DEVELOPMENT OF HOMOGENEOUS NUMERICAL PLATFORM FOR 3D THROUGH PROCESS SIMULATION OF SELECTIVE LASER MELTING CONSIDERING CHANGES OF AGGREGATIVE STATES

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ABSTRACT
A novel numerical platform for through process modelling of multi-material SLM is discussed. The paper presents recent results on modelling of the powder removal operation focusing on gas flow and the loose powder particles entrained in the flow linked to the physical associated processes within a frame of the holistic platform allowing for multiphysics simulations and based entirely on homogeneous numerical methods such as CA and LBM avoiding unnecessary interfaces between different modules. The qualitative results reflect a typical approach for particle local removal in multi-material SLM.

NOMENCLATURE
Roman letters
b = number of vectors in velocity model
$\boldsymbol{e}$ = phase space variable - velocity (vector)
$\{\boldsymbol{e}_i, i = 1,\ldots,b\}$ = set of discrete velocities, velocity model
$f, f_i(\boldsymbol{x},t)$ = distribution function
g = gravitational acceleration
m = mass factor
t = time
Δt = time step
$\boldsymbol{v}$ = fluid (gas) velocity
w_i = weights for calculation of equilibrium distribution function
$\boldsymbol{x}$ = coordinates of the lattice nodes (or cells),
$\Delta\boldsymbol{x}$ = cell size, resolution of the model space velocity

Greek symbols
ρ = fluid density
τ = relaxation time
Ω = collision operator

Subscripts
i = i^{th} component of the velocity model
x = horizontal vector component
y = vertical vector component

Superscripts
eq = equilibrium
in = input stream
p = particle
out = output stream

INTRODUCTION
The rapid expansion of additive manufacturing (AM) in recent years favoured demand and development of advanced numerical tools for modelling and optimisation of such complicated processes, which very often deal with different materials in different states of matter, such as multi-material selective laser melting (SLM). There are several numerical models considering different aspects of particle powder bed generation, heat exchange, and transfer, phase transformation, melting, and solidification [1-3]. The problems, however, appear when a holistic through process approach is required. Complicated interfaces between different components of the suggested multiscale models based on heterogeneous numerical methods almost eliminate the possibility of full scale through process modelling due to arising difficulties and limitations.
The holistic numerical platform discussed in this work is based on cellular automata (CA) and Lattice Boltzmann methods (LBM). The platform is developed as a part of the modelling led approach for studying and optimisation the interaction between different physical mechanisms in multi-material laser-assisted AM. The proposed approach is based entirely on homogeneous methods eliminating the complicated interfaces allowing for modelling

several physical events occurring in sequence or simultaneously. They include a powder bed deposition, laser energy absorption, and heating of the powder bed by the moving laser beam leading to powder melting or sintering, fluid flow in the melted pool, flow through partly or not melted material, and solidification. The concept of the holistic numerical approach and principles of the calculation platform has been discussed earlier [4]. Recently, several modules have been developed and combined for the modelling. The number of physical processes and phenomena that can be modelled simultaneously is defined by the number of variables associated with the point, site, cell, or node in the same domain. An implementation of a new process requires the addition of only new variables and appropriate algorithms. The applied computation method, known as frontal CA, allows for multiple algorithmic accelerations. While parallel programming environment using Computer Unified Device Architecture (CUDA) developed by NVIDIA is the most appropriate for LBM applications due to its specific algorithmic structure. The applied environment makes LBM a highly efficient and productive method expanding the area of its potential applications.

HOLISTIC MODEL OF SLM

The principles of the multiphysics modelling approach in the development of the entire SLM process are discussed in our previous publications [4-7]. Fig.1 represents the proposed diagram of the entire process divided by stages according to the associated physical phenomena connected with the corresponding mathematical models that constitute the holistic SLM process model. The diagram includes new items marked by green colour, namely: the powder removal operation linked to the physical associated process and the model. The details of adding these elements into the holistic model are considered in this study.

Some characteristics of the powder bed generation (PBG) model supported by the initial results can be found elsewhere [4,5] while a simplified model of the heat transfer currently used in the holistic model is discussed in [6,7]. The named two models are based on the CA method. Other models, namely the fluid flow with the free surface and the thermal model are based on LBM [6,7]. The referenced above models operate in the 2D domain although their three-dimensional counterparts are currently under development.

