Modelling, Validation, and Design for Additive Manufacturing

Applications of numerical methods to 3D printing processes

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Outline

- Introduction
- Adaptive Isogeometric Analysis for Heat Transfer Problems
- Physical Modelling and Experimental Validations
- Functionally Graded Material Design for Additive Manufacturing
- Conclusions

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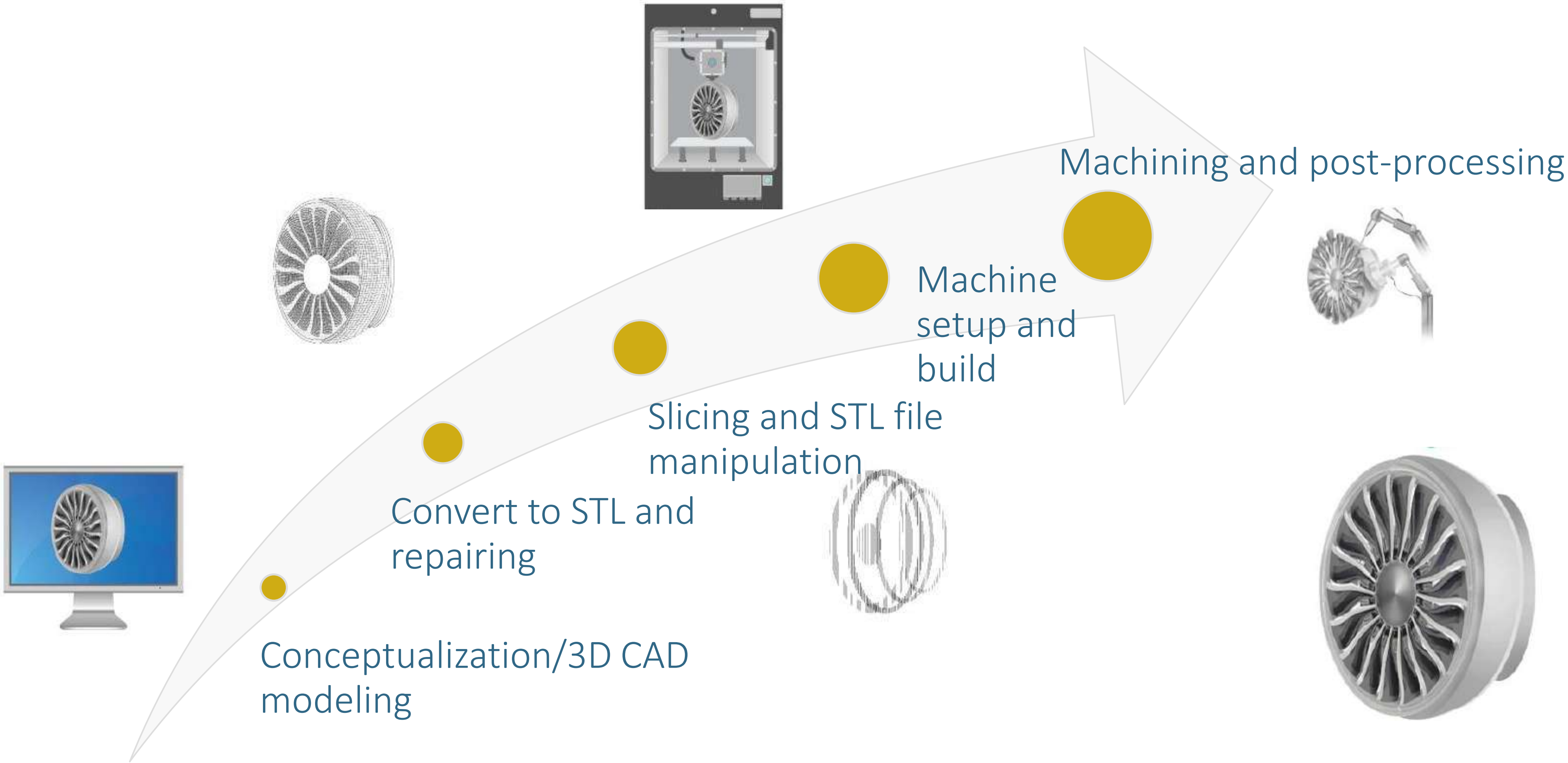
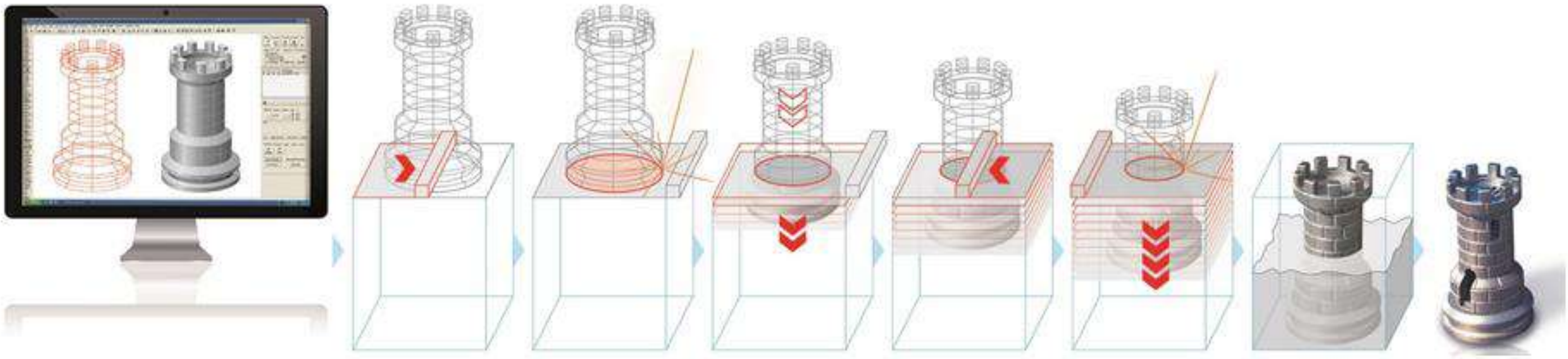
Additive Manufacturing generic production process



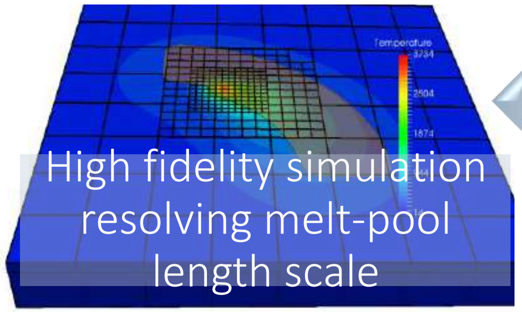
Laser powder bed fusion process



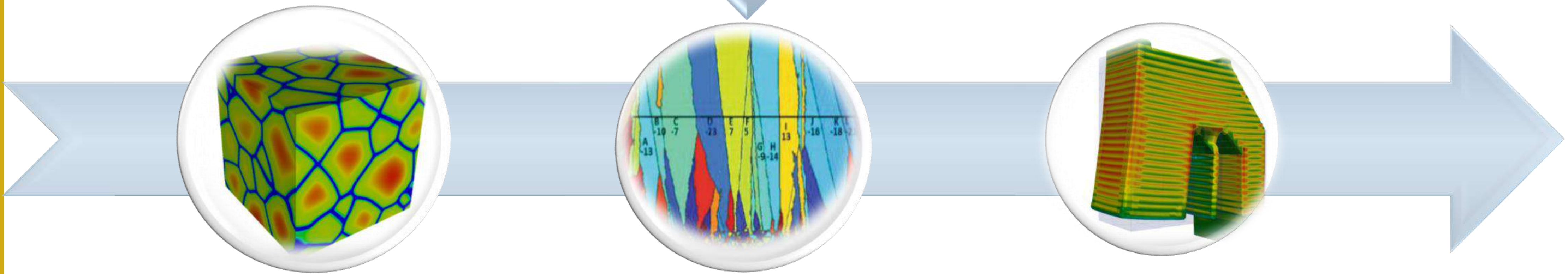
3D virtual model | Powder coating | Laser exposure | Platform lowering | Powder coating | Repeat layer cycles | Powder removal | Final artifact

Image source: EOS Gmbh

LPBF Numerical simulations: Multi-scale



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



Micro($\sim 10^{-6}$m) Meso($\sim 10^{-4}$m) Macro($\sim 10^{-2}$m)

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Why adaptive isogeometric analysis?

- The multi-scale nature of the problem calls for **adaptive numerical scheme** where refinement and coarsening can be efficiently performed.

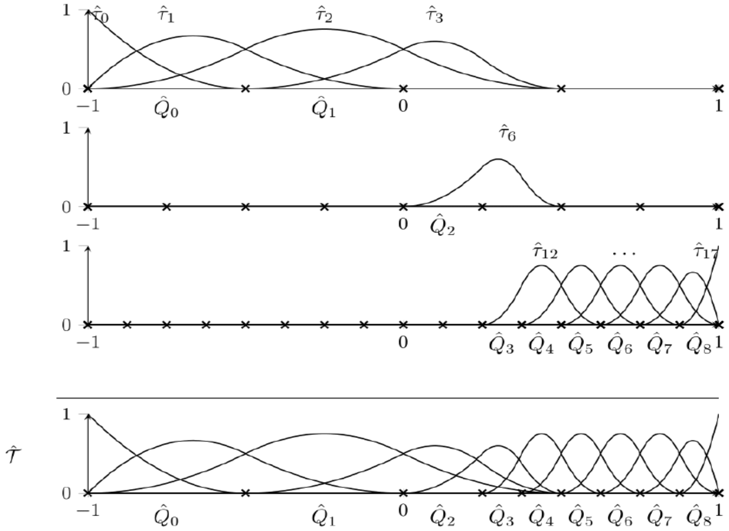
- The high temperature gradients in the vicinity of the melt-pool regions can be well-approximated by means of high-order basis functions.

- **Goal**: Develop a multi-level, high-order and adaptive numerical method suitable to simulate heat transfer problems with a localized moving heat source.

Adaptive IGA for heat transfer problems

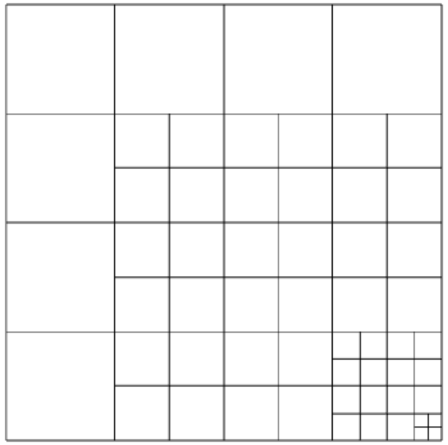
Truncated Hierarchical B-splines (THB-splines)

THB-splines can be employed as a basis for adaptive isogeometric analysis, reducing interactions between different levels in the spline hierarchy.



