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1st Winter School on

Trends on Additive Manufacturing for Engineering Applications

SIRAMM

Simulation for additive manufacturing: opportunities and challenges

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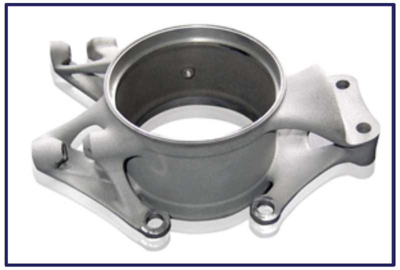
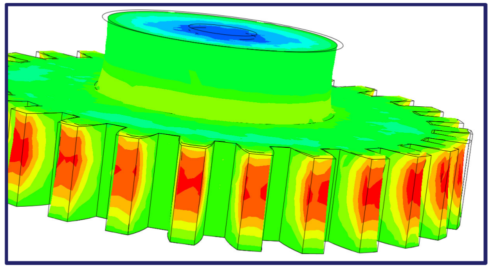
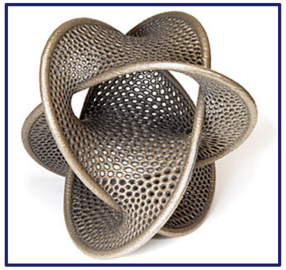





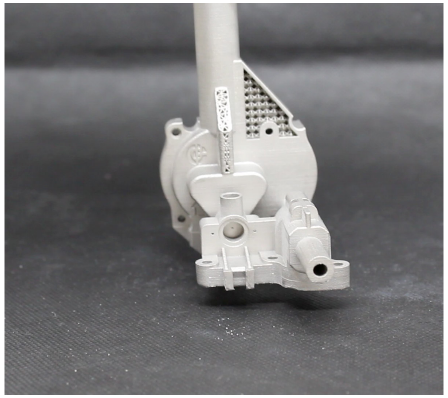
Presentation outline

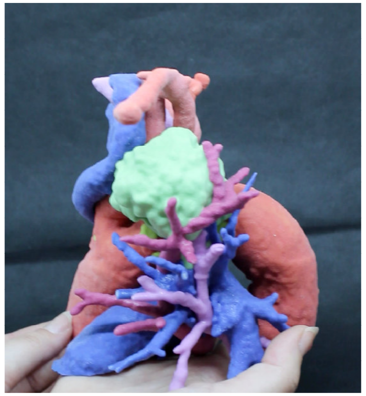
- **Introduction**
  - AM - 3DP: advantages, open problems
- **Design for additive**
  - Phase-field topology optimization: gradient material
  - Adaptive isogeometric analysis
  - Phase-field topology optimization: single material
- **Process simulations**
  - Immersed boundary approach
    - Melt pool: high fidelity simulations
    - Part-scale: low fidelity simulations
  - Two-level method
- **Product simulations**
  - Lattice components
  - Industrial components
- **Future activities & directions**
  - Innovative processes and materials
- **Conclusion**

AM: advantages / disadvantages / impact

Advantages

- Produce complex geometries: close to free-form flexibility
- Produce single device made of multiple components (assembling more parts into a single one)
- Combine different devices and geometries in a single printing batch
- Green technology: reduced waste
- Accelerate design-testing-production process chain (even in our labs)

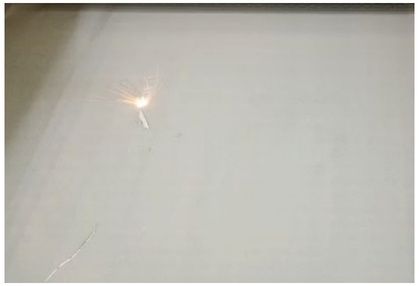


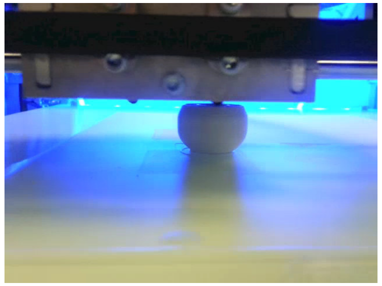


Disadvantages

- Need of support materials (technology dependent)
- Very localized physics (multi-scale problem, technology dependent)

- Low speed (still a limitation)
- High cost (still a limitation)
- Interaction with further production steps (subtractive or finishing)





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- Introduction
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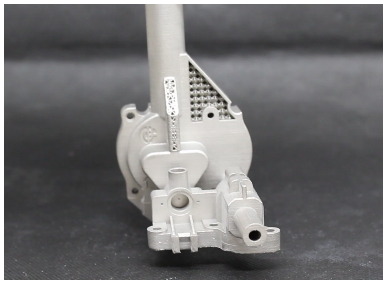
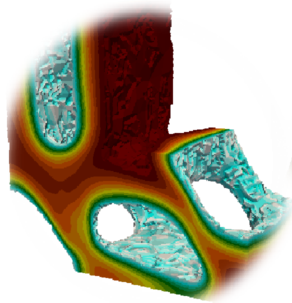
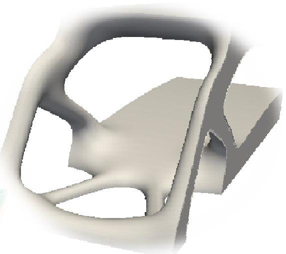
Design for additive: challenges

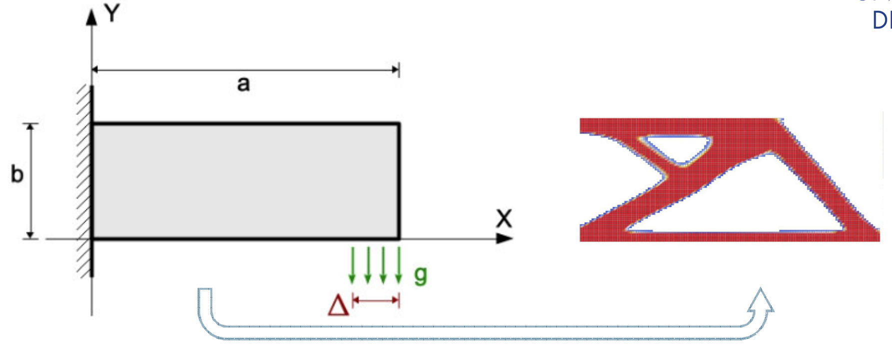
- **Close-to-freeform** flexibility requiring **novel design approaches**
- **Topology** and **shape optimization** as tools for **design**, focusing on product functionality and production constraints

Phase-field topology optimization (PF top-opt)

Topology optimization: goal
- Optimal distribution of given amount of material
- Minimize structure compliance (i.e., maximize stiffness)

Phase-field Method:
- No filtering methods required (cfr. SIMP approaches)



Limit discussion to for linear elastic problems
Introduce standard elastic problem in a domain Ω

$$\begin{aligned} \mathrm{div}[\mathbb{C}\,\boldsymbol{\varepsilon}(\mathbf{u})] &= \mathbf{b} \quad \text{in} \quad \Omega \\ \mathbf{u} &= \mathbf{0} \quad \text{on} \quad \Gamma_D \\ [\mathbb{C}\,\boldsymbol{\varepsilon}(\mathbf{u})] &= \mathbf{t} \quad \text{on} \quad \Gamma_N \end{aligned}$$

