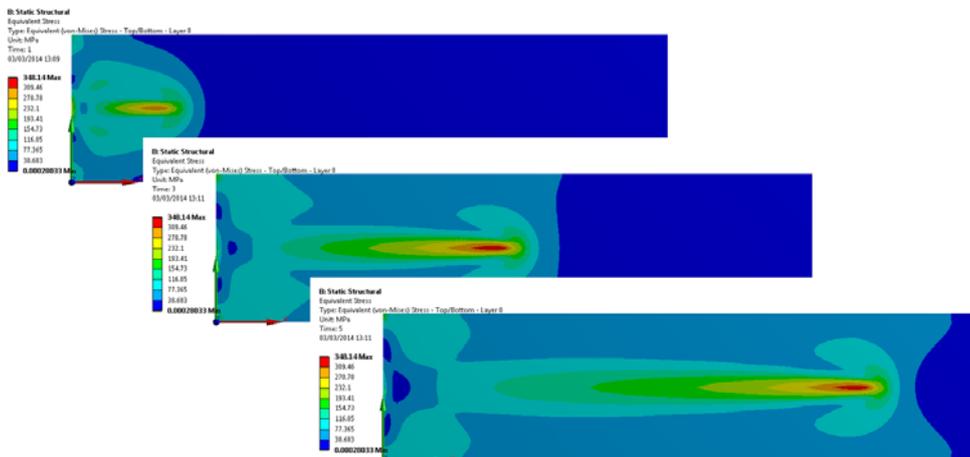


Figure 9 - Transient equivalent stress (residual stress due to heat build-up) at 1s, 3s and 5s: 2-way TSI

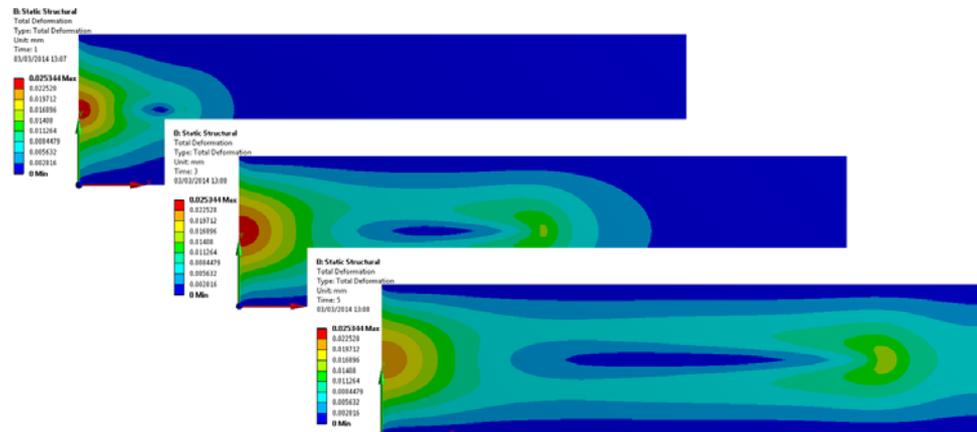


Figure 10 – Transient deformation due to heat build-up at 1s, 3s and 5s

5 Discussion

The escalating industrial interest in Additive Layer Manufacturing is clearly manifested in an increasing volume of academic publications which are computational in nature. A large percentage of these publications are looking at the melt pool and residual stresses using a variety of modelling techniques.

In addition to a brief and by no means exhaustive review of computational modelling of AM processes, focussing on the Selective Laser Melting of metal powder-bed processes, four computational case studies have been presented in the previous section.

The first case looked at using thermo-fluidic simulation using FLUENT at a millimetric scale of the melt pool to understand the internal convection which is generated by temperature-dependent surface tension – the Marangoni convection cells. The results qualitatively agree with [42], and would suggest that in a melt-pool which is dominated by Marangoni convection, that gas bubbles could be trapped if they were to be entrained, and retained during solidification. Hence, this study looks at one of the root causes of a specific type of porosity.

The second and third cases looked at a thermo-fluidic simulations using FLUENT and Lattice-Boltzmann on a micrometric scale. In these simulations, the powder particles are treated in their entirety, and inter-particulate heat transfer is numerically calculated (conduction/radiation/convection). These simulations also aim to provide predictions of porosity as a function of laser power input and speed, as shown in Figure 6, differentiating between porosity emanating from un-melted zones, gas trapping/entrainment and shrinkage porosity.

However these micro-scale simulations can also be used to understand the critical melt-pool dimensions and defects such as balling. These findings relate to previous work [48, 49, 50], where the inclusion of Marangoni convection in models increases the melt-pool aspect ratio by up to 150%, with the melt-pool able to spread wider than the laser diameter, but with a shallower depth giving higher aspect ratios than thermal-only based simulations.