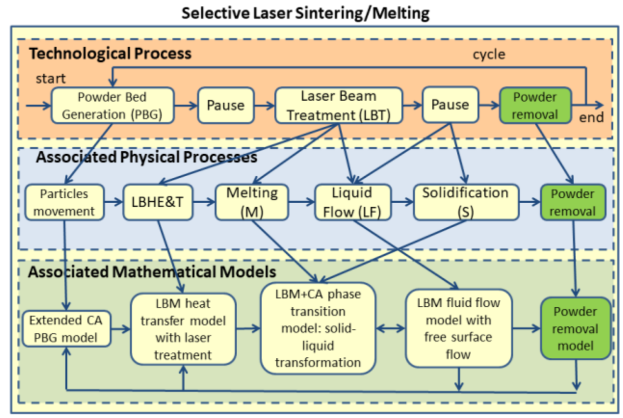


Figure 1
Diagram of the SLM process linked to the associated physical phenomena and the mathematical models

In this paper, we discuss the new model taking into consideration removing the loose powder particles from the powder bed. As a part of the homogeneous numerical platform, the model is aimed to support optimization of the multiple material SLM (MMSLM) systems similar to the one developed at the University of Manchester comprising a powder bed delivery mechanism spreading the main building powder material with point by point micro vacuum material removing system [8]. It has been designed for selective, precise single layer powder removal at specific locations combining with several dry powder dispensers depositing powders according to the designed pattern. The model development considering gas flow and the loose powder particles entrained in the flow is also based on LBM and it is the main focus of this study.

Gas flow model for powder removal: The MMSLM process dealing with two or more materials in the manufacturing of complex multi-material structural elements faces new challenges. The challenges are connected not only with the significant differences in the material properties but also with the necessity of removal of one powder material to clear a place for delivery of another one. The removal happens at different stages of the manufacturing process, namely during the generation of the multi-material powder bed and/or after completion of the SLM consecutive processing stages. After generation of the powder bed (an example is presented in Fig.2) and completion of the SLM single processing stage (Fig 3), some of the untreated powder material should be removed. To simulate this operation and process, a new model of powder removal is developed in two variants. The first one simply rewove untreated particles from the modelled space. The second variant has been developed to analyze the effectiveness of the loose particle removal operation. It is developed in the 2D version.

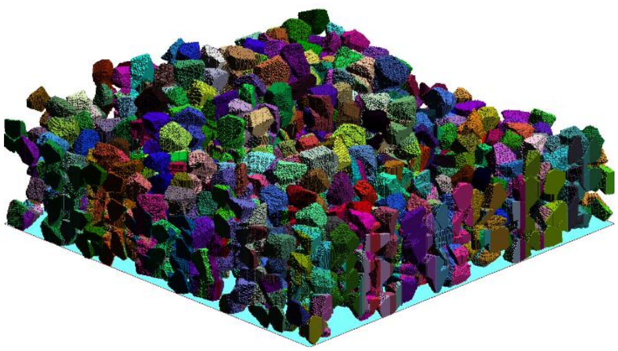
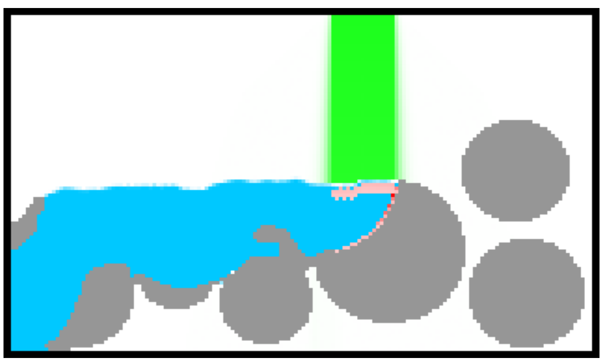


Figure 2
Modelling results: deposition of 1200 particles on the area of 600×600 cells