Admissible meshes

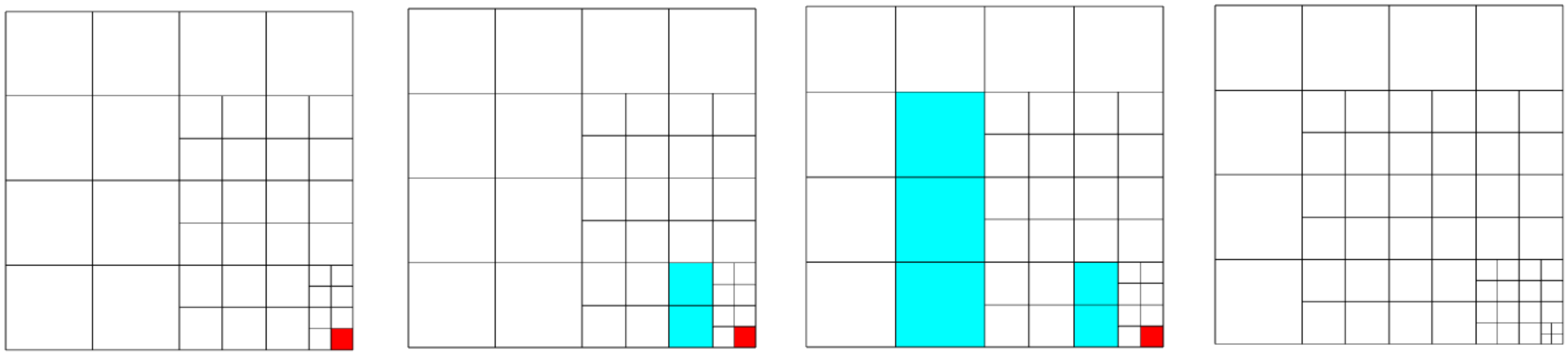
A hierarchical mesh is admissible of class *m* if, for each element *Q*, the functions that do not vanish in *Q* belong to at most *m* successive levels



Giannelli, C., Jüttler, B., Speeler, H., THB-spline: the truncated basis for hierarchical splines, Comp. Aided Geom. Design. (2012)

Admissible adaptive mesh

- **Admissible refinement algorithm: Recursively** refine the elements in the refinement neighborhood of the marked elements.

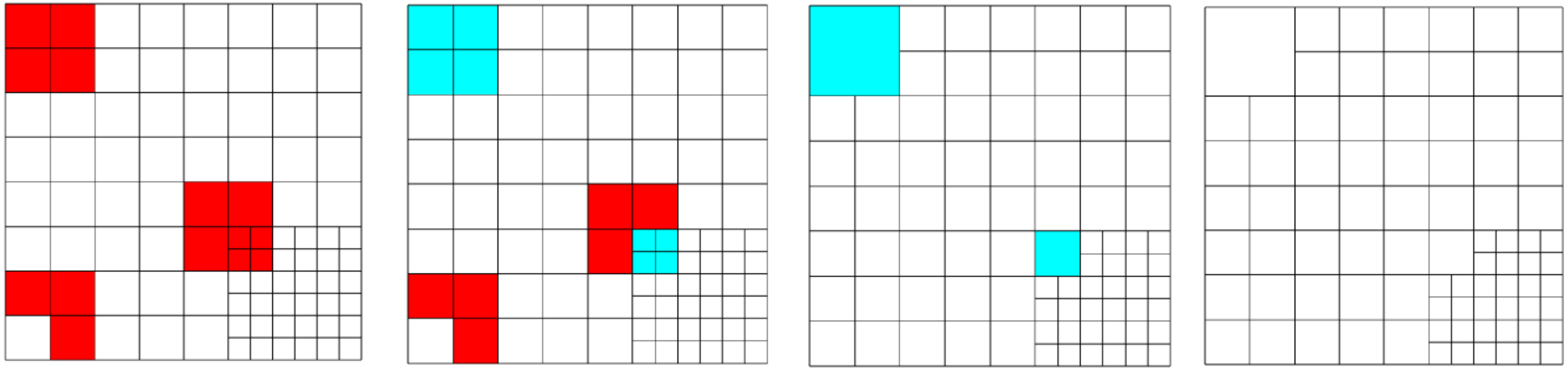


The final mesh automatically fulfills admissibility requirements!

A. Buffa, C. Giannelli, Adaptive isogeometric methods with hierarchical splines: Error estimator and convergence, Mathematical Models and Methods in Applied Sciences 26 (2016) 1–25

Admissible adaptive mesh

- **Admissible mesh coarsening:** A **recursive algorithm** to efficiently perform coarsening and at the same time automatically fulfills the admissibility requirements.



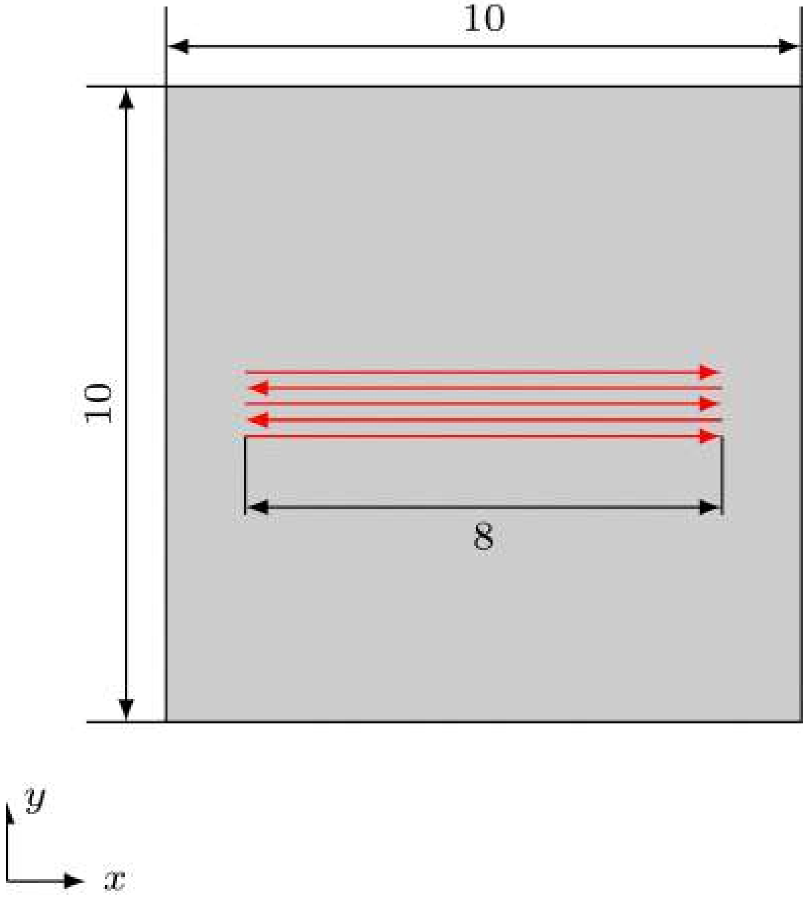
The final mesh automatically fulfills admissibility requirements!

Carraturo, M., Giannelli, C., Reali, A., Vazquez, R., Suitably graded THB-spline refinement and coarsening: Towards an adaptive isogeometric analysis of additive manufacturing processes, CMAME (2019)

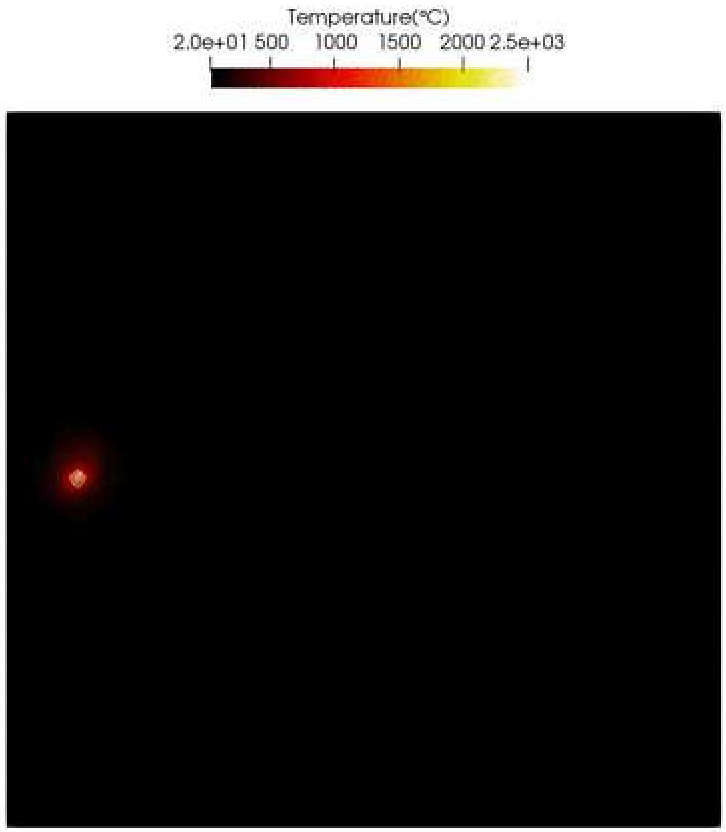
Numerical example 2D

- Process parameters:
  - Laser power = 190 [W]
  - Laser speed = 800 [mm/s]
  - Laser radius = 0.05[mm]
  - Hatch distance = 0.05[mm]
  - Initial temperature = 25°

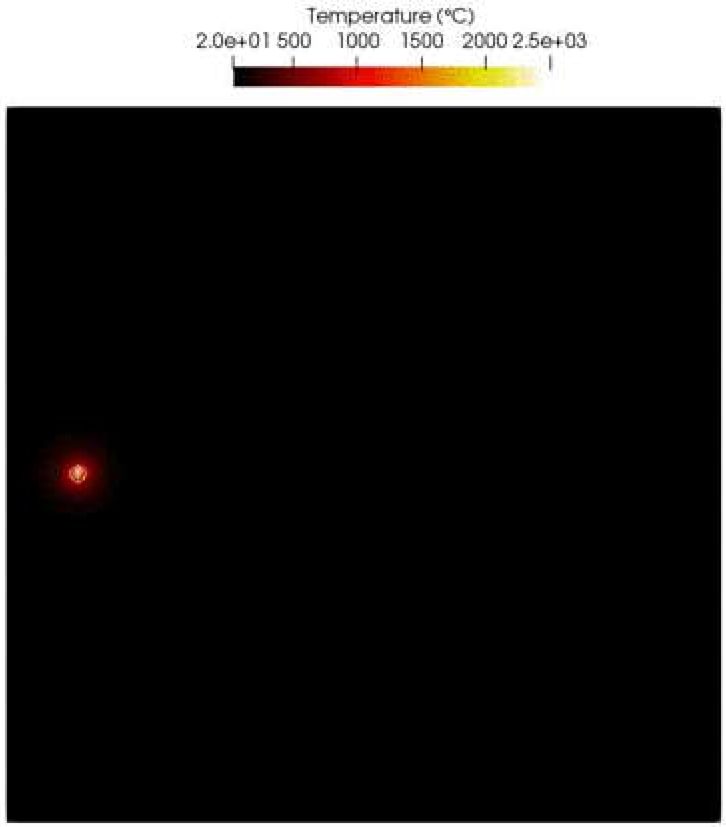
- Material parameters:
  - Absorptivity = 0.33
  - Conductivity = 29 [mW/m/K]
  - Heat capacity = 650 [J/kg/K]
  - Density = 8440[kg/m^3]



