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Numerical modeling of additive manufacturing: some thermomechanical aspects

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STEEL SIM 2021

October, virtual conference

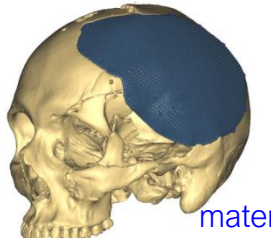
Introduction: L-PBF (laser beam melting)

Benefits…

- Direct manufacturing of complex parts, based on CAD description
- Reduced time to market
- Light post-forming processes
- Wide application range in terms of materials

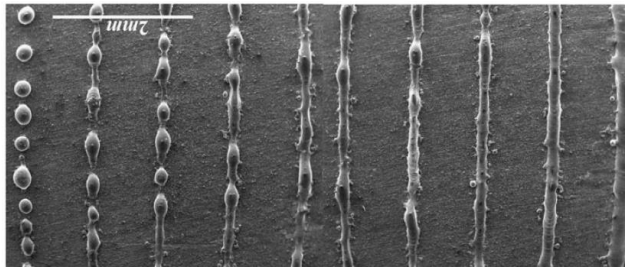
sirris.be

autodesk.fr

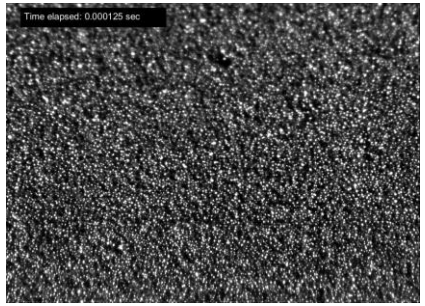


materialise.com

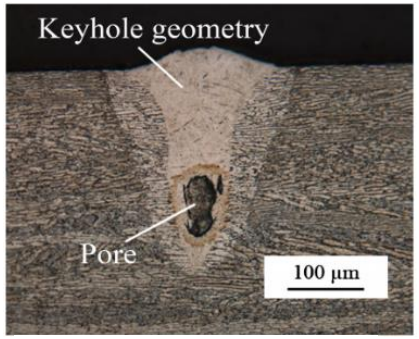
▶ *… but defects, at various scales, as results of complex multiphysics*



"Balling", 316L, Li *et al*. 12

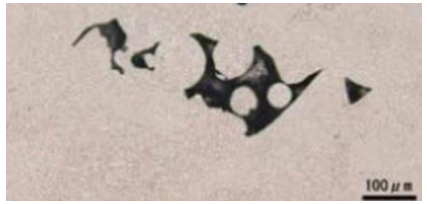


Vaporization and denudation, Bidare *et al*. 18

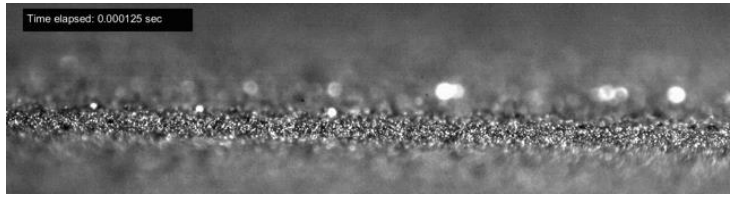


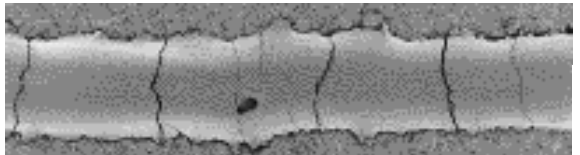
Porosities, Gong *et al*. 14

Cracks, Mercelis & Kruth 06



Lack of fusion, Ti-6-4, Bandyopadhyay & Traxel 18

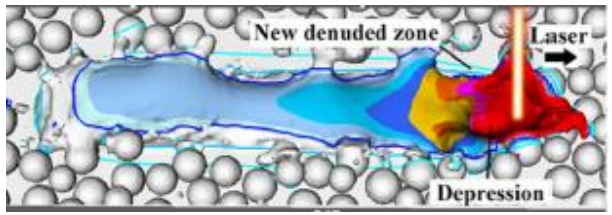




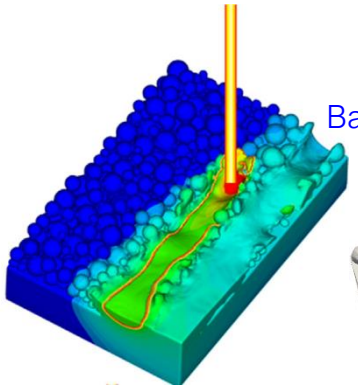
Microcracks Al_2O_3, Moniz *et al*. 19

Numerical modeling: which scale?

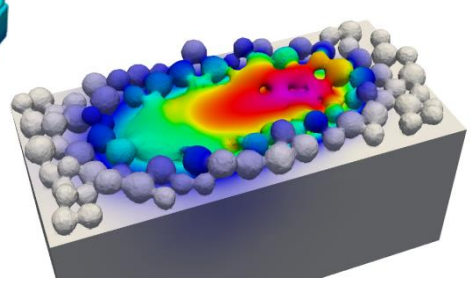
Particles scale – "microscopic"



Khairallah *et al*. 16



Bayat & Hattel 19

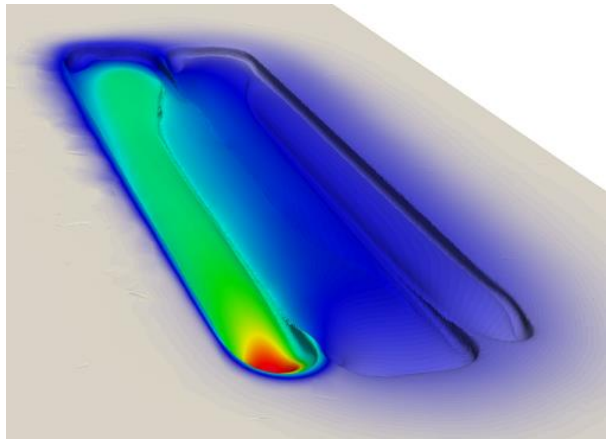


Zhang *et al*. 19, CEMEF

- *Interaction laser – powder particles*
- *Formation of melted zone, porosities*
- *Influence of powder granulometry distribution*

- *Very high computing time*

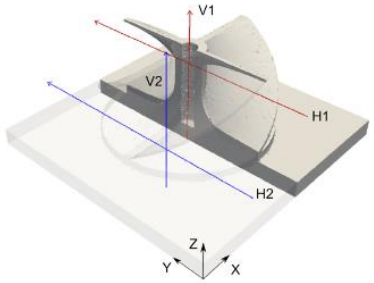
Track scale – Continuous powder bed "mesoscopic"

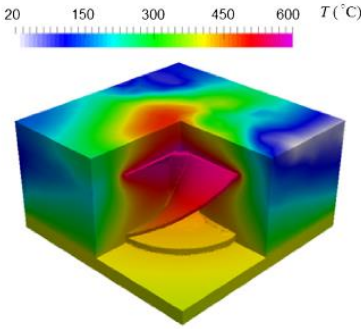


- *Interaction laser – powder bed*
- *Balling, keyhole*
- *Shape of elementary deposits* (tracks)
- *Stress formation* in the wake of the melted zone
- *Hot cracking*

Objective Simulate L-PBF at **meso-** and **macro-scale** by FEM

Part scale "macroscopic"





Zhang et al. 19, CEMEF

- *Temperature* distribution
- *Distortions and stress*, during and after processing
- *Cold cracking* (solid state)

Khairallah, Anderson, Rubenchik, King, *Acta Materialia* 2016
Bayat, Mohanty, Hattel, *Heat and Mass Transfer* 2019

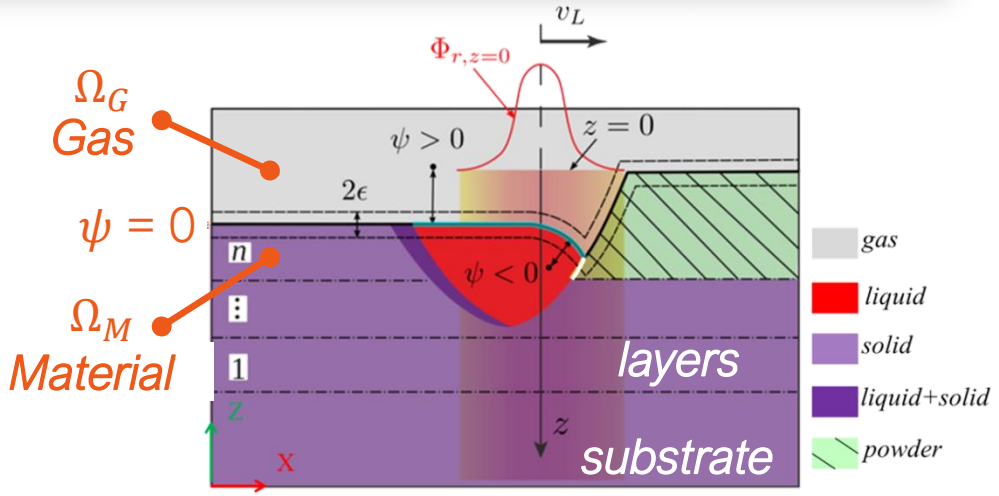
Outline of the presentation

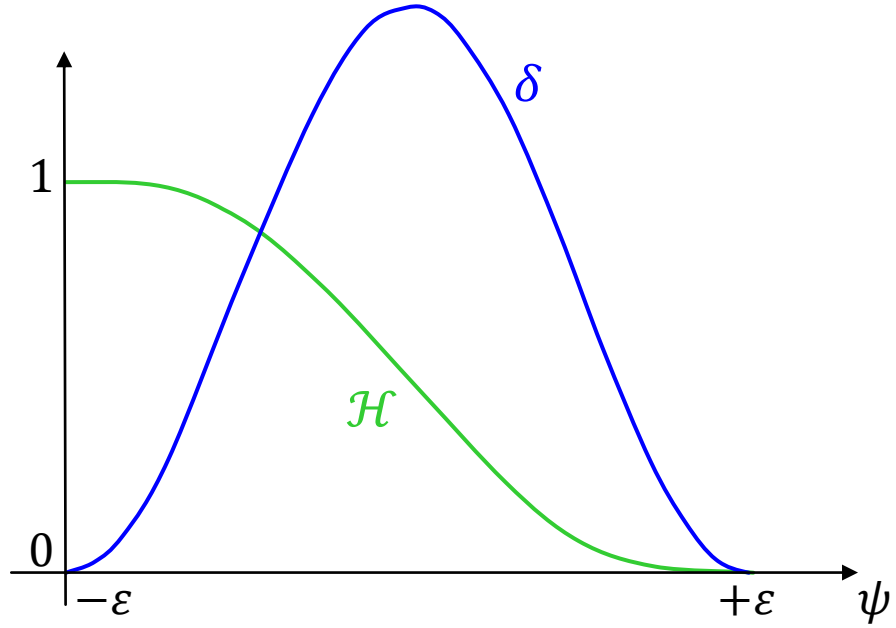
- L-PBF: Numerical simulation at the scale of elementary tracks
  - Thermohydraulics
    - Comparison with experimental testing, and validation
  - Thermomechanics
    - Focus on cracking risks: "cold" cracking, and solidification cracking
    - How to combine thermohydraulics and solid mechanics?
    - How to identify material behavior in processing conditions?
- Conclusions & perspectives

Meso approach: thermohydraulics

Meso approach for L-PBF

- Level set framework for unsteady thermohydraulics
  - Domains
    - Multiphased domain : the material Ω_M
    - Monophased domain : gas Ω_G
  - Interface between domains Ω_M and Ω_G
    - Signed distance function ψ. Interface: $\psi = 0$
    - Smooth Heaviside function $\mathcal{H}$ in the transition zone $\pm\varepsilon$
  - Mixed quantities
    - In the transition zone : $\{\chi\} = \mathcal{H}\langle\chi\rangle^M + (1-\mathcal{H})\,\chi^G$
    - In the material : $\langle\chi\rangle^M = \sum_{phases\ j} g_M^j\,\chi^j$
  - Smoothed Dirac function $\delta = \dfrac{\partial\mathcal{H}}{\partial\psi}$





Thermo-hydraulics: main features

Thermal Solver

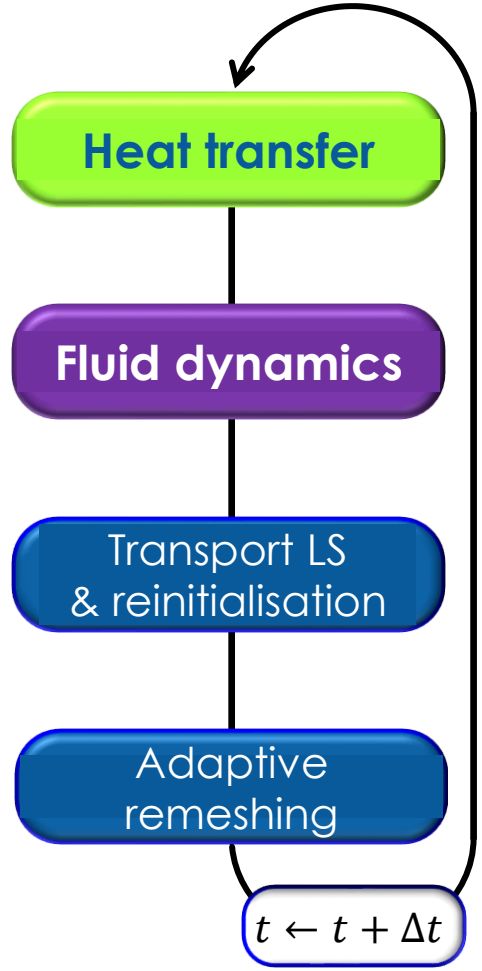
- Laser interaction
  - Heat input in surface on opaque liquids: Gaussian or "top-hat" distribution (+ CSF method, $\times \delta$)
  - Heat input in volume on semi-transparent liquids, or on powder bed: Beer-Lambert model

$$\frac{d\phi}{dz} = -\alpha\phi \qquad \dot{Q}(z) = -\frac{d\phi}{dz} = \phi_{r,z=0}\alpha \exp\left(-\int_0^z \alpha dz\right)$$

  - Heat loss, due to possible vaporization
- Models for apparent conductivity of powder beds

Navier-Stokes Solver (compressible)

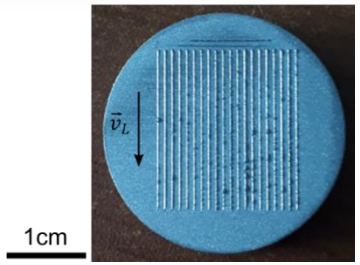
- Newtonian behavior
  - Transition powder / melted liquid: variation of $\langle\rho\rangle^M$ on a predefined interval ΔT
  - Laminar flow (Re < 1000)
- Applied forces
  - Gravity: $\{\rho\}\,\mathbf{g}$
  - Surface tension, including Marangoni: $\mathbf{f}_{ST} = \gamma\kappa_t\mathbf{n}_l + \frac{\partial\gamma}{\partial T}\nabla_s T$ ($\times \delta$)
  - Recoil pressure, due to possible vaporization