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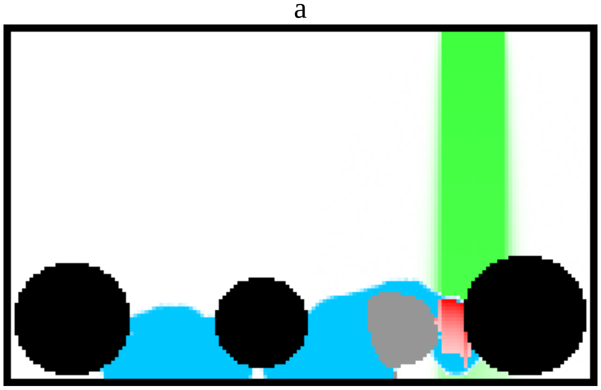


b

Figure 3
Simulation results illustrating SLM of one (a) and two (b) different materials in a single layer. Note green colour represents laser beam, shades of pink and red - heat transfer intensity, blue – the liquid state, grey and black – the solid state of materials

The model uses the same principles, algorithms as the other LBM submodels of the SLM holistic model. The main blocks of the LBM for gas flow are shown in Fig.4. The D2Q9 velocity model is applied for this task, thus there are 9 components of the distribution function in two dimensions.

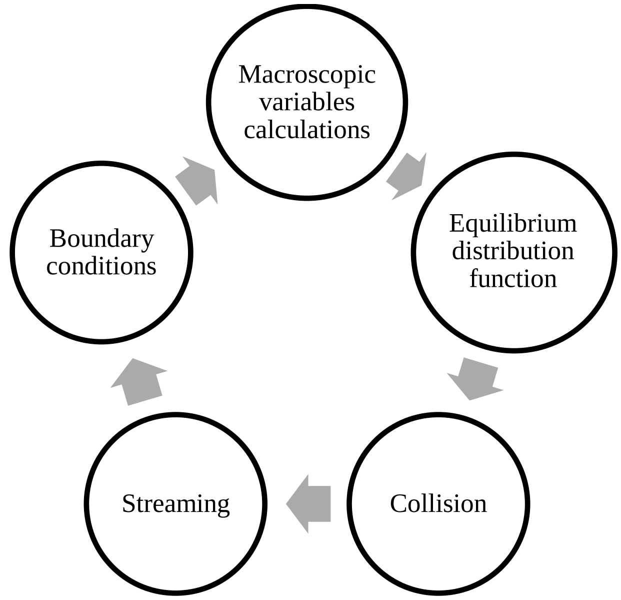


Figure 4
Block-diagram of the calculations of the gas flow model based on LBM

A macroscopic variables calculations block allows for obtaining the density of a gas ρ and velocity $\boldsymbol{v}$ calculated at every node of the modelled space:

$$\rho = \sum_{i=0}^{b} f_i \quad (1)$$

$$\rho\boldsymbol{v} = \sum_{i=0}^{b} f_i \mathbf{e}_i \quad (2)$$

Then, the equilibrium distribution function is obtained:

$$f_i^{\text{eq}} = w_i \rho[1 + 3\boldsymbol{e}_i \cdot \boldsymbol{v} + 4.5(\boldsymbol{e}_i \cdot \boldsymbol{v})^2 - 1.5\boldsymbol{v} \cdot \boldsymbol{v}] \quad (3)$$

The collision operation can be described by the following equation (with the Bhatnagar-Gross-Krook collision operator [45]):

$$f_i^{\text{out}} = f_i^{\text{in}} + \Omega_i = f_i^{\text{in}} + \frac{\Delta t}{\tau}[f_i^{\text{eq}} - f_i^{\text{in}}] \quad (4)$$

Streaming is simply the transfer of the appropriate component of the distribution function to the neighbouring node according to the velocity vector:

$$f_i^{\text{in}}(\boldsymbol{x} + \boldsymbol{e}_i, t + \Delta t) = f_i^{\text{out}}(\boldsymbol{x}, t) \quad (5)$$

