

A unified fluid-solid formulation for thermo-mechanical problems using the PFEM: application to LPBF

WCCM-ECCOMAS 2026

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Introduction

Particle Finite Element Method

Particle Finite Element Method (PFEM)¹ $\rightarrow$ Lagrangian FEM + remeshing

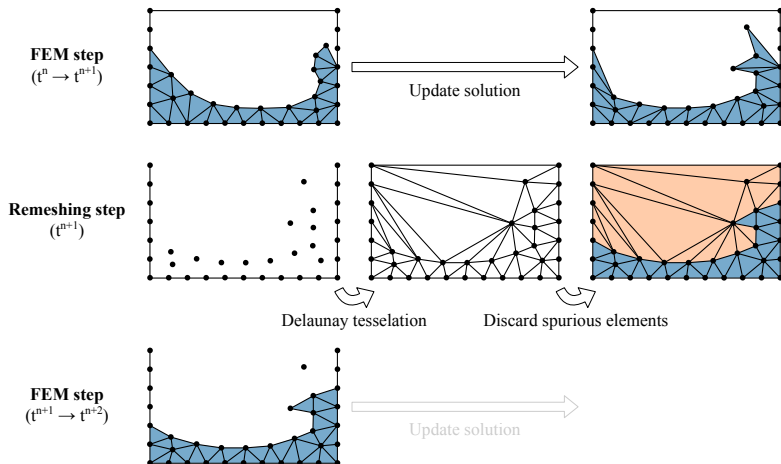


Figure 1: Diagram of a PFEM simulation

¹S. R. Idelsohn, E. Oñate, and F. Del Pin. "The particle finite element method: a powerful tool to solve incompressible flows with free-surfaces and breaking waves". In: *Int. J. Numer. Methods Eng.* 61.7 (2004), pp. 964–989. DOI: 10.1002/nme.1096.

Laser Powder Bed Fusion

Laser Powder Bed Fusion (LPBF) → additive manufacturing process used to create complex parts by selectively melting metal powder layer by layer

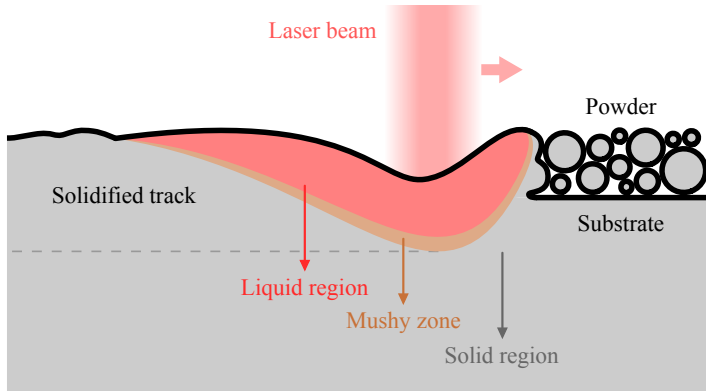


Figure 2: LPBF process (mesoscale)

Aim → predict shape, residual stresses and defects from process parameters (e.g. laser power, scanning speed, powder layer thickness and packing density)

Numerical framework

Spatial discretization (1)

Mixed velocity-pressure-temperature formulation:

- Momentum balance equation:

$$\rho \dot{\mathbf{v}} - \nabla \cdot \boldsymbol{\sigma} - \rho \mathbf{b} = 0$$

- Mass conservation equation:

$$\frac{1}{K} \dot{p} - \alpha_V \dot{T} + \nabla \cdot \mathbf{v} = 0$$

- Heat equation:

$$\rho c_v \dot{T} + \nabla \cdot \mathbf{q} - R = 0$$

Same conservation equations for solids and fluids → **unified formulation**

Domain discretized using **first-order mixed ($\mathbf{v} - p - T$) finite elements**

One material per element

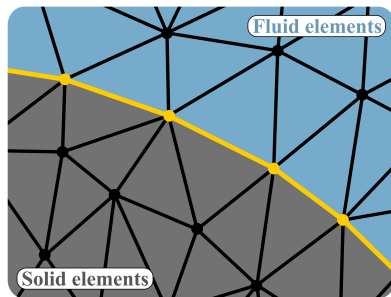


Figure 3: Numerical interface between solid and fluid sub-domains

Spatial discretization (2)