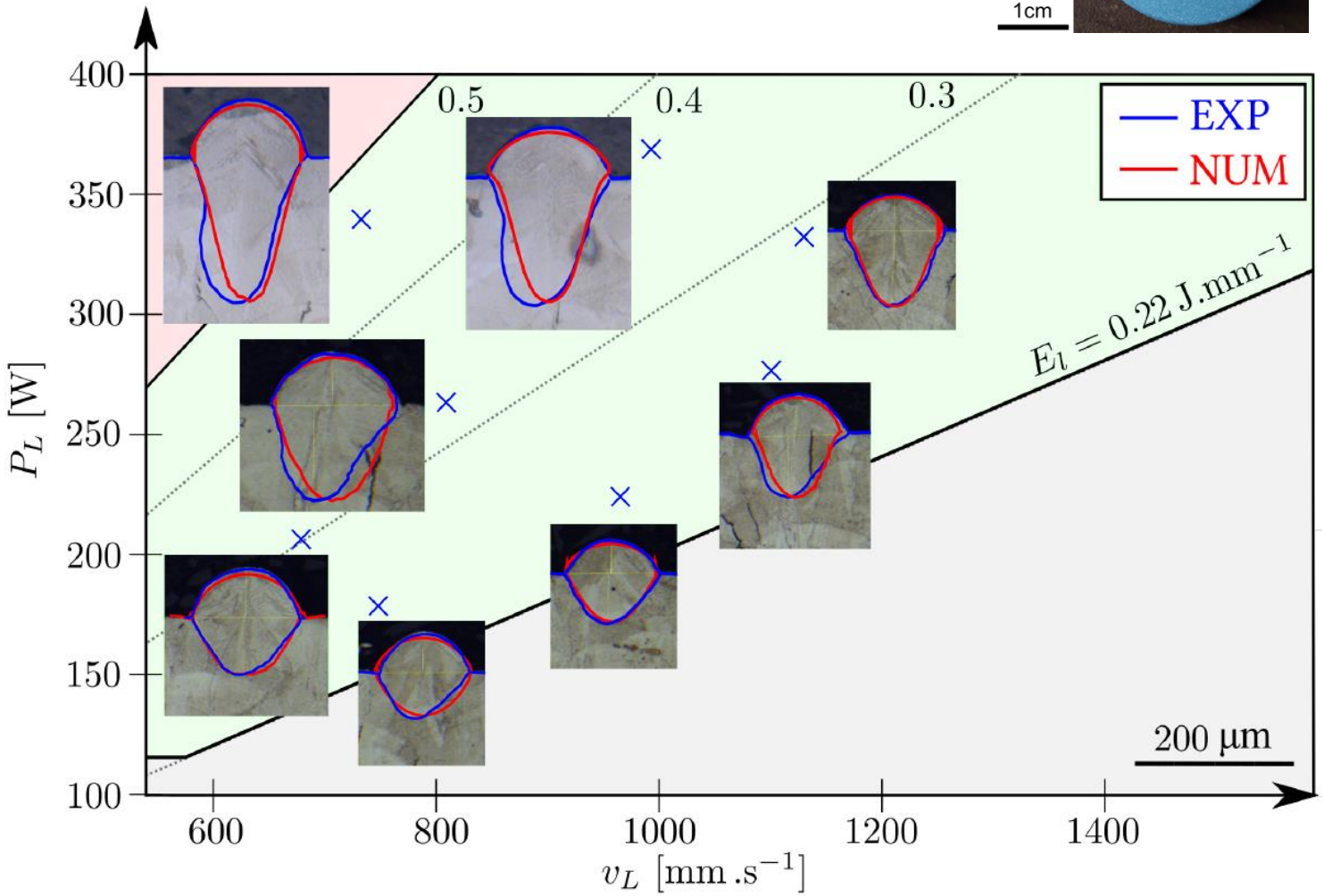


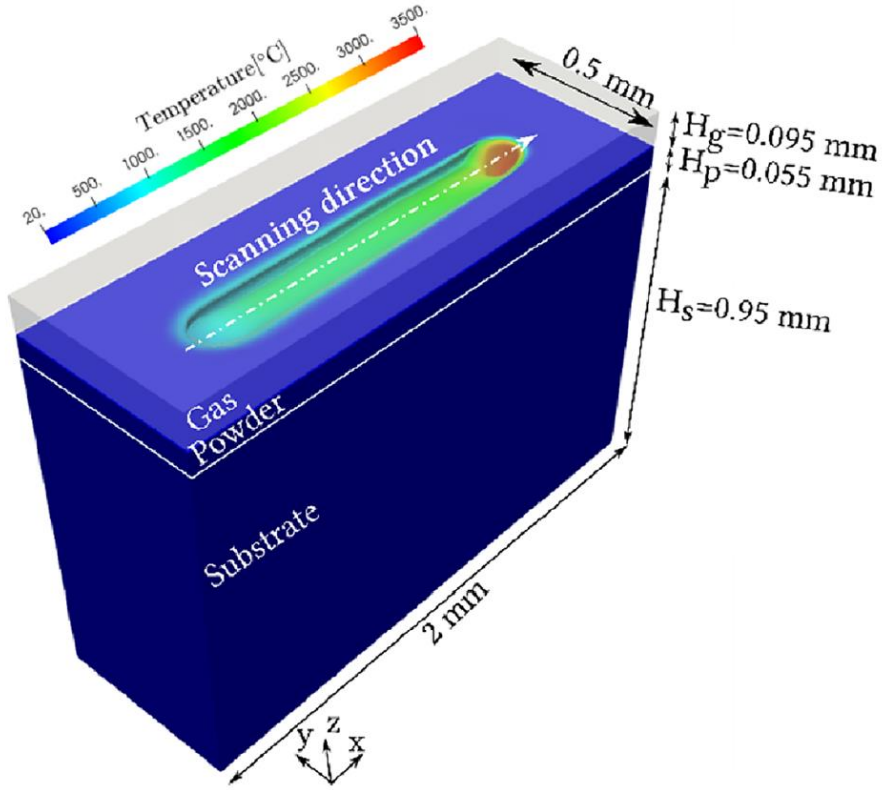
Chen, Guillemot, Gandin, Bellet, Additive Manufacturing 2017
Queva, Guillemot, Moriconi, Metton, Bellet, Additive Manufacturing 2020

Simulation *vs* experiments for metals: IN738

Experiments: PhD of David Grange, 2020
Centre des Matériaux – Mines Paristech







Numerical simulation: PhD of Alexis Queva, 2021, CEMEF

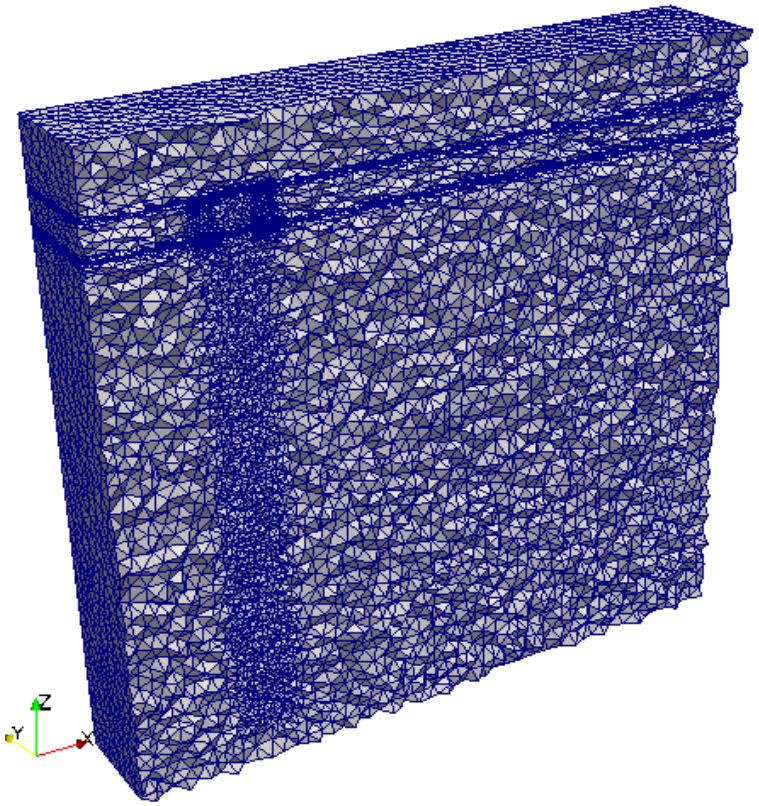
Dynamic mesh adaptation

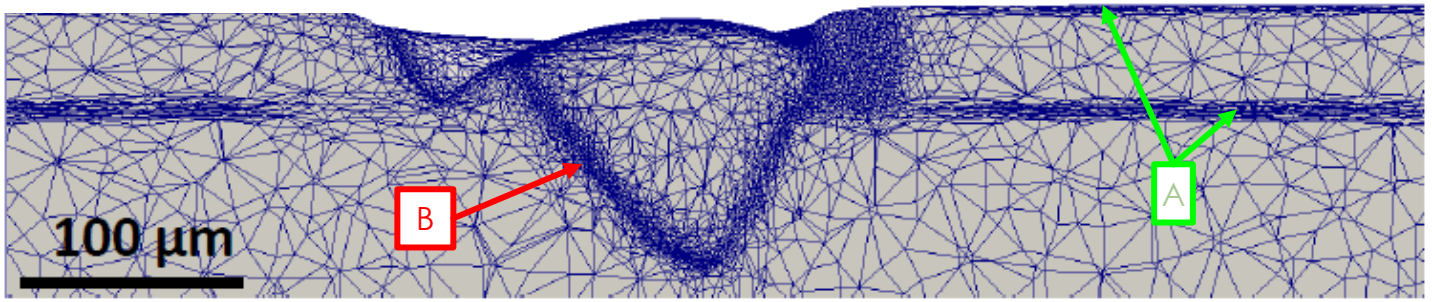
Multi-objective mesh adaptation
Coupez, J. Comp. Physics 2011
based on:

- Density (A)
- & Liquid fraction (B)
- & laser interaction zone

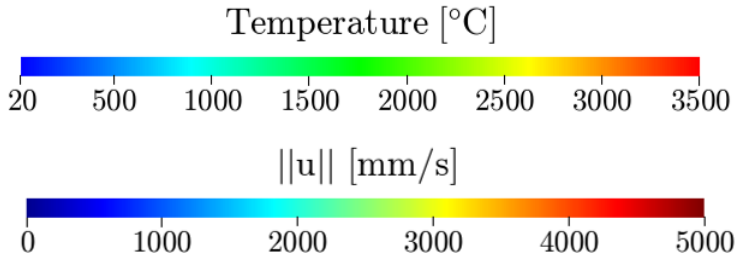
Background size: 50 µm
Min size : 0.5 µm
Remeshing period 10 μs

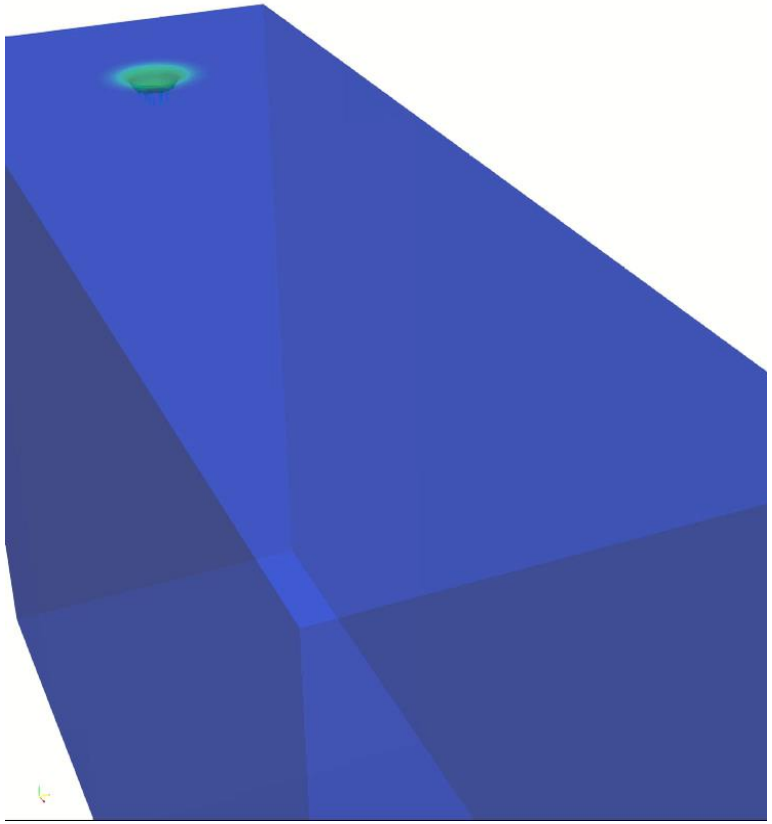
$N_{Elts}(t_0) = 2.1$ M
$N_{Elts}(t_{end}) = 2.6$ M