There are three kinds of boundary conditions applied in the model. The first one is the bounce-back boundary conditions:

$$f_i(\boldsymbol{x} + \boldsymbol{e}_i, t + \Delta t) = f_{\bar{i}}(\boldsymbol{x}, t) \quad (6)$$

where $\bar{i}$ defines reverse direction: $\boldsymbol{e}_{\bar{i}} = -\boldsymbol{e}_i$.
The other boundary conditions are symmetrical and open with the density of a gas defined as constant.
The focus of this study as stated above is the simulation of the gas flow allowing for local removal of the loose

particles. Hence, the model should contain equations describing the motion of the particles entrained in the gas stream. The particles of different mass and sizes are considered in the simulation although they are assumed to be small enough to influence the gas flow. Then, applying Newton's laws of motion to the linear motion of a particle of constant mass, the following equations for the horizontal and vertical components of velocity can be obtained:

$$v_x^{\mathrm{p}}(t+1) = m v_x^{\mathrm{p}}(t) + (1-m) v_x(t) \quad (7)$$

$$v_y^{\mathrm{p}}(t+1) = m v_y^{\mathrm{p}}(t) + (1-m) v_x(t) - g \quad (8)$$

where $m = 0$ corresponds to zero mass while $m = 1$ is associated with a very high-mass particle. The gravitational factor g depends not only on the modelling parameters such as lattice size, time step and g_{max} but also on the particle size because of gas resistance: $g = 0$ when $m = 0$, and $g = g_{\mathrm{max}}$ when $m = 1$.

A particle location is not discretized in relation to the lattice site and remains a continuous variable. A new position is calculated according to Euler's integration scheme:

$$x^{\mathrm{p}}(t+1) = x^{\mathrm{p}}(t) + \frac{u_x^{\mathrm{p}}(t+1) + u_x^{\mathrm{p}}(t)}{2} \quad (9)$$

$$y^{\mathrm{p}}(t+1) = y^{\mathrm{p}}(t) + \frac{u_y^{\mathrm{p}}(t+1) + u_y^{\mathrm{p}}(t)}{2} \quad (10)$$

RESULTS AND DISCUSSION

The results concerning the modelling of the loose particles local removal are discussed below. The presented results are mainly qualitative and the case study allows for evaluation of the quality and correctness of the numerical solution. Quantitative adaptation and complete model verification will be done gradually after gathering results of comparison with reliable data and using the developed simulation code for modelling of different aspects concerning the specific SLM processes. One of the modelled spaces is shown in Fig.5 reflecting a typical device for the particle local removal similar to a micro vacuum cleaner but having an additional element for air (gas) inflation.

The boundaries at the top of the area and also the left and right ones are open boundaries with a constant density (pressure). The external pressure at the left and right open boundaries is equal to atmospheric pressure ($\rho = 1$) while pressure at the inner and outer parts of the top boundary can be set above and under the chosen atmospheric pressure. The system allows for tracing gas inflows and outflows correspondently. The other boundaries are simulated as obstacles with the bounce-back rule. The wall configuration, relevant sizes, gas pressure can be varied during the analysis to achieve optimal conditions of the particle removal process.

Figs 6-12 present the obtained results in the form of horizontal (the left picture) and vertical (the right one) velocity components. The gas streams directed to the right and the top are shown by shades of red colour while those directed to the left and the bottom are represented by shades of blue colour. The trajectories of moving particles are also shown in the figures. The size of the particle is one of the main determinants of the removal system. The trajectories of the particles of three different sizes are simulated in this case study. Violet trajectories correspond to very small particles ($m = 0$), green ones represent medium and blue trajectories are related to the biggest particles. To start with, only "vacuum" cases were analyzed (Figs.7-9). In these cases, a gap between a vacuum tube and the surface is a crucial parameter. If the gap is too small an inflowing gas flow is too weak to entrain the particles in the flow (Fig.7). An increasing gap is accompanied by increasing gas flow and the removal device becomes more effective (Fib.8). When the gap becomes too big, the device can remain effective (Fig.9a) although turbulences that can appear in the tube can lead to asymmetrical flow and instabilities. In situations like this, the effectiveness of the device drops significantly even for a highly symmetrical case. It has to be noted that the results illustrated in Fig.9 represent the 2D simulation case. They are likely to be different for 3D model configurations. The observed instabilities are typical for wider tubes and are diminished when the tube diameter becomes narrower (Fig.10).

