Cost effective digital twin of directed energy deposition additive manufacturing

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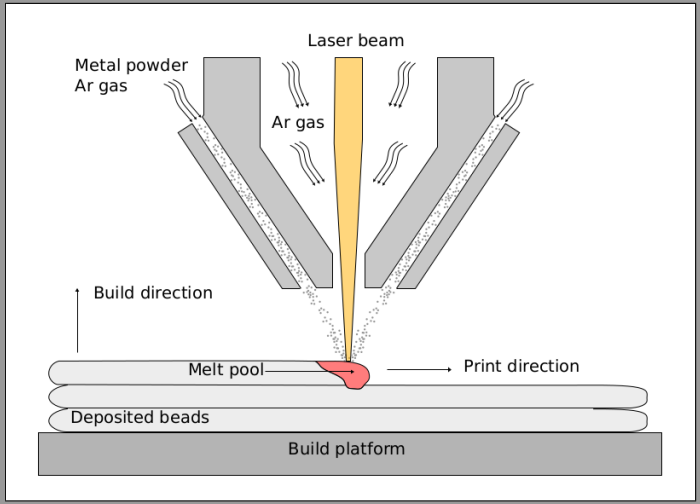
Directed energy deposition additive manufacturing



Fast and **part-scale** numerical simulations for **optimization** of process parameters

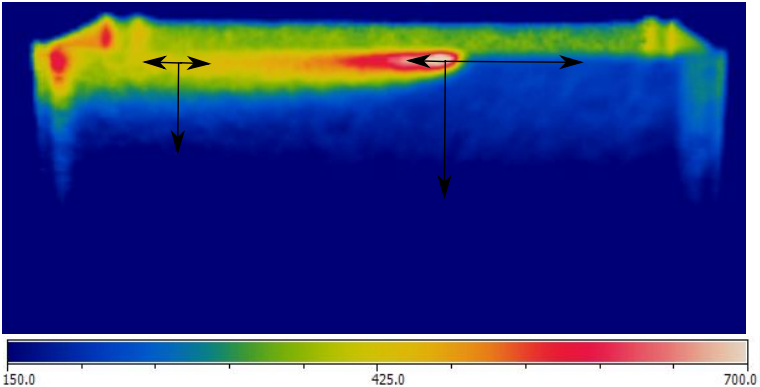
Thermal analysis

Microstructure

Residual stresses

Thermal analysis

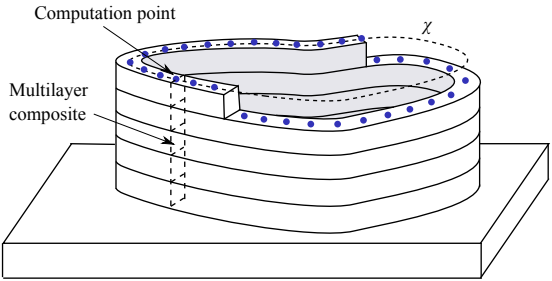
- **Assumptions** **Neglecting** horizontal heat flux



D. Weisz-Patrault, **Additive Manufacturing** 31, 100990, 2019

Thermal analysis

- **Assumptions** **Neglecting** horizontal heat flux



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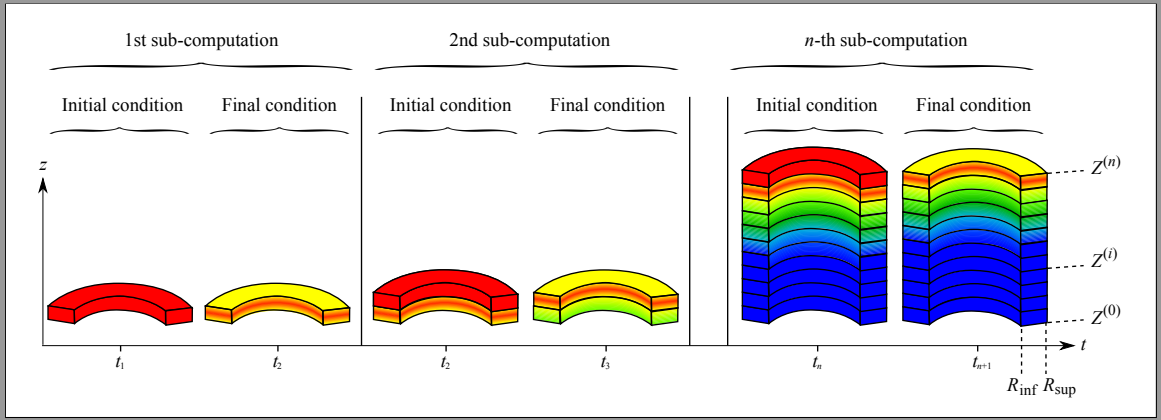
Thermal analysis



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Thermal analysis

$$\frac{\partial^2 T^{(i)}}{\partial r^2} + \frac{1}{r}\frac{\partial T^{(i)}}{\partial r} + \frac{\partial^2 T^{(i)}}{\partial z^2} - \frac{1}{D^{(i)}}\frac{\partial T^{(i)}}{\partial t} = -\frac{Q^{(i)}(t)}{\lambda^{(i)}}$$

- **Boundary conditions**

$$(a): \begin{cases} \widehat{\lambda}\dfrac{\partial T^{(i)}}{\partial r} = H\left(T^{(i)} - T_{\mathtt{ext}}\right) & r = R_{\mathtt{inf}} \quad (1 \leq i \leq n) \\ \widehat{\lambda}\dfrac{\partial T^{(i)}}{\partial r} = -H\left(T^{(i)} - T_{\mathtt{ext}}\right) & r = R_{\mathtt{sup}} \quad (1 \leq i \leq n) \end{cases}$$

$$(b): \begin{cases} \lambda^{(1)}\dfrac{\partial T^{(1)}}{\partial z} = H_{\mathtt{pla}}\left(T^{(1)} - T_{\mathtt{pla}}\right) & z = Z^{(0)} \\ \lambda^{(n)}\dfrac{\partial T^{(n)}}{\partial z} = -H\left(T^{(n)} - T_{\mathtt{ext}}\right) & z = Z^{(n)} \end{cases}$$

$$(c): \begin{cases} T^{(i)} = T^{(i+1)} & z = Z^{(i)} \quad (1 \leq i \leq n-1) \\ \lambda^{(i)}\dfrac{\partial T^{(i)}}{\partial z} = \lambda^{(i+1)}\dfrac{\partial T^{(i+1)}}{\partial z} & z = Z^{(i)} \quad (1 \leq i \leq n-1) \end{cases}$$