Numerical example 2D

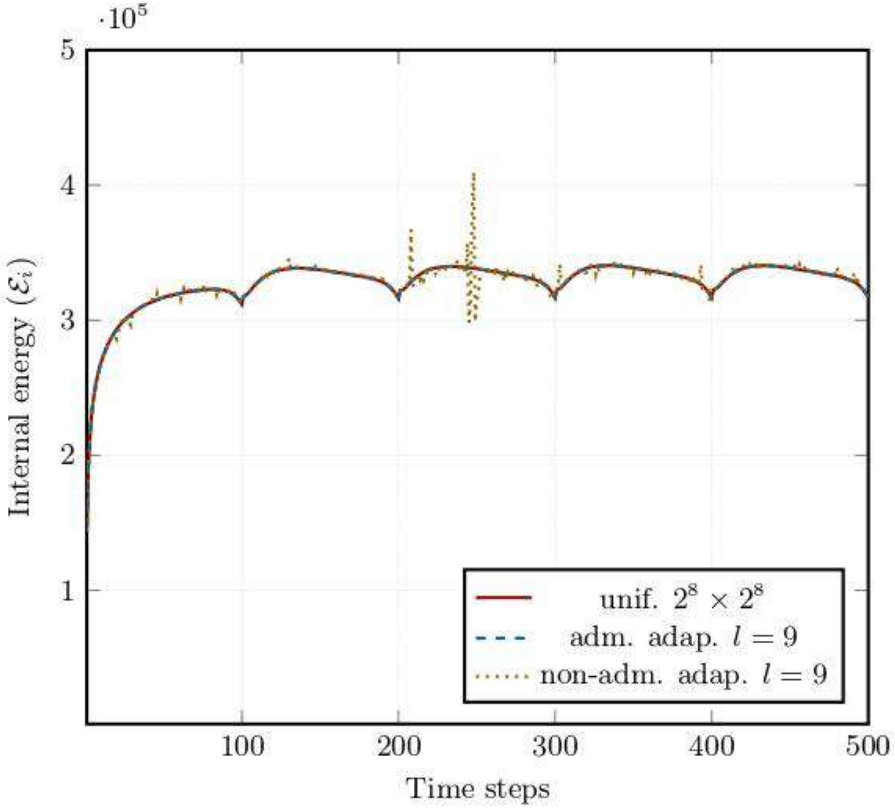


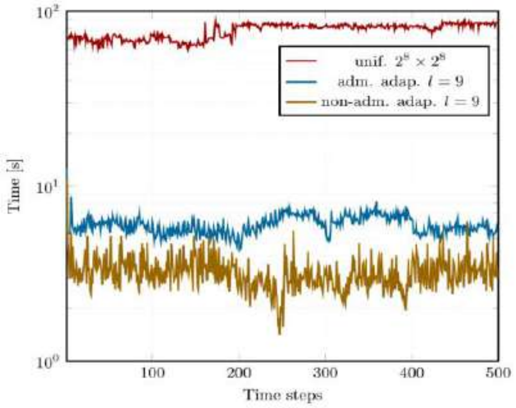
Non-admissible grid

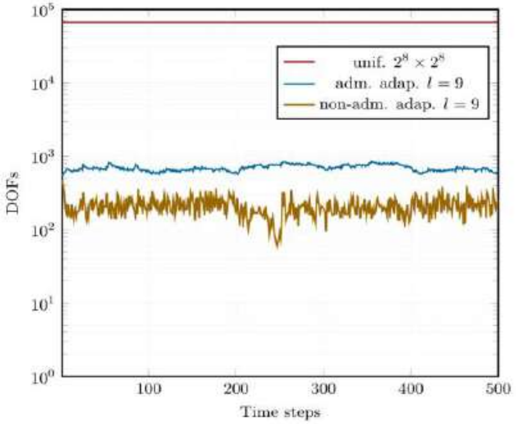


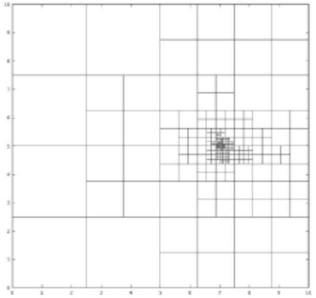
Admissible grid

Numerical example 2D

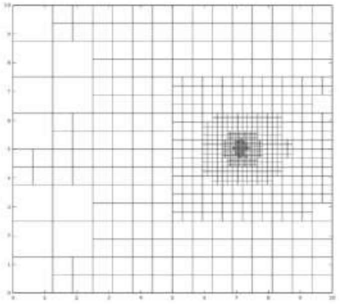








Non-admissible



Admissible

Carraturo, M., Giannelli, C., Reali, A., Vazquez, R., Suitably graded THB-spline refinement and coarsening: Towards an adaptive isogeometric analysis of additive manufacturing processes, CMAME (2019)

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Physical modelling

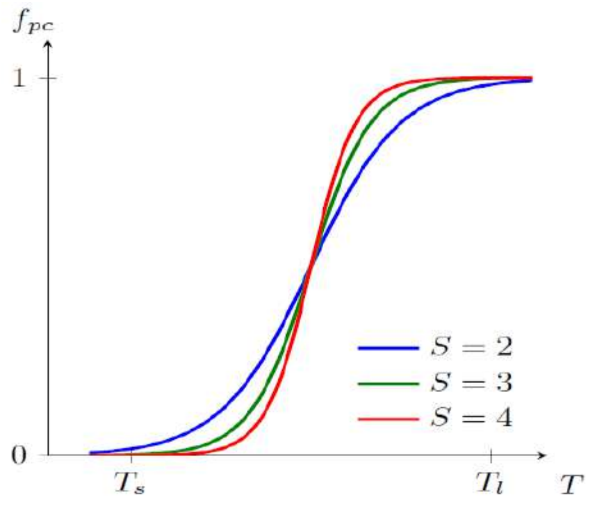
- **Temperature-based phase-change model:**
  - Heat equation is expressed in terms of enthalpy (H) and temperature (T):

$$\frac{\partial H}{\partial t} - \nabla(k\nabla T) = Q \qquad \text{in} \quad \Omega$$

$$-k\nabla T = q \qquad \text{on} \quad \Gamma_N$$

$$H(t) = \int_{T_{ref}}^{T} \rho c(T) dT + \rho L f_{pc}(T) = H^c + H^l$$

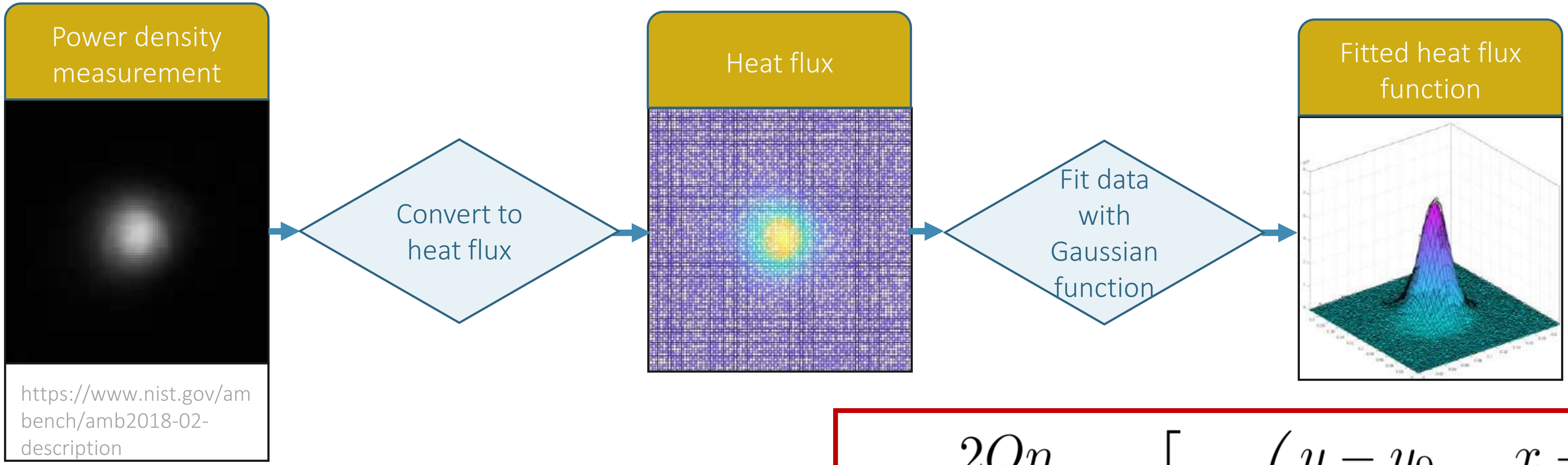
$$f_{pc}(T) = \frac{1}{2}\left[\tanh\left(S\frac{2}{T_l - T_s}\left(T - \frac{T_s - T_l}{2}\right)\right) + 1\right]$$



Celentano, D., Oñate, E. and Oller, S. (1994), A temperature-based formulation for finite element analysis of generalized phase-change problems. Int. J. Numer. Meth. Engng.

Physical modelling

- **Energy input from power density measurements:**



$$q = \frac{2Q\eta}{\pi r^2} \exp\left[-2\left(\frac{y-y_0}{r^2} + \frac{x-x_0}{r^2}\right)\right]$$

Physical modelling

- Anisotropic conductivity: allows to partially consider melt-pool dynamics in the model.

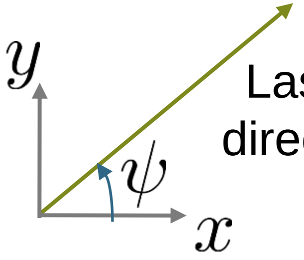
$$\frac{\partial H}{\partial t} - \operatorname{div}(\mathbf{K}^A \nabla T) = Q$$

$$\mathbf{K}^A = \mathbf{R}\mathbf{K}^O\mathbf{R}^T$$

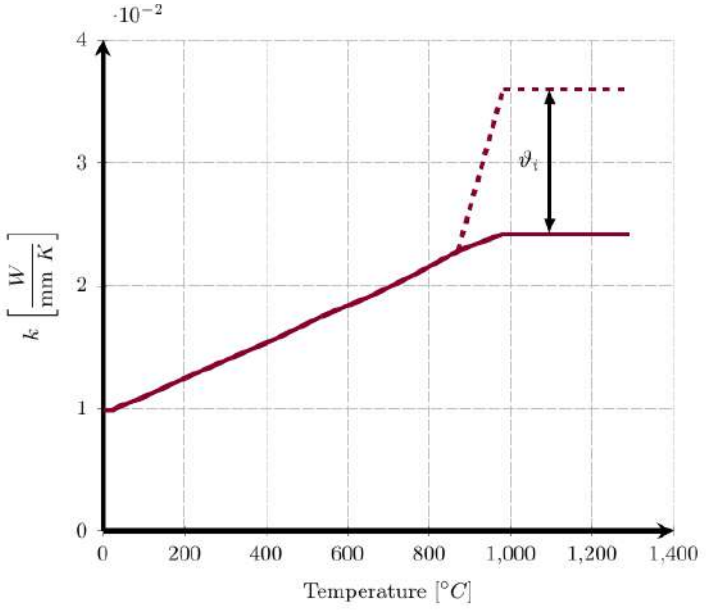
$$k(\theta)\begin{bmatrix} \vartheta_x & 0 & 0 \\ 0 & \vartheta_y & 0 \\ 0 & 0 & \vartheta_z \end{bmatrix}$$

Rotation matrix

$$\begin{bmatrix} cos(\psi) & -sin(\psi) & 0 \\ sin(\psi) & cos(\psi) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$



Laser direction

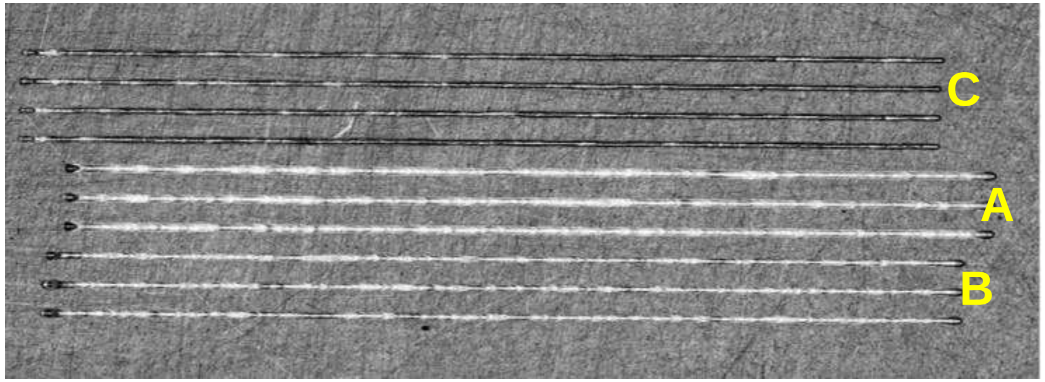


Kollmannsberger, S., Carraturo, M., Auricchio, F. and Reali, A. (2019), Accurate Prediction of Melt Pool Shapes in Laser Powder Bed Fusion by the Non-Linear Temperature Equation Including Phase Changes. IMMI.