Objective

Minimize structure compliance:

$$\int_{\Omega} \mathbf{b}\cdot\mathbf{u}\, d\Omega + \int_{\Gamma_N} \mathbf{t}\cdot\mathbf{u}\, d\Gamma$$

properly distributing material in Ω

Introduce description of meso-structure (variable density, lattice):
- Obtain a graded design, i.e., structure with varying density

Acknowledgments: M.Carraturo, E.Rocca, A.Reali (UniPV & IMATI-CNR), **E.Bonetti** (Università di Milano & IMATI-CNR), **D.Hömberg** (WIAS Institute Berlin)

Publications:

- Carraturo, Rocca, Bonetti, Hömberg, Reali, FA. *Graded-material design based on phase-field and topology optimization*. Computational Mechanics, Vol. 64, 1589–1600 (2019)
- FA, Bonetti, Carraturo, Hömberg, Reali, Rocca. *A phase-field based graded-material topology optimization with stress constraint*. *M3AS*, Vol. 30 (08), 1461–1483 (2020)

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Phase-field topology optimization: gradient multi-material

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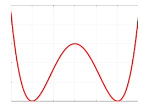
- Phase-field variables
  φ : material presence $\quad 0 \leq \varphi \leq 1 \quad$ [$\varphi = 0$: no material, $\varphi = 1$: material]
  χ : material features (scalar quantity=density) $\quad 0 \leq \chi \leq \varphi \quad$ [$\chi = 0$: material B, $\chi = \varphi$: material A]

- Material elasticity continuously varies from a soft ($\mathbb{C}_B$) to a stiff material ($\mathbb{C}_A$) $\quad \mathbb{C} = \mathbb{C}_B \chi + \mathbb{C}_A (1 - \chi)$

- Classical topology optimization: minimize compliance, complemented with a perimeter measure

$$\mathcal{J}(\phi, \mathbf{u}) = \int_{\Omega} \phi\, \mathbf{b} \cdot \mathbf{u}(\phi)\, d\Omega + \int_{\kappa_N} \mathbf{t} \cdot \mathbf{u}(\phi)\, d\Gamma + \kappa_\phi \int_{\Omega} \left| \gamma_\phi \|\nabla \phi\|^2 + \frac{1}{\gamma_\phi} \psi_0(\phi) \right| d\Omega$$

Double-well potential



$$\psi_0(\phi) = (\phi - \phi^2)^2$$

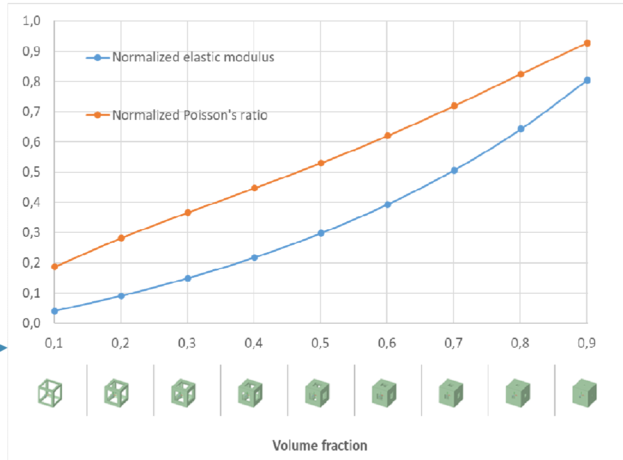
- New topology optimization: Introduce extra-penalization for the gradient of second scalar field χ

$$\mathcal{J}^M(\phi, \mathbf{u}, \chi) = \mathcal{J} + \kappa_\chi \int_{\Omega} \gamma_\chi \|\nabla \chi\|^2\, d\Omega$$

- Introduce volume constraint & complementary problem (equilibrium)

$$\mathcal{L}^M(\phi, \mathbf{u}, \chi) = \mathcal{J}^M + \lambda \left[\int_{\Omega} (\phi - \bar{v})\, d\Omega \right] + \mathcal{S}^M$$

$$\mathcal{S}^M(\phi, \mathbf{u}, \chi, \mathbf{p}) = \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{u}) : \mathbb{C}(\phi, \chi)\, \boldsymbol{\varepsilon}(\mathbf{p})\, d\Omega - \int_{\Gamma_N} \mathbf{g} \cdot \mathbf{p}\, d\Gamma$$



- Elastic tensors also from homogenization on a lattice RVE with periodic BCs

Phase-field gradient top-opt: approx & solution scheme

- Minimization process
  - Allen-Cahn gradient flow, i.e. steepest descent pseudo-time stepping method, with time-step increment τ

$$\frac{\gamma_\phi}{\tau}\int_\Omega (\phi_{n+1}-\phi_n)\; v_\phi \, d\Omega + \kappa_\phi\, \gamma_\phi \int_\Omega \nabla\phi \cdot \nabla v_\phi d\Omega + \;\dots = 0$$

$$\frac{\gamma_\chi}{\tau}\int_\Omega (\chi_{n+1}-\chi_n)\; v_\chi \, d\Omega + \kappa_\chi\, \gamma_\chi \int_\Omega \nabla\chi \cdot \nabla v_\chi d\Omega + \;\dots = 0$$

  - Alternate solution of gradient flow and equilibrium problem

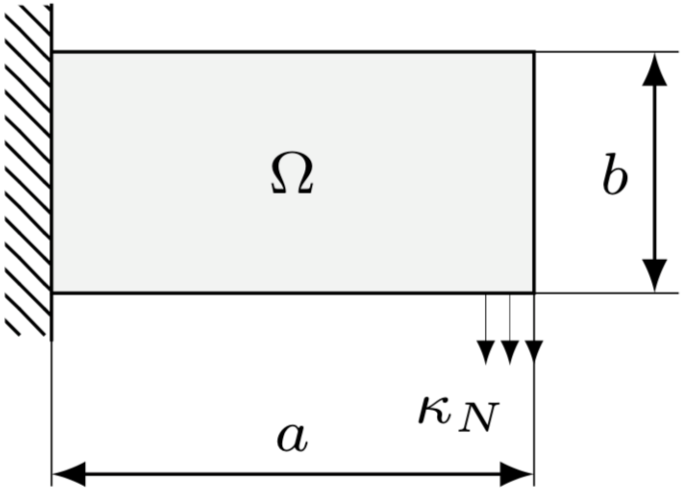
- Finite element approximation of fields
  - Discretize domain using quads
  - Piecewise linear basis functions (except that for global fields)