- **Initial condition**

$$T^{(i)}(r, z, t = t_n) = T^{(i)}_{\mathtt{ini}}(r, z)$$

$$T_{\mathrm{dep}} = \frac{I\,\eta\,R_{\mathrm{beam}}}{\sqrt{2\pi}\lambda_{\mathrm{liq}}}\arctan\left(\frac{\sqrt{8D_{\mathrm{liq}}t_{\mathrm{beam}}}}{R_{\mathrm{beam}}}\right)$$

D. Bäuerle (2003)

D. Weisz-Patrault, **Additive Manufacturing** 31, 100990, 2019

Thermal analysis

$$\boxed{\frac{\partial^2 T^{(i)}}{\partial r^2} + \frac{1}{r}\frac{\partial T^{(i)}}{\partial r} + \frac{\partial^2 T^{(i)}}{\partial z^2} - \frac{1}{D^{(i)}}\frac{\partial T^{(i)}}{\partial t} = -\frac{Q^{(i)}(t)}{\lambda^{(i)}}}$$

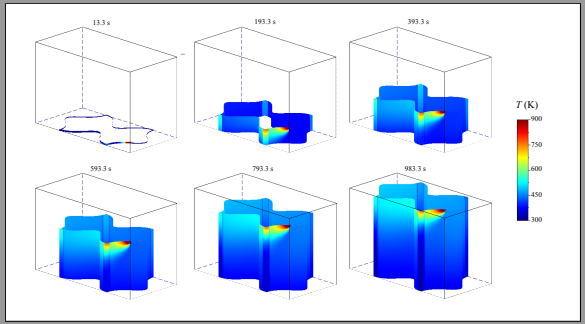
$$T_h^{(i)}(r,z,t) = \sum_{j=1}^{N_j}\sum_{k=1}^{N_k} \Theta_{j,k}\left(a_j J_0(\alpha_j r) + \widetilde{a}_j Y_0(\alpha_j r)\right)\left(b_{j,k}^{(i)}\cos(\beta_{j,k}^{(i)} z) + \widetilde{b}_{j,k}^{(i)}\sin(\beta_{j,k}^{(i)} z)\right)\exp\left(-D^{(i)}\left(\alpha_j^2 + \left(\beta_{j,k}^{(i)}\right)^2\right)(t-t_n)\right)$$

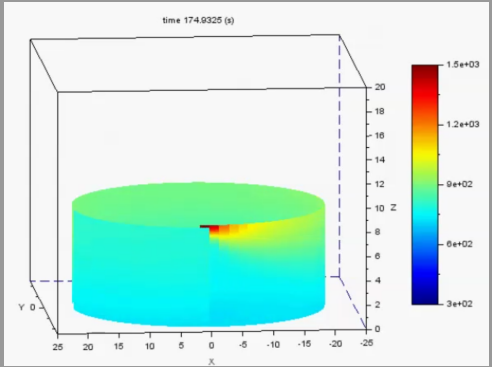
Où $\beta \mapsto \det\left[\underline{\underline{K}}(\beta)\right]$

$$\begin{pmatrix}
K_{1,1} & K_{1,2} & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
K_{2,1} & K_{2,2} & K_{2,3} & K_{2,4} & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
K_{3,1} & K_{3,2} & K_{3,3} & K_{3,4} & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & K_{4,3} & K_{4,4} & K_{4,5} & K_{4,6} & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & K_{5,3} & K_{5,4} & K_{5,5} & K_{5,6} & \cdots & 0 & 0 & 0 & 0 \\
 & & & & & & \vdots & & & & \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & K_{2n-2,2n-3} & K_{2n-2,2n-2} & K_{2n-2,2n-1} & K_{2n-2,2n} \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & K_{2n-1,2n-3} & K_{2n-1,2n-2} & K_{2n-1,2n-1} & K_{2n-1,2n} \\
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & K_{2n,2n-1} & K_{2n,2n}
\end{pmatrix}$$

D. Weisz-Patrault, **Additive Manufacturing** 31, 100990, 2019

Thermal analysis





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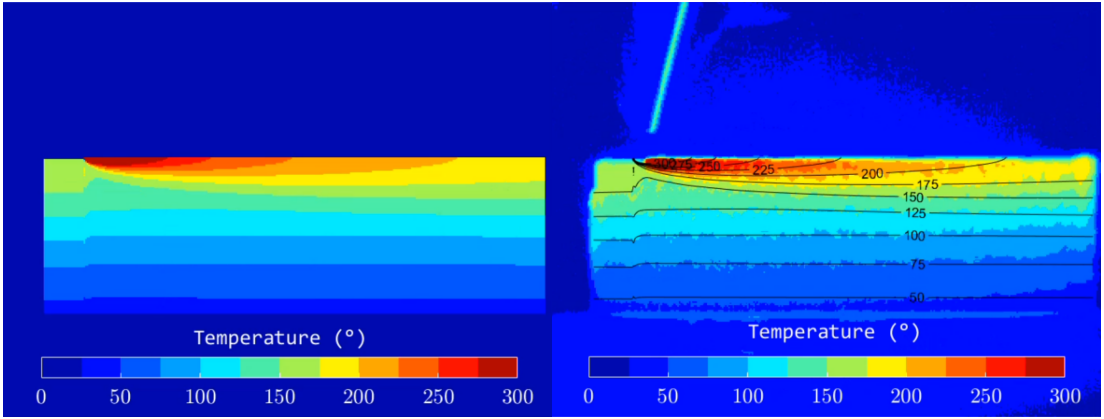