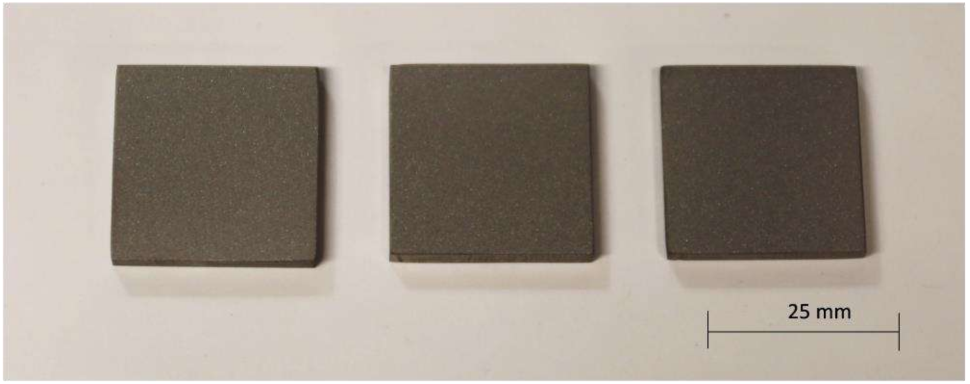
Experimental validation (AMBench2018)

- Adjacent, independent laser scans using 3 different combinations (case A, B, and C) of laser power and speed

- Material:INCONEL 625 (a Nickel-based superalloy widely used in AM applications)
- No powder is involved



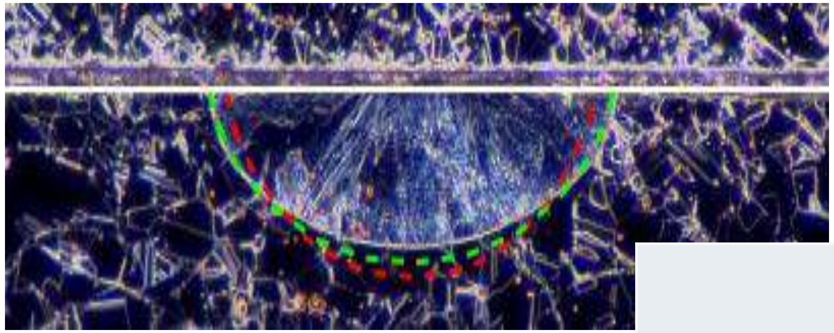
Source: https://www.nist.gov/ambench/amb2018-02-description

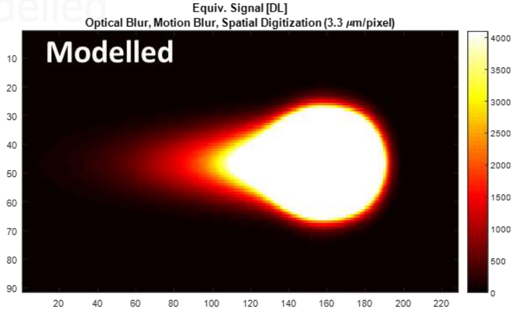


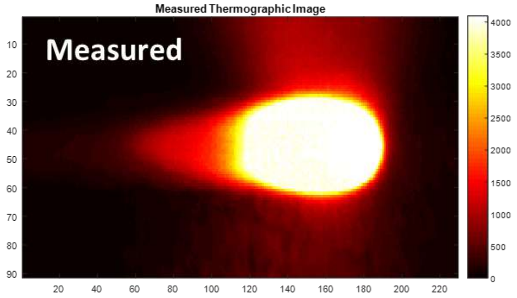
Source: https://www.nist.gov/ambench/amb2018-02-description

Experimental validation (AMBench2018)

- *Ex-situ* measurements of the melt-pool cross section
- *In-situ* measurements of the melt-pool length.







Case	Numeric length [μm]	Measured length [μm]	Length Δ[%]
A	671.8	659	1.94
B	783	782	0.13
C	732.2	754	2.89

Kollmannsberger, S., Carraturo, M., Auricchio, F. and Reali, A. (2019), Accurate Prediction of Melt Pool Shapes in Laser Powder Bed Fusion by the Non-Linear Temperature Equation Including Phase Changes. IMMI.

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Phase-field topology optimization

Objective:

- Minimize the compliance (i.e., maximize the stiffness) of the structure for linear elastic problems
- Obtain a functionally graded lattice design with varying density

Phase-field Method:

- No filtering methods required (cfr. SIMP approaches)
- No function re-initialization required (cfr. Level-set method)

Carraturo, M., Rocca, E., Bonetti, E., Hömberg, D., Reali, A. and Auricchio, F. (2019). Graded-material design based on phase-field and topology optimization. *Computational Mechanics*, 1-12.

Phase-field topology optimization

Objective

Minimize the compliance of the structure defined as:

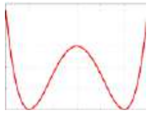
$$\int_{\Gamma_N} \mathbf{g} \cdot \mathbf{u}(\varphi, \chi) \mathrm{d}\Gamma$$

- Phase-field variables

$0 \leq \varphi \leq 1 \quad a.e.\ in\ \Omega$ — Defines the material regions

$0 \leq \chi \leq \varphi \quad a.e.\ in\ \Omega$ — Defines the density of the material

- Extended objective functional



Double-well potential

$$\mathcal{J}^{\varepsilon}(\mathbf{u}, \varphi, \chi) = \underbrace{\kappa_{\varphi} \int_{\Omega} \left(\frac{\mathcal{W}(\varphi)}{\varepsilon_{\varphi}} + \varepsilon_{\varphi} \frac{|\nabla \varphi|^2}{2} \right) \mathrm{d}x}_{\text{Free-energy functional}} + \underbrace{\kappa_{\chi} \int_{\Omega} \varepsilon_{\chi} \frac{|\nabla \chi|^2}{2} \mathrm{d}x}_{\text{Density gradient term}} + \int_{\Gamma_N} \mathbf{g} \cdot \mathbf{u} \mathrm{d}x$$

Phase-field topology optimization

Objective

Minimize the extended objective functional:

$$\mathcal{J}^{\varepsilon}(\mathbf{u}, \varphi, \chi)$$

under the constraints:

- Volume constraint is introduced using the Lagrange multiplier $\lambda_\varphi \in \mathbb{R}$

$$\Longrightarrow \lambda_\varphi \left(\int_\Omega \varphi \mathrm{d}x - \int_\Omega m_\varphi \mathrm{d}x \right) =: \lambda_\varphi M_\varphi = 0$$

- Mass constraint is introduced using the Lagrange multiplier $\lambda_\chi \in \mathbb{R}$ and controlled by a mass fraction parameter $m_\chi < m_\varphi$ defining the target mass fraction in the optimized structure w.r.t. the mass of the initial volume filled with purely bulk material.

Phase-field topology optimization

Objective

Minimize the extended objective functional:

$$\mathcal{J}^{\varepsilon}(\mathbf{u}, \varphi, \chi)$$

under the constraints:

- The mechanical equilibrium equations are satisfied:

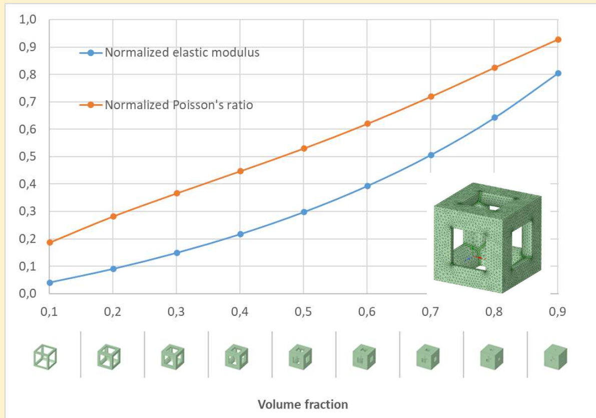
$$-\nabla \cdot \boldsymbol{\sigma} = \mathbf{0} \quad \text{in } \Omega$$

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{g} \quad \text{on } \Gamma_g$$

$$\mathbf{u} = \mathbf{u}_0 \quad \text{on } \Gamma_d$$

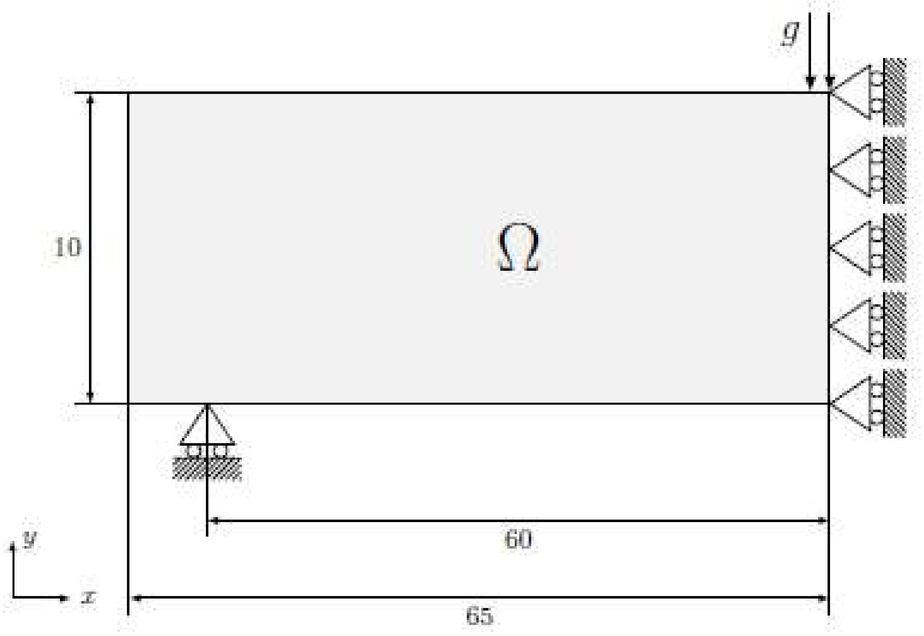
$$\boldsymbol{\sigma} = \mathbb{C}(\varphi, \chi) : \boldsymbol{\varepsilon}(\mathbf{u}) \quad \text{in } \Omega$$