The final case study shows modelling efforts to predict thermal residual stresses during a single run of the laser over a plate, using two different thermal-structural coupling schemes in ANSYS workbench. Further work remains to be done with this model to incorporate further build layers in the vertical direction.

This work has only touched briefly on a number of other areas which are being looked at computationally, such as multi-scale, discrete-element modelling, component topological optimisation and prediction of material properties. However, to a certain extent all computational models need validation in order to be trusted in a predictive capacity.

As the various laser-based processes are rapidly evolving, earlier experimental thermo-mechanical validation using lower laser speeds and powers, such as [22, 24, 51] may still be applicable in the early stages of computational model development, but there needs to be a constant re-validation of case studies with new data to match the new machine capabilities. Furthermore, post-mortem examination of built parts, or studies using lower melting point materials cannot replace an in-situ thermal imaging visualisation or x-ray tomography of the melt-pool, particularly for complex powder-based systems.

Another under-developed area which is critical to accurate computational modelling is the measurement of thermo-physical properties especially for powder-materials, such as thermal conductivity, but also liquid metal surface tension and absorptivity, which are so influential in the melt-pool simulations and characteristics.

6 Conclusions

A review of the state-of-the-art in computational modelling of the Additive Layer Manufacturing (ALM) process, specifically those involving the selective melting of metal powder has been presented.

A description of models being developed at Swansea University and case studies of applications has also been presented. In line with efforts at other commercial and academic organisations, these efforts are currently focusing on:

- thermal modelling at the microscale (at the level of the powder)
- thermal modelling at the macroscale (at the level of the build plate)
- residual stress modelling at the macroscale

These models are at the early stages of development, and the links between the multiple scales are yet to be created, but they are already being used as aids in understanding the occurrence of key process defects such as porosity and balling at a fundamental level.

7 Acknowledgements

The work described in this paper was carried out as part of the Advanced Sustainable Manufacturing Technologies (ASTUTE) project (ref. numb. 80380). ASTUTE has been part-funded by the European Regional Development Fund through the Welsh Government, and the authors would like to acknowledge this funding.

The authors also wish to acknowledge involvement on the AMAZE Project, co-funded by the European Commission in the 7th Framework Programme (Contract #FoF.NMP.2012-4-313781), by the European Space Agency and by the individual partner organisations.

Finally, the authors would like to thank Renishaw, and specifically Dr Chris Sutcliff, Ben Robinson and Dr Ben Ferrar for the ongoing discussions on laser-based powder bed process simulation.

8 Bibliography

- [1] T. Wohlers and T. Gornet, "History of Additive Manufacturing," Wohler Associates, Inc., Fort Collins, Colorado, 2012.
- [2] T. Wohlers and T. Caffrey, "Additive Manufacturing: Going Mainstream," *Manufacturing Engineering*, pp. 67-73, June 2013.
- [3] P. Li, D. M. Maijer, T. C. Lindley and P. D. Lee, "A through process model of the impact of in-service loading, residual stress, and microstructure on the final fatigue life of an A356 automotive wheel," *Materials Science and Engineering A*, vol. 460–461, p. 20–30, 2007.
- [4] C.-A. Gandin and A. Jacot, "Modeling of precipitate-free zone formed upon homogenization in a multi-component alloy," *Acta Materialia*, vol. 55, p. 2539–2553, 2007.
- [5] J. W. Kang, T. J. Wang, T. Y. Huang and B. C. Liu, "Though process numerical simulation of a heavy hydroturbine blade casting," *IOP Conf. Series: Materials Science and Engineering (MCWASP XIII)*, vol. 33, pp. 1-8, 2012.
- [6] J.-M. Drezet, M. Gremaud and M. Rappaz, "State-of-the-art in the Modelling of Aluminium and Copper Continuous Casting Processes," in *Continuous Casting*, John Wiley & Sons, 2006, pp. 151-160.
- [7] J. W. Elmer, S. M. Allen and T. W. Eager, "Microstructural Development during Solidification of Stainless Steel Alloys," *Metallurgical Transactions A*, vol. 20A, pp. 2117-2131, 1989.