D. Weisz-Patrault et al., **Additive Manufacturing** 56, 102903, 2022

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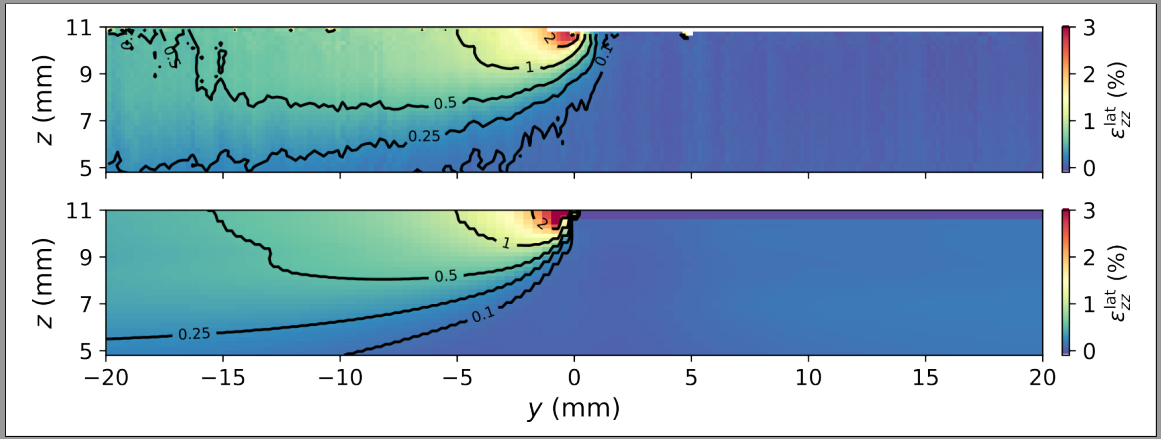
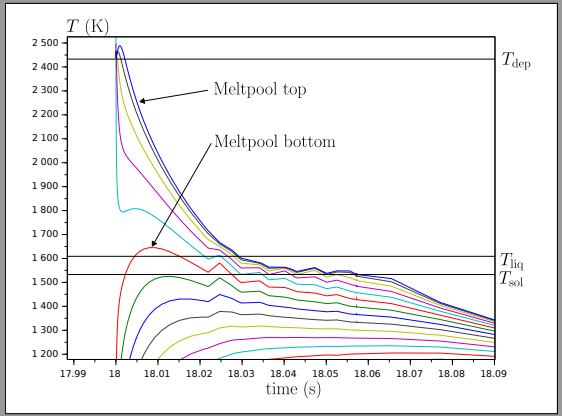
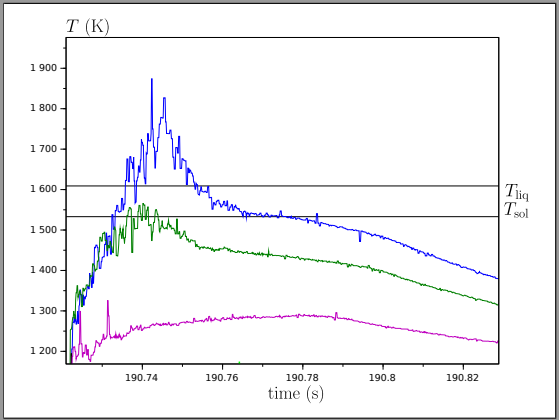


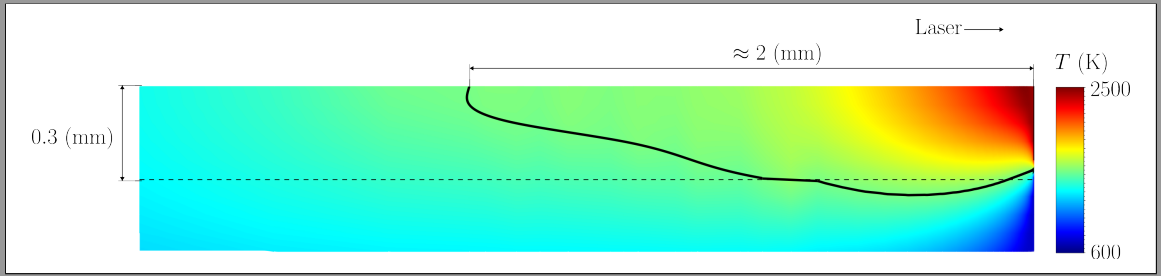
S. Gaudez et al., **Additive Manufacturing** 101, 104674, 2025

Thermal analysis



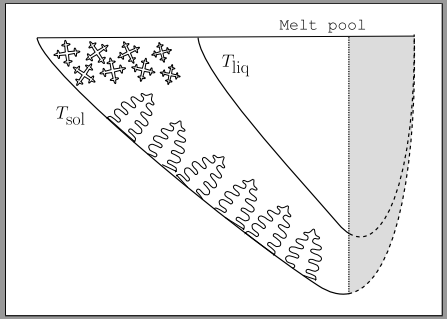


Thermal analysis



Microstructure

- Liquid/solid interface
  - **Normal velocity** $v = \alpha \Delta T^{\beta}$
  - **Local** computations of T, c_j, κ
  - **Very fine** scale of **dendrites**
- Numerical methods
  - Level-set
  - Phase-field
  - Dendritic needle network
  - Cellular automaton
- Difficulties in engineering
  - Significant **computation time**
  - **Random** crystal orientations of **equiaxed grains**