Obtained from **asymptotic homogenization** on a lattice RVE with periodic BCs



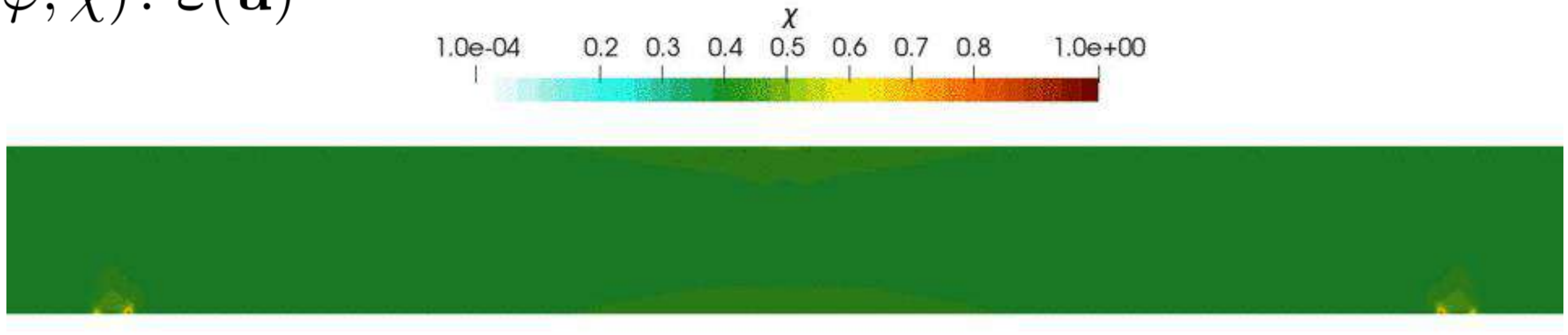
MBB 2D example

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

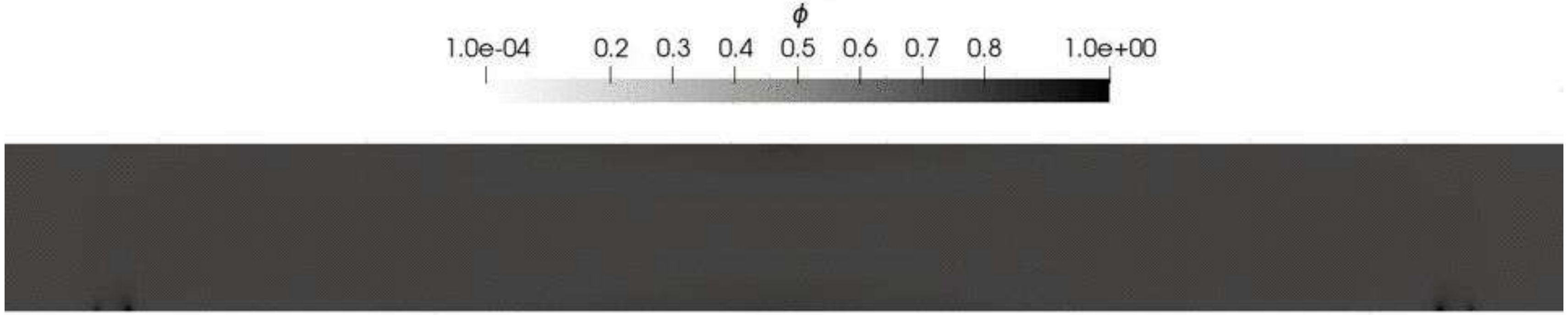


MBB 2D example

$$\boldsymbol{\sigma} = \mathbf{C}(\varphi, \chi) : \boldsymbol{\varepsilon}(\mathbf{u})$$

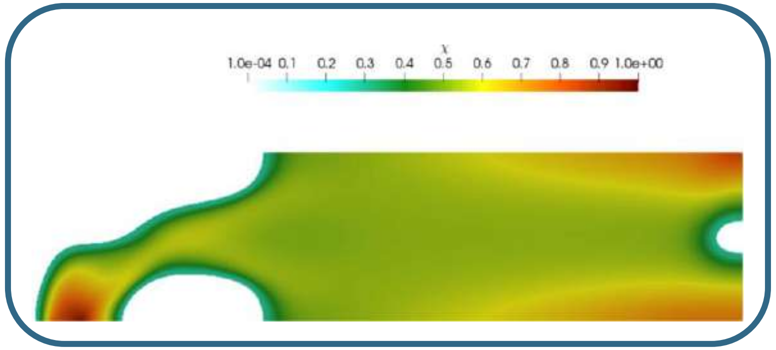


χ

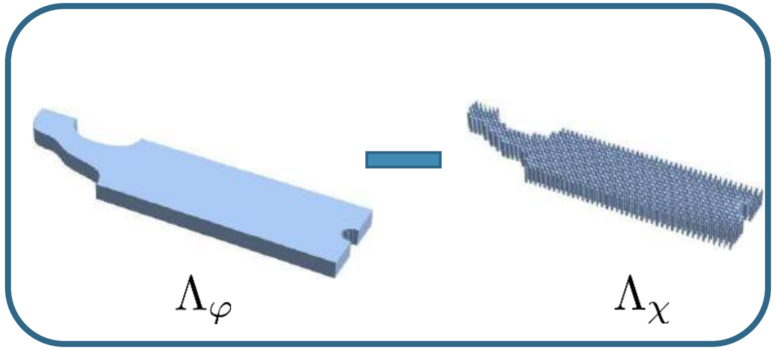


φ

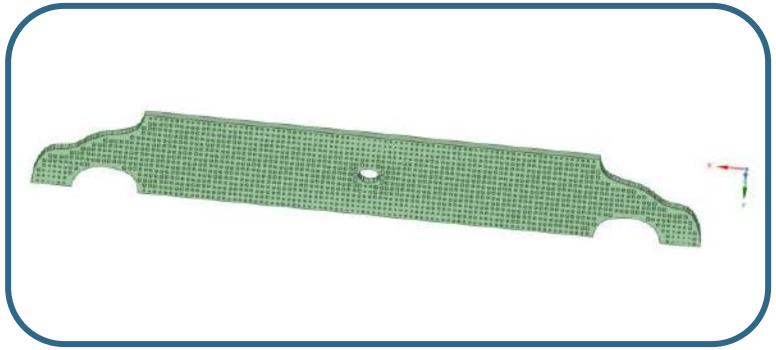
From numerical analysis to 3D printing



Discrete map of field variables



Generate 3D virtual model

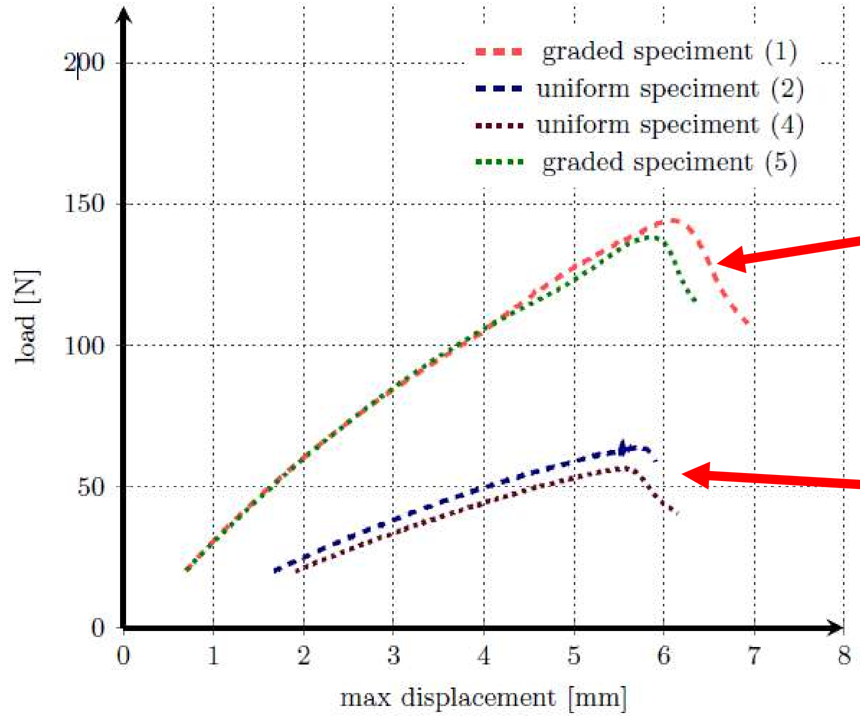


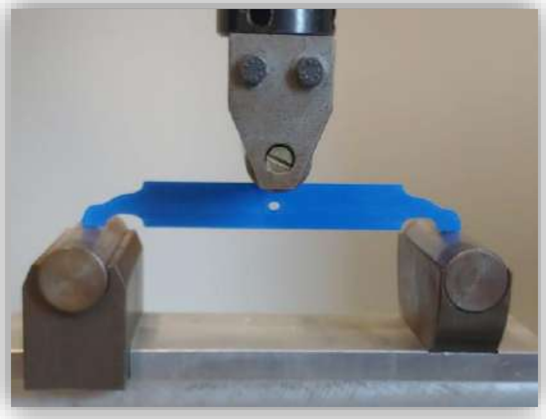
3D printing

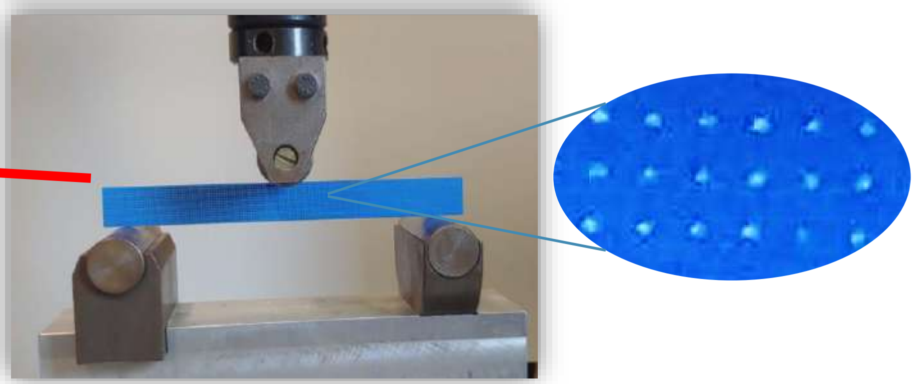
Alaimo G., Carraturo M., Rocca E., Reali A., Auricchio F., Functionally graded material design for plane stress structures using phase field method, II International Conference on Simulation for Additive Manufacturing - Sim-AM 2019

Experimental measurements

- **Objective:** Evaluate the improvement in terms of max. displacements obtained in the optimized specimen w.r.t. a uniform specimen of the same weight.