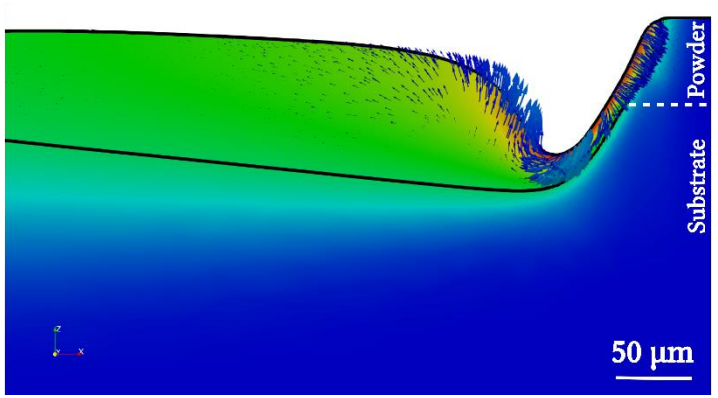


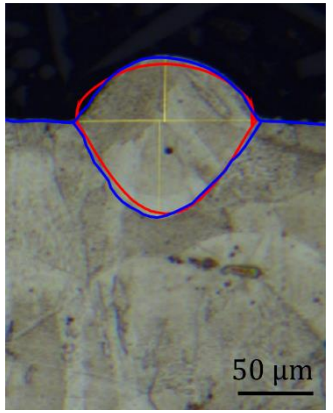


IN738, $\phi_L = 100$ µm

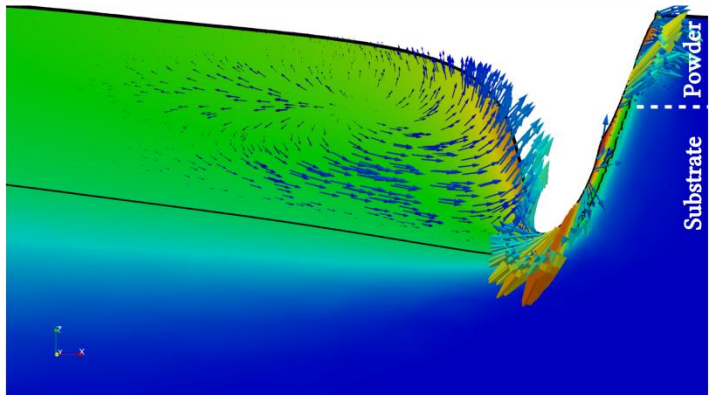


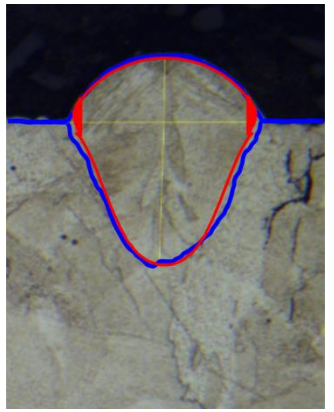




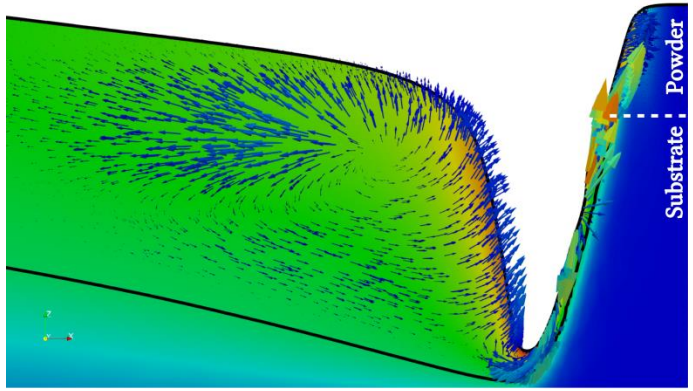


$P_L = 230$ W, $v_L = 960$ mm/s
0.24 J/mm
$A = 0.70$





$P_L = 320$ W, $v_L = 1100$ mm/s
0.29 J/mm
$A = 0.79$



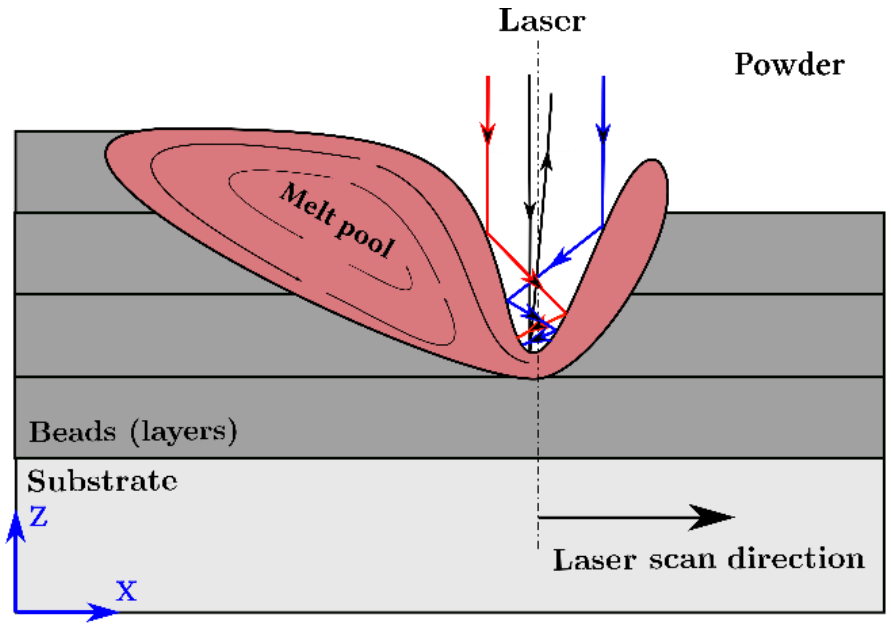
$P_L = 340$ W, $v_L = 730$ mm/s
0.47 J/mm
$A = 0.82$

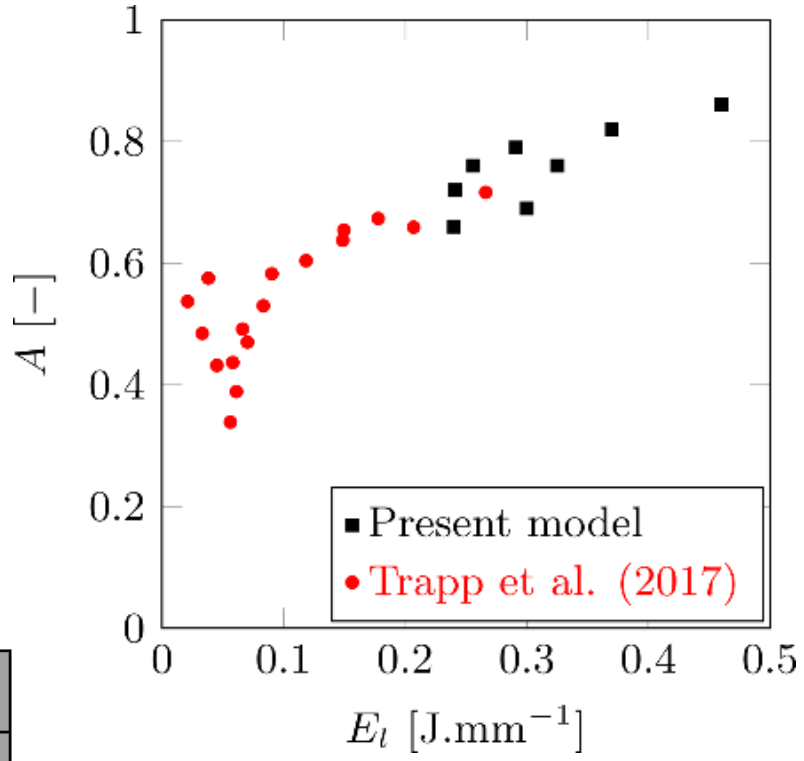
Grange, Queva, Guillemot, Colin, Bartout, Bellet,
J Mater Proc Tech 2021

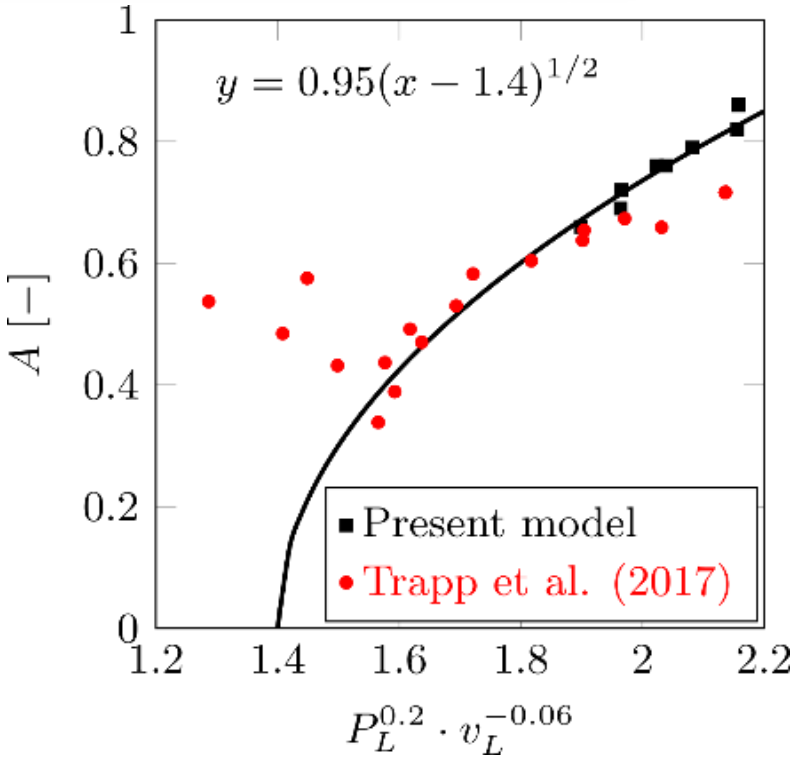
Evaluation of the absorption coefficient

- Augmentation of A with keyhole formation

$$E_l = \frac{P_L}{v_L} \nearrow \implies \text{keyhole} \nearrow \implies A \nearrow$$







$$A = 0.95\sqrt{{P_L}^{0.2}{v_L}^{-0.06} - 1.4}$$

with P_L [W] and v_L [mm s^{-1}]

Trapp *et al*. (TU Dresden, Lawrence Livermore), Appl Mat Today 2017
Grange, Queva, Guillemot, Colin, Bartout, Bellet, J Mater Proc Tech 2021

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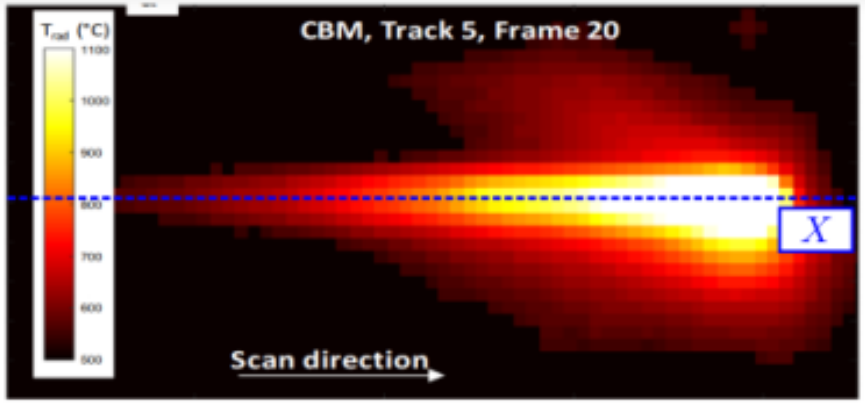
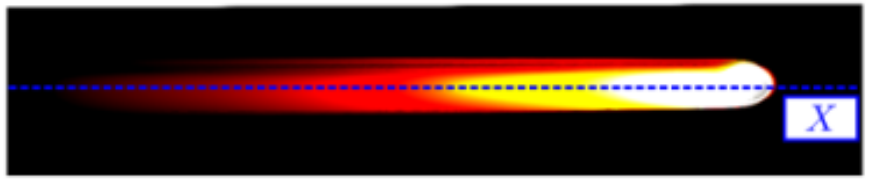
Thermal validation for metals: IR imaging

- Temperature distribution
- Extension of melt pool

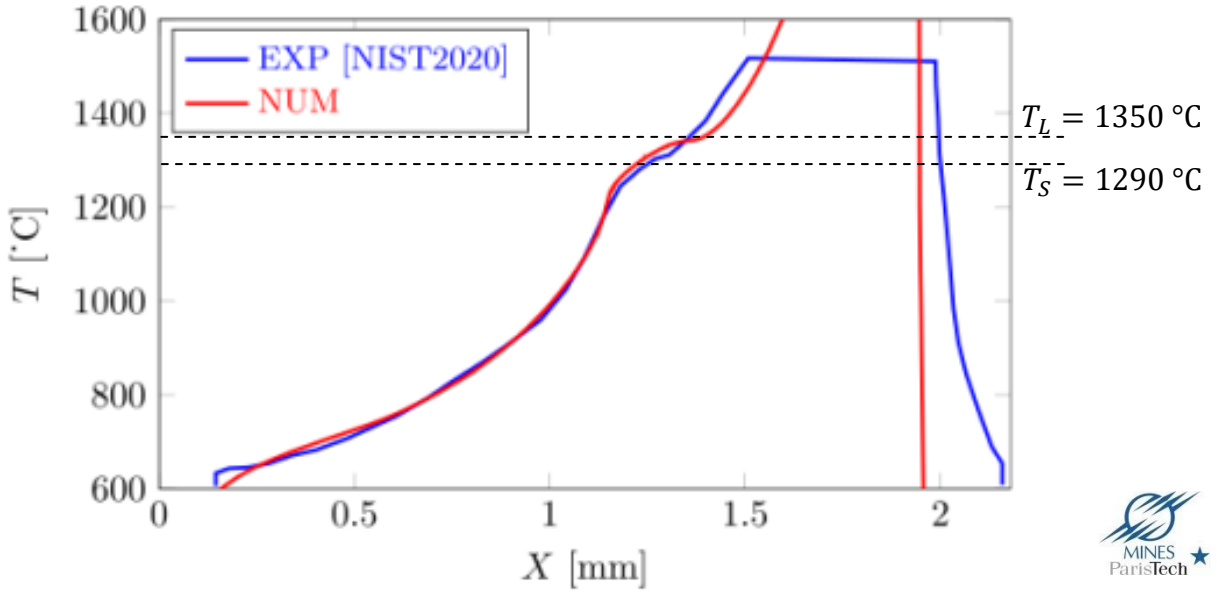
Experimental
NIST: Lane *et al*. 2020



IN625
$P_L = 195$ W
$v_L = 800$ mm s^{-1}
$\phi_L = 100$ µm



Modelling



Extension to multiple tracks…

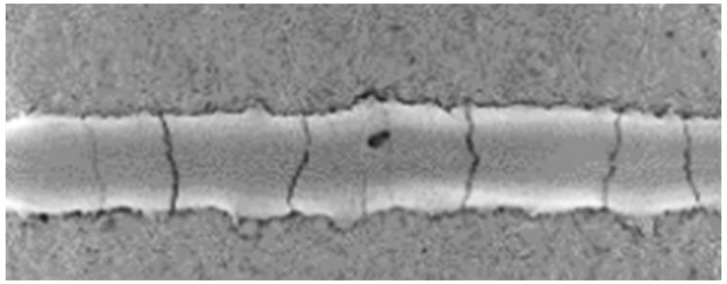
IN718
3 layers of a lattice pillar
9 tracks per layer
1 mm^2

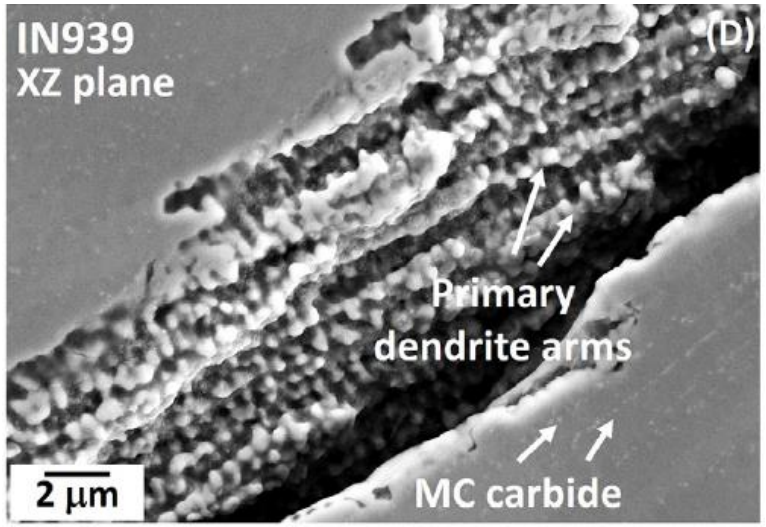
Meso approach: solid mechanics

Why solid mechanics at the meso scale?