Q Dollé, D Weisz-Patrault, **Computational Materials Science**, 2024

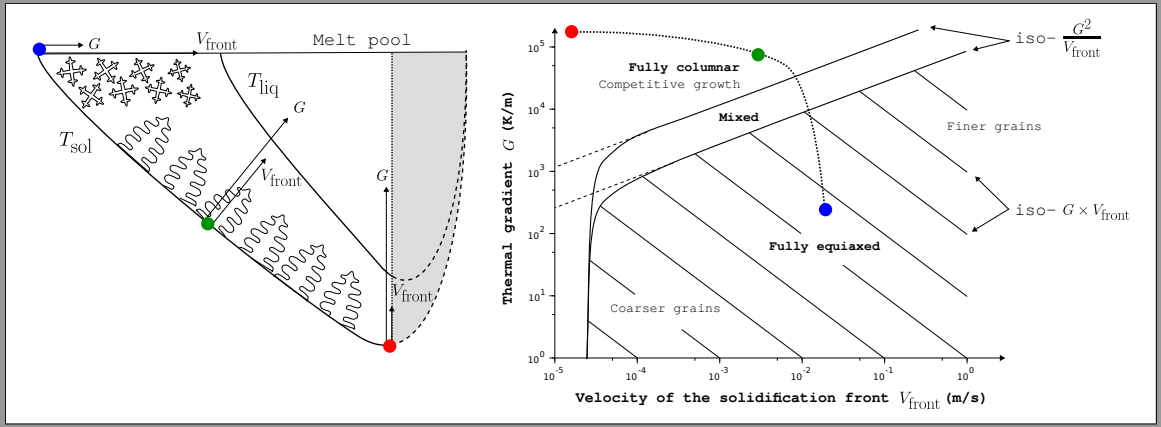
Microstructure

- Model requirements
  - No description of **individual dendrites**
  - Description of **grains** (families of dendrites)
  - **Average** phenomena
  - **Very fast** computations
- Model features
  - **Solidification maps**
  - **Solidification front** velocity vs. **dendritic** velocity
  - **Favorably oriented grain** selection criterion
  - Voronoi **tessellation** construction **procedure**

Q Dollé, D Weisz-Patrault, **Computational Materials Science**, 2024

Microstructure

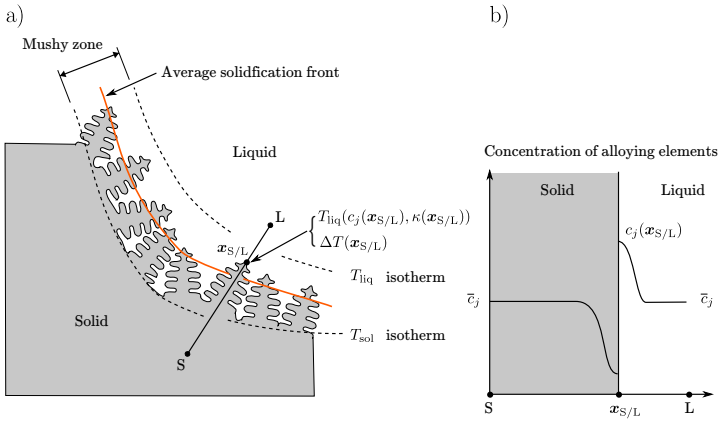
Solidification maps



Q Dollé, D Weisz-Patrault, **Computational Materials Science**, 2024

Microstructure

Average solidification front



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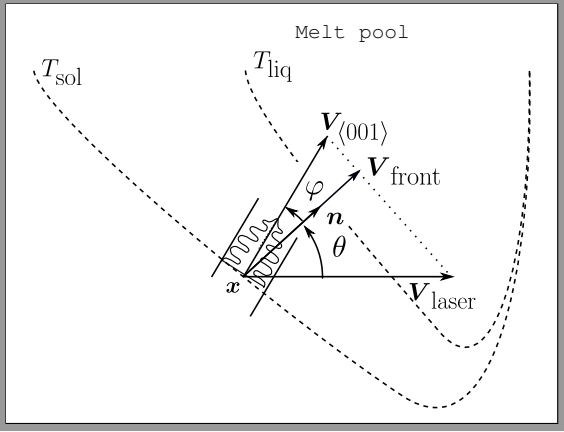
Microstructure

Solidification front velocity vs. **Dendritic velocity**

$$\begin{cases} \underline{V}_{\text{front}}(\underline{x}) = |\underline{V}_{\text{beam}}| \cos\theta(\underline{x})\underline{n}(\underline{x}) \\ \underline{V}_{\text{front}}(\underline{x}) = \left|\underline{V}_{\langle 001\rangle}(\underline{x})\right| \cos\varphi(\underline{x})\underline{n}(\underline{x}) \end{cases}$$

$$\left|\underline{V}_{\langle 001\rangle}(\underline{x})\right| = |\underline{V}_{\text{beam}}| \frac{\cos\theta(\underline{x})}{\cos\varphi(\underline{x})}$$



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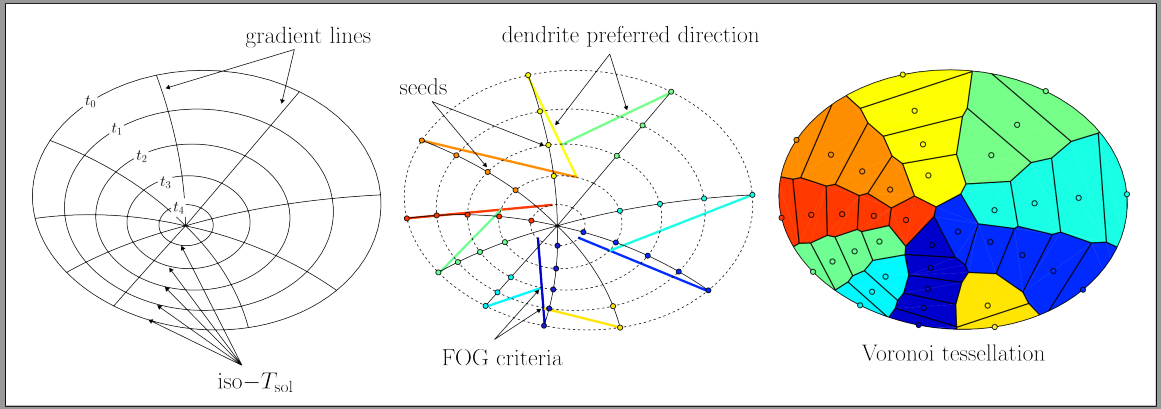
Microstructure