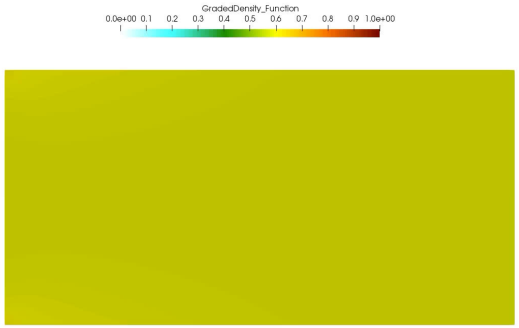
- Adopt a two-step algorithm
  - solve equilibrium to get displacement vector
  - solve Allen-Cahn gradient flow to get phase-field, material field, Lagrange multiplier vectors
  - rescale to fulfilling constraints

```
input  : Q, Q_φ, Q_χ, Q_λ, φ_0, χ_0
output: Optimal topology
φ_n ← φ_0
χ_n ← χ_0
while (Δ_φ ≥ tol or Δ_χ ≥ tol) and n ≤ max_iter do
    ũ_{n+1} ← solve(26)
    (φ̃*_{n+1}, χ̃*_{n+1}, λ̃_{n+1}) ← solve(27)
    φ̃_{n+1} ← rescale (φ̃*_{n+1}) to [0, 1]
    χ̃_{n+1} ← rescale (χ̃*_{n+1}) to [0, φ]
    update(Δ_φ and Δ_χ)
    φ_n ← φ_{n+1}
    χ_n ← χ_{n+1}
end
```

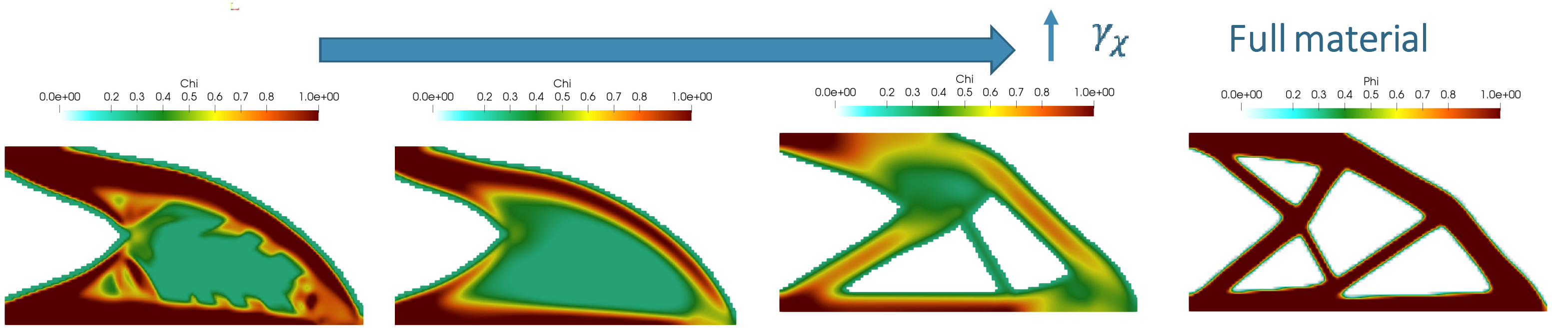
- Use Δϕ L2-norm increments as convergence criteria

Phase-field gradient top-opt: examples





Grey = no material
Color (different than grey) = material
Different color = different materials



Sensitivity study for γ_χ

Increasing penalty gradient material, structures closer to *black-and-white* solution

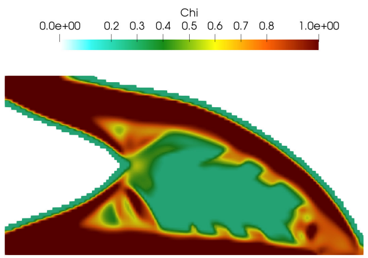
- Multi-material distribution very different from single-material topology (right figure) for small values of γ_χ
- Voids present in single-material structure replaced by areas of soft material in multi-material structure
- When thickness of diffuse interface is too small compared to element size, solution does not converge

Phase-field gradient top-opt: examples

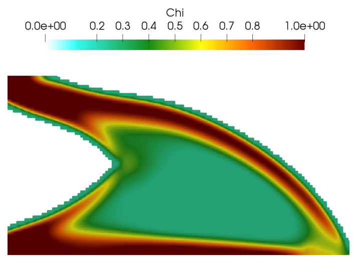
Sensitivity study for γ_χ

↑ γ_χ Full material

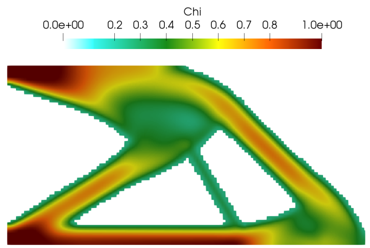
Grey = no material
Color = material
Different color = different materials



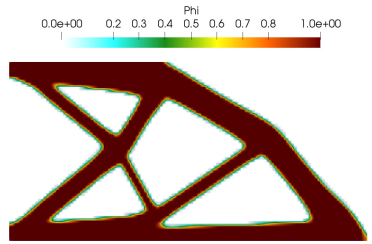
$\gamma_\chi = 0.001$



$\gamma_\chi = 0.01$



$\gamma_\chi = 0.1$



full material

- Volume fraction index m_ϕ : to estimate material volume
- Material fraction index m_χ : to estimate material amount (density)

$$m_\phi = \frac{1}{\Omega}\int_\Omega \phi \, d\Omega$$

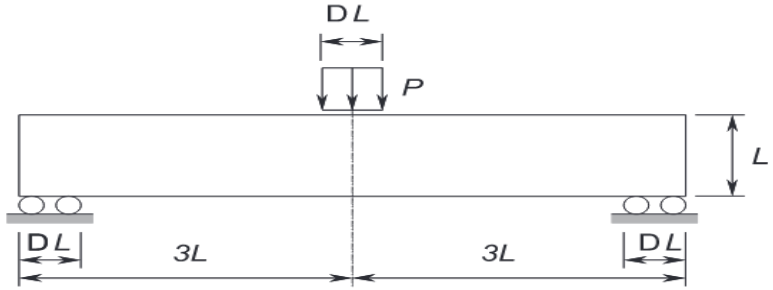
$$m_\chi = \frac{1}{\Omega}\int_\Omega \chi \, d\Omega$$

γ_χ	Compliance	m_χ	Converge?
0.001	105.3	0.380	NO
0.005	122.9	0.265	YES
0.01	133.0	0.245	YES
0.02	141.9	0.230	YES
0.05	154.0	0.225	YES
0.1	165.4	0.201	YES

Employing a softer material decreases body compliance, leading to heavier structures compared to the homogeneous material case

Phase-field gradient top-opt: MBB example

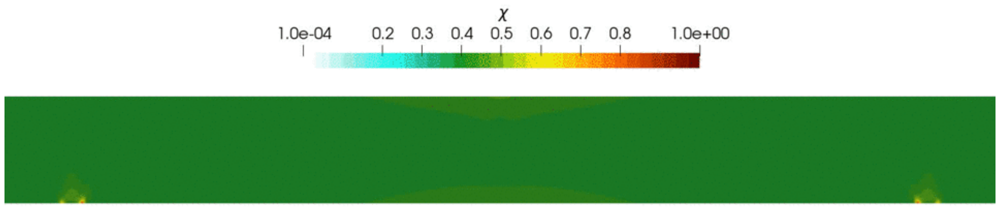
- Messerschmitt-Bölkow-Blohm (MBB) beam
  - Applied force = 25 N
  - Material: RGD851 rigid polymer from Stratasys (E=2.3 GPa and ν=0.3)
  - 3D printer machine: Stratasys Objet 260 Connex 3
  - Volume fraction = 0.6
  - Mass fraction = 0.4