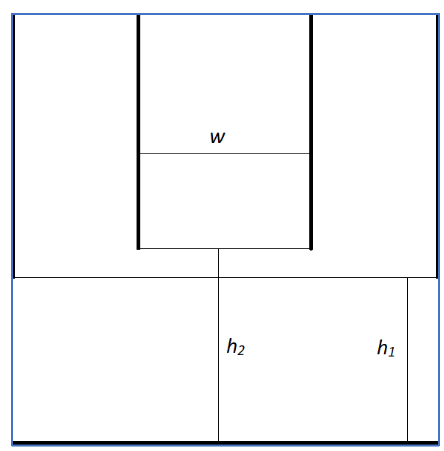


Figure 5
Modelling domain with boundaries

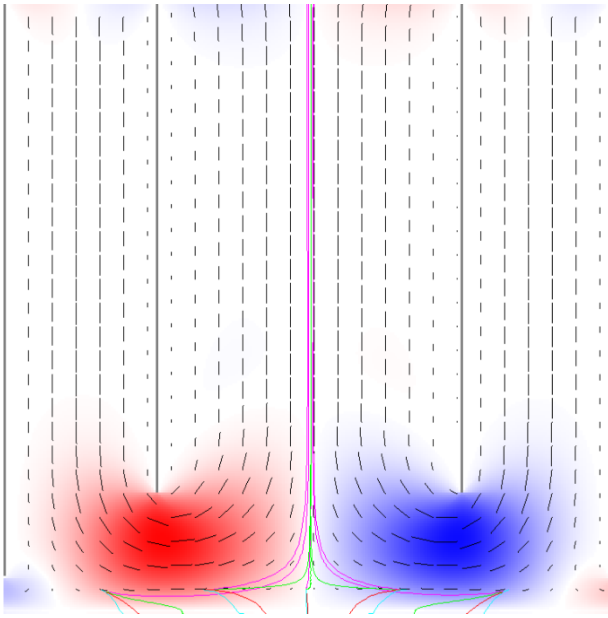


Figure 6
Gas streams and trajectories of moving particles predicted by the LBM model

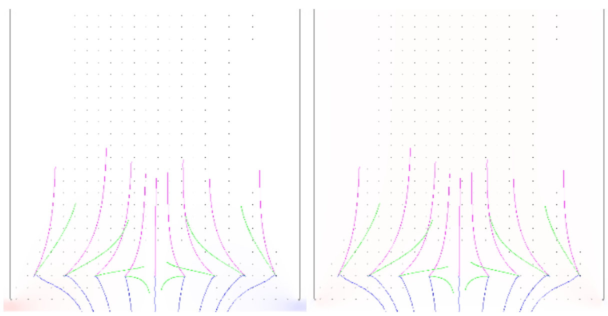


Figure 7
Modelling results: the case of the vacuum only with a small gap

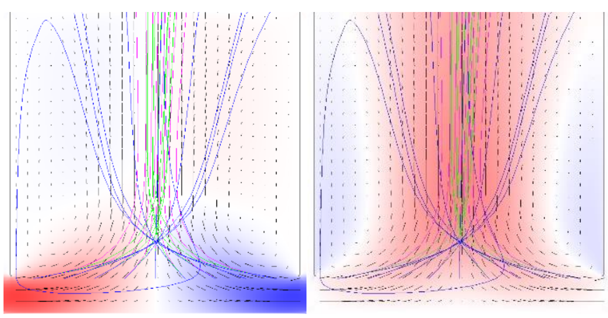
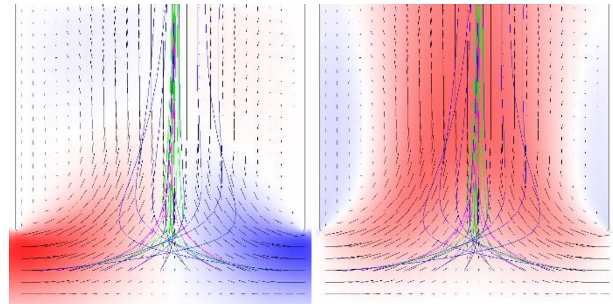