Voronoi tessellation construction procedure



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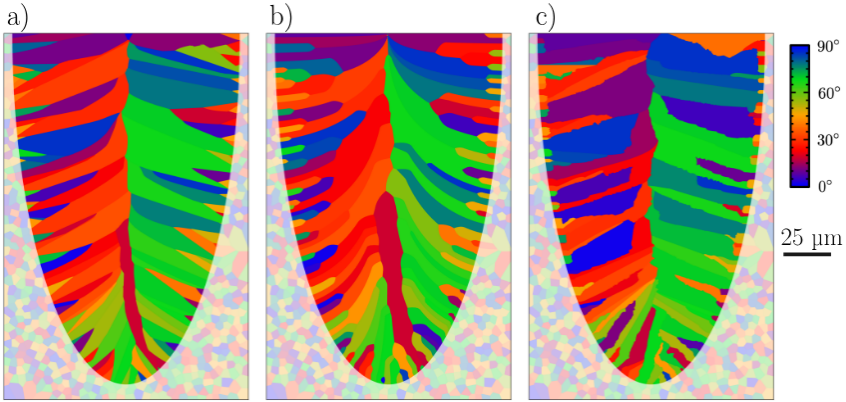
Microstructure

Validation vs. other numerical methods



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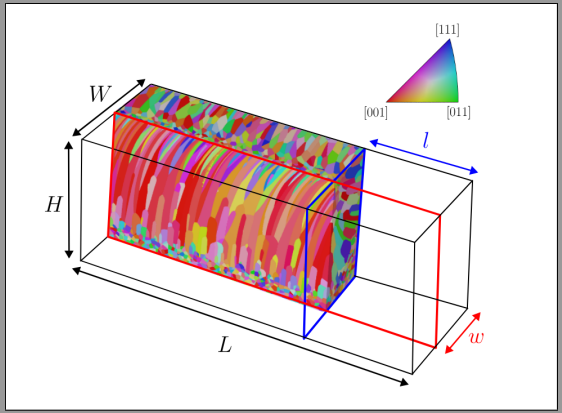
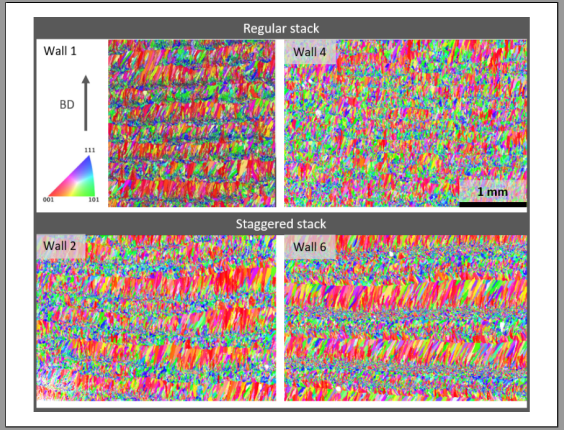
Microstructure

Validation vs. experiments





M Bréhier et al., **Rapid Prototyping Journal**, 2024

Microstructure

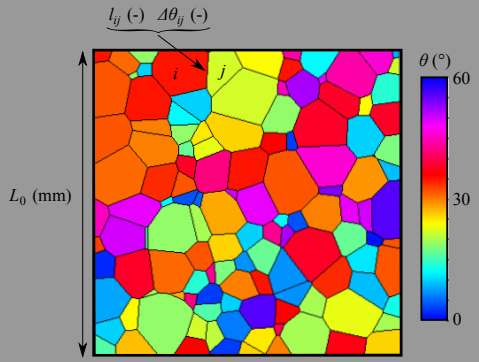
Croissance de grain

Planar hexagonal crystals

- FFC $\langle 1,1,1 \rangle$
- Orientation : 1 angle
- Periodicity 60°

Oriented tessellations

- $\underline{x}, \underline{y}$: coordinates of seeds
- $\underline{w}$: weights
- $\underline{\theta}$: crystal orientations
- $\underline{\alpha} = \left(\underline{x}, \underline{y}, \underline{w}, \underline{\theta}\right)$: meso state



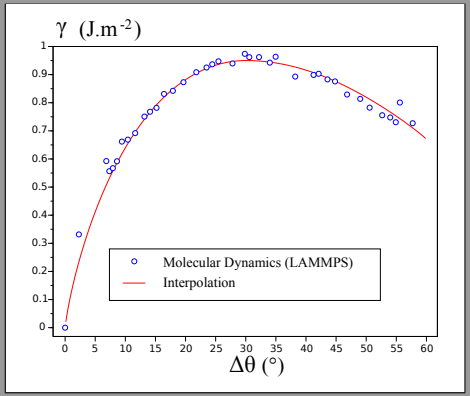
S Sakout et al., **Acta Materialia**, 2020

