

# KISSAM Simulation Software for Additive Manufacturing

# 3D simulation of electron beam melting process with adaptive mesh refinement at mesoscale level



### Powder bed fusion processes simulation at mesoscale (melt-pool) level



### Underlying physical models in KiSSAM

- Hydrodynamic solver based on Thermal Lattice Boltzmann Method with Volume of Fluid free surface tracking
- Phase transition solid/liquid
- Surface tension and wetting
- Marangoni convection
- Dumping drag force in mushy zone
- Recoil pressure, mass and energy losses due to the strong evaporation from the liquid surface
- Radiation cooling
- Convection cooling
- Evaporated metal and chamber gas flow tracking
- Heat cooling and conduction in the bulk far from the melt-pool
- Ray tracing with multiple reflections (for laser beam) and MC simulation of electron trajectories with elastic and inelastic scattering in metal (for electron beam)
- Sensors and detectors photodiode response simulation
- Grain microstructure simulation at solidification same as CAFE model (in progress)
- Powder bed packing DEM solver with knife movement (fork of BlazeDEM project)



#### **Free surface Temperature Lattice Boltzmann Method**



Volume of Fluid method for free surface tracking

Advanced modern method

- Suitable for massively parallel systems such as GPGPUs
- Liquid surface is explicitly tracked
- Modelling of the interaction with solid
- Describes heat transfer flows (both thermal conductivity and convection)

$$\frac{\partial f}{\partial t} + \vec{v} \frac{\partial f}{\partial \vec{x}} = \Omega(f, f')$$

$$f(\vec{x},\vec{v},t) \to f_{ijk}(\vec{x},t);\, i,\, j,\, k=-1,0,1;$$

$$\rho = \int fm \, \mathrm{dv} \qquad \qquad \rho = \sum_{i} f_{i}$$

$$\rho \overline{u} = \int fm \overline{v} \, \mathrm{dv} \qquad \qquad \rho \overline{u} = \sum_{i} \overline{e_{i}} f_{i}$$



Numerical scheme cell



Curvature calculation scheme

### **Adaptive Mesh**

- Melt pool is fitted by a fine mesh (3-5 µm resolution).
- Fluid dynamics is simulated in a small region around the melt pool (~ 1 mm).
- Heat transfer is simulated in a large domain (~ 1 cm) with adaptive mesh step.
- Geometry of the powder and melted metal is stored as high resolution sparse volumetric data in the whole region.

### **Electron beam Monte-Carlo ray tracing simulation**

Elastic scattering (approximation of the screened Rutherford scattering):

$$\frac{d\sigma(\theta)}{d\Sigma} = \frac{Z(Z+1)e^4}{p^2v^2} \frac{1}{\left(1+\cos\theta+2\beta\right)^2}, \quad \beta = \left(\frac{\hbar Z^{1/3}}{pa_B}\right)^2$$

$$=\frac{2\beta(1+\beta)p^2v^2A}{2\pi N_A\rho Z(Z+1)e^4}$$

Inelastic scattering

( the differential energy loss (stopping power) due to the electron-electron scattering ):

Λ

$$\frac{dE}{ds} = -785 \frac{\rho Z}{AE} \ln \left(\frac{1.166E}{J}\right) [\text{eV/Å}]$$

#### Every trajectory consists of straight line segments

segment length:  $L_r = -\Lambda \log R_1$ energy deposition per segment:  $L_r \frac{dE}{ds}$  polar  $\theta$  and azimuthal  $\varphi$  angles of collision:

$$R_{2} = \frac{\int_{0}^{\theta} \frac{d\sigma(\theta')}{d\theta'} \sin \theta' d\theta'}{\int_{0}^{\pi} \frac{d\sigma(\theta')}{d\theta'} \sin \theta' d\theta'}$$

$$\varphi = 2\pi R_{3}$$
backscattering
heat
deposition

 $R_{\prime}, R_{2}, R_{3}$  are uniformly distributed random numbers

#### Multiple trajectories are simulated every time step

### **Power of back-scattered electrons**



Absorption profile in a 70µm Ti sphere for 60 kV beam

Part of backscattered electrons during the simulation of powder melting

# Powder simulation using the discrete element method

- Powder packing in the PBF process may have significant impact on the quality of the manufactured detail
- Powder dynamics can be simulated using the discrete element method (DEM)
  - numerical method of solving the ODE of dynamics of a system many spherical rigid bodies (particles) with respect to the wall boundaries and moving objects
  - Gravity, friction, elastic forces are taken into account
    - Hertz-Mindlin contact model to calculate the elastic forces acting on each particle
      - Amontons-Coulomb friction law
- The substrate relief is approximated from the previous layer (or some initial substrate relief is assumed)
- Powder particle dynamics is simulated till steady-state solution is obtained
- Particle data is sent to the main simulation module

$$\frac{d^2 \boldsymbol{p}_i}{dt^2} = \boldsymbol{f}_i$$
$$\boldsymbol{I}_i \frac{d\boldsymbol{\omega}_i}{dt} + \boldsymbol{\omega} \times \boldsymbol{H} = \boldsymbol{t}_i$$
$$\boldsymbol{f}_i = \sum \boldsymbol{f}_i^s + \sum \boldsymbol{f}_i^b$$
$$\boldsymbol{t}_i = \boldsymbol{r}_i \times \boldsymbol{f}_i^s$$