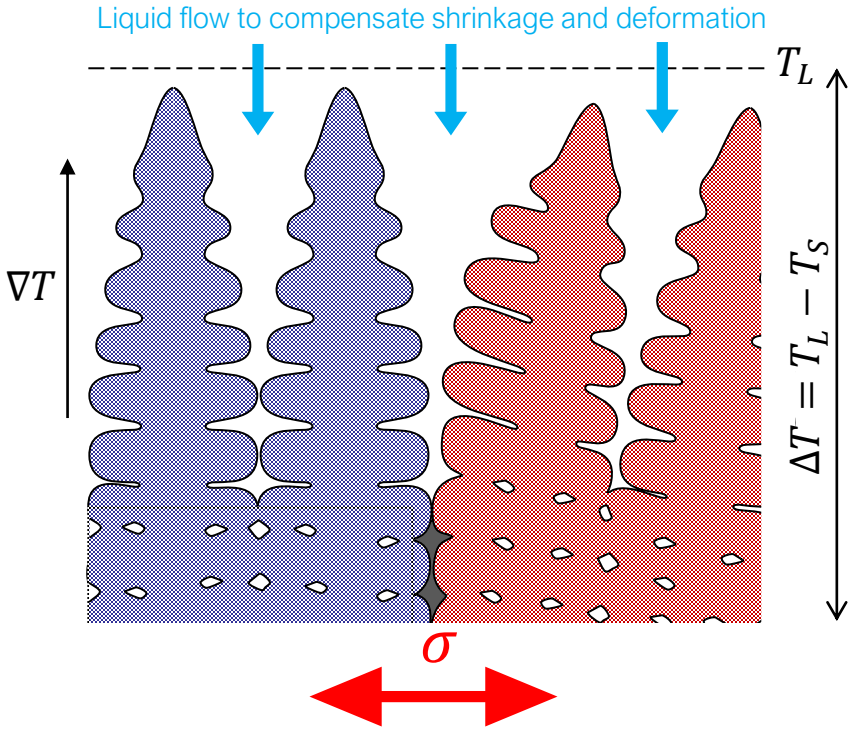
- *Required for analysis of*
  - Cold cracking
  - Solidification cracking

  } result of local stress build-up in the wake or the laser, at the rear of the melt pool





Tang *et al.*, Acta Mater 2021



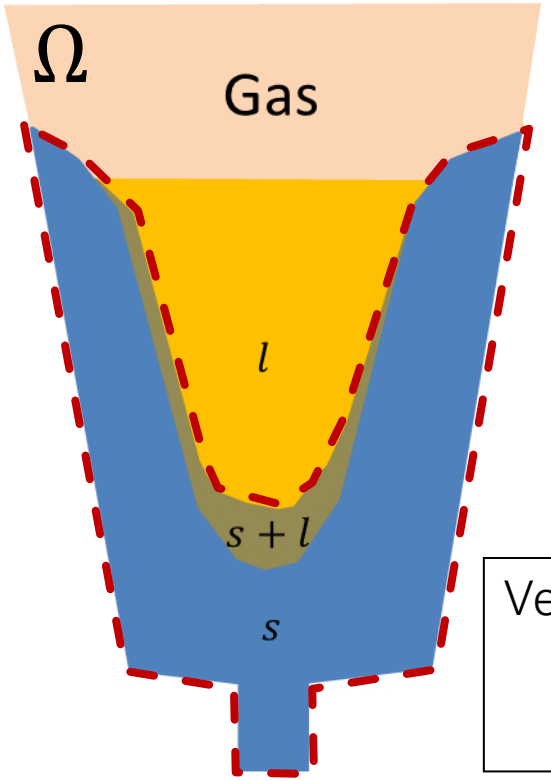
What is needed:

- *A solver for solid mechanics*
- *A constitutive model + material data*
- *A criterion for cracking*

Concurrent solid and fluid resolution

- PhD Shaojie Zhang (2020)

STEP I: solid mechanics



- **Solid:** elastic-viscoplastic
- **Mush:** non-Newtonian fluid, homogenized
- **Liquid & Gas:** Newtonian fluids, augmented viscosity

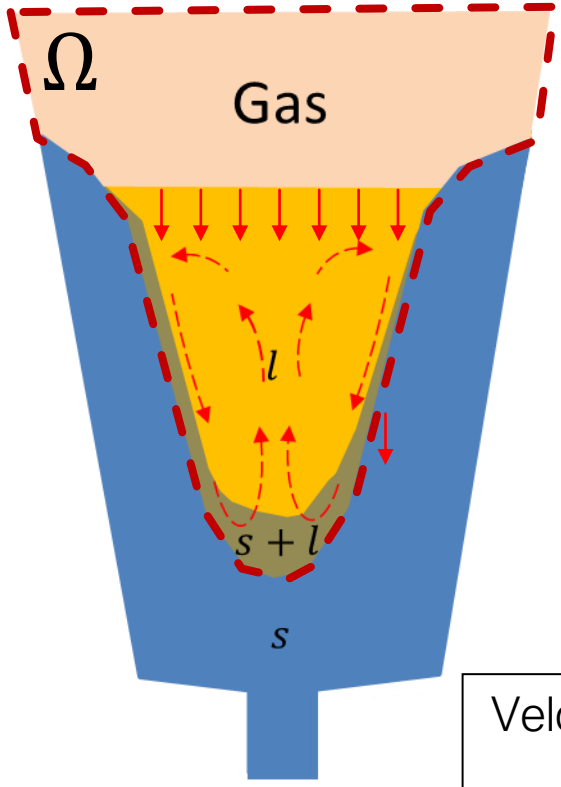
Velocity and pressure **calculated on the whole domain Ω**:

$(\mathbf{v}_{\mathrm{I}}, p_{\mathrm{I}})$

→ In the solid and the mush:

$\mathbf{v}_{\mathrm{I}}, \boldsymbol{\sigma}_{\mathrm{I}}, \boldsymbol{\varepsilon}_{\mathrm{I}}$

STEP II: fluid mechanics



- **Navier-Stokes eqs., spatially averaged** (2-phase in the mush)
- **Darcy** terms
- **Compressibility** (solidification shrinkage)
- **Liquid:** nominal viscosity
- **Solid**: Newtonian, arbitrary high viscosity

Velocity and pressure **calculated on the whole domain Ω**:

$(\mathbf{v}_{\mathrm{II}}, p_{\mathrm{II}})$

→ In the mush, the liquid and the gas: $\mathbf{v}_{\mathrm{II}}, p_{\mathrm{II}}$

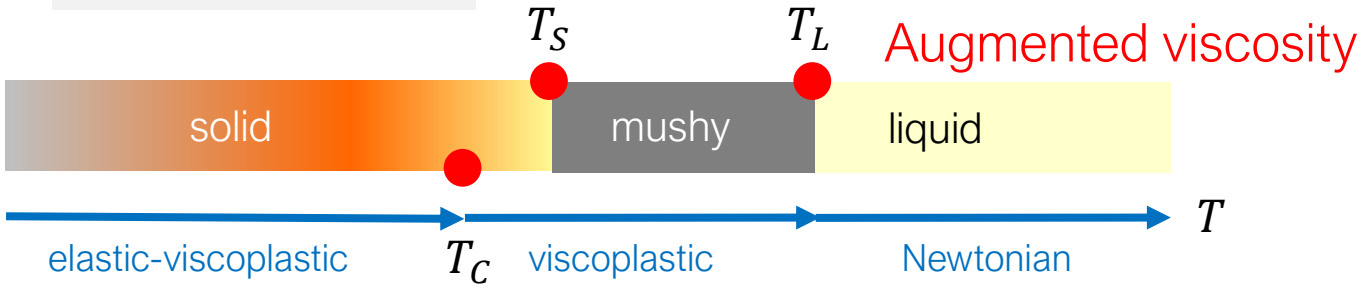
S. Zhang, Guillemot, Gandin, Bellet, Comp Meth Appl Mech Eng 2019
S. Zhang, Guillemot, Gandin, Bellet, Metall Mater Trans B 2021

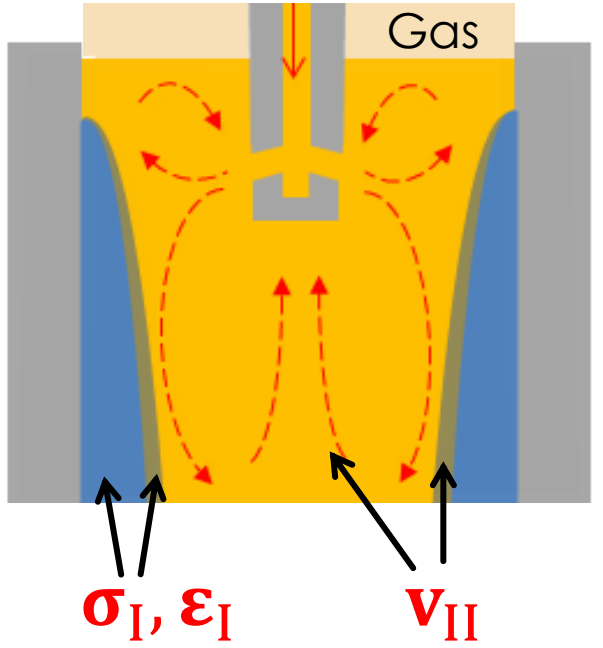
STEP I: solid mechanics

Non-linear

$$\begin{cases} \nabla \cdot \mathbf{s} - \nabla p + \rho \mathbf{g} = 0 \\ \nabla \cdot \mathbf{v} = \mathrm{tr}(\dot{\boldsymbol{\varepsilon}}_{th}) + H(T_C - T)\mathrm{tr}(\dot{\boldsymbol{\varepsilon}}_{el}) \end{cases} \rightarrow (\mathbf{v}_\mathrm{I}, p_\mathrm{I})$$

$$H(T_C - T) = \begin{cases} 0 & T > T_C \\ 1 & T \leq T_C \end{cases}$$





STEP II: fluid mechanics

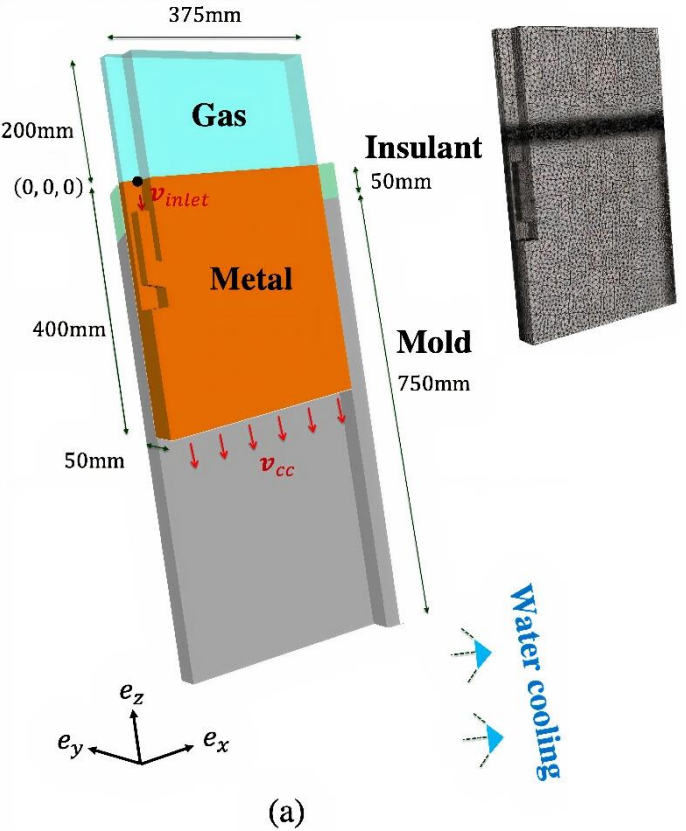
Nominal viscosity

Linear !

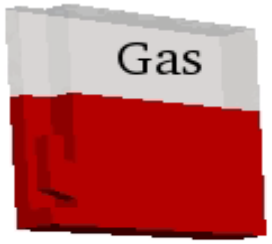
$$\begin{cases} \langle\rho\rangle^l \left(\dfrac{\partial\langle\mathbf{v}^l\rangle}{\partial t} + \dfrac{1}{g^l}(\nabla\langle\mathbf{v}^l\rangle)\langle\mathbf{v}^l\rangle\right) = -g^l\nabla\langle p\rangle^l + \nabla\cdot\langle\mathbf{s}^l\rangle - g^l\mu^l K^{-1}\left(\langle\mathbf{v}^l\rangle - g^l\langle\mathbf{v}\rangle^s\right) + g^l\langle\rho\rangle^l\mathbf{g} \\ \nabla\cdot\langle\mathbf{v}^l\rangle = -\dfrac{1}{\langle\rho\rangle^l}\left(\dfrac{\partial\langle\rho\rangle^M}{\partial t} + \langle\mathbf{v}^l\rangle\cdot\nabla\langle\rho\rangle^l + \nabla\cdot\left(g^s\langle\rho\rangle^s\langle\mathbf{v}\rangle^s\right)\right) \end{cases} \rightarrow (\mathbf{v}_\mathrm{II}, p_\mathrm{II})$$

$\mathbf{v}_\mathrm{I}$ as an input:

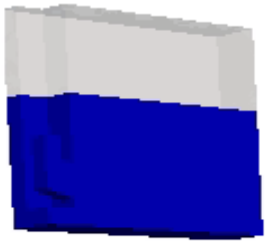
in fully solid regions,	in Darcy term,	in mass conservation,
$\mathbf{v}_{\mathrm{II}_{\mathrm{imp}}} = \mathrm{v}_\mathrm{I}$	$g^l\langle\mathbf{v}\rangle^s = \mathbf{v}_\mathrm{I}$	$\langle\mathbf{v}\rangle^s = \mathbf{v}_\mathrm{I}$

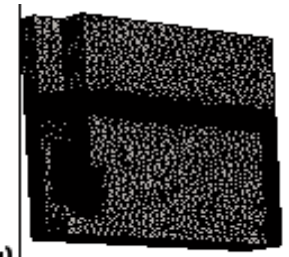


(a)