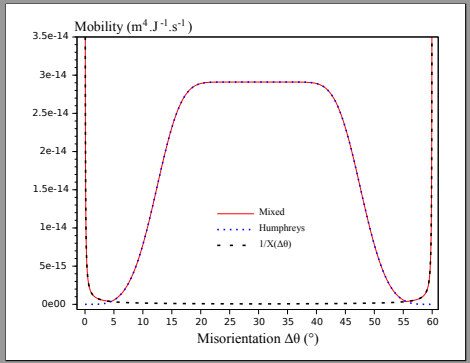
Microstructure

Grain growth

$$\gamma(T, \Delta\theta) = (G(T)/G(0))\gamma(0, \Delta\theta)$$

$$D(T, \Delta\theta, v^*) = [v^*]^2 / m_{CD}(T, \Delta\theta)$$

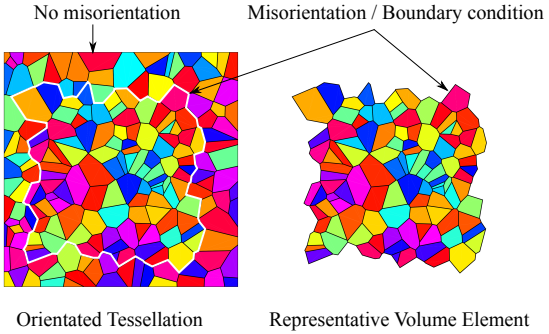




S Sakout et al., **Acta Materialia**, 2020

Microstructure

Grain growth



S Sakout et al., **Acta Materialia**, 2020

Microstructure

Grain growth

Total energy in the polycrystal

$$\mathcal{E}(T,\underline{\alpha}) = L_0 \sum_{(i,j)\in I_{\mathrm{RVE}}} l_{ij}\gamma_{ij}$$

Total dissipation in the polycrystal

$$\mathcal{D}(T,\underline{\alpha},\underline{v}^*) = L_0 \sum_{(i,j)\in I_{\mathrm{RVE}}} l_{ij}D^*_{ij}$$

S Sakout et al., **Acta Materialia**, 2020

Microstructure

Grain growth

$$\underline{\dot{w}}_{\text{meso}} = \begin{cases} \underset{\underline{\dot{w}} \in \mathbb{R}^n}{\texttt{argmax}}\, \mathcal{D}(T, \underline{\alpha}, \underline{\dot{w}}) \\ \texttt{s.t.} \quad : \quad \mathcal{D}(T, \underline{\alpha}, \underline{\dot{w}}) + \dot{\mathcal{E}}(T, \underline{\alpha}) = 0 \\ \qquad\qquad \dfrac{\partial M}{\partial \underline{w}} \cdot \underline{\dot{w}} = 0 \end{cases}$$

$$\boxed{\underline{\dot{w}}_{\text{meso}} = -\frac{m(T)}{L_0^3} \underline{\underline{M}}_{\text{meso}}(\underline{\alpha}) \cdot \frac{\partial \mathcal{E}_{\text{meso}}(T, \underline{\alpha})}{\partial \underline{w}}}$$

S Sakout et al., **Acta Materialia**, 2020

Microstructure

Grain growth

Residual stresses

- Finite Element Analysis (Cast3m)
  - **Incremental computation** (mass addition)
  - **Thermal** loading using **eigenstrain**
  - **Shell** elements

$$\Delta \underline{\underline{\varepsilon}}_k^{\text{th}}(\underline{x}) = \alpha \left(T_k(\underline{x}) - T_{k-1}(\underline{x})\right) \underline{\underline{I}}$$

  - **Temperature** dependent **material properties**

$$E(T) = E_0 \left(1 - \beta_E \left(T - T_0\right)\right)$$

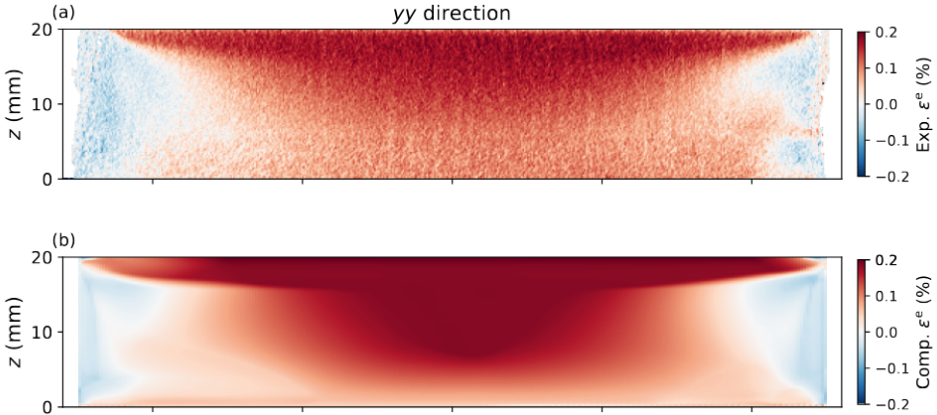
$$\mu(T) = \mu_0 \left(1 - \beta_\mu \left(T - T_0\right)\right)$$

$$\sigma_Y(T) = \sigma_0 \left[1 + \beta \exp -\gamma(T - T_0)\right]$$

D. Weisz-Patrault et al., **Additive Manufacturing** 56, 102903, 2022

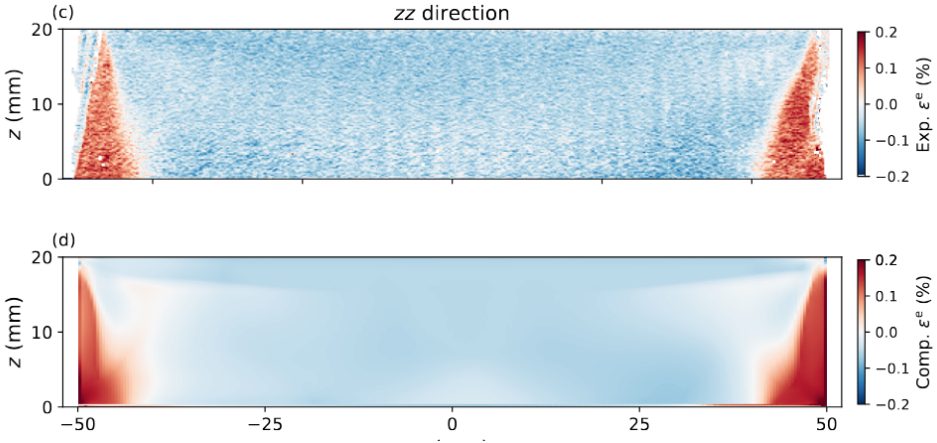
P. Margerit et al., **Additive Manufacturing** 37, 101664, 2021