Scheme of Hertz-Mindlin contact model (picture from [Capozzi et al (2018). Data in Brief. doi:22.10.1016/j.dib.2018.12.061])



Scheme of multilayer calculation: (a) PBF simulation, (b) solidified layer representation, (c) powder generation for the next layer. Lines mean data dependencies

# Fast GPU DEM solver

- The solver is developed based on Blaze-DEMGPU open source DEM code core
  - Blaze-DEMGPU algorithms and data structures improved
  - Some bugs fixed
- Code is optimised and extended for the PBF powder generation
  - Initial setup of a particle "cloud" with a given size distribution
  - Substrate reader from the STL format
    - Python scripts for STL substrate decimation based on the vtk library routines are developed
  - Verlet algorithm for substrate discrete elements i.e. triangles of its fast GPU implementation
  - A moving blade for the powder alignment is introduced
- Code has performance more than 10<sup>10</sup> discrete elements per second
- 5mm x 5mm layer can be simulated in ~ 1–2 hours using the particles with mean size 40 µm Simulation of powder

Nicolin Govender, Daniel N. Wilke, Schalk Kok. Blaze-DEMGPU: Modular high performance DEM framework for the GPU architecture, SoftwareX, V. 5, 2016, P. 62-66, https://doi.org/10.1016/j.softx.2016.04.004



Simulation of powder packing 6mm x 1mm x 80 µm. Yellow is a moving blade. Powder particles are colored by their velocity magnitude. Simulation time ~ 30 mins.

# **High Performance Computing**

KiSSAM is a high performance software with multiple presets for the purposes of powder bed fusion in additive manufacturing.

Typical performance is 0.5 – 1 hr per 1 ms of scanning time

Here are some sample setups modeled on a single GeForce RTX 3090 24 GB GPGPU and total simulation times.



Bulk samples ~1 week

Single tracks on a plate ~ 1h





### **KiSSAM on web cloud**

#### www.kissam.cloud





Showing Image /results/output\_33/rendered3D/pic95000.png



#### Single track on plate ???? P=1500W Speed=1.0 m/s



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Hatched layer Ti6Al4V Power =1680.0 W Speed = 4.27 m/s

Bulk sample Ti6Al4V Power = 2208 W Speed = 5.854 m/s

Automated multilayer procedure:

- post-process geometry output;
- simulate powder deposition;
- rasterize powder particles onto fine mesh;
- continue PBF simulation.

Bulk sample Ti6Al4V Power = 2208 W Speed = 5.854 m/s

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# Thin wall

Left column: longitudinal cross-section of the wall. Right: video of the melt pool dynamics during the EB-PBF process for all the layers.

Powder too strong wetting ( $\theta_{pow} = 10^\circ$ ) leads to the melt pool spill, wall widening and decreasing the melt depth causing.







Example of the thin wall manufacturing failure due to the melt pool balling.



# Conclusion

KiSSAM is GPU-based software for additive manufacturing simulations of melt-pool scale. The code allows to:

- Identify scanning regime defects: balling, keyholing, etc.
- Inspect melted sample morphology: roughness, porosity.
- Virtually build overhangs, thin walls, fine structures.
- Get temperature history, portion of absorbed energy.

On a desktop workstation with at least one high-end GPU, it is possible to:

- Simulate in full 3D
- Resolve small powder particles, sintering and pores on a fine mesh
- Perform multi-layer simulations
- Get detailed process maps (hundreds of experiments) in a few days



# **Related papers**

- Zakirov, A., Belousov, S., Bogdanova, M., Korneev, B., Stepanov, A., Perepelkina, A., ... & Potapkin, B. (2020). Predictive modeling of laser and electron beam powder bed fusion additive manufacturing of metals at the mesoscale. *Additive Manufacturing*, *35*, 101236
- Nakapkin, D. S., Zakirov, A. V., Belousov, S. A., Bogdanova, M. V., Korneev, B. A., Stepanov, A. E., ... & Meshkov, A. (2019). Finding optimal parameter ranges for laser powder bed fusion with predictive modeling at mesoscale. In *Sim-AM 2019: II International Conference on Simulation for Additive Manufacturing* (pp. 297-308). CIMNE.
- EBAM-2023 poster KiSSAM 3D simulation of electron beam melting process with adaptive mesh refinement at mesoscale level



### Morphology during multilayer melting



#### 1<sup>st</sup> layer



2<sup>nd</sup> layer



#### 3<sup>rd</sup> layer





4<sup>th</sup> layer



#### 5<sup>th</sup> layer