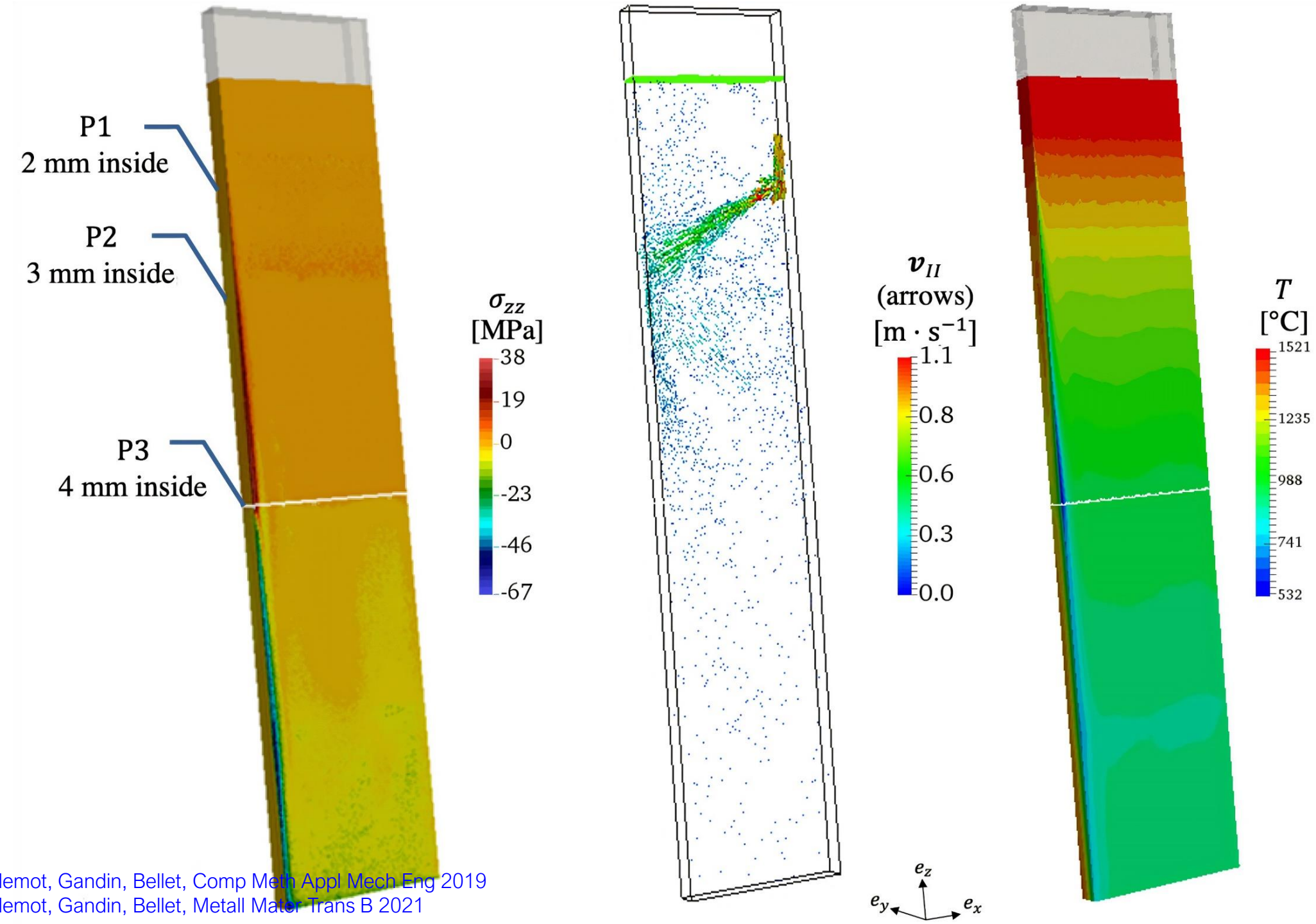
Metal





Time: 0 s

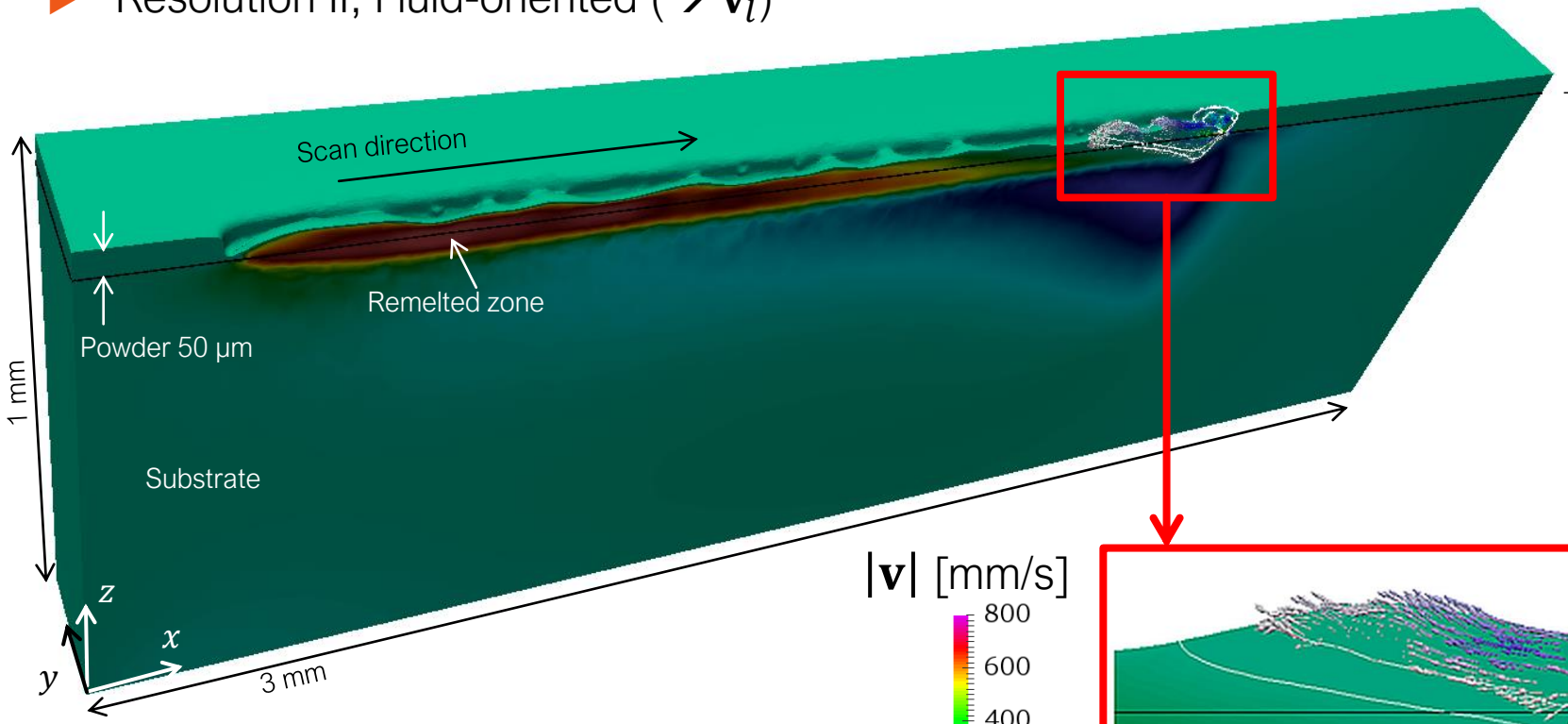
S. Zhang, Guillemot, Gandin, Bellet, Comp Meth Appl Mech Eng 2019
S. Zhang, Guillemot, Gandin, Bellet, Metall Mater Trans B 2021

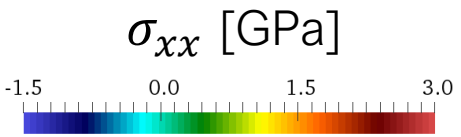


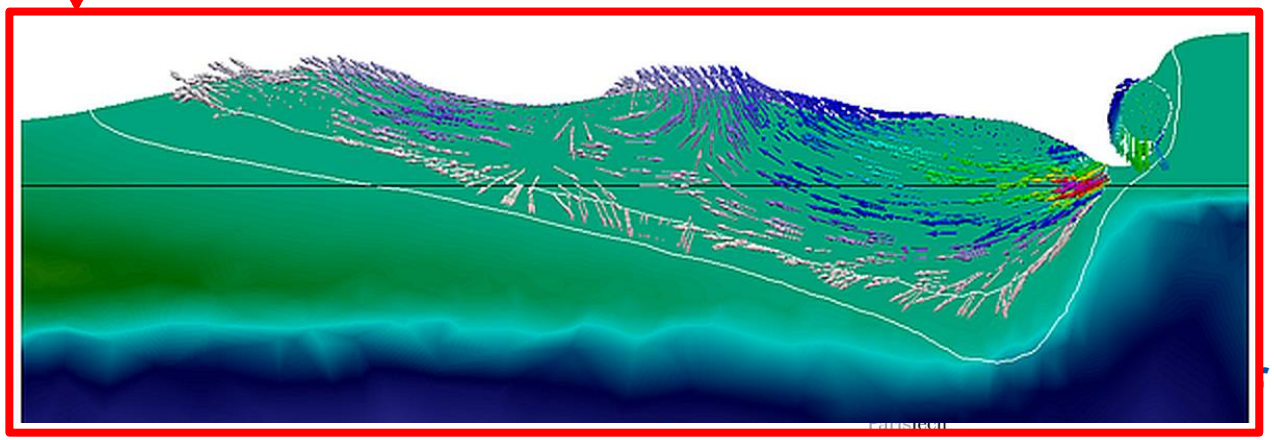
S. Zhang, Guillemot, Gandin, Bellet, Comp Meth Appl Mech Eng 2019
S. Zhang, Guillemot, Gandin, Bellet, Metall Mater Trans B 2021

Results : solid thermomechanics + fluid flow in melted zone

- *Ceramic L-PBF*
- *Two-step mechanical resolution, at each time step, on the whole domain*
  - Resolution I, Solid-oriented(→ $\mathbf{v}_s, \boldsymbol{\sigma}$)
  - Resolution II, Fluid-oriented (→ $\mathbf{v}_l$)