Figure 8
Modelling results: the case of the vacuum only with a medium gap



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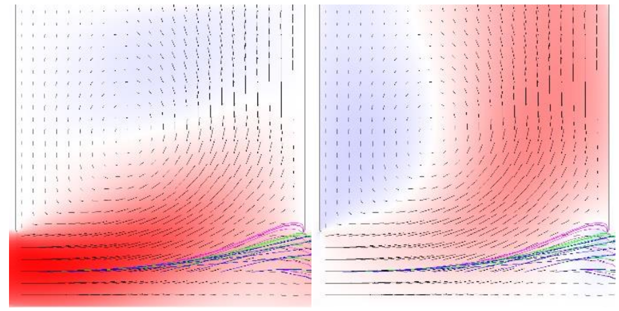

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Figure 9
Modelling results: the case of the vacuum only with a big gap. Stable (a) and unstable (b) flows

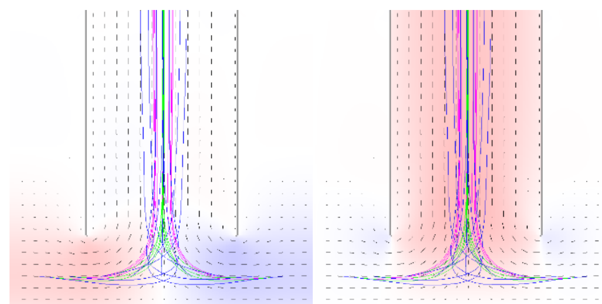

Figure 10
Modelling results: the case of the vacuum only with a big gap and narrow tube

Considering the simulation results from the technological point of view, we can conclude that efficient control of the particles removal by using the device with only vacuum function is fraught with difficulties. It is due to the high dependence of the device effectiveness on the gap, which is difficult to maintain at an optimal level. As can be seen in Fig 8 and 9, some movement in the opposite direction and turbulences can appear within the tube. It is possible to enforce such movement by the application of an additional inflow channel with much higher gas pressure. Some simulation results are presented in Fig. 6, 11 and 12. A simple liner shape is less effective because of a strong gas stream in a downward direction (Fig.6). The device becomes more effective in the presence of the stream in the horizontal direction. It is possible to obtain more effective design options by using different profiles of the internal and external tubes. This would have the additional advantage that the two-tube solution makes the control of the minimal gap between the external tube and the surface much easier.

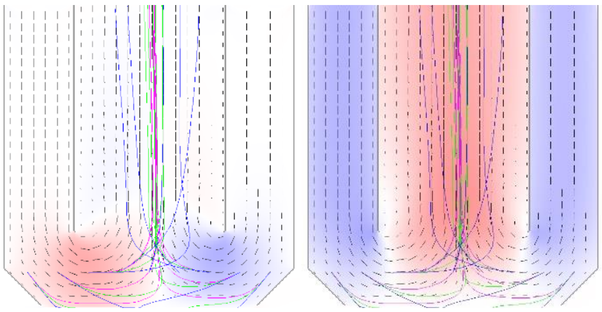

Figure 11
Modelling results showing inflows and outflows for different tube profiles and higher pressure. The 1st case.

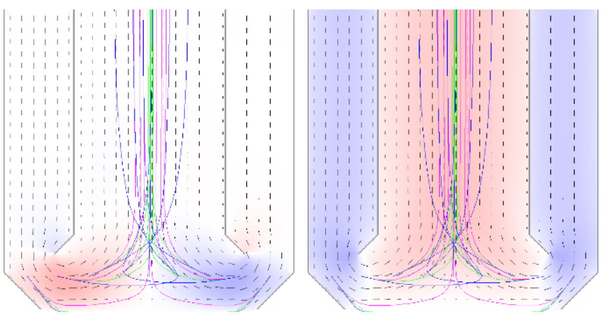

Figure 12
Modelling results showing inflows and outflows for different tube profiles and higher pressure. The 2nd case.

CONCLUSIONS

The presented case studies allow for evaluation of the quality and correctness of the numerical solution concerning modelling of the loose particles local removal during a multi-material SLM process. The developed model concerning the gas flow and loose powder particles entrained into the flow is a part of the holistic numerical platform allowing for multiphysics simulation of a multi-material SLM process. The platform is developed with the aim to be based entirely on homogeneous numerical methods such as CA and LBM avoiding unnecessarily complicated interfaces between different modules. It has also been shown in this study that more effective design options of the particle removal device can be achieved by using different profiles of the internal and external two-tube system.

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