Residual stresses



S. Gaudez et al., **Additive Manufacturing** 101, 104674, 2025

Residual stresses



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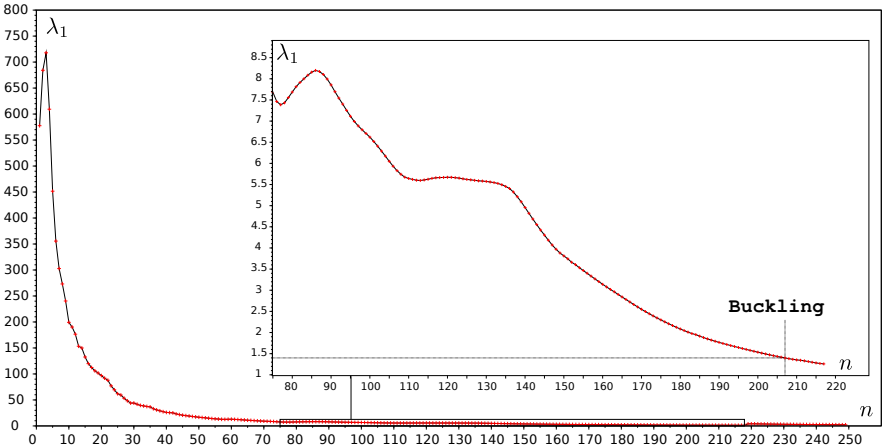
Residual stresses



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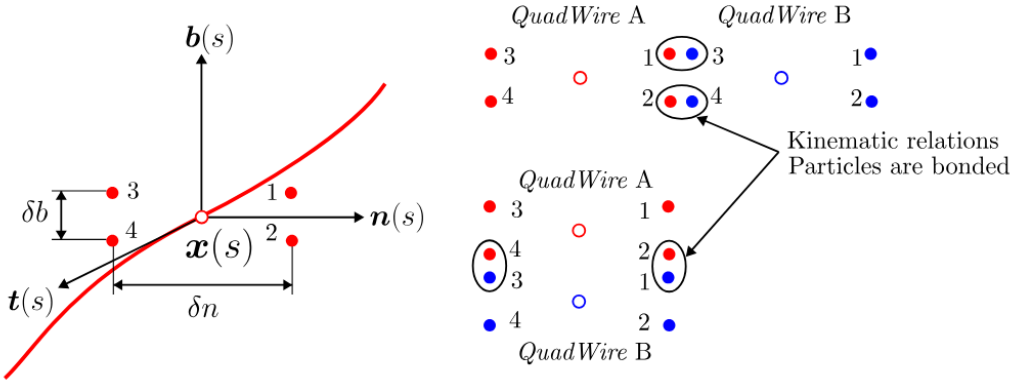
Residual stresses



L. Preumont et al., **CMAME**, 427, 117010, 2024

Residual stresses

$$\mathrm{PVI} = \int_0^l \sum_{k=1}^{4} \left(\underline{f}_k(s).\underline{v}_k^*(s) - \underline{F}_k(s).\underline{v}_k^{*\prime}(s) \right) \mathrm{d}s$$

Consistency condition

$$\begin{aligned}\mathrm{PVI} \quad &= \int_0^l \Bigg(\underline{m}_n(s).\frac{\delta^n \underline{v}^*(s)}{\delta_n} + \underline{m}_b(s).\frac{\delta^b \underline{v}^*(s)}{\delta_b} + \underline{m}_\times(s).\frac{\delta^\times \underline{v}^*(s)}{\delta_n\,\delta_b} - \underline{F}(s).\underline{v}^{*\prime}(s) \\ &\quad - \underline{M}_n(s).\frac{\delta^n \underline{v}^{*\prime}(s)}{\delta_n} - \underline{M}_b(s).\frac{\delta^b \underline{v}^{*\prime}(s)}{\delta_b} - \underline{M}_\times(s).\frac{\delta^\times \underline{v}^{*\prime}(s)}{\delta_n\,\delta_b} \Bigg) \mathrm{d}s\end{aligned}$$

with

$$a = \frac{a_1 + a_2 + a_3 + a_4}{4} \qquad \delta^n a = \frac{a_1 + a_2 - a_3 - a_4}{2}$$

$$\delta^b a = \frac{a_1 - a_2 + a_3 - a_4}{2} \qquad \delta^\times a = a_1 - a_2 - a_3 + a_4$$

Residual stresses

Internal power

$$\mathrm{PVI} = -\int_0^l \left(\dot{\underline{\underline{\xi}}}^*(s) : \underline{\underline{\Sigma}}(s) + \dot{\underline{\underline{\underline{\chi}}}}^*(s) \vdots \underline{\underline{\underline{M}}}(s) + \dot{\underline{\gamma}}^*(s).\underline{M}_\times(s) \right) \mathrm{d}s$$

Thermodynamic balance equation

$$\underline{\underline{\Sigma}}(s) : \dot{\underline{\underline{\xi}}}(s) + \underline{\underline{\underline{M}}}(s) \vdots \dot{\underline{\underline{\underline{\chi}}}}(s) + \underline{M}_\times(s).\dot{\underline{\gamma}}(s) - \rho(s) \left(\dot{\psi}(s) + \dot{T}(s)\, e_S(s) \right) - \frac{T'(s)\, q(s)}{T(s)} = D(s)$$