- [8] W. Hofmeister, M. Griffith, M. Ensz and J. Smugeresky, "Solidification in Direct Metal Deposition by LENS Processing," *Journal of Materials*, pp. 30-34, 2001.
- [9] M. Sun and J. Beaman, "A Three Dimensional Model for Selective Laser Sintering," in *Solid Freeform Fabrication Symposium*, Austin, Texas, USA, 1991.
- [10] E. M. Weissman and M. B. Hsu, "A Finite Element Model of Multi-Layered Laser Sintered Parts," in *Solid Freeform Fabrication Symposium*, Austin, Texas, USA, 1991.
- [11] J. C. Nelson, N. K. Vail and J. W. Barlow, "Laser Sintering Model for Composite Materials," in *Solid Freeform Fabrication Symposium*, Austin, Texas, USA, 1993.
- [12] R. Chin, J. Beuth and C. Amon, "Thermomechanical modeling of successive material deposition in layered manufacturing," in *Solid Freeform Fabrication Symposium*, Austin, Texas, USA, 1996.
- [13] L. Flach, D. A. Klostennan, R. P. Chartoff, R. Prototype, O. Rapid, P. Process and D. Consortium, "A THERMAL MODEL FOR LAMINATED OBJECT MANUFACTURING (LOM)," in *Solid Freeform Fabrication Symposium*, Austin, Texas, USA, 1997.
- [14] N. W. Klingbeil, J. L. Beuth, R. K. Chin and C. H. Amon, "Measurement and Modeling of Residual Stress-Induced Warping in Direct Metal Deposition Processes," in *Solid Freeform Fabrication Symposium*, 1998.
- [15] K. Dai and L. Shaw, "Thermal and Stress Modeling of Laser Fabrication of Multiple Material Components," in *Solid Freeform Fabrication Symposium*, 2001.
- [16] S. Das and H. Chung, "A Model of Laser-Powder Interaction in Direct Selective Laser Sintering of Metals," in *Solid Freeform Fabrication Symposium*, 2001.

- [17] A. O. F. Niebling, "ANALYZING THE DMLS-PROCESS BY A MACROSCOPIC FE-MODEL," in *Solid Freeform Fabrication Symposium*, 2002.
- [18] T. Chen and Y. Zhang, "METAL POWDER LAYER ON TOP OF MULTIPLE SINTERED LAYERS," in *Solid Freeform Fabrication Symposium*, 2003.
- [19] T. Chen and Y. Zhang, "Numerical Simulation of Two-dimensional melting and resolidification of a two-component metal powder layer in selective laser sintering process," *Numerical Heat Transfer, Part A*, vol. 46, pp. 633-649, 2004.
- [20] K. Dai and L. Shaw, "Finite element analysis of the effect of volume shrinkage during laser densification," *Acta Materialia*, vol. 53, pp. 4743--4754, oct 2005.
- [21] K. Dai and L. Shaw, "Thermal and mechanical finite element modeling of laser forming from metal and ceramic powders," *Acta Materialia*, vol. 52, pp. 69--80, jan 2004.
- [22] K. Dai, X. Li and L. L. Shaw, "Comparisons between Thermal Modeling and Experiments in Laser-Densified Dental Powder Bodies," in *Solid Freeform Fabrication Symposium*, 2003.
- [23] H. Pan and F. Liou, "Modeling of the metal powder flow with carrier gas in coaxial nozzle for direct laser deposition process," in *Solid Freeform Fabrication Symposium*, 2004.
- [24] L. Wang, S. Felicelli and J. Craig, "Thermal Modelling and Experimental Validation in the LENS Process," in *Solid Freeform Fabrication Symposium*, Austin, Texas, USA, 2007.
- [25] F. Liou, Z. Fan, H. Pan, K. Slattery, M. Kinsella and J. Newkirk, "Modeling and Simulation of A Laser Deposition Process," 2007.
- [26] R. Acharya, R. Bansal, J. J. Gambone, P. Cilino and S. Das, "COMPUTATIONAL MODELING AND EXPERIMENTAL VALIDATION OF MICROSTRUCTURAL DEVELOPMENT IN SUPERALLOY CMSX-4 PROCESSED THROUGH SCANNING

- LASER EPITAXY," in *Solid Freeform Fabrication Symposium*, 2012.
- [27] T. T. Diller and J. Beaman, "Thermal Model of the Build Environment for Polyamide Powder Selective Laser Sintering," 2010.
- [28] B. Cheng and K. Chou, "MELT POOL GEOMETRY SIMULATIONS FOR POWDER-BASED ELECTRON BEAM ADDITIVE MANUFACTURING," in *Solid Freeform Fabrication Symposium*, 2013.
- [29] K. Zeng, D. Pal and B. Stucker, "A Review of Thermal Analysis Methods in Laser Sintering and Selective Laser Melting," in *Solid Freeform Fabrication Symposium*, Austin, Texas, USA, 2012.
- [30] E. Attar and C. Korner, "Lattice Boltzmann method for dynamic wetting problems," *Journal of Colloid and Interface Science*, vol. 335, p. 84–93, 2009.
- [31] C. Korner, E. Attar and P. Heintl, "Mesoscopic simulation of selective beam melting processes," vol. 211, pp. 978--987, 0 0 2011.
- [32] C. Korner, A. Bauereiß and E. Attar, "Fundamental consolidation mechanisms during selective beam melting of powders," *Modelling Simul. Mater. Sci. Eng.*, vol. 21, pp. 1-18, 2013.
- [33] M. Markl, R. Ammer, U. Ljungblad, U. Råde and C. Körner, "Electron Beam Absorption Algorithms for Electron Beam Melting Processes Simulated by a Three-Dimensional Thermal Free Surface Lattice Boltzmann Method in a Distributed and Parallel Environment," *Procedia Computer Science*, vol. 18, pp. 2127-2136, 2012.
- [34] W. Jiang, K. Dalgarno and T. Childs, "Finite Element Analysis of Residual Stresses and Deformations in Direct Metal SLS Process," in *Solid Freeform Fabrication Symposium*, Austin, Texas, USA, 2012.
- [35] A. K. Ibraheem, B. Derby and P. J. Withers, "Thermal and Residual Stress Modelling of the Selective Laser Sintering Process," *Materials Research Society Symposium Proceedings*, vol. 758, pp. 47-52, 2002.