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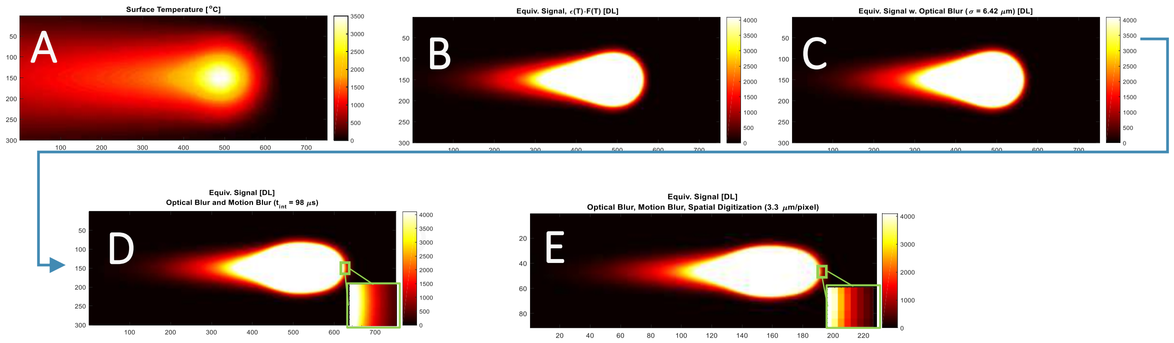
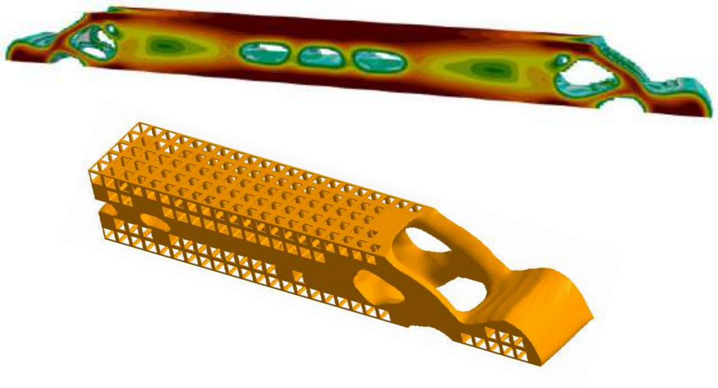
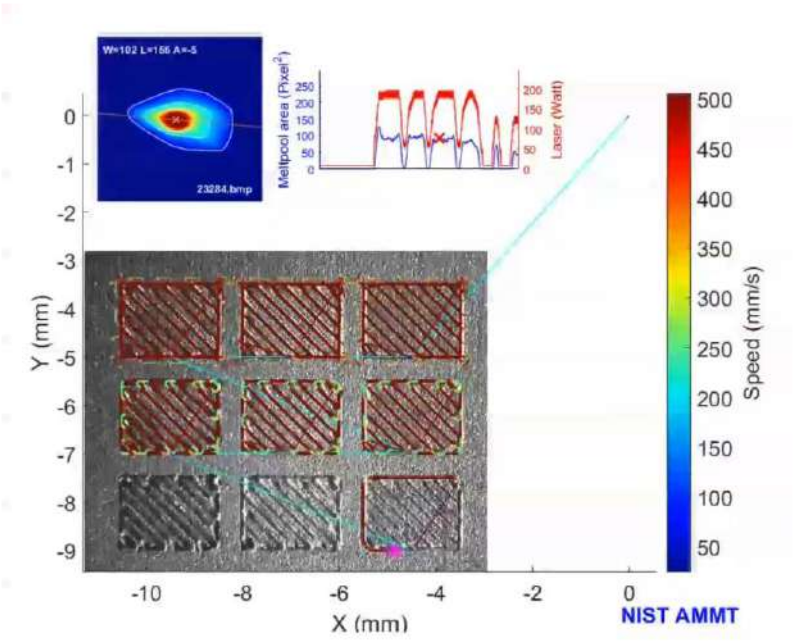
Conclusions

- **Adaptive IGA** is an attractive methodology to deal with heat transfer problem with moving heat source.
- A thermal model based on a **data fitting** of power density measurements and **anisotropic conductivity** is validated w.r.t. thermal camera measurements.
- A **phase-field topology optimization** approach can be used to design **functionally graded lattice structures** with higher stiffness compared to uniform lattice structures of the same weight.

Further outlook







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Dr.-Ing. habil. Stefan Kollmannsberger
Technical University of Munich

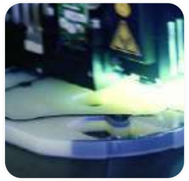
The 7 categories of AM (ASTM/ISO)

Fused deposition modeling (FDM)

- Materials: ABS, ceramics
- Applications: tissue/scaffolds

Binder jetting

- Materials: polymers, ceramics, and metals
- Applications: arts, prototyping



Material jetting

- Materials: polymers
- Applications: electrical and chemical industry

Vat Photopolymerization

- Materials: polymers
- Applications: coating and printing industry

Sheet lamination

- Materials: metals
- Applications: prototyping

Direct energy deposition (DED)

- Materials: metals
- Applications: repairing/joining metal components

Laser powder bed fusion (LPBF)

- Materials: metals
- Applications: aerospace and biomedical industry

Laser powder bed fusion features

Benefits:

- Complex geometries
- Better material properties
- Higher accuracy and surface finish

Drawbacks:

- High residual stresses induced by the process
- Needs of supports
- High costs

LPBF Numerical simulations: Challenges

- Complex geometrical features

LPBF Numerical simulations: Challenges

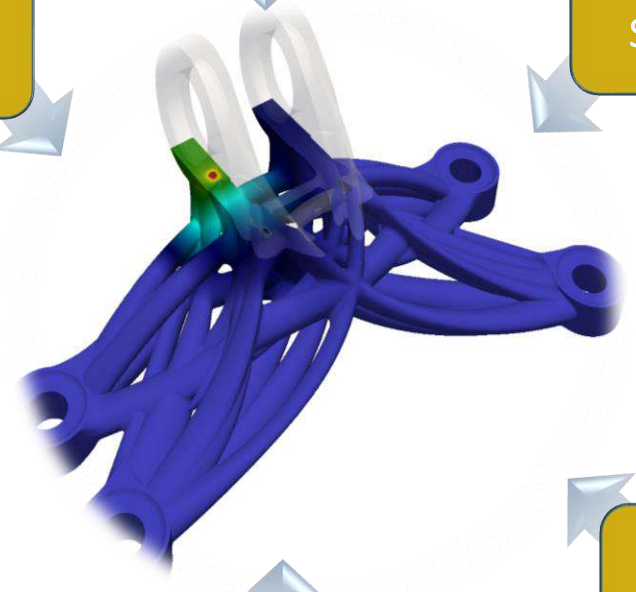
- Complex physics

Radiation

Multi-material

Melting & Solidification

Plasticity



Particle scattering

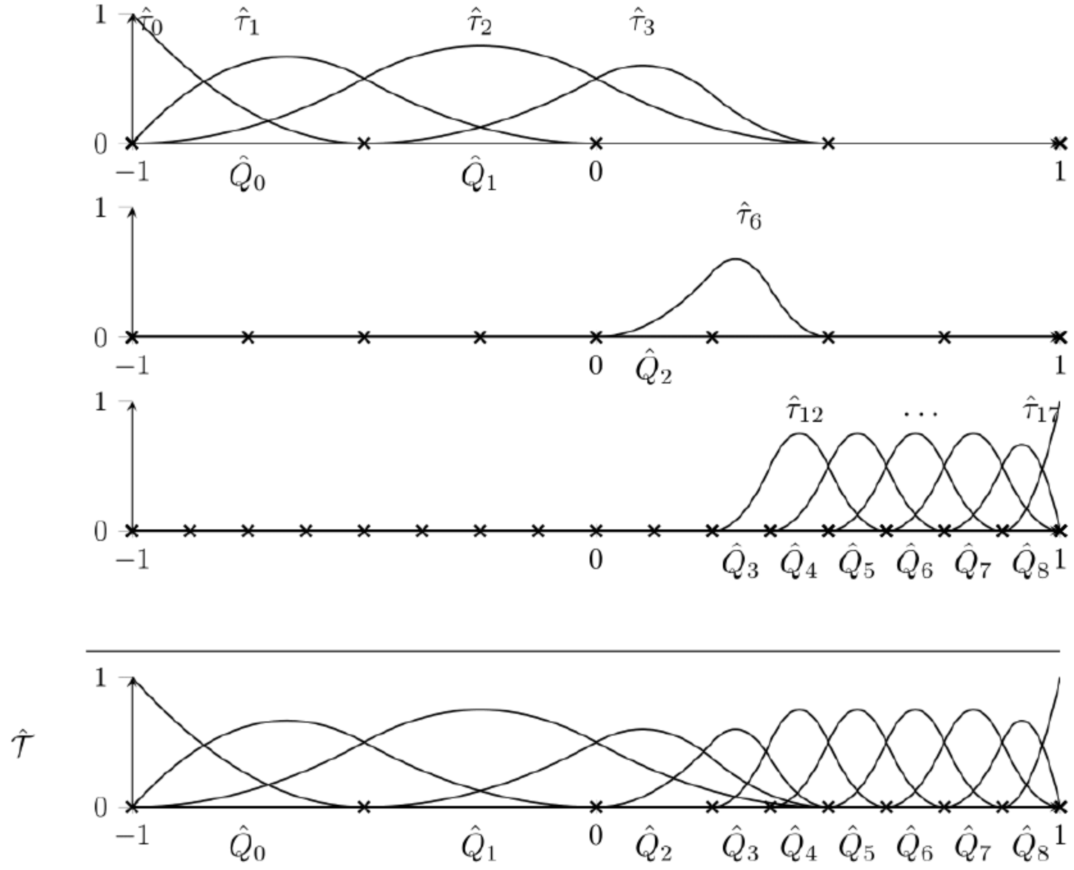
Phase-change

Marangoni effects

Convection

THB-splines features

- **Key features**:
  - Local Linear independence
  - Local and compact support
  - Two scale relation
  - Partition of unity
  - Non-negativity



Adaptive IGA

- From Buffa and Giannelli (2016) we take the definitions of multilevel *support extension* and *refinement neighborhood* of an active element *Q* of level *l*:

  - Definition support extension: the support of B-splines of level *k* which do not vanish on the element *Q*

$$S(\hat{Q},k) := \left\{ \hat{Q}' \in \hat{G}^k : \exists \hat{\beta} \in \hat{\mathcal{B}}^k, \mathrm{supp}\hat{\beta} \cap \hat{Q}' \neq \emptyset \wedge \mathrm{supp}\hat{\beta} \cap \hat{Q} \neq \emptyset \right\}.$$

  - Definition refinement neighborhood: set of elements of level *l − m + 1* with a child in the support extension of *Q*.

$$\mathcal{N}_r(\hat{Q},m) := \left\{ \hat{Q}' \in \hat{\mathcal{G}}^{\ell-m+1} : \exists \hat{Q}'' \in S(\hat{Q},\ell-m+2), \hat{Q}'' \subseteq \hat{Q}' \right\}.$$

Adaptive IGA

- Definition *coarsening neighborhood* of an element *Q* of level *l :* the set including all the active elements of level *l+m* which are in the support extension of the children of the element *Q*:

$$\mathcal{N}_c(\hat{\mathcal{Q}}, \hat{Q}, m) := \left\{ \hat{Q}' \in \hat{\mathcal{G}}^{\ell+m} : \exists\, \hat{Q}'' \in \hat{\mathcal{G}}^{\ell+1} \text{ and } \hat{Q}'' \subset \hat{Q}, \text{ with } \hat{Q}' \subset S(\hat{Q}'', \ell+1) \right\}.$$

- Property: When the coarsening neighborhood of an element to be re-activated turns out to be empty it ensures that all the re-activated functions are fully truncated on level *l+1*.