Momentum balance equation

$$\mathbf{M} \dot{\mathbf{v}} + \mathbf{F}_{\text{int}} - \mathbf{F}_{\text{ext}} = \mathbf{0}$$

$$\mathbf{M}_e = \int_{\mathbb{V}_e} \rho \mathbf{N}_v^T \mathbf{N}_v \, d\mathbb{V}$$

$$\mathbf{F}_{\text{int},e} = \int_{\mathbb{V}_e} \mathbf{B}^T (\hat{\mathbf{s}} - \hat{\mathbf{I}} \mathbf{N} \mathbf{p}_e) \, d\mathbb{V}$$

$$\mathbf{F}_{\text{ext},e} = \int_{\mathbb{V}_e} \rho \mathbf{N}_v^T \mathbf{b} \, d\mathbb{V} + \int_{\mathbb{S}_{t,e}} \mathbf{N}_v^T \bar{\mathbf{t}} \, d\mathbb{S}$$

Mass conservation equation

$$\mathbf{C} \dot{\mathbf{p}} - \mathbf{E} \dot{\mathbf{T}} + \mathbf{D} \mathbf{v} + \mathbf{S}_f + \mathbf{S}_s = \mathbf{0}$$

$$\mathbf{C}_e = \int_{\mathbb{V}_e} \frac{1}{K} \mathbf{N}^T \mathbf{N} \, d\mathbb{V}$$

$$\mathbf{E}_e = \int_{\mathbb{V}_e} \alpha_V \mathbf{N}^T \mathbf{N} \, d\mathbb{V}$$

$$\mathbf{D}_e = \int_{\mathbb{V}_e} \mathbf{N}^T \hat{\mathbf{I}}^T \mathbf{B} \, d\mathbb{V}$$

Heat equation

$$\mathbf{H} \dot{\mathbf{T}} + \mathbf{K} \mathbf{T} - \mathbf{S}_R - \mathbf{S}_q = \mathbf{0}$$

$$\mathbf{H}_e = \int_{\mathbb{V}_e} \rho c_v \mathbf{N}^T \mathbf{N} \, d\mathbb{V}$$

$$\mathbf{K}_e = \int_{\mathbb{V}_e} k \nabla \mathbf{N}^T \nabla \mathbf{N} \, d\mathbb{V}$$

$$\mathbf{S}_{R,e} = \int_{\mathbb{V}_e} \mathbf{N}^T R \, d\mathbb{V}, \quad \mathbf{S}_{q,e} = \int_{\mathbb{S}_{q,e}} \mathbf{N}^T \bar{q} \, d\mathbb{S}$$

Time integration

Residuals of the momentum, mass and heat equations (**implicit scheme**):

$$\mathbf{R}_v^{n+1} = \mathbf{M}^{n+1} \dot{\mathbf{v}}^{n+1} + \mathbf{F}_{\text{int}}^{n+1} - \mathbf{F}_{\text{ext}}^{n+1}$$

$$\mathbf{R}_p^{n+1} = \mathbf{C}^{n+1} \dot{\mathbf{p}}^{n+1} - \mathbf{E}^{n+1} \dot{\mathbf{T}}^{n+1} + \mathbf{D}^{n+1} \mathbf{v}^{n+1} + \mathbf{S}_s^{n+1} + \mathbf{S}_f^{n+1}$$

$$\mathbf{R}_T^{n+1} = \mathbf{H}^{n+1} \dot{\mathbf{T}}^{n+1} + \mathbf{K}^{n+1} \mathbf{T}^{n+1} - \mathbf{S}_R^{n+1} - \mathbf{S}_q^{n+1}$$

Available time integration schemes: backward Euler, Newmark and generalized- α

Staggered thermo-mechanical solver:

- Thermal step:

$$\mathbf{K}_{\text{th}}^{n+1(i)} \Delta \mathbf{T} = -\mathbf{R}_T^{n+1(i)} \rightarrow \mathbf{T}^{n+1(i+1)} = \mathbf{T}^{n+1(i)} + \Delta \mathbf{T}$$

- Mechanical step (**monolithic velocity-pressure system**):

$$\mathbf{K}_{\text{mech}}^{n+1(i)} \begin{bmatrix} \Delta \mathbf{v} \\ \Delta \mathbf{p} \end{bmatrix} = - \begin{bmatrix} \mathbf{R}_v^{n+1(i)} \\ \mathbf{R}_p^{n+1(i)} \end{bmatrix} \rightarrow \begin{aligned} \mathbf{v}^{n+1(i+1)} &= \mathbf{v}^{n+1(i)} + \Delta \mathbf{v} \\ \mathbf{p}^{n+1(i+1)} &= \mathbf{p}^{n+1(i)} + \Delta \mathbf{p} \end{aligned}$$

The **thermal** and **mechanical steps** are performed iteratively until convergence

Phase change – Material models

Simple expression of the liquid fraction:

$$f_l(T) = \begin{cases} 0 & \text{if } T \leq T_s \\ \frac{T - T_s}{T_l - T_s} & \text{if } T_s < T < T_l \\ 1 & \text{if } T_l \leq T \end{cases}$$