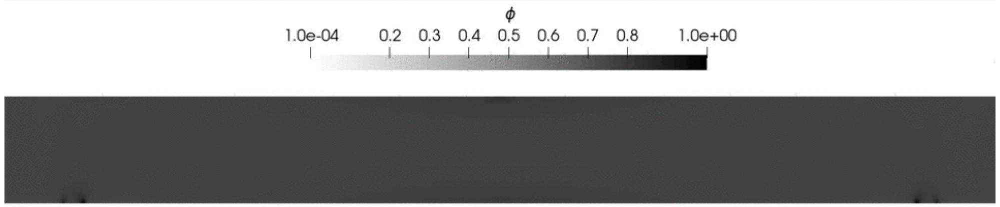
Messerschmitt-Bolkow-Blohm GmbH;Paytenet al.1998; Bulmanet al.2001

- Results
  1. Black-and-white structure indicates material presence
  2. Density continuously re-distributed within material region

χ



φ



Acknowledgments: **G.Alaimo, M.Carraturo, E.Rocca, A.Reali** (UniPV & IMATI-CNR)

Publications: Alaimo, Carraturo, Rocca, Reali, FA. *Functionally graded material design for plane stress structures using phase field method*, II International Conference on Simulation for Additive Manufacturing - Sim-AM 2019

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Phase-field gradient top-opt: numerics, 3D printing & experiments

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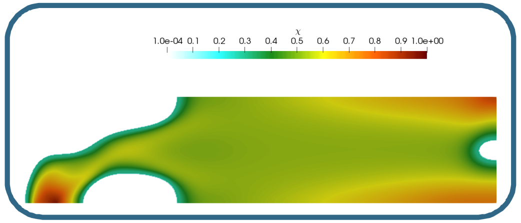
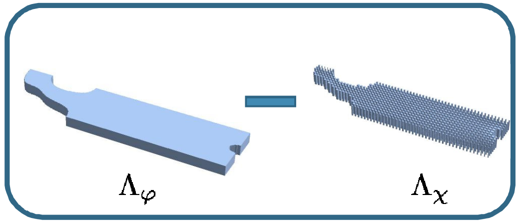
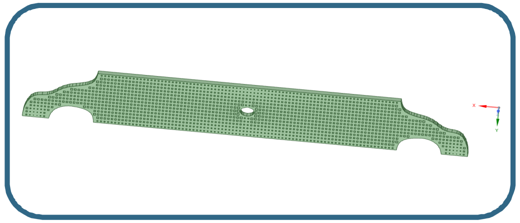
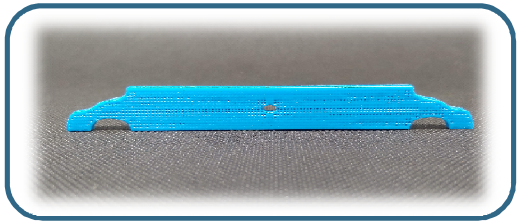
Objective: evaluate optimized versus uniform (same weight) specimen in terms of max. displacements

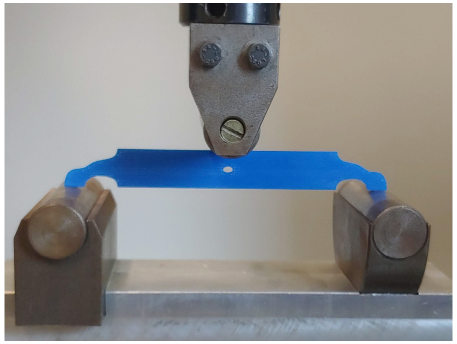


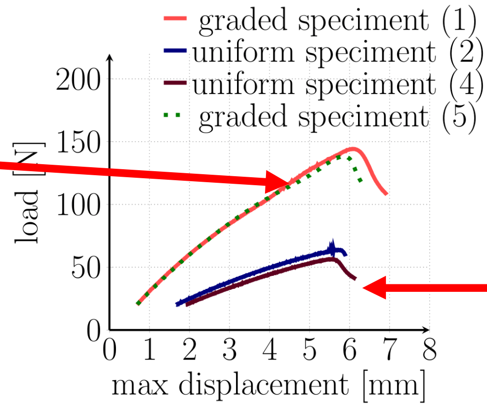


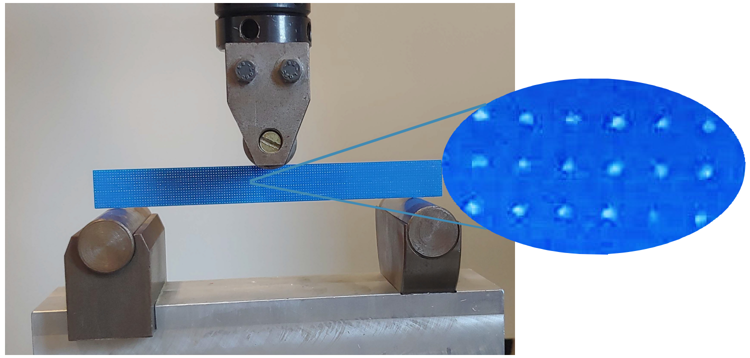




Discrete map of field variables → Generate 3D virtual model → 3D printing







Results: for the same load, we observe a **reduction of 50%** as max. displacement

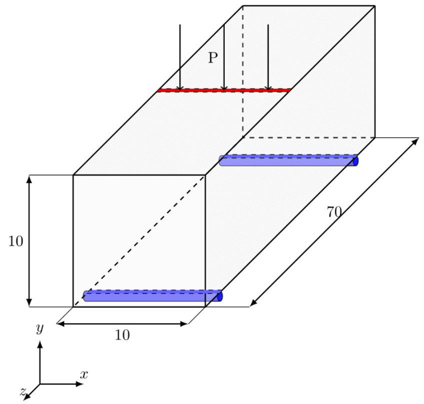
Special thanks to: G.Alaimo (ProtoLab) & S.Marconi (3D4Med)

Acknowledgments: G.Alaimo, M.Carraturo, E.Rocca, A.Reali (UniPV & IMATI-CNR)

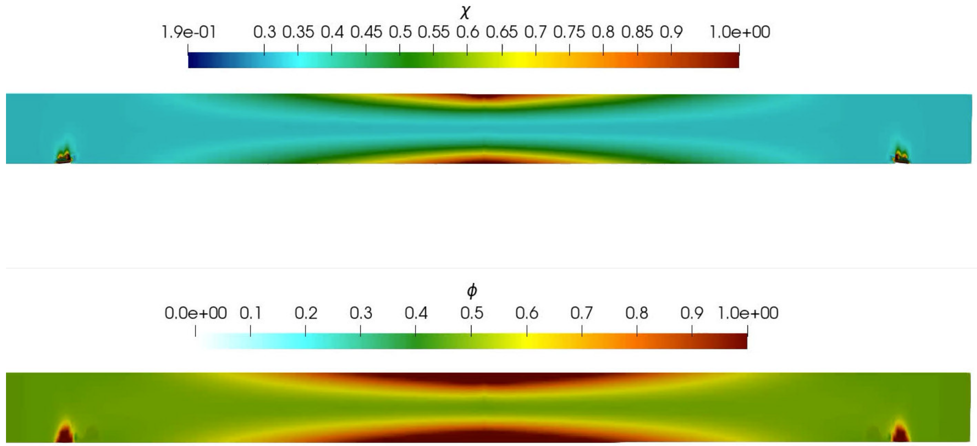
Publications: Alaimo, Carraturo, Rocca, Reali, FA *Functionally graded material design for plane stress structures using phase field method*, II Int.Conf. Simulation for AM - Sim-AM 2019