Adaptive IGA

Algorithm 5 `coarsen`

Input: $\mathcal{Q}$, $\mathcal{M}_c$, m
Output: $\mathcal{Q}$

for $Q \in \mathcal{M}_c$ **do**
  $\mathcal{R}_c \leftarrow \mathcal{R}_c \cup$ `get_parent`(Q)
end for
for $Q \in \mathcal{R}_c$ **do** ▷ This loop must be done from the finest to the coarsest level
  $Q_c \leftarrow$ `get_children` (Q)
  if $(Q_c \subset \mathcal{M}_c$ **and** $\mathcal{N}_c(\mathcal{Q}, Q, m) = \emptyset)$ **then**
    update $\mathcal{Q}$ by activating Q and removing its children Q_c
  end if
end for

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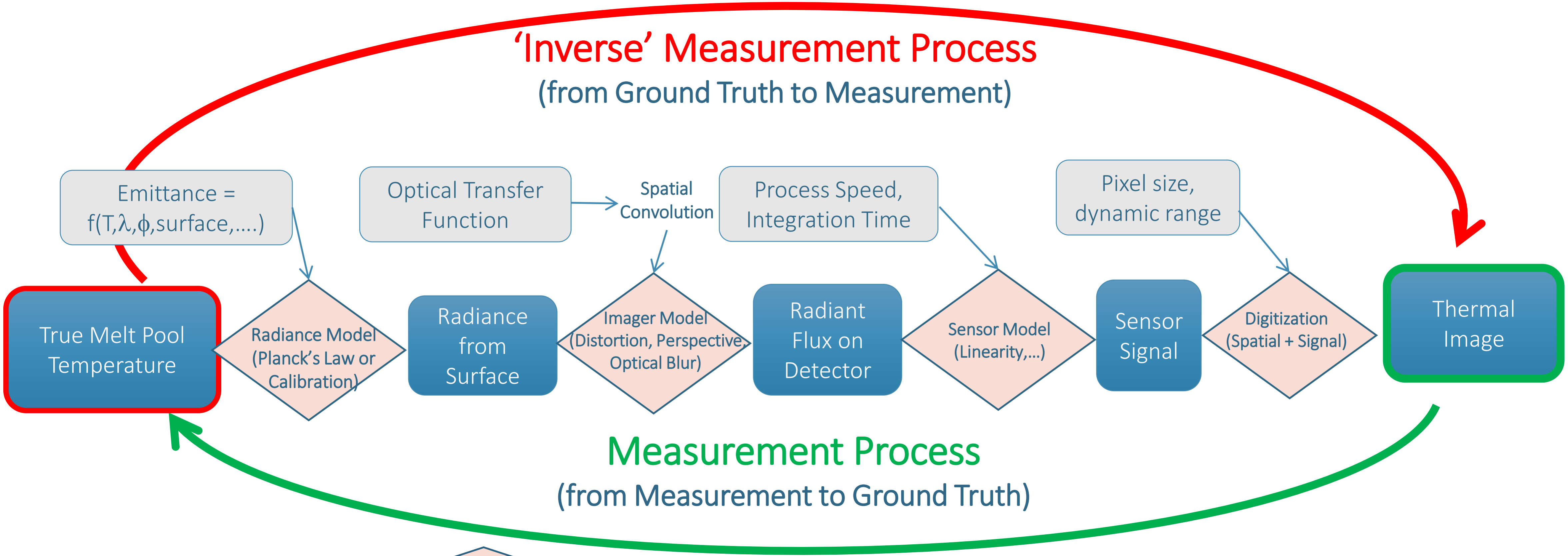
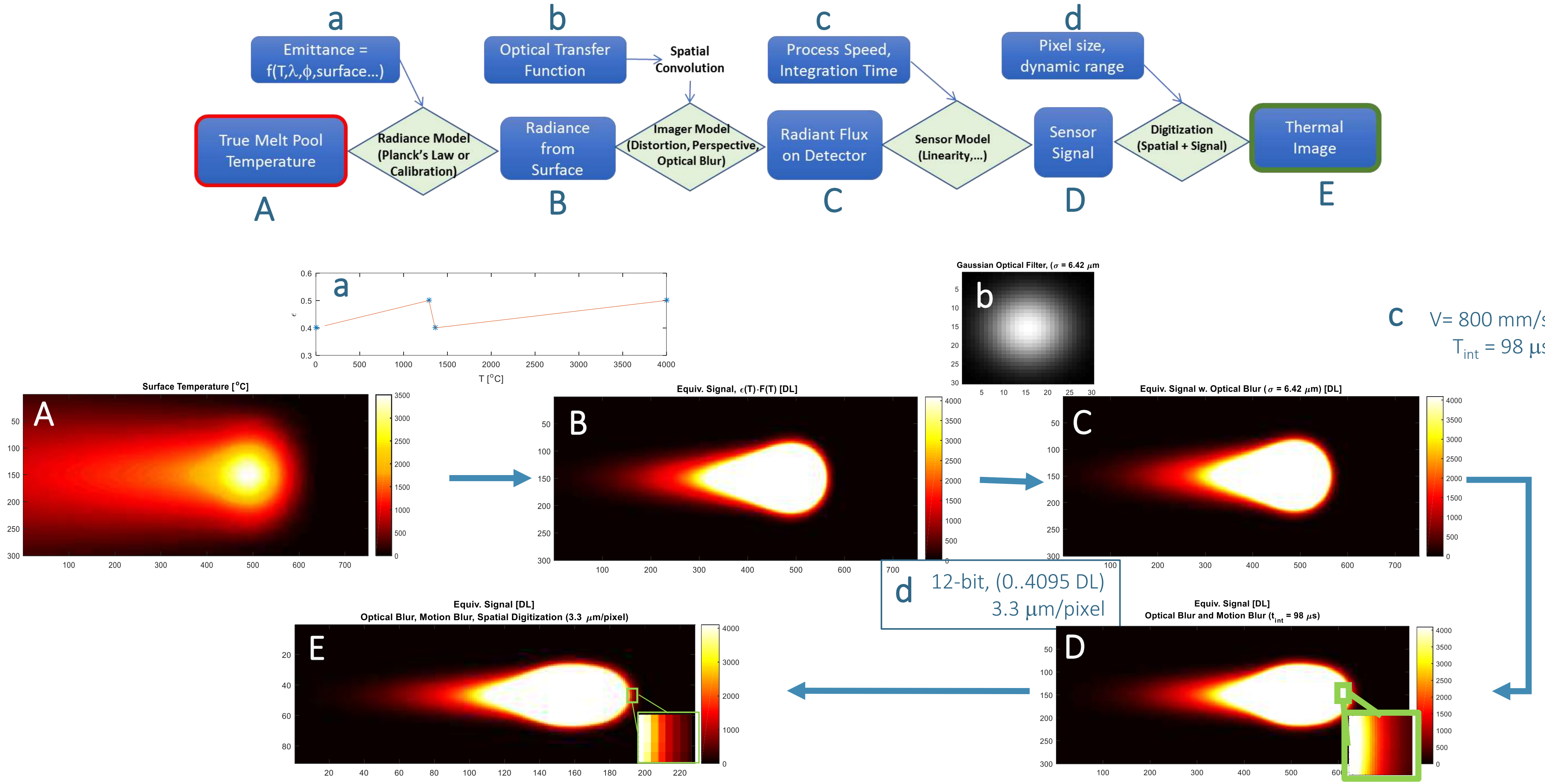
Thermografic measurement model



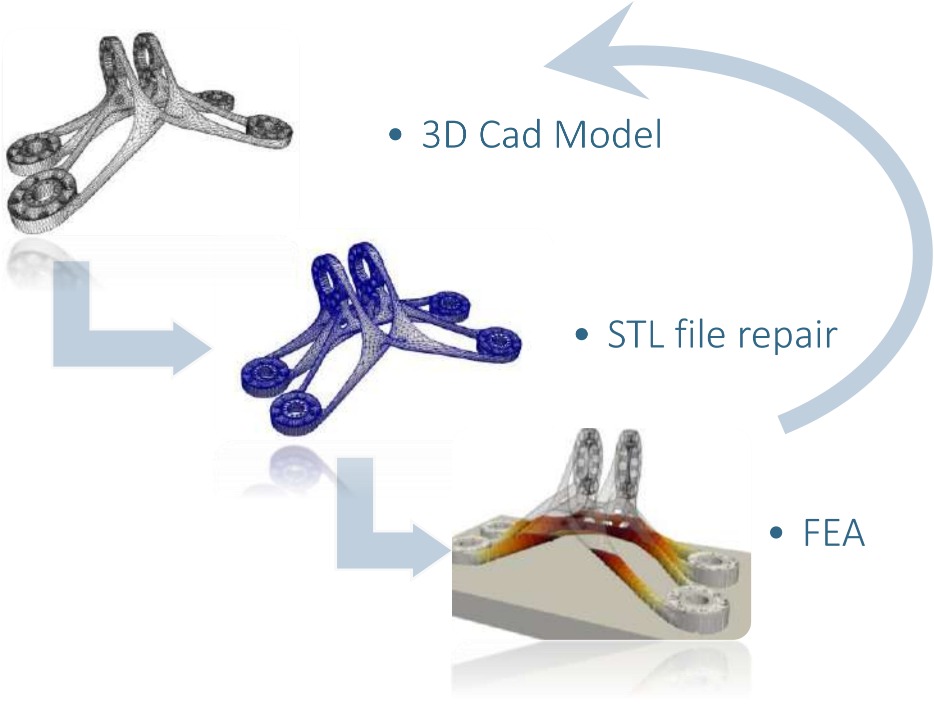
- Some functions are difficult or impossible to reverse
- Some inputs are difficult to measure

Thermografic measurement model



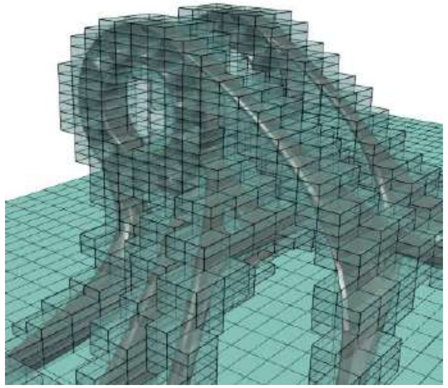
Part-scale Additive Manufacturing Thermal Process Simulations using the Finite Cell Method