Choice of material models depending on the liquid fraction:

- Solid region ($f_l = 0$): thermo-elasto-visco-plastic solid model
- Mushy zone ($0 < f_l < 1$): non-Newtonian power-law fluid model
- Liquid region ($f_l = 1$): Newtonian fluid model

Reminder: fluid and solid material models are tied to finite elements

Consistency with choice of material models:

- $f_l = 0 \rightarrow$ solid elements
- $f_l > 0 \rightarrow$ fluid elements

Phase change – Element transformation

Enforce the choice of material model $\rightarrow$ transform elements from fluid to solid and/or vice versa

After each FEM step, elements are transformed based on their average nodal temperature:

$$\bar{T}_e = \frac{1}{N} \sum_i^N T_i$$

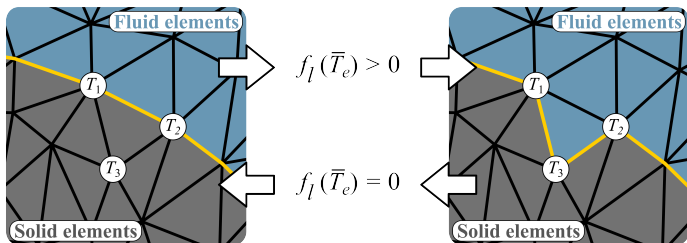


Figure 4: Criteria for the solid-to-fluid and fluid-to-solid element transformations.

Phase change – Summary

Appropriate choice of model parameters → smooth transition in material behavior across the mushy zone

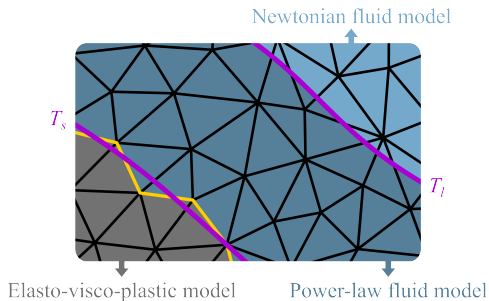


Figure 5: Materials models across the mushy zone. The numerical interface between fluid and solid elements is represented by the yellow line.

Numerical interface → approximation of the solidus isothermal

Remeshing for fluid-solid interaction problems

Remeshing algorithm:

- Edge-splitting/level-set based **mesh adaptation**²
- **Constrained tessellation** for interface tracking

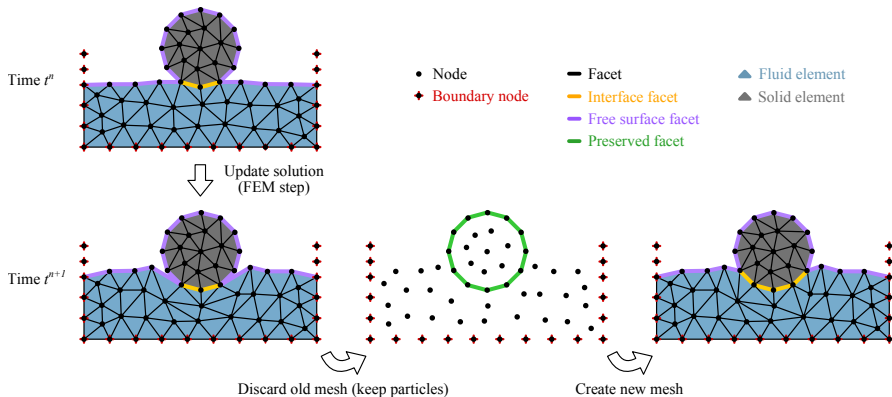


Figure 6: Base remeshing algorithm for fluid-solid interaction problems

²M. Lacroix et al. "An efficient level set-based mesh adaptation for the particle finite element method". In: *Comput. Meth. Appl. Mech. Eng.* 450 (2026), p. 118644. DOI: 10.1016/j.cma.2025.118644.

This method is presented in ...

Computer Methods in Applied Mechanics and Engineering 459 (2026) 119074



Contents lists available at ScienceDirect

Comput. Methods Appl. Mech. Engrg.

journal homepage: www.elsevier.com/locate/cma



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³D. Bogucki et al. “A unified fluid-solid formulation for thermo-mechanical problems using the Particle Finite Element Method: Application to metal additive manufacturing”. In: *Comput. Meth. Appl. Mech. Eng.* 459 (2026), p. 119074. DOI: 10.1016/j.cma.2026.119074.