Phase-field gradient top-opt: 3D extension

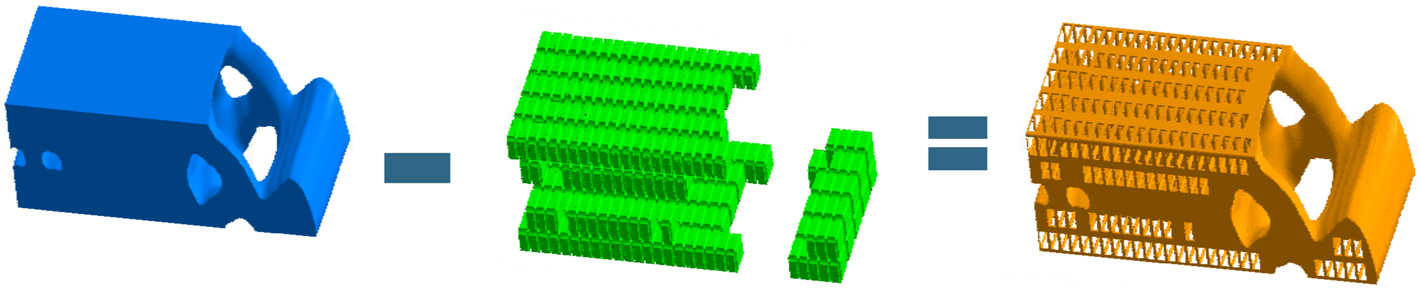
- Objective: extend 2D workflow to 3D structures to evaluate the performance of the optimization for a 3D case
- Example: MBB-beam problem



Optimize structure using phase-field gradient top-opt



Slicing & 3D model reconstruction



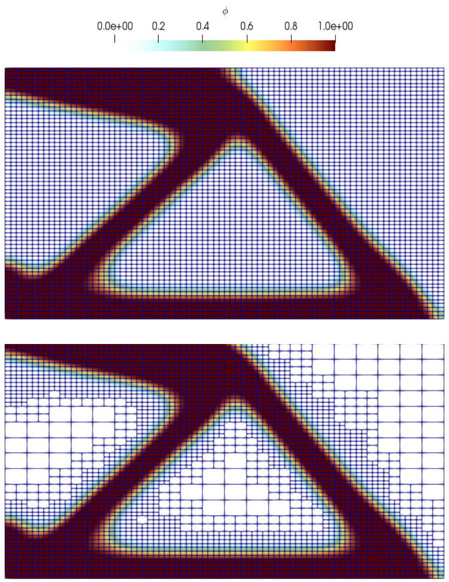
On-going work...

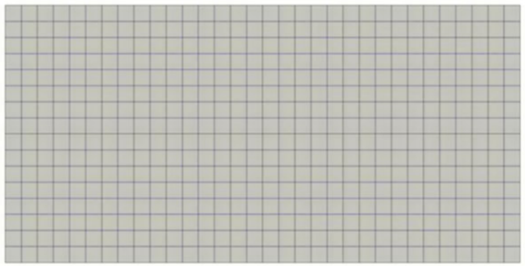
3D printing & Experiment

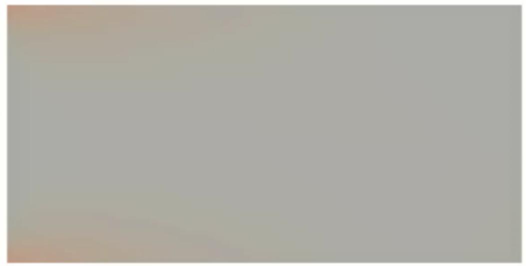
Phase-field single material top-opt: adaptive isogeometric analysis

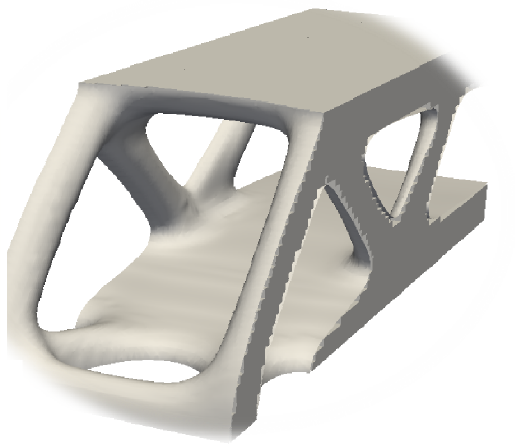
- **Idea:** Approximate mechanical and phase-field solution space using IGA, since higher continuity of IGA basis functions very effective for phase-field methods
- Adaptive Isogeometric Analysis as presented in **Henning et al. 2016** allows to **locally concentrate the computational effort** at the material interface **without any loss of accuracy**
- Single material

Work in progres…









- 60% reduction in terms of DOFs
- 40% less CPU time
- Higher improvement are likely expected for the 3D case…

TECHNISCHE UNIVERSITÄT DRESDEN

Acknowledgments: Markus Kästner, Paul Henning, Leonhard Heindel (TU Dresden), **M.Carraturo, A.Reali** (UniPV & IMATI-CNR)

Publications: Henning, Heindel, Carraturo, Reali, FA, Kästner. *Projection Methods in Adaptive Isogeometric Analysis and its Application to Topology Optimization,* Proceedings in Applied Mathematics and Mechanics (*accepted*).

Phase-field single-material top-opt: new formulations

Single material, hence single scalar field ϕ

Volume-constrained formulation:

- Formulation including compatibility, constitutive, equilibrium equation into a single functional

$$\mathcal{L}^{vc}(\phi, \boldsymbol{u}, \boldsymbol{\varepsilon}, \boldsymbol{\sigma}) = \mathcal{J}(\phi, \boldsymbol{u}) + \kappa_b \mathcal{B}(\phi) - \mathcal{E}^{el}(\boldsymbol{\varepsilon}, \phi) + \int_\Omega \boldsymbol{\sigma} : (\boldsymbol{\varepsilon} - \nabla^s \mathbf{u})\, d\Omega + \lambda \left[\int_\Omega (\phi - \bar{v})\, d\Omega \right]$$

ϕ bounding — Elastic energy — Hu-washizu — Volume constraint

With

$$\mathcal{B}(\phi) = \int_\Omega b(\phi)\, d\Omega \quad with \quad b(\phi) = \begin{cases} (\phi - 1)^2/2 & if \quad \phi > 1 \\ 0 & if \quad 0 \le \phi \le 1 \\ \phi^2/2 & if \quad \phi < 0 \end{cases} \qquad \mathcal{E}^{el}(\boldsymbol{\varepsilon}, \phi) = {}^1\!/_2 \int_\Omega \mathbb{C}(\phi)\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon}\, d\Omega$$

- No need of re-normalizing volume fraction
- All eqns into a single functional, i.e. possible monolithic solution schemes

Volume-minimization formulation:

Not imposing a constraint on volume but looking for volume minimization

$$\mathcal{L}^{vm}(\phi, \boldsymbol{u}, \boldsymbol{\varepsilon}, \boldsymbol{\sigma}) = \mathcal{J}(\phi, \boldsymbol{u}) + \kappa_b \mathcal{B}(\phi) - \mathcal{E}^{el}(\boldsymbol{\varepsilon}, \phi) + \int_\Omega \boldsymbol{\sigma} : (\boldsymbol{\varepsilon} - \nabla^s \mathbf{u})\, d\Omega + \frac{\kappa_v}{2} \left[\int_\Omega \phi^2 d\Omega \right]$$

Volume minimization

Results

- Relation between $\mathcal{L}^{vc}$ and $\mathcal{L}^{vm}$: possible to show that they return the same solution
- Second approach is not a saddle point problem but a true minimization (improved convergence properties)

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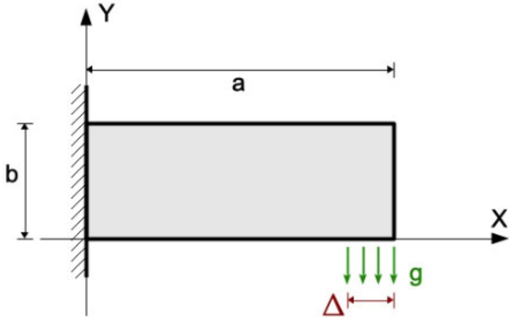
Acknowledgments: E.Rocca, A.Reali (UniPV & IMATI-CNR), U.Stefanelli (University of Vienna), M.Marino (University of Roma Tor Vergata)

Publications: Marino. FA, Reali, Rocca, Stefanelli (2020), *Mixed variational formulations for structural topology optimization based on phase-field,* submitted

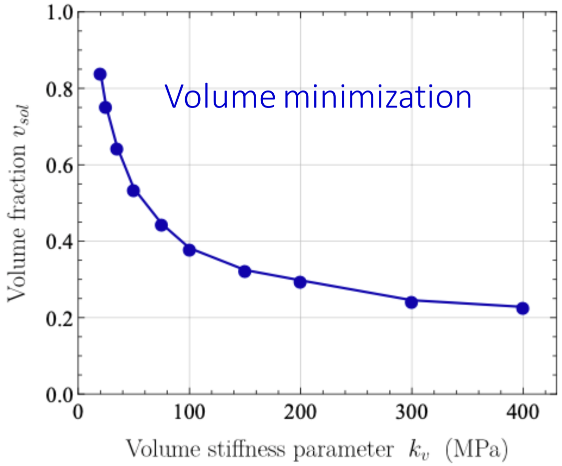
Phase-field single-material top-opt: new formulation results

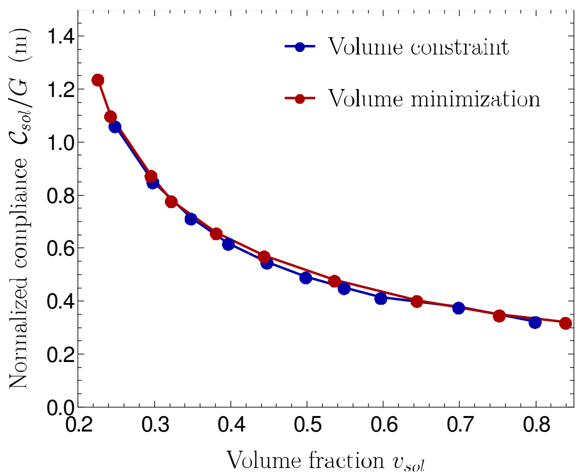
Accurate and extensive numerical investigation

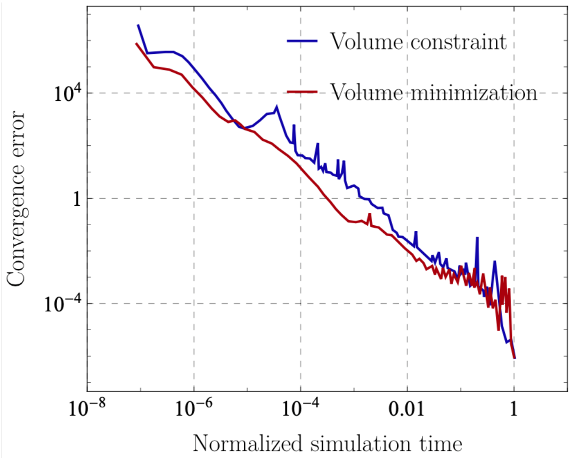


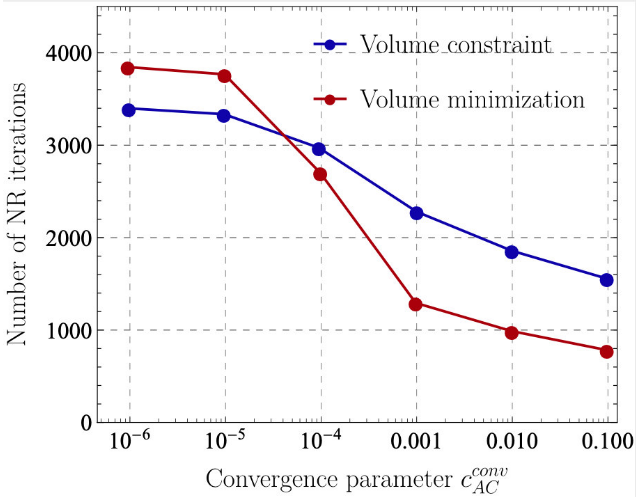
- Increasing volume stiffness reduces volume fraction
- Solutions from two formulations are identical in terms of compliance C_{sol} and interface perimeter P_{sol} for the same value of final volume fraction

- Volume minimization shows improved convergence
  - error decreases more monotonically (!)
- Volume minimization converges faster in terms of
  - simulation time
  - number of Newton iterations



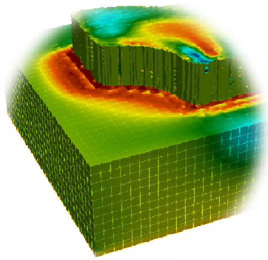


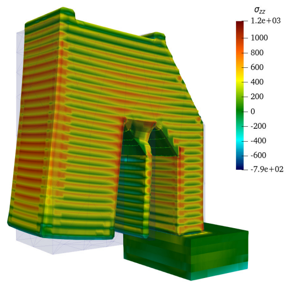




Process simulations: challenges

- **Large scale range** both in space and time
- **Complex physical phenomena** to be modeled
- Predict defects due to process