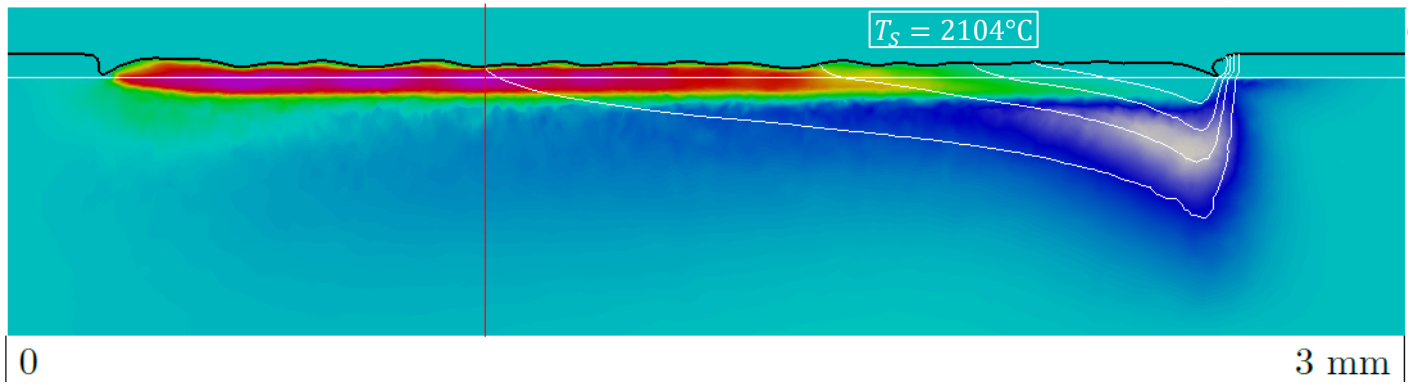




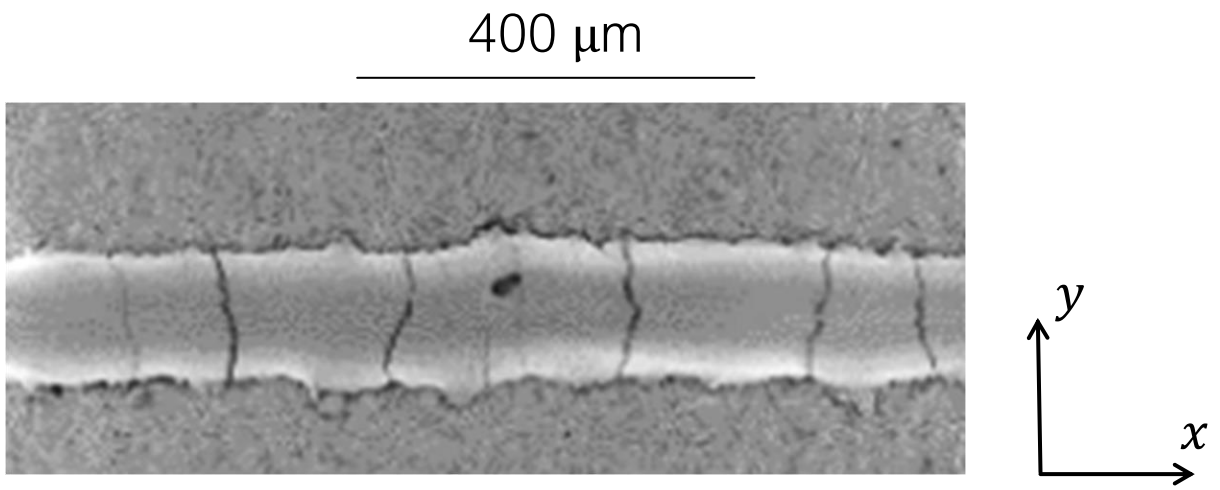


Stress generated, and impact of additional heating

- Fusion laser $P_L = 84$ W, $\phi_L = 100$ µm, $v_L = 300$ mm s^{-1}

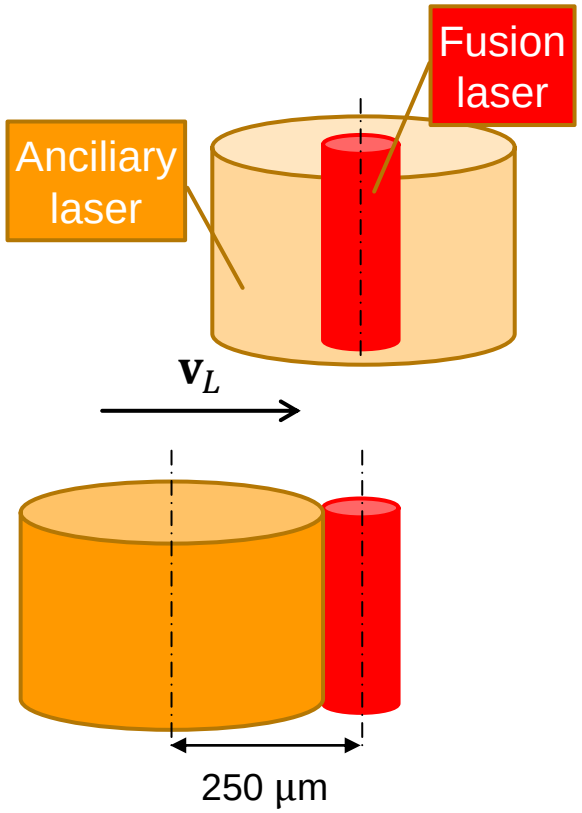


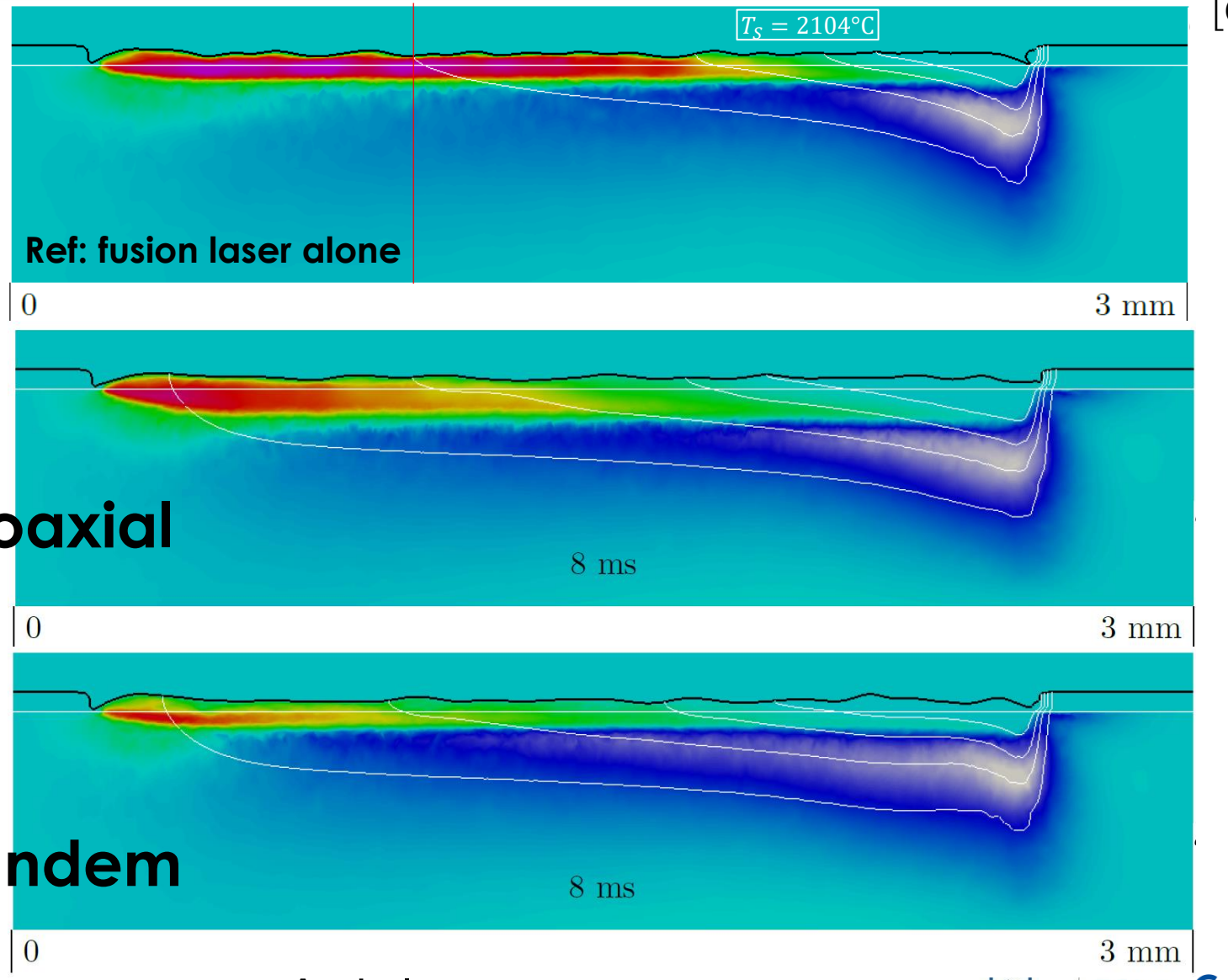
Axial stress σ_{xx}



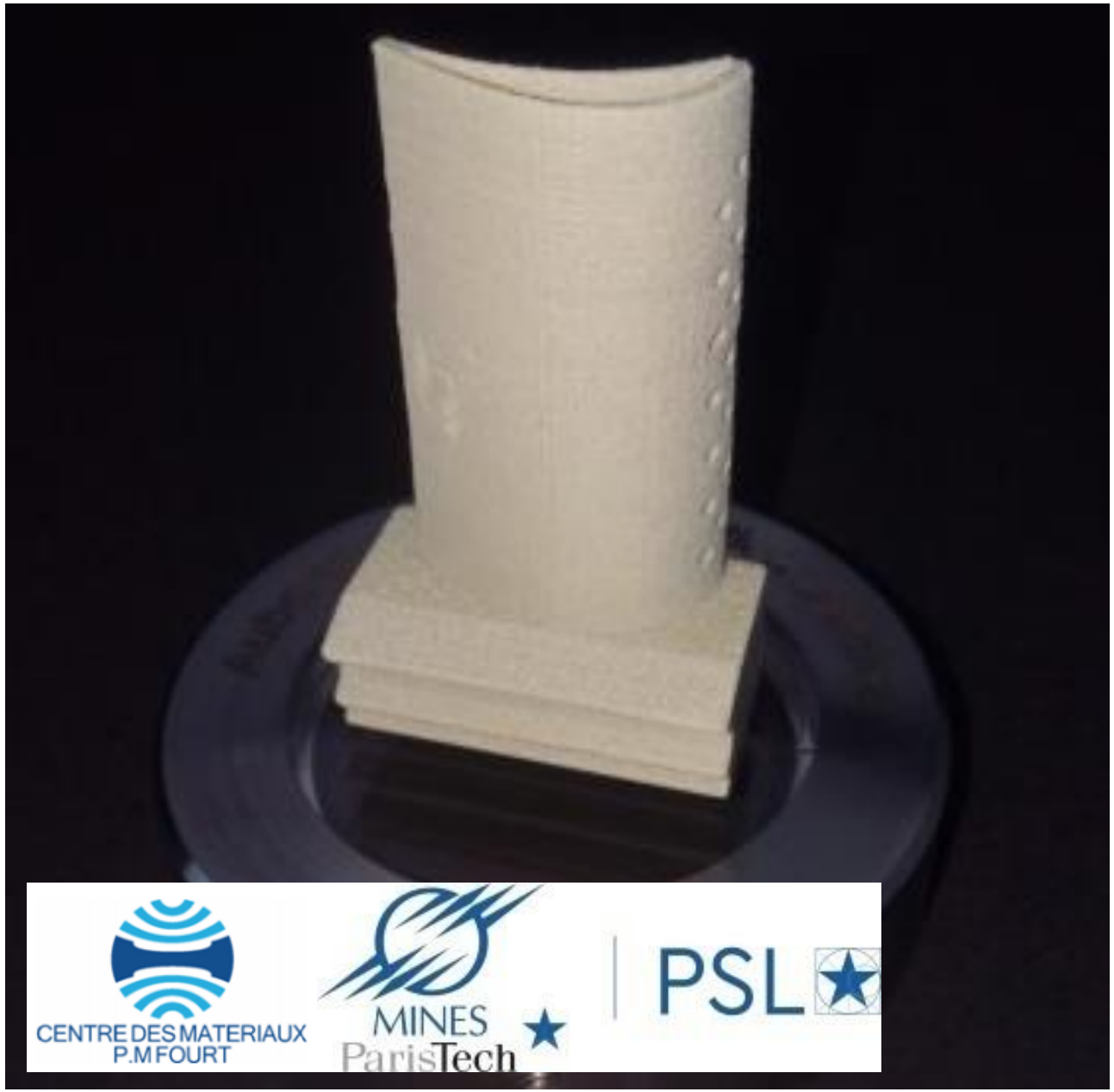
Stress generated, and impact of additional heating

- Fusion laser $P_L = 84$ W, $\phi_L = 100$ µm, $v_L = 300$ mm s^{-1}
- 2nd laser $P_L = 60$ W, $\phi_L = 400$ µm





Axial stress σ_{xx}

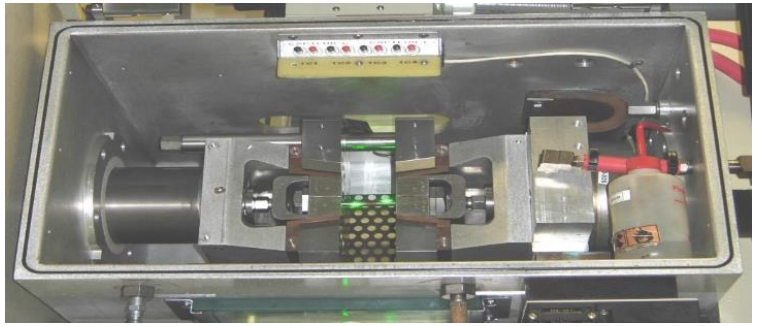

CENTRE DES MATERIAUX
P.M FOURT
MINES
ParisTech
PSL

Mechanical characterization, for metals, at high temperature, for L-PBF simulation

High temperature mechanical characterization

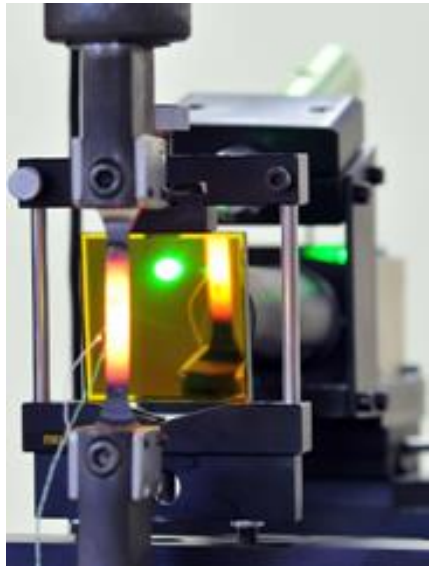
Testing under resistive heating

- ✓ Gleeble® machines
- ✓ Specific machines, lab-customized



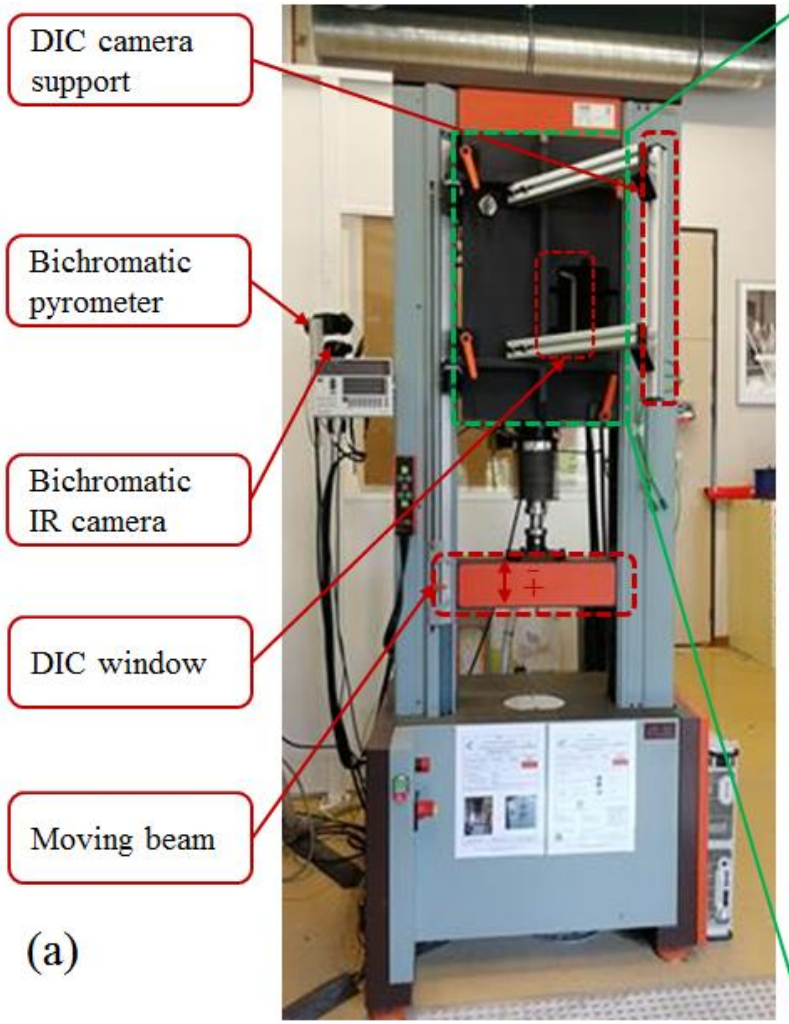
Gleeble® machine

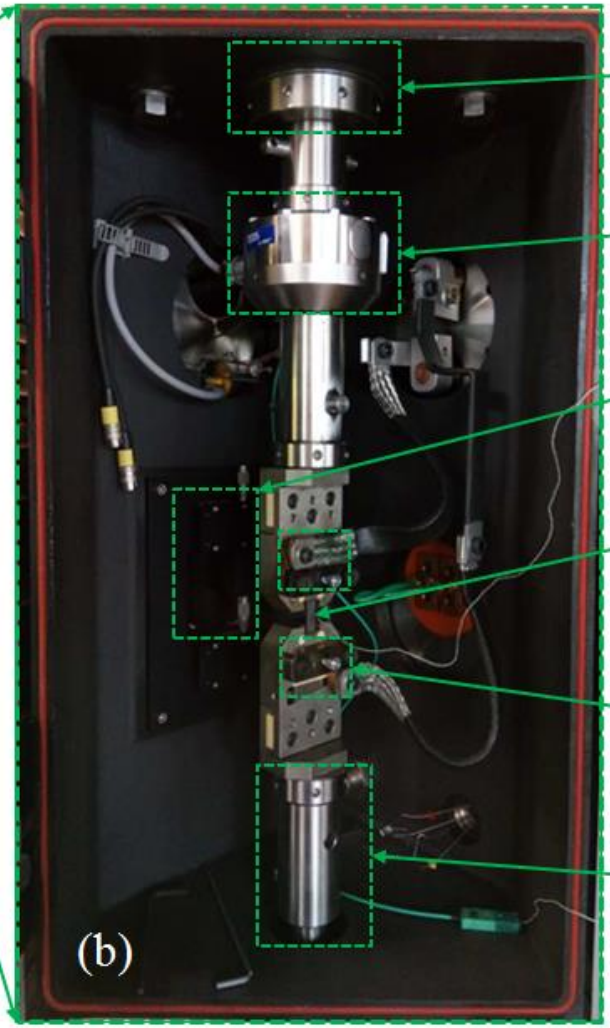
"Old" TABOO (CEMEF)



- PhD Feng Gao (2021)