Numerical examples

Illustrative example

Steel beam melting

Melting of a steel beam → PFEM example proposed by Franci et al. 2017

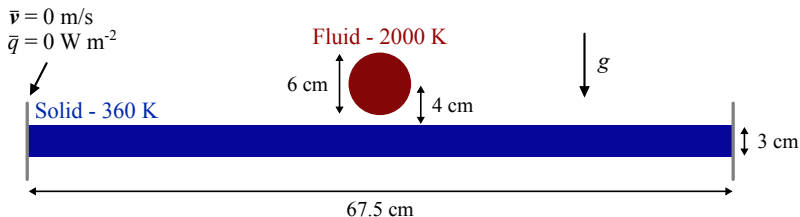


Figure 7: Initial configuration and boundary conditions

⁴A. Franci et al. "PFEM formulation for thermo-coupled FSI analysis. Application to nuclear core melt accident". In: *Comput. Meth. Appl. Mech. Eng.* 325 (2017), pp. 711–732. DOI: 10.1016/j.cma.2017.07.028.

Melting of a bare substrate

Static laser test (2D axisymmetric) – Setup

Thermo-fluid-solid simulation of a static laser on a bare substrate of Inconel 718 considering:

- Vaporization effects (recoil pressure + heat loss)
- Marangoni forces (surface tension)

Uniform laser beam:

$$\bar{q}_{L,z} = \begin{cases} -a \frac{P_L}{\pi R_L^2} \left(1 - e^{-\frac{t}{\tau_m}}\right) & \text{if } r \leq R_L \\ 0 & \text{if } r > R_L \end{cases}$$

with

- Laser power: $P_L = 471.24 \text{ W}$
- Laser radius: $R_L = 50 \text{ }\mu\text{m}$
- Characteristic time: $\tau_m = 30 \text{ }\mu\text{s}$
- Absorptivity: $a = 0.3$

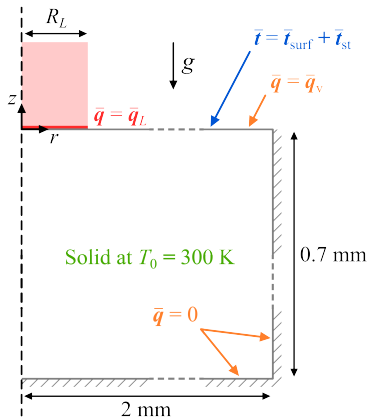


Figure 8: Initial configuration and boundary conditions

Static laser test (2D axisymmetric) – Snapshots

Simulation time: 60 μs

Time-step size: $\sim 2.5 \times 10^{-2} \mu\text{s}$

Number of nodes: $\sim 5,000$

Number of elements: $\sim 10,000$

Computation time: $\sim 15 \text{ min}$

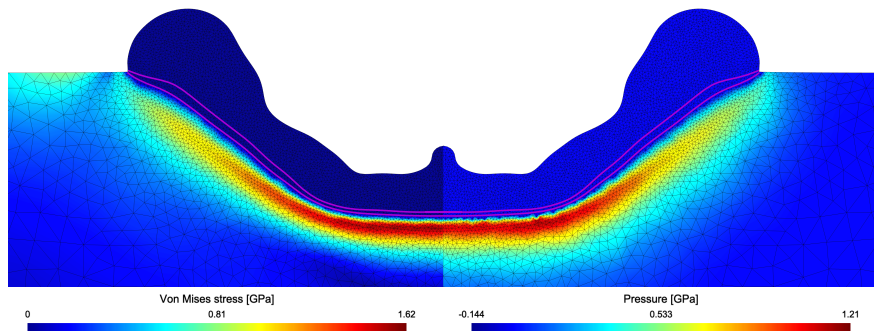


Figure 9: Von Mises stress distribution (left); pressure distribution (right). Zoom on the region of interest at $t = 60 \mu\text{s}$.

Static laser test (2D axisymmetric) – Verification

Comparison of the melt pool shape with fluid-only simulation results from the literature^{5,6}

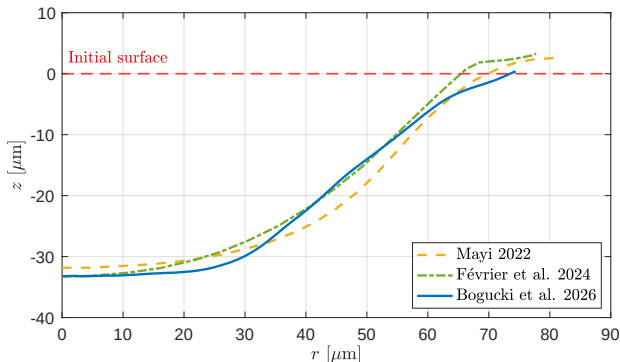


Figure 10: Shape of the melt pool (i.e. $T = 1521$ K isothermal) at $t = 60 \mu\text{s}$.