- [36] M. F. Zaeh and G. Branner, "Investigations on residual stresses and deformations in selective laser melting," *Production Engineering*, vol. 4, no. 1, pp. 35-45, 2010.
- [37] J. Ding, P. Colegrove, J. Mehnen, P. M. Sequeira Almeida, F. Wang and S. Williams, "Thermo-mechanical analysis of Wire and Arc Additive Layer Manufacturing process on large multi-layer parts," *Computational Materials Science*, vol. 50, no. 12, pp. 3315-3322, 2011.
- [38] P. Mercelis and J.-P. Kruth, "Residual stresses in selective laser sintering and selective laser melting," *Rapid Prototyping Journal*, vol. 12, no. 5, pp. 254-265, 2006.
- [39] H. Zhang, Q. Zhou and Y. Zheng, "A multi-scale method for thermal conduction simulation in granular materials," *Computational Materials Science*, vol. 50, no. 10, pp. 2750-2758, 2011.
- [40] D. Pal, N. Patil, M. Nikoukar, K. Zeng, H.-K. K. and B. Stucker, "An Integrated Approach to Cyber-Enabled Additive Manufacturing using Physics based, Coupled Multi-scale Process Modeling," in *Solid Freeform Fabrication Symposium*, Austin, Texas, USA, 2013.
- [41] N. Keller and V. Ploshikhin, "Multi-Scale FEM Simulation of Selective Laser Melting Process," in *European Altair Technology Conference*, Torino, Italy, 2013.
- [42] G. Gladush and I. Smurov, *Physics of Laser Materials Processing - Theory and Experiment*, Moscow, Russia: Springer Series in Materials Science, 2011.
- [43] A. V. Gusarov, M. Pavlov and I. Smurov, "Residual Stresses at Laser Surface Remelting and Additive Manufacturing," *Physics Procedia*, vol. 12, pp. 248--254, jan 2011.
- [44] A. V. Gusarov and I. Smurov, "Two-dimensional numerical modelling of radiation transfer in powder beds at selective laser melting," *Applied Surface Science*, vol. 255, pp. 5595--5599, mar 2009.

- [45] A. V. Gusarov and I. Smurov, "Modeling the interaction of laser radiation with powder bed at selective laser melting," *Physics Procedia*, vol. 5, pp. 381--394, jan 2010.
- [46] V. R. Voller and C. Prakash, "A Fixed-Grid Numerical Modeling Methodology for Convection-Diffusion Mushy Region Phase-Change Problems," *Int. J. Heat Mass Transfer*, vol. 30, pp. 1709-1720, 1987.
- [47] I. Roberts, C. J. Wang, R. Esterlein, M. Stanford and D. J. Mynors, "A three-dimensional finite element analysis of the temperature field during laser melting of metal powders in additive layer manufacturing," *Int. J. Machine Tools and Manufacture*, vol. 49, no. 12-13, pp. 916-923, 2009.
- [48] Y. P. Lei, H. Murakawa, Y. W. Shi and X. Y. Li, "Numerical Analysis of the competitive influence of Marangoni flow and evaporation on heat surface temperature and molten pool shape in laser surface remelting," *Computational Materials Science*, vol. 21, pp. 276-290, 2001.
- [49] S. Safda, L. Li and M. A. Sheikh, "Numerical analysis of the effects of non-conventional laser beam geometries during laser melting of metallic materials," *J. Phys. D: Appl. Phys.*, vol. 40 , p. 593--603, 2007.
- [50] B. S. Koo, Simulation of Melt Pool Penetration and Fluid Flow Behaviour During Welding, Lehigh University, Bethlehem, USA: PhD Thesis, 2013.
- [51] L. Van Belle, G. Vansteenkiste and J.-C. Boyer, "Comparisons of numerical modelling of the Selective Laser Melting," *Key Engineering Materials*, vol. 1067, pp. 504-506, 2012.