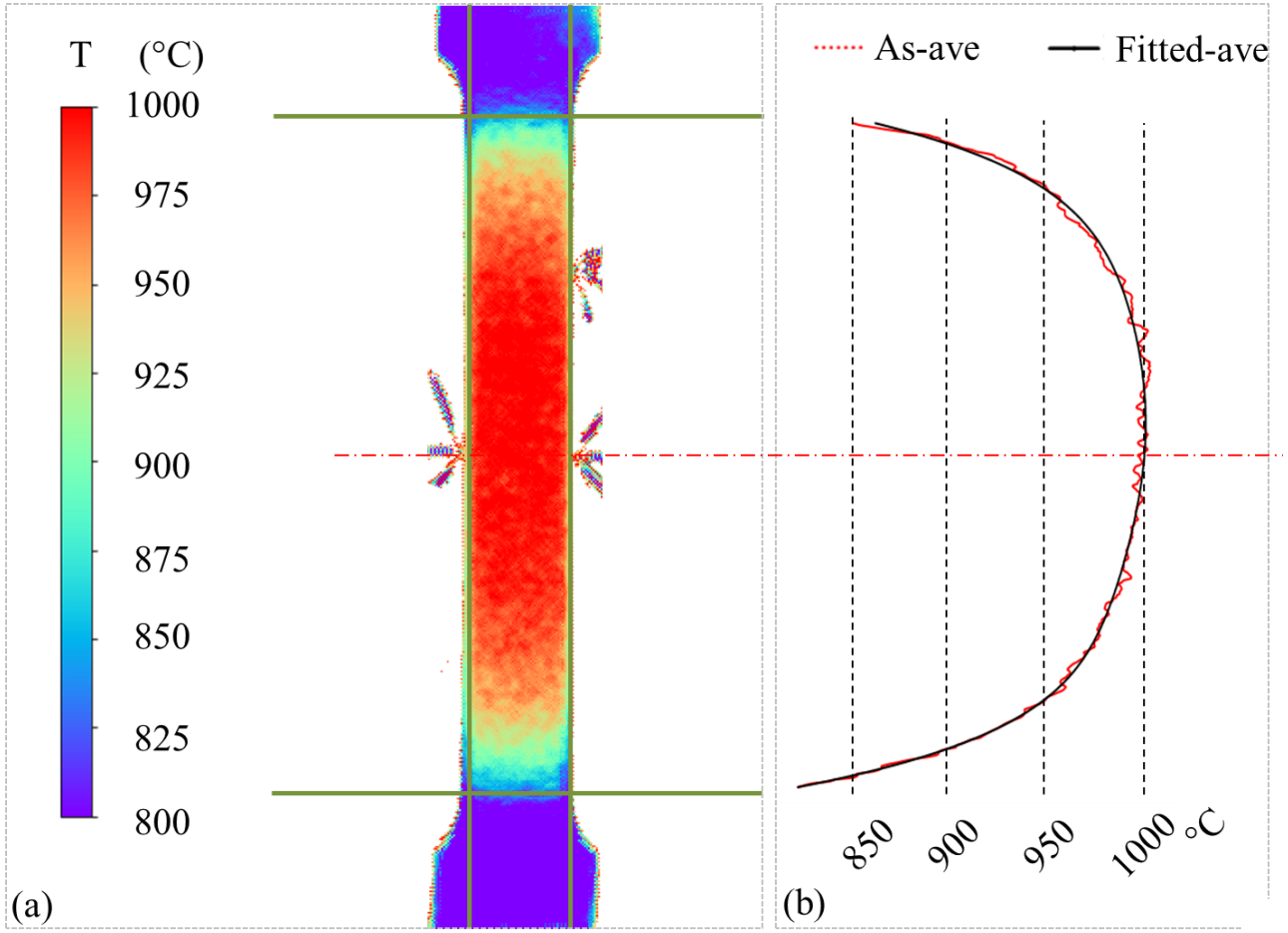
"New" DEDIMET





High temperature mechanical characterization

Superalloy IN718, as-fabricated by L-PBF

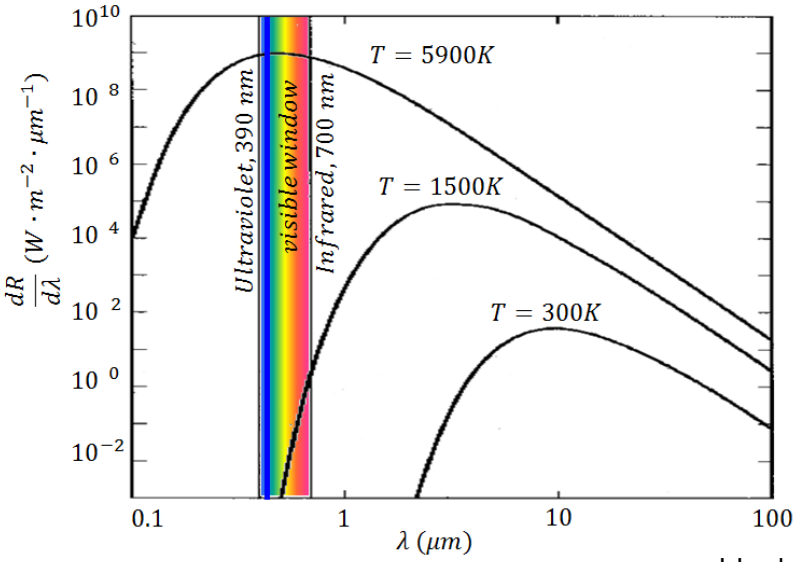


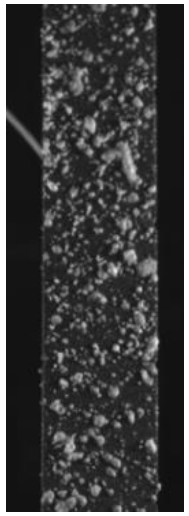
Infra-red imaging

- Testing in presence of ∇T → non-uniform! → inverse analysis, by FEM

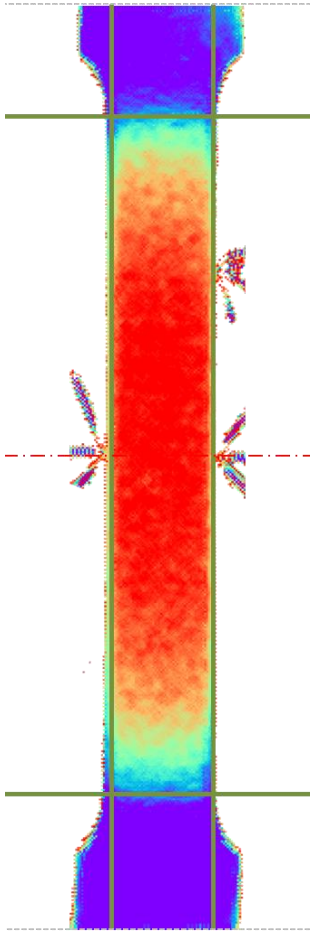
High temperature mechanical characterization

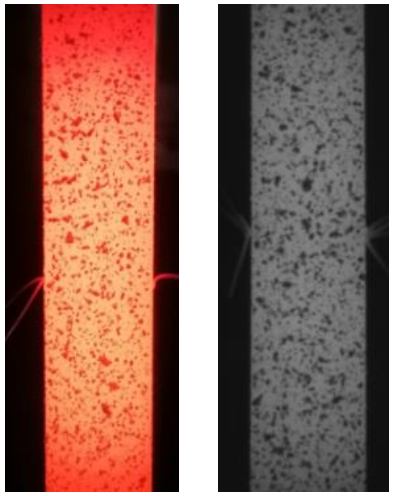
- Specific DIC technique



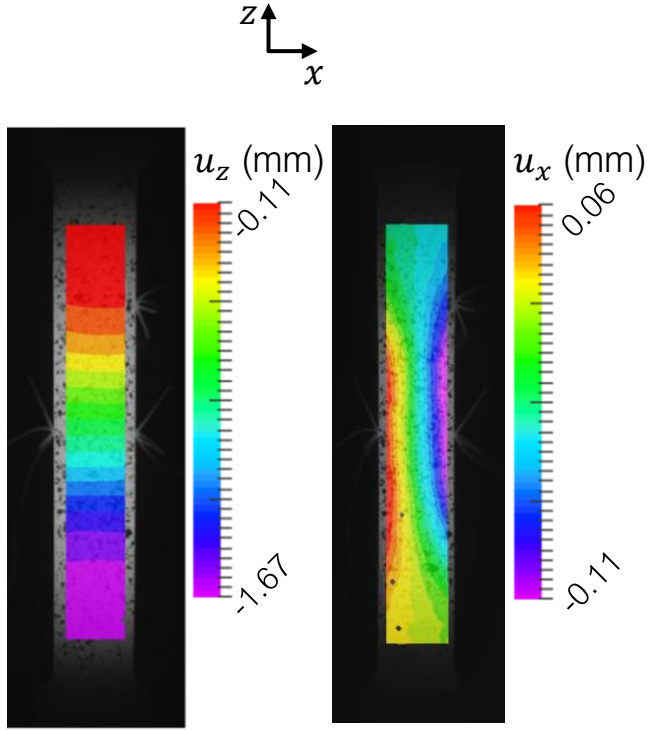


Under blue lighting
< 900 °C





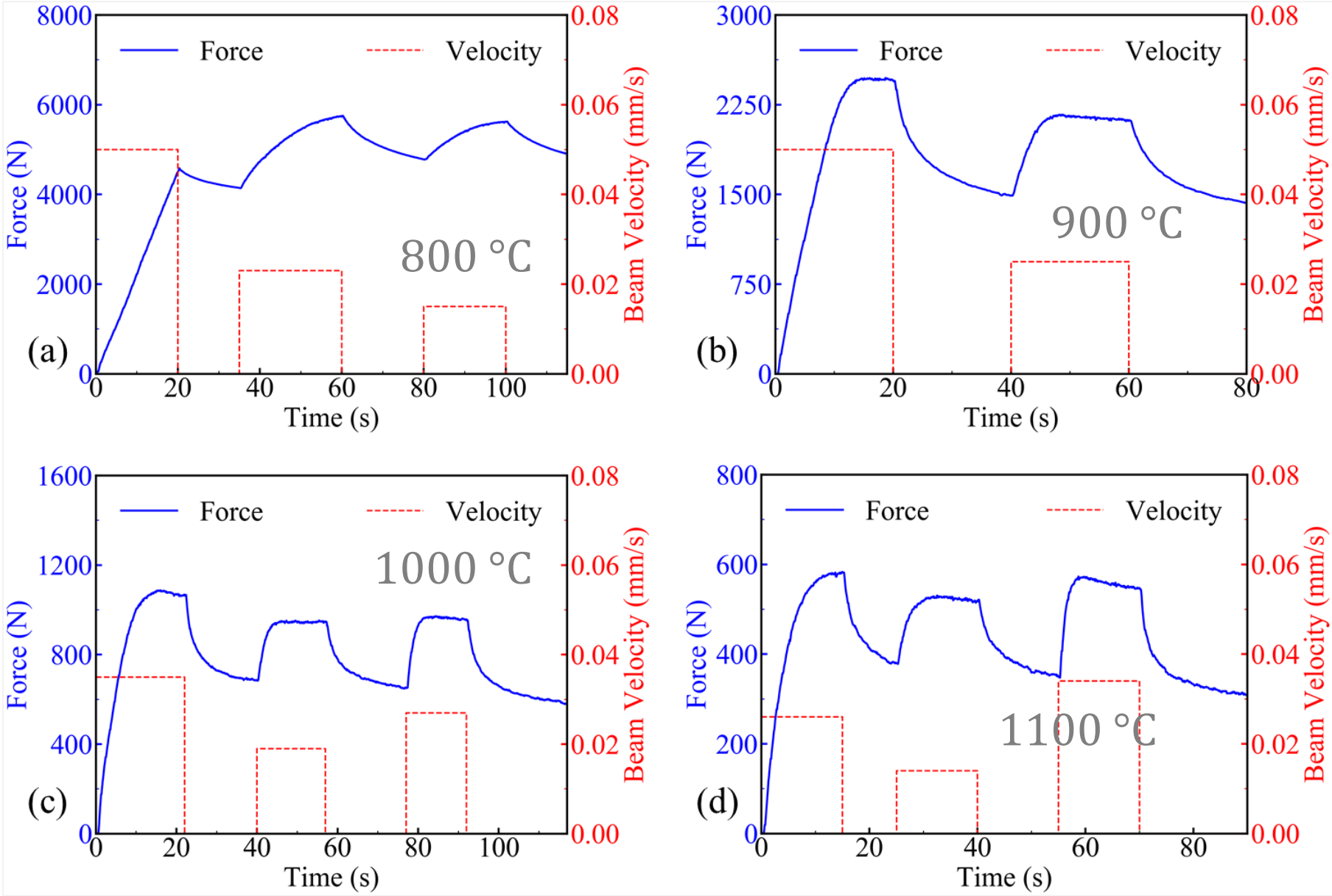
Self-emitting
> 800 °C



Post-treatment VIC-3D

How to identify an elastic-viscoplastic model?

- Experimental data base
  - ✓ Successive tractions and relaxations



How to identify an elastic-viscoplastic model?

- Selection of a candidate model

$$\begin{cases} \dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{th} + \dot{\boldsymbol{\varepsilon}}^{el} + \dot{\boldsymbol{\varepsilon}}^{vp} \\ \dot{\boldsymbol{\varepsilon}}^{th} = \alpha(T)\dfrac{dT}{dt}\mathbf{I} \\ \dot{\boldsymbol{\varepsilon}}^{el} = \dfrac{1+\nu}{E}\dot{\boldsymbol{\sigma}} - \dfrac{\nu}{E}\mathrm{tr}(\dot{\boldsymbol{\sigma}})\mathbf{I} \\ \dot{\boldsymbol{\varepsilon}}^{vp} = \dfrac{3}{2\bar{\sigma}}\left\langle \dfrac{\bar{\sigma} - \sigma_s(\bar{\varepsilon}, T)}{K(T)} \right\rangle^{\frac{1}{m}} \mathbf{s} \end{cases}$$

$$\sigma_s(\bar{\varepsilon}, T) = \left(\sigma_{Y,ref} + Q_{r,ref}\left(1 - \exp\left((-b\bar{\varepsilon})\right)\right)\right)\exp\left(\frac{Q_1}{R_g T} - \frac{Q_1}{R_g T_{ref}}\right)$$

$$K(T) = K_{ref}\exp\left(\frac{Q_2}{R_g T} - \frac{Q_2}{R_g T_{ref}}\right)$$

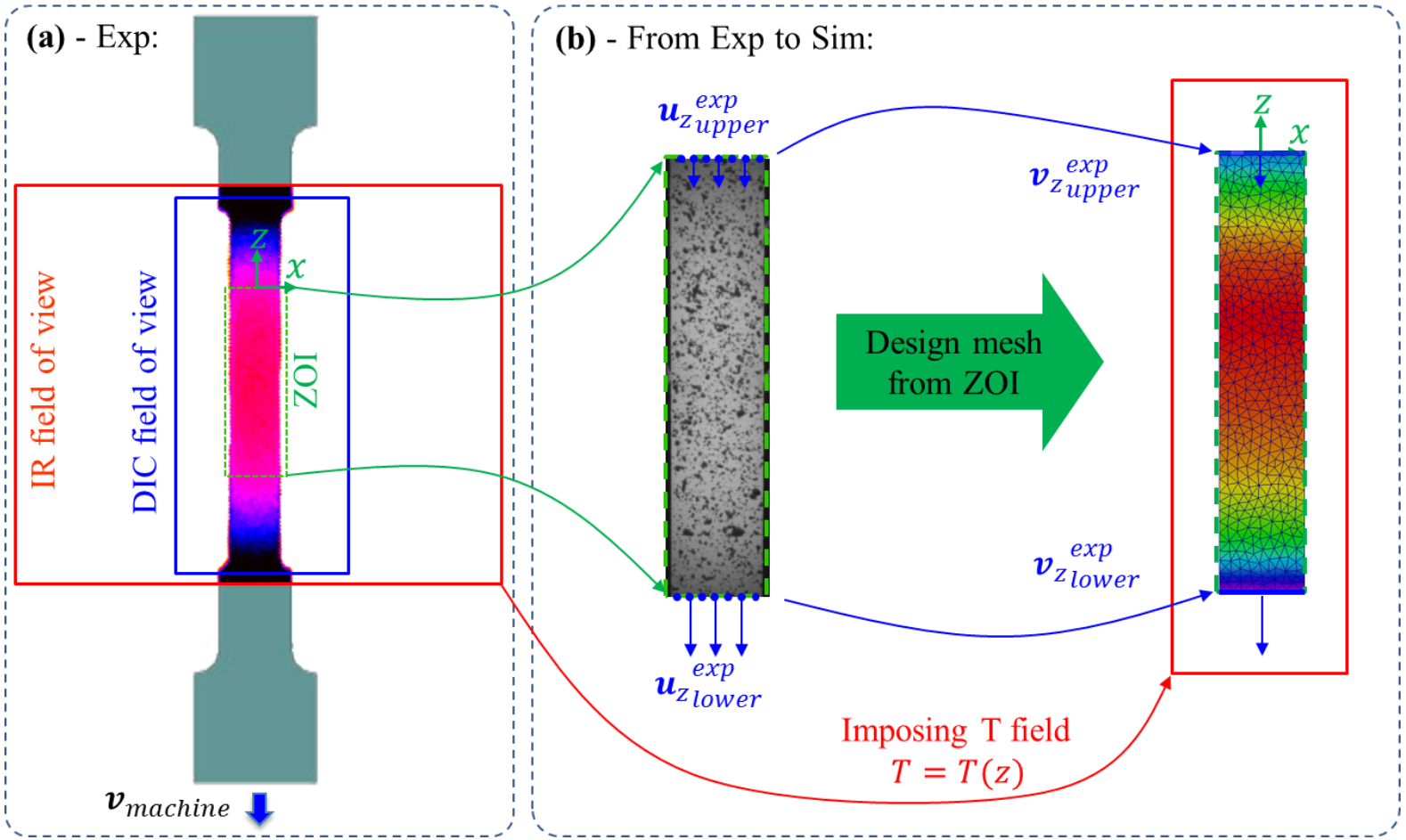
$$\bar{\sigma} = \underbrace{\left(\sigma_{Y,ref} + Q_{r,ref}\left(1 - \exp\left((-b\bar{\varepsilon})\right)\right)\right)\exp\left(\frac{Q_1}{R_g T} - \frac{Q_1}{R_g T_{ref}}\right)}_{\sigma_s} + \underbrace{K_{ref}\dot{\bar{\varepsilon}}^{m}\exp\left(\frac{Q_2}{R_g T} - \frac{Q_2}{R_g T_{ref}}\right)}_{\sigma_{overstress}}$$