⁵Y. Mayi. "Compréhension et simulation des phénomènes physiques affectant la fabrication additive en SLM". Ph.D. Thesis. HESAM Université, 2021. URL: <https://hal.science/tel-03612996>.

⁶S. Février et al. "Simulation of melt pool dynamics including vaporization using the particle finite element method". In: *Comput. Mech.* (2024). DOI: 10.1007/s00466-024-02571-4.

Laser track test (3D) – Setup

Thermo-fluid-solid simulation of a laser track on a bare stainless steel substrate (neglecting vaporization effects and Marangoni forces)

Gaussian laser beam:

$$\bar{q}_{L,z} = \begin{cases} -a \frac{2P_L}{\pi R_L^2} e^{-\frac{2r^2}{R_L^2}} & \text{if } r \leq R_L \\ 0 & \text{if } r > R_L \end{cases}$$

with

- Laser power: $P_L = 45 \text{ W}$
- Laser radius: $R_L = 50.97 \text{ }\mu\text{m}$
- Absorptivity: $a = 0.3$
- Scanning speed: $V_L = 30 \text{ cm/s}$

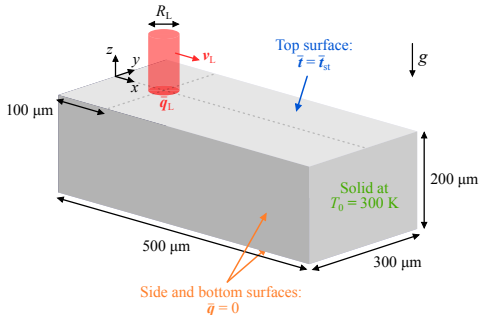


Figure 11: Initial configuration and boundary conditions

Laser track test (3D) – Snapshots

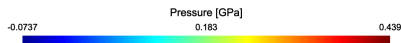
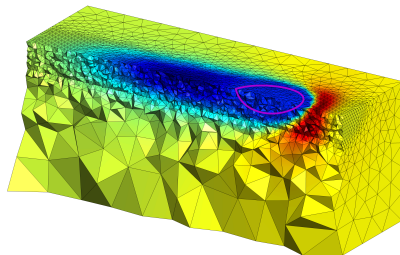
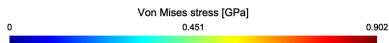
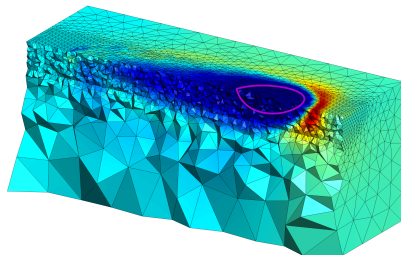
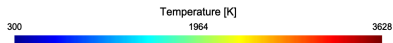
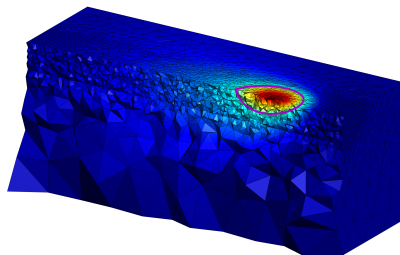
Simulation time: 1 ms

Time-step size: $\sim 5 \times 10^{-2} \mu\text{s}$

Number of nodes: $\sim 20,000$

Number of elements: $\sim 100,000$

Computation time: $\sim 15 \text{ h}$



Laser track test (3D) – Verification

Comparison of the melt pool shape with experimental and numerical results from the literature^{7,8}

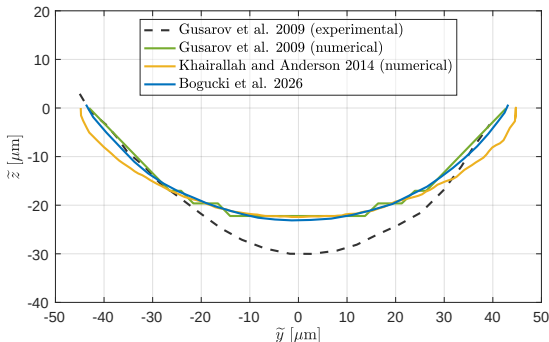


Figure 13: Comparison of the shape of the melt pool perpendicular to the scanning direction (i.e. $T = 1700$ K isothermal for the numerical results; dark line for the experimental result) with experimental and numerical results.