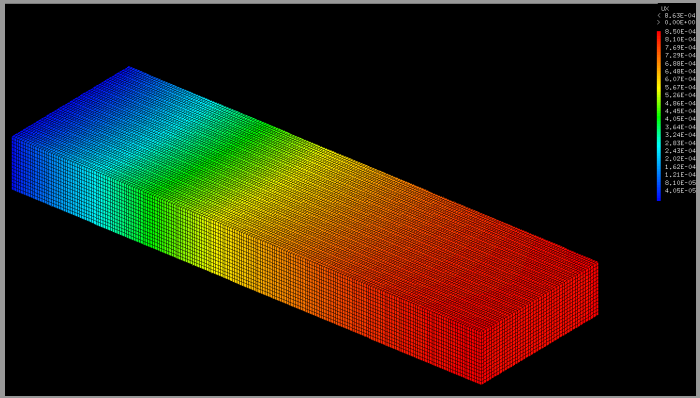
Thermo-elastic behavior

$$\begin{cases} \underline{\underline{\Sigma}} = \underline{\underline{\underline{\underline{R}}}}^{\xi} : \left(\underline{\underline{\xi}} - \underline{\underline{\alpha}}^{\xi} \Delta T \right) + \underline{\underline{\underline{\underline{R}}}}^{\xi\chi} \vdots \underline{\underline{\underline{\chi}}} + \underline{\underline{\underline{R}}}^{\xi\gamma}.\underline{\gamma} \\ \underline{\underline{\underline{M}}} = \underline{\underline{\underline{\underline{R}}}}^{\chi} \vdots \left(\underline{\underline{\underline{\chi}}} - \underline{\underline{\underline{\alpha}}}^{\chi} \Delta T \right) + \underline{\underline{\xi}} : \underline{\underline{\underline{\underline{R}}}}^{\xi\chi} + \underline{\underline{\underline{R}}}^{\chi\gamma}.\underline{\gamma} \\ \underline{M}_\times = \underline{\underline{R}}^{\gamma}.\left(\underline{\gamma} - \underline{\alpha}^{\gamma} \Delta T \right) + \underline{\underline{\xi}} : \underline{\underline{\underline{R}}}^{\xi\gamma} + \underline{\underline{\underline{\chi}}} : \underline{\underline{\underline{\underline{R}}}}^{\chi\gamma} \end{cases}$$

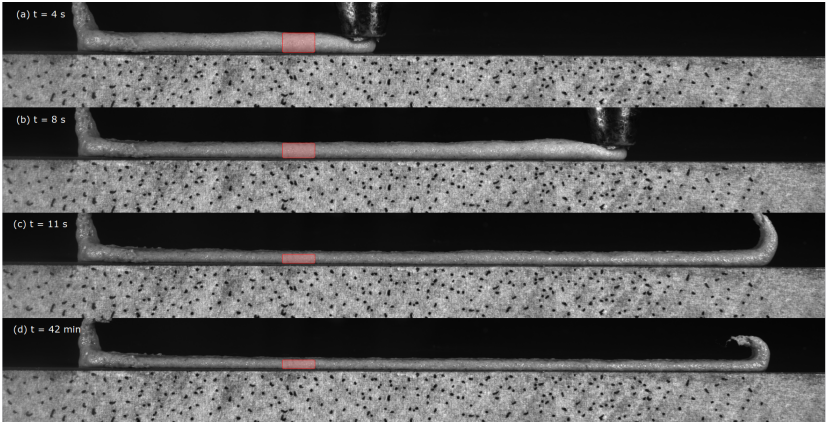
Residual stresses

Stiffness identification

$$J(p) = \frac{1}{2} \int_0^l \left(\rho\, \psi(s) - \rho^{3\mathrm{D}}\, \psi^{3\mathrm{D}}(s) \right)^2 \mathrm{d}s$$



Residual stresses



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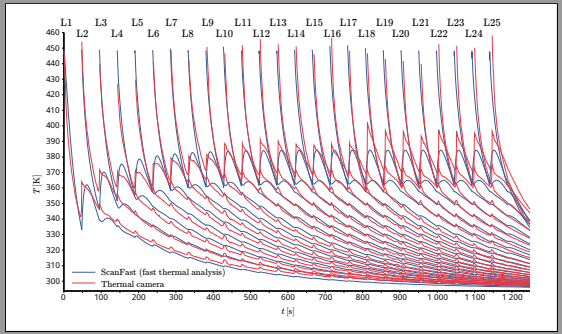
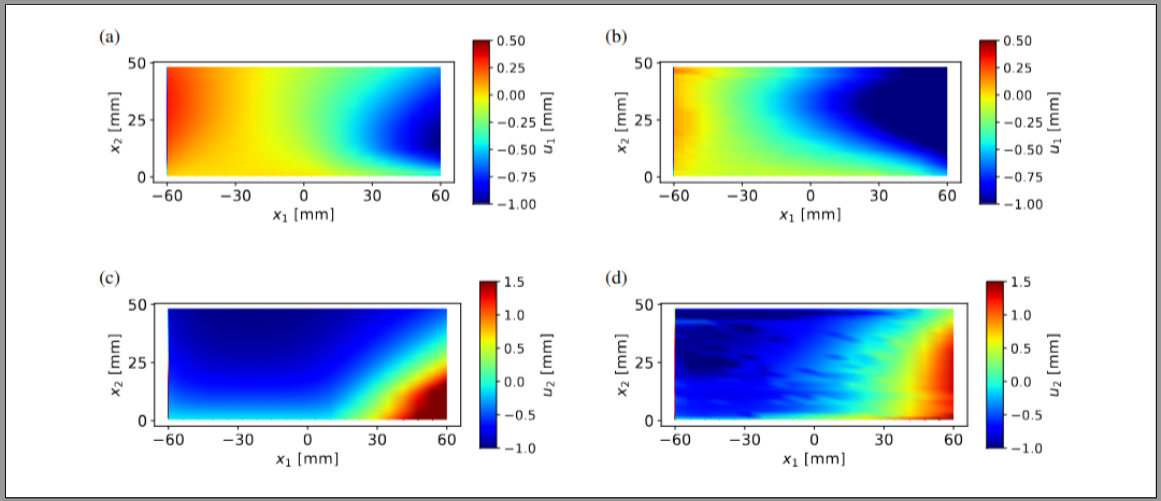
Residual stresses



Residual stresses



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Questions ?