✓ A set of parameters to identify

$$\mathbf{p} = \{\sigma_{Y,ref}, Q_{r,ref}, b, K_{ref}, m, Q_1, Q_2\}$$

How to identify an elastic-viscoplastic model?

▶ Local inverse analysis procedure



Cost function to be minimized:

$$\min_{\mathbf{p}} f_c = \sum_{i=1}^{N} \omega_i \frac{\sum_{j=1}^{M_i} \left| F_{i,j}^{sim}(\mathbf{p}) - F_{i,j}^{exp} \right| \Delta t_{i,j}}{\sum_{j=1}^{M_i} F_{i,j}^{exp} \Delta t_{i,j}}$$

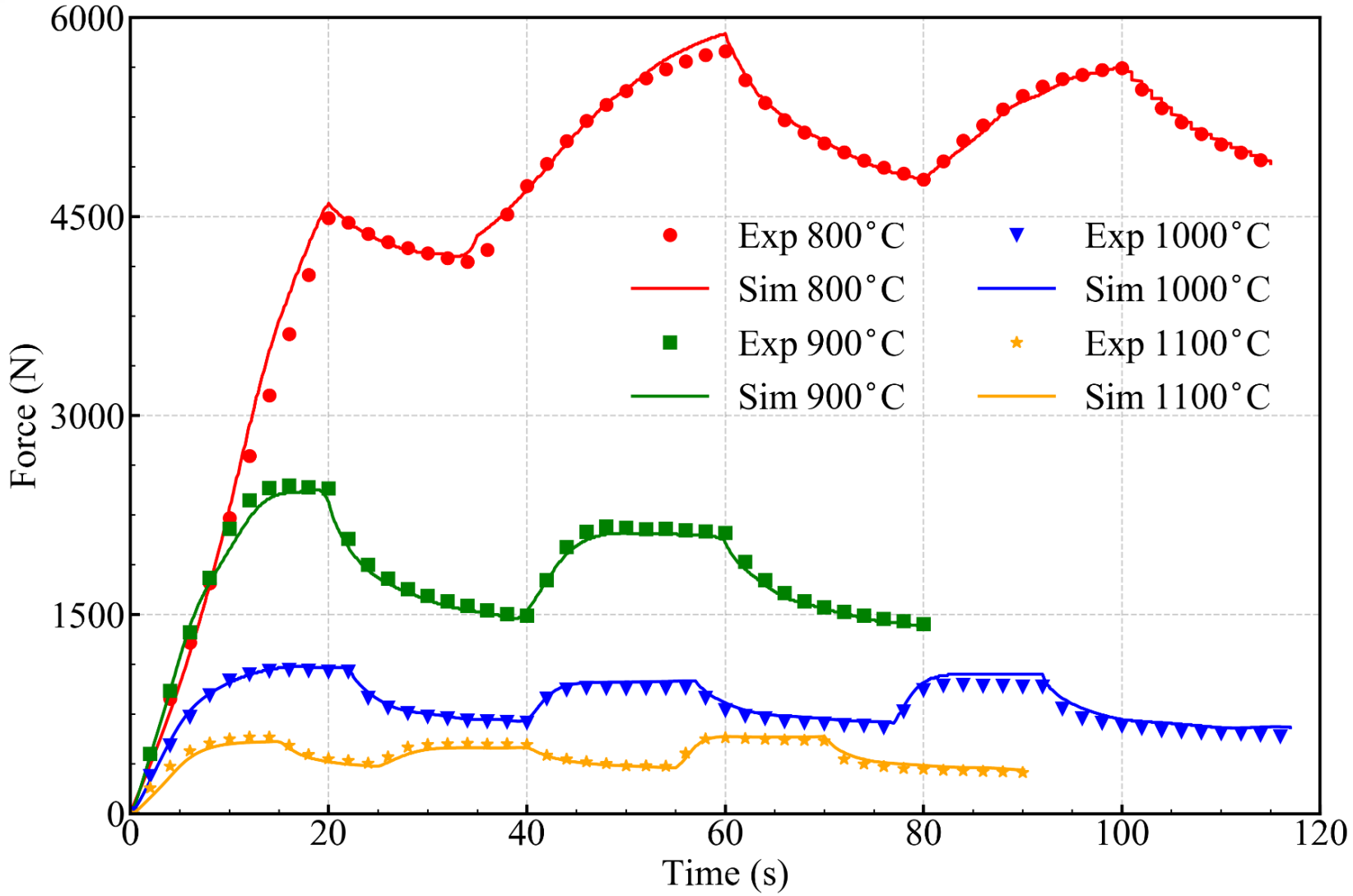
Optimisation algorithm: MOOPI (CEMEF)

- Meta-model (response surface)
- Defined by kriging
- Minimization by combining genetic algor. and BFGS

Roux *et al.*, Arch Mech Eng 2020

Gao, Macquaire, Y. Zhang, Bellet, Strain, under review, 2021

Results: force *vs* time at different temperatures

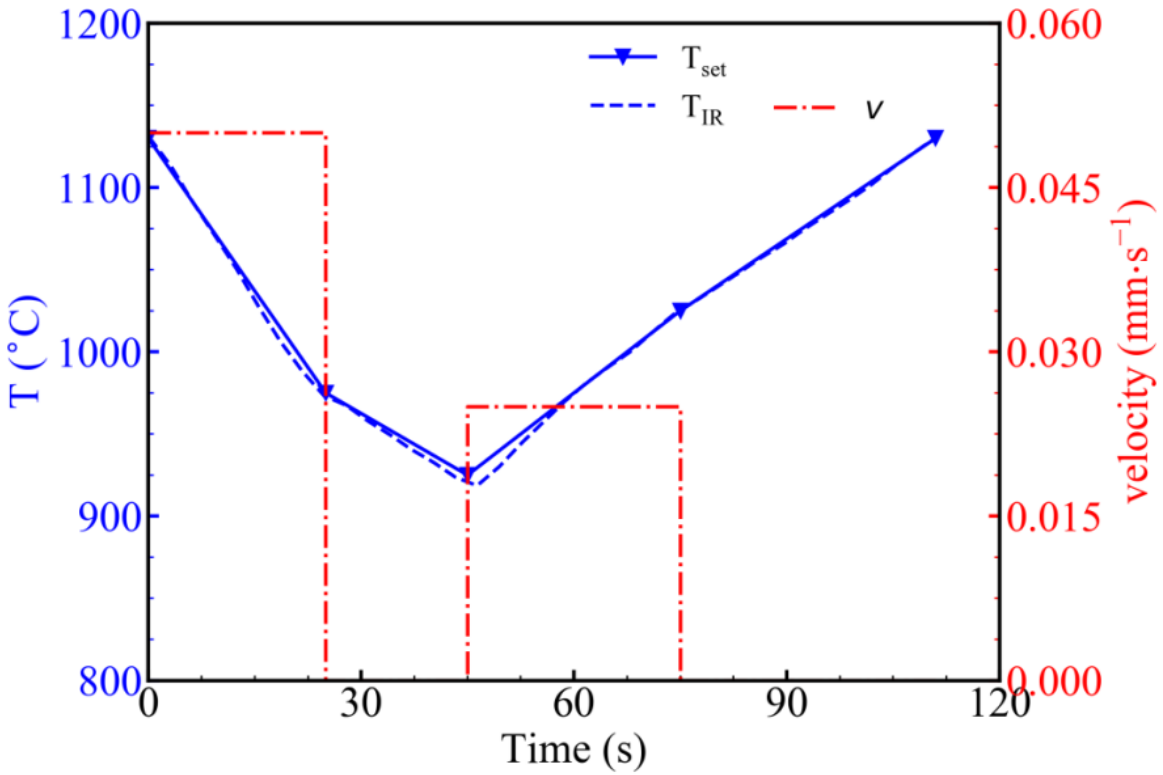


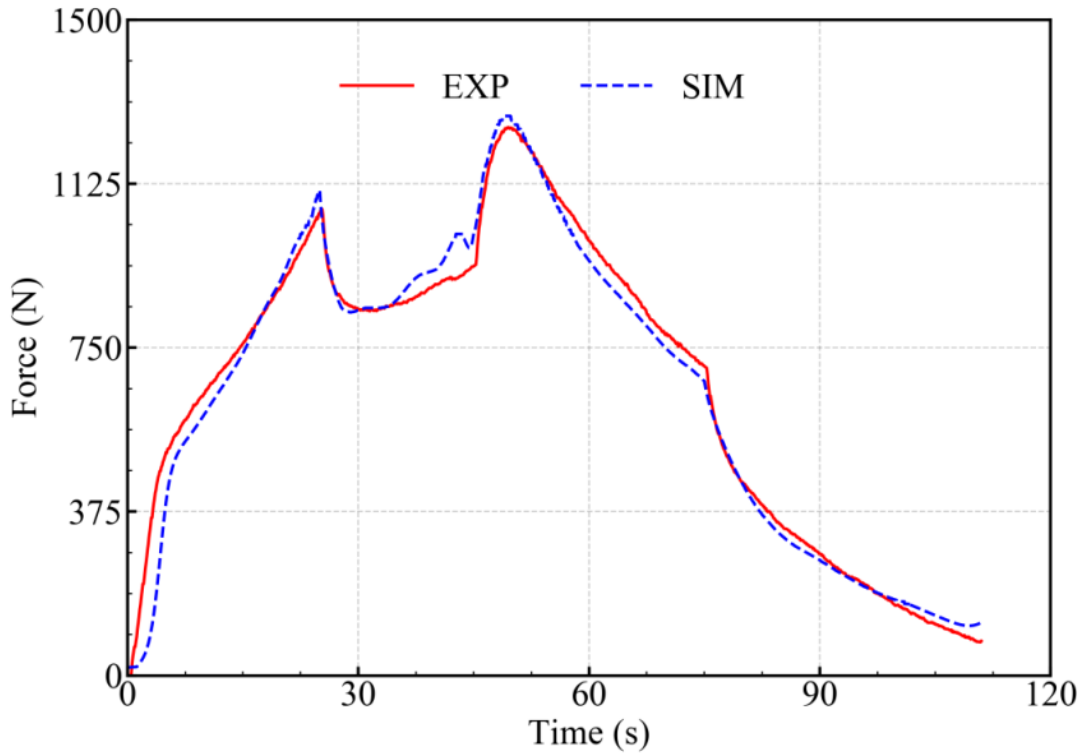
Superalloy IN718, as-fabricated by L-PBF

$\mathbf{p_{opt}}$
$\sigma_{Y,ref} = 107$ MPa
$Q_{r,ref} = 83$ MPa
$b = 367$
$Q_1 = 157$ kJ mol^{-1}
$K_{ref} = 1118$ MPa
$m = 0.252$
$Q_2 = mQ_{vp} = 77$ kJ mol^{-1}

Gao, Macquaire, Y. Zhang, Bellet, Strain, under review, 2021

Check for a non-constant temperature case



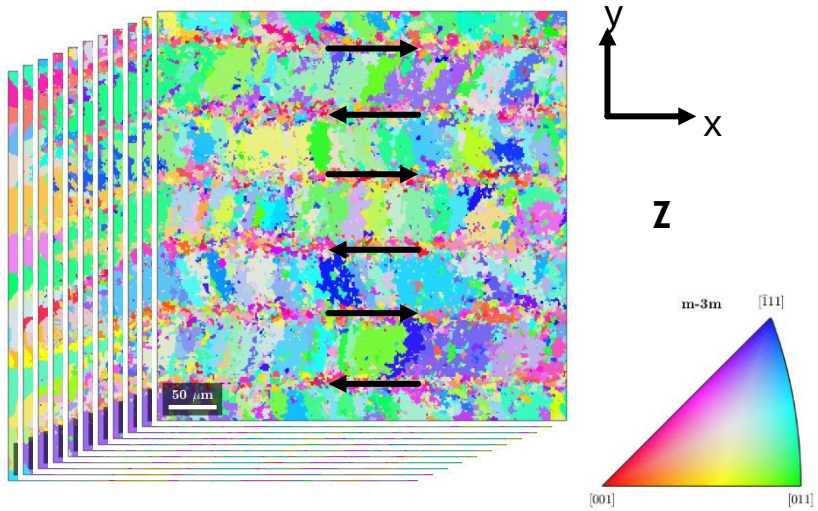


Gao, Macquaire, Y. Zhang, Bellet, Strain, under review, 2021

Conclusions

- Finite element and level set approach, to model thermohydraulics in L-PBF
- Concurrent resolution of solid mechanics, in view of determining adequate process windows
- Local inverse modelling to identify the mechanical behavior of metallic alloys in L-PBF processing conditions

- Not discussed here
  - Accounting for anisotropy
- Next steps
  - Cracking prediction…
  - … enriched by coupling with simulation of microstructure formation
    - Grain structure prediction by CA-FE modelling
    - Phases formation in very fast solidification conditions, by CalPhaD (Thermocalc)-based models



Camus, Gandin, Guillemot, 2021 CEMEF

Thank you for your attention !

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