⁷A. V. Gusarov et al. "Model of Radiation and Heat Transfer in Laser-Powder Interaction Zone at Selective Laser Melting". In: *J. Heat Transf.* 131.7 (2009), p. 072101. DOI: 10.1115/1.3109245.

⁸S. A. Khairallah and A. Anderson. "Mesoscopic simulation model of selective laser melting of stainless steel powder". In: *J. Mater. Process. Technol.* 214.11 (2014), pp. 2627–2636. DOI: 10.1016/j.jmatprotec.2014.06.001.

LPBF single track

LPBF single track (3D) – Setup

Simulation of the LPBF process with Inconel 718 substrate and powder (considering **vaporization effects** and **Marangoni forces**)

Laser parameters:

- Gaussian beam
- Laser power: 190 W
- Laser diameter: 80 μm
- Scanning speed: 1.56 m/s

Substrate geometry:

- Length: 1000 μm
- Width: 300 μm
- Height: 200 μm

Powder bed geometry:

- Height: 30 μm
- Packing density: ~ 0.45

Initial particle distribution generated with the open-source packing generator software RCPGenerator

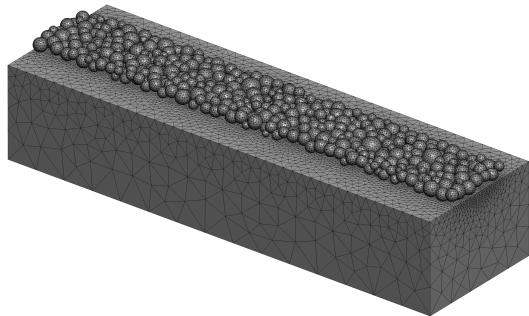


Figure 14: Initial mesh

LPBF single track (3D) – Snapshots (1)

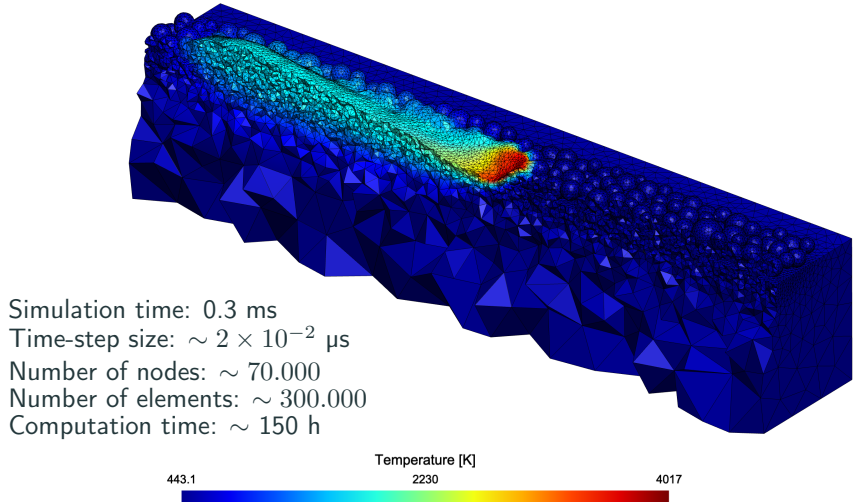


Figure 15: Temperature distribution at $t = 0.3 \text{ ms}$

LPBF single track (3D) – Snapshots (2)

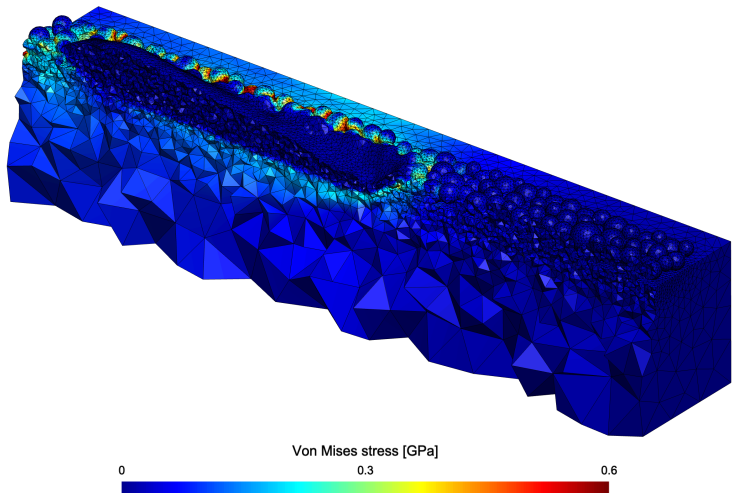


Figure 16: Von Mises stress distribution at $t = 0.3$ ms

LPBF single track (3D) – Snapshots (3)