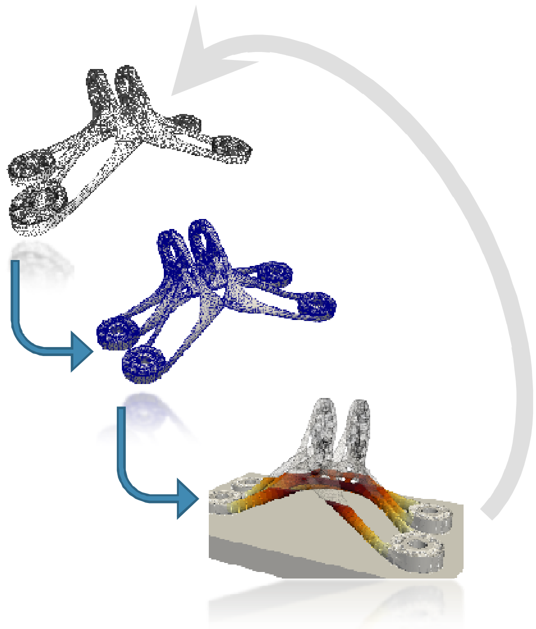




LPBF-AM process simulations

Focus on the most industrially relevant technology: laser powder bed fusion for metal components (LPBF)

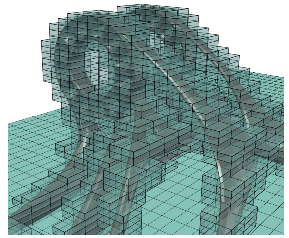
Standard AM-design process

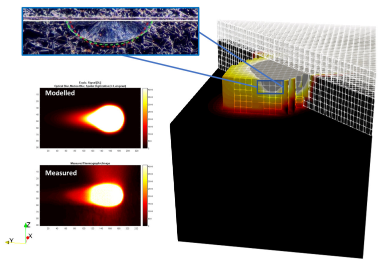


- 3D virtual model is developed within a CAD environment
- Geometry to be repaired
- Conform mesh generated
- Finite element analysis of the process
- To update the geometry, need to go back to CAD software and start procedure once again …

AM-design-through-analysis

- Thermo-mechanical analyses can be performed directly on CAD models
- STL repair step required only once the final design ready to be printed
- Remarkable computational speed-up for multi-layer high-fidelity analyses of complex geometrical features





Acknowledgments: Ernst Rank, Stefan Kollmannsberger, John Jomo, Ali Özcan, Nils Zander (TUM), **M.Carraturo, A.Reali** (UniPV & IMATI-CNR)

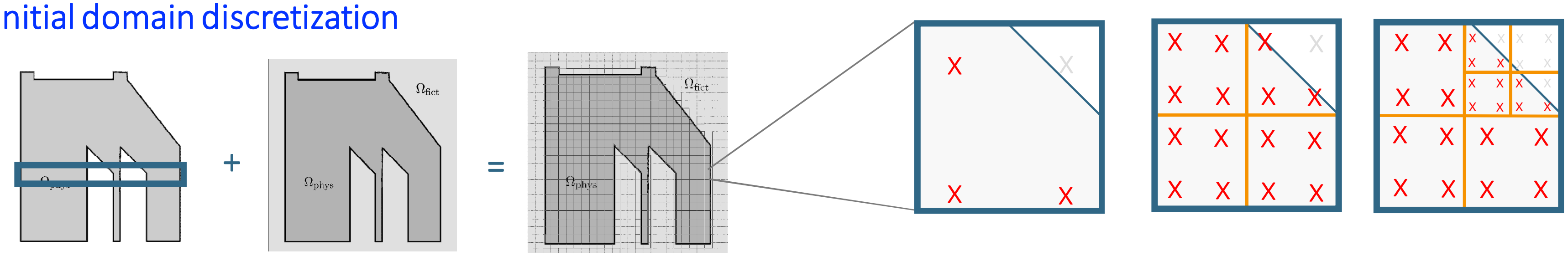
Publications:

- Kollmannsberger, Özcan, Carraturo, Zander, Rank. *A hierarchical computational model for moving thermal loads and phase changes with applications to selective laser melting.* CAMWA, Vol. 75 (5), 1483-1497 (2018)
- Carraturo, Jomo, Kollmannsberger, Reali, FA, Rank. *Modeling and experimental validation of an immersed thermo-mechanical part-scale analysis for laser powder bed fusion processes.* Additive Manufacturing, Vol. 36, 101498 (2020)

Immersed boundary approach for growing domain

The Finite Cell Method (FCM)

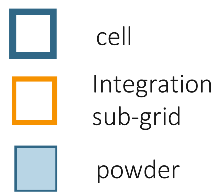
- Initial domain discretization



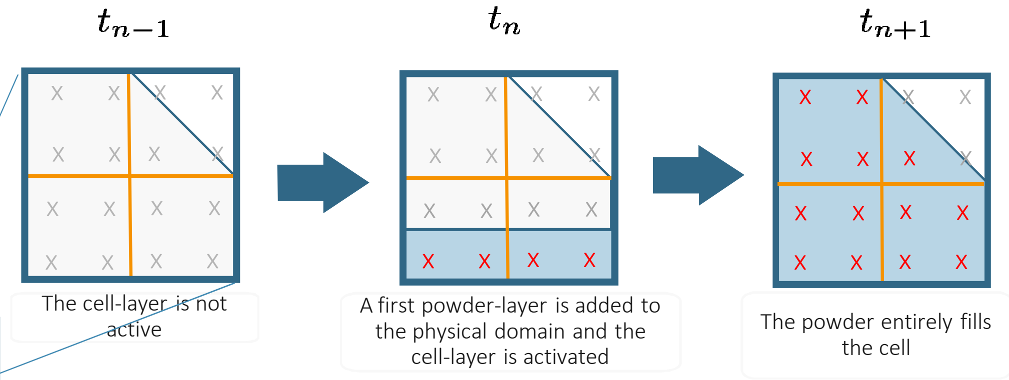
- ➢ **Weak form modified** using a parameter α evaluated at Gauss points
- ➢ Integration points distributed on **sub-cells** to accurately integrate over discontinuities at boundaries

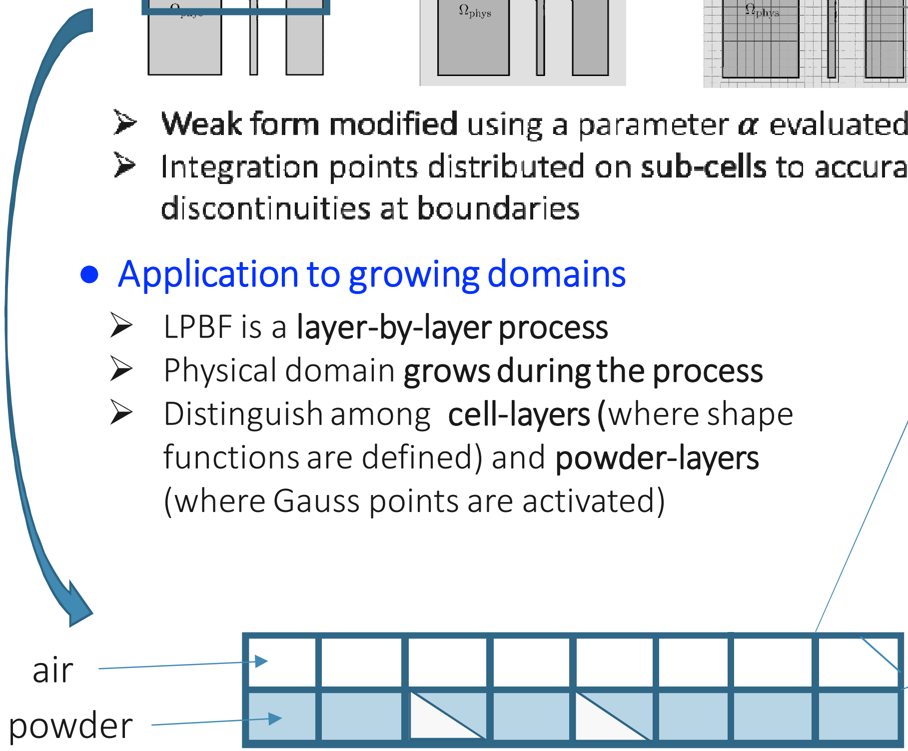
$$\alpha(\mathbf{x})\, a(\mathbf{u},\mathbf{v}) = l\,(\mathbf{v})$$

with $\alpha(\mathbf{x}) = \begin{cases} 1 : & \forall \mathbf{x} \in \Omega_{phys} \\ 0 : & \forall \mathbf{x} \notin \Omega_{phys} \end{cases}$