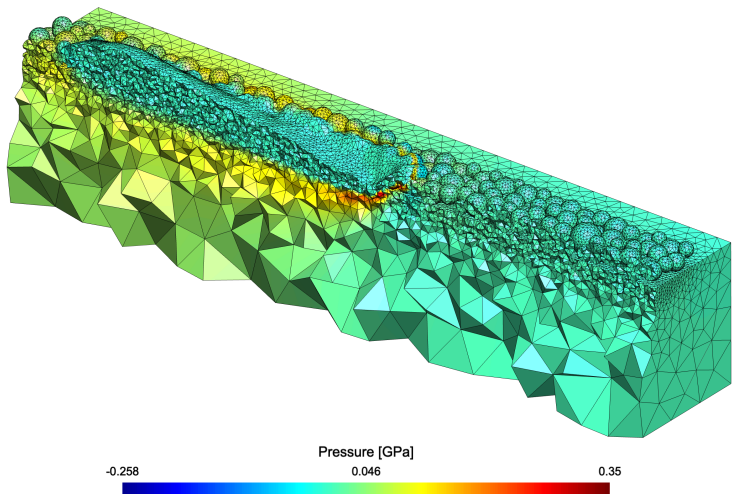


Figure 17: Pressure distribution at $t = 0.3$ ms

Conclusion

Conclusion and future works

Current **capabilities** of our **PFEM framework**:

- Thermo-fluid-solid simulations
- Vaporization effects
- Marangoni forces
- **Laser-fluid-solid interaction**
- **Phase change**
- **Application** to single track **LPBF** experiments

Future works:

- Further **experimental validation**
- Explicit time integration
- Laser reflections
- Solid microstructure and crystal plasticity

Thank you for your attention!

Feel free to contact me at dorian.bogucki@uliege.be for additional information

Dorian Bogucki acknowledges the funding from Wallonia-Brussels
Federation – Concerted Research Actions, Belgium



Martin Lacroix acknowledges the research project TiNTHyN, as
part of the Win4Excellence program – convention 2310142,
Walloon Region of Belgium



Appendices

Generalized- α scheme (1)

Generalized- α scheme used for all conservation equations with a single set of parameters (γ , α_m and α_f)

Computation of the residuals:

$$\begin{aligned} \mathbf{R}_v^{n+1} &= \alpha_m \mathbf{M}^{n+1} \dot{\mathbf{v}}^{n+1} + \alpha_f (\mathbf{F}_{\text{int}}^{n+1} - \mathbf{F}_{\text{ext}}^{n+1}) + (1 - \alpha_m) \mathbf{M}^n \dot{\mathbf{v}}^n + (1 - \alpha_f) (\mathbf{F}_{\text{int}}^n - \mathbf{F}_{\text{ext}}^n) \\ \mathbf{R}_p^{n+1} &= \alpha_m (\mathbf{M}_\tau^{n+1} \dot{\mathbf{v}}^{n+1} + \mathbf{C}^{n+1} \dot{\mathbf{p}}^{n+1} - \mathbf{E}^{n+1} \dot{\mathbf{T}}^{n+1}) + \alpha_f (\mathbf{D}^{n+1} \mathbf{v}^{n+1} + \mathbf{D}_\tau^{n+1} \mathbf{p}^{n+1} + \mathbf{C}_\beta^{n+1} \mathbf{p}^{n+1} - \mathbf{F}_\tau^{n+1}) \\ &\quad + (1 - \alpha_m) (\mathbf{M}_\tau^n \dot{\mathbf{v}}^n + \mathbf{C}^n \dot{\mathbf{p}}^n - \mathbf{E}^n \dot{\mathbf{T}}^n) + (1 - \alpha_f) (\mathbf{D}^n \mathbf{v}^n + \mathbf{D}_\tau^n \mathbf{p}^n + \mathbf{C}_\beta^n \mathbf{p}^n - \mathbf{F}_\tau^n) \\ \mathbf{R}_T^{n+1} &= \alpha_m \mathbf{H}^{n+1} \dot{\mathbf{T}}^{n+1} + \alpha_f (\mathbf{K}^{n+1} \mathbf{T}^{n+1} - \mathbf{S}_R^{n+1} - \mathbf{S}_q^{n+1}) + (1 - \alpha_m) \mathbf{H}^n \dot{\mathbf{T}}^n + (1 - \alpha_f) (\mathbf{K}^n \mathbf{T}^n - \mathbf{S}_R^n - \mathbf{S}_q^n) \end{aligned}$$

Computation of the time derivatives of the unknowns:

$$\begin{aligned} \dot{\mathbf{v}}^{n+1} &= \frac{\mathbf{v}^{n+1} - \mathbf{v}^n}{\gamma \Delta t} - \frac{1 - \gamma}{\gamma} \dot{\mathbf{v}}^n \\ \dot{\mathbf{p}}^{n+1} &= \frac{\mathbf{p}^{n+1} - \mathbf{p}^n}{\gamma \Delta t} - \frac{1 - \gamma}{\gamma} \dot{\mathbf{p}}^n \\ \dot{\mathbf{T}}^{n+1} &= \frac{\mathbf{T}^{n+1} - \mathbf{T}^n}{\gamma \Delta t} - \frac{1 - \gamma}{\gamma} \dot{\mathbf{T}}^n \end{aligned}$$

Update of the positions:

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \Delta t \mathbf{v}^n + \Delta t \gamma (\mathbf{v}^{n+1} - \mathbf{v}^n)$$

Generalized- α scheme (2)

Choice of the parameters $\rightarrow$ parameters for first-order problems:

$$\alpha_m = \frac{3 - \rho_\infty}{2(1 + \rho_\infty)}, \quad \alpha_f = \frac{1}{\rho_\infty + 1}, \quad \gamma = \frac{1}{2} + \alpha_m - \alpha_f$$

- $\rightarrow$ Second-order accuracy only for fluids
- $\rightarrow$ Still well suited to solids¹⁰

¹⁰C. Kadapa, W.G. Dettmer, and D. Perić. "On the advantages of using the first-order generalised-alpha scheme for structural dynamic problems". In: *Comput. Struct.* 193 (2017), pp. 226–238. DOI: 10.1016/j.compstruc.2017.08.013.

Phase change – Material models (cont'd)

Table 1: Material models and parametrization considered in the phase transformation model.

Solid elements	Fluid elements	
State variables: s , α , $\bar{\varepsilon}_{vp}$ and ρ	No state variables	
Elasto-visco-plastic model (solid region)	Power-law fluid model (mushy zone)	Newtonian fluid model (liquid region)
$\overset{\nabla}{\sigma} = \mathcal{H} : (\mathbf{D} - \mathbf{D}_{vp} - \mathbf{D}_{th}) + \dot{\mathcal{H}} : (\mathcal{H}^{-1} : \sigma)$ $\overset{\nabla}{\alpha} = \frac{2}{3} h_k \mathbf{D}_{vp} + \frac{\dot{h}_k}{h_k} \alpha$ $\mathbf{D}_{vp} = \frac{\sqrt{2}}{2} \left\langle \frac{\bar{\sigma} - \sigma_y}{\sqrt{3} K_S \bar{\varepsilon}_{vp}^{n_S}} \right\rangle^{\frac{1}{m_S}} \mathbf{N}$ $\mathbf{D}_{th} = \frac{\tilde{\alpha}_V}{3} \dot{T} \mathbf{I}$	$\sigma = 2 K_F \dot{\gamma}^{m_F - 1} \text{dev}(\mathbf{D}) - p \mathbf{I}$ $\rho = \rho(p, T)$	$\sigma = 2 K_F \text{dev}(\mathbf{D}) - p \mathbf{I}$ $\rho = \rho(p, T)$
Elasto-visco-plastic model $\leftrightarrow$ power-law fluid model (at $T = T_s$)	Power-law fluid model $\leftrightarrow$ Newtonian fluid model (at $T = T_l$)	
$\sigma_y(T) = 0, \quad h_k(T) = 0$ $K_S(T) = K_F(T), \quad n_S(T) = 0, \quad m_S(T) = m_F(T)$	$m_F(T) = 1$	

Thermal expansion coefficient for solids

Pressure part of the stress-strain relationship of the thermo-elasto-visco-plastic model:

$$\begin{aligned}\dot{p} &= -K(T) (D_{ii} - (D_{\text{th}})_{ii}) + \frac{\dot{K}(T)}{K(T)} p \\ &= -K(T) \left(\nabla \cdot \mathbf{v} - \tilde{\alpha}_V(T) \dot{T} \right) + \frac{\dot{K}(T)}{K(T)} p\end{aligned}$$

Using $\dot{K} = \frac{dK}{dT} \frac{dT}{dt} = \frac{dK}{dT} \dot{T}$, the pressure part can be rewritten as:

$$\frac{1}{K(T)} \dot{p} - \left(\tilde{\alpha}_V(T) + \frac{1}{K^2(T)} \frac{dK}{dT}(T) p \right) \dot{T} + \nabla \cdot \mathbf{v} = 0$$

which is equivalent to the mass conservation equation where the volumetric thermal expansion coefficient is defined as:

$$\alpha_V(p, T) = \tilde{\alpha}_V(T) + \frac{1}{K^2(T)} \frac{dK}{dT}(T) p$$