- Application to growing domains
  - ➢ LPBF is a **layer-by-layer process**
  - ➢ Physical domain **grows during the process**
  - ➢ Distinguish among **cell-layers** (where shape functions are defined) and **powder-layers** (where Gauss points are activated)





Immersed boundary approach for growing domain: different scale approaches

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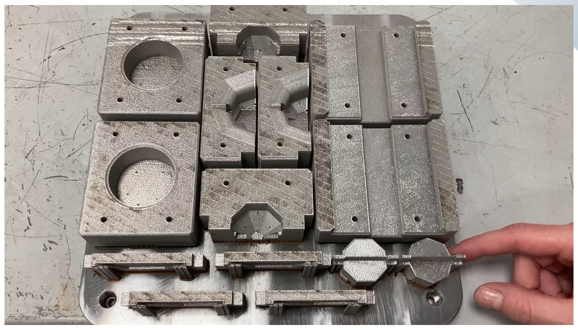
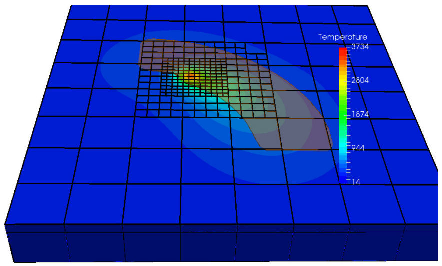
- Due to problem complexity, need to choose a-priori solution scale
- Choose quantities of interested

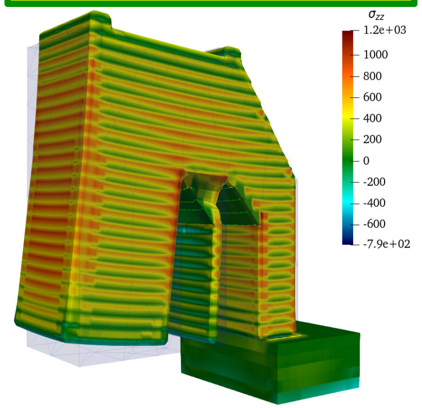
Input parameters	Range values
Laser power	100÷1000 [W]
Laser speed	0.2÷1.5 [m/s]
Laser spot radius	25÷100 [μm]



Melt-pool analysis
High-fidelity simulation



Part-scale analysis
Low-fidelity simulation



Objective
- Predict **temperature and stress state** at the **melt-pool length-scale** (element size ~ 10μm)
- Evaluate melt-pool shape and cooling rate

Model features
- **Few laser strokes** can be simulated (10÷100 mm length)
- Powder is included in the model
- Phase-change has to be taken into account

Objective
- Predict **part deflection** after base plate removal
- Evaluate **residual stresses** in the final component

Model features
- **Complete process** is simulated (including post-processing steps, e.g. part removal)
- Powder modeled as conduction BC, not included in the domain
- Latent heat usually neglected

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Immersed boundary for melt pool: thermal problem

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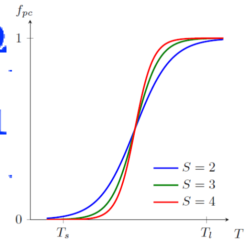
- Heat transfer equation

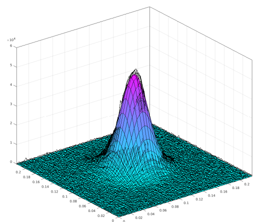
$$\rho c\dot{T} + \rho L\dot{f}_{pc} - \nabla(k\nabla T) = 0 \quad \text{in} \quad \Omega$$

$$f_{pc} = \frac{1}{2}\left[\tanh\left(S\frac{2}{T_l - T_s}\left(T - \frac{T_s + T_l}{2}\right)\right) + 1\right]$$



- Initial conditions

$$T(\mathbf{x}, t) = T_0 \quad \text{at} \quad t = 0$$



- Boundary conditions

$$k\nabla T(\mathbf{x}, t)\cdot\mathbf{n} = q^s + q^L \quad on \quad \Gamma_N$$

Radiation heat flux: $q^s = \sigma\epsilon(T^2 + T_e^2)(T_e^2 - T^2)$

Laser heat source: $q^L = \dfrac{2Q\eta}{\pi\rho^2}\exp\left[-2\left(\dfrac{y - y_0}{r^2} + \dfrac{x - x_0}{r^2}\right)\right]$

Obtained fitting measured data with a gaussian distribution

- Mechanical equation

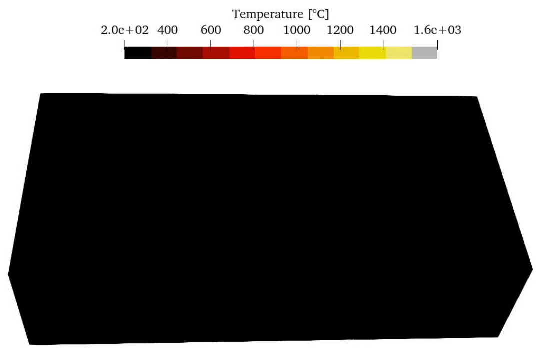
$$\nabla\cdot\boldsymbol{\sigma} + \mathbf{b} = \mathbf{0}$$

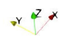
$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{th} + \boldsymbol{\varepsilon}^{el} + \boldsymbol{\varepsilon}^{pl}$$

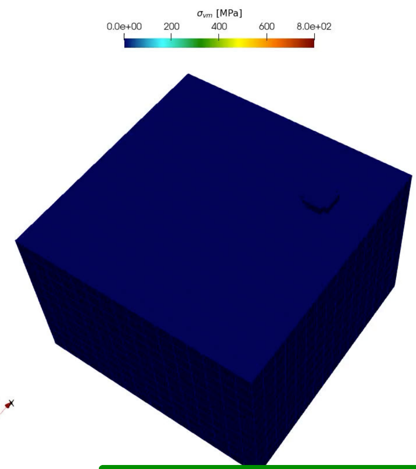
$$\boldsymbol{\varepsilon}^{th} = \alpha^{th}\Delta T\mathbf{I}$$

$$\boldsymbol{\varepsilon}^{pl} = \dot{\gamma}\frac{\partial\Phi}{\partial\boldsymbol{\sigma}}$$

$$\Phi = \sigma_{vm} - \sigma_y(\gamma, T) \leq 0$$







Thermal problem

Mechanical problem