Standard AM-design process



FCM AM-*design-through-analysis*

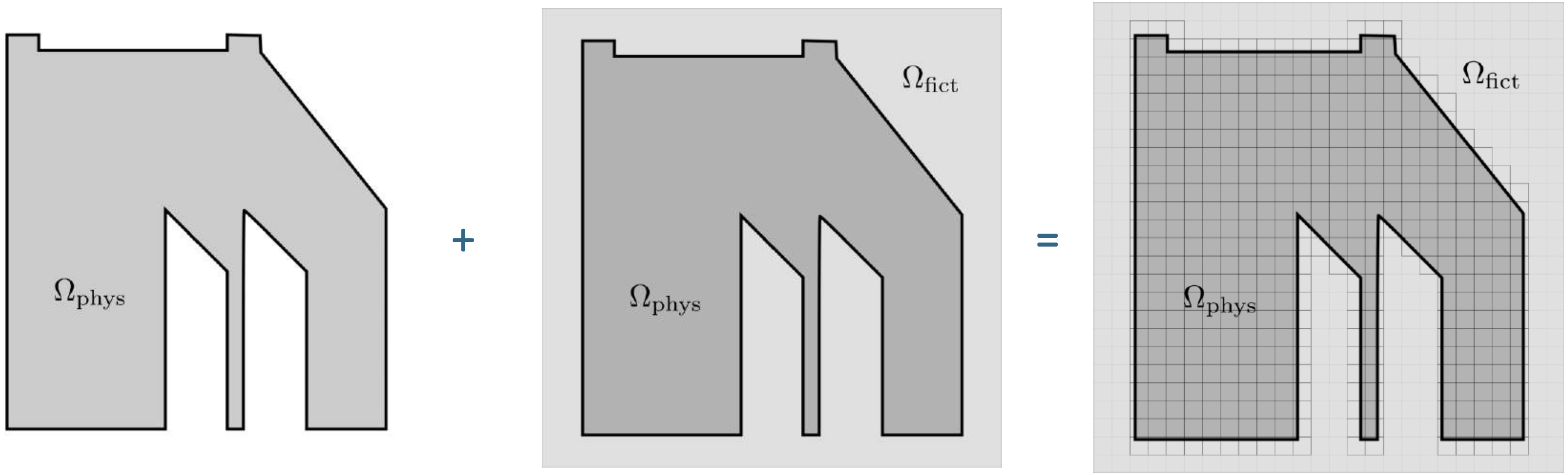
- The thermo-mechanical analysis is performed directly on the CAD model.



- The STL repair step is required only once the final design is ready to be printed.

FCM for growing domain

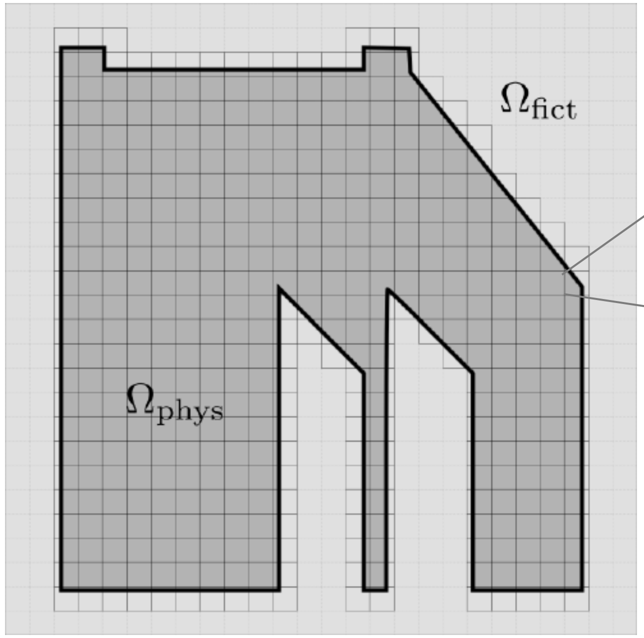
- Initial domain discretization

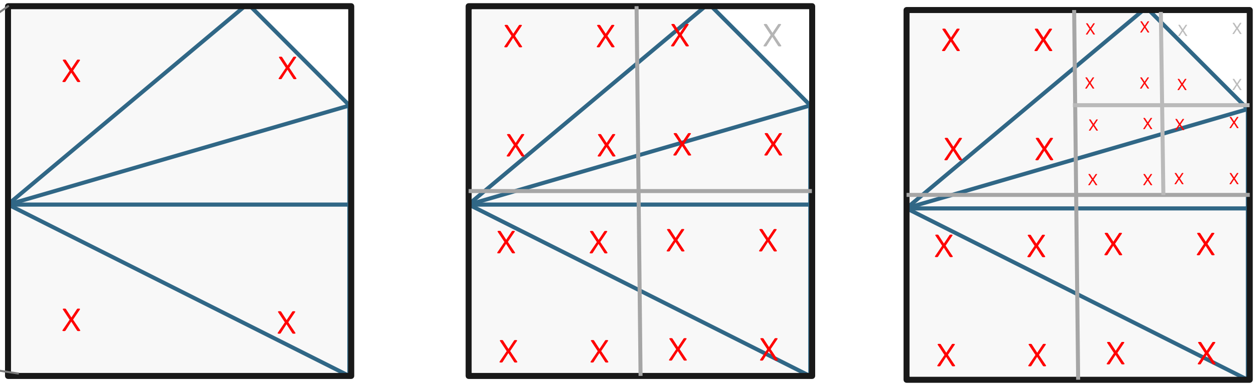


$$\alpha(\boldsymbol{x}) \cdot a(\boldsymbol{u}, \boldsymbol{v}) = l(\boldsymbol{v}) \qquad \alpha(\boldsymbol{x}) = \begin{cases} 1 & : \quad \forall \boldsymbol{x} \in \Omega_{phys} \\ 0 & : \quad \forall \boldsymbol{x} \in \Omega_{fict} \end{cases}$$

FCM for growing domain

- Numerical integration using Quad/Octree partitioning





Other integration schemes could be used:

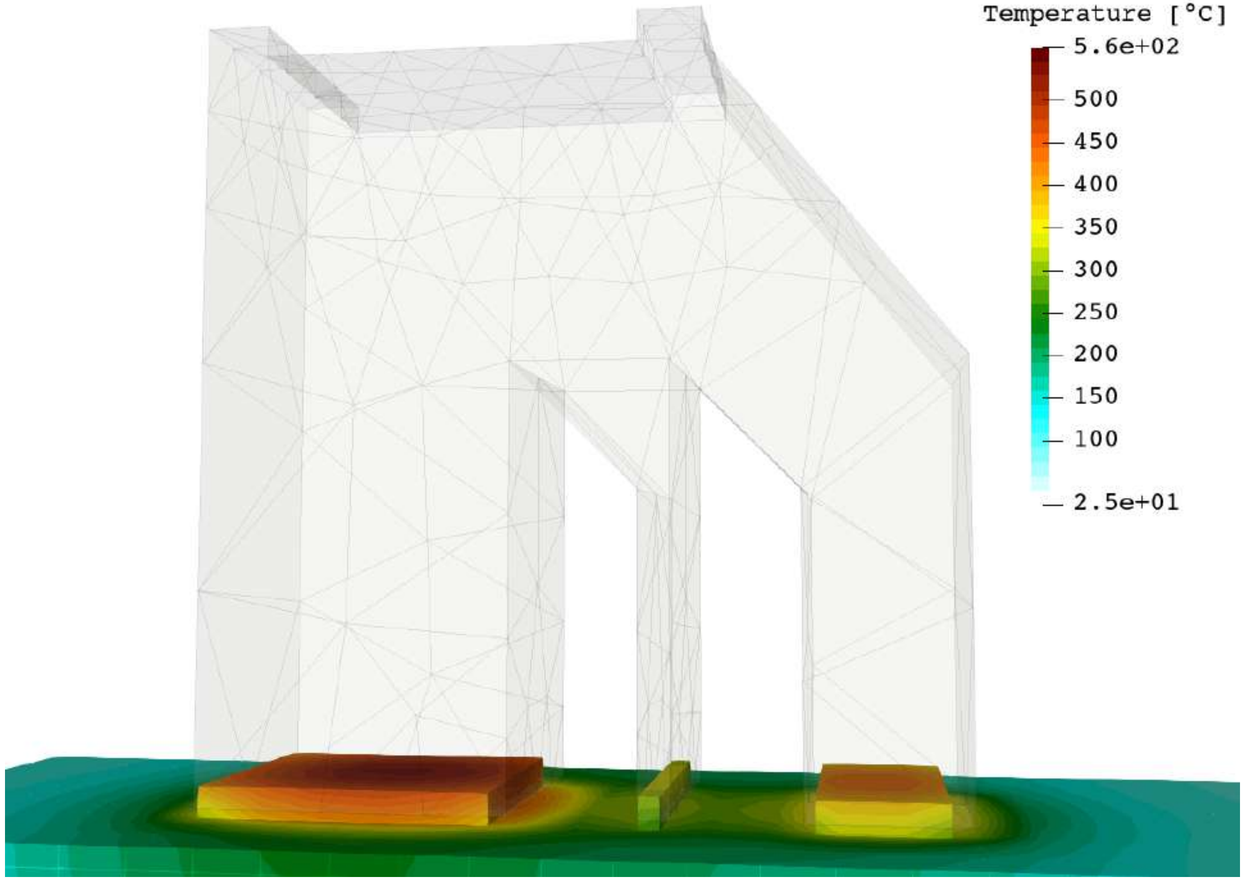
- Smart-Octree (Kudela et al. 2016)
- Moment fitting (Hubrich et al. 2016)
- Etc…

FCM for growing domain

- We distinguish between two different kind of layers:

    1. ***Cell layer***: the layer of the finite cells supporting the basis functions

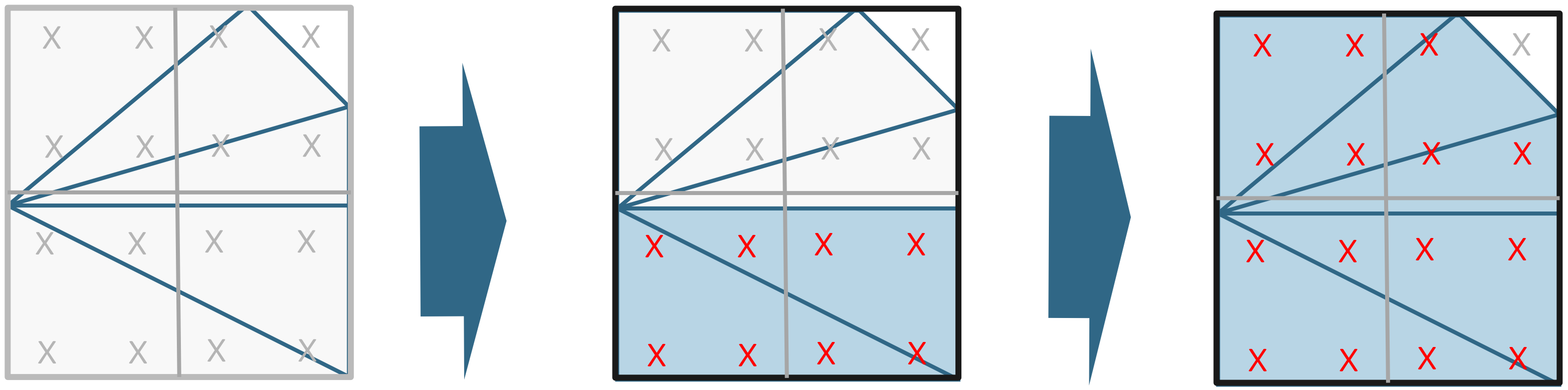
    2. ***Powder (or physical) layer***: it corresponds to the actual layer of powder spread by the machine



FCM for growing domain

- Growing domain

t_{n-1} $\quad$ t_n $\quad$ t_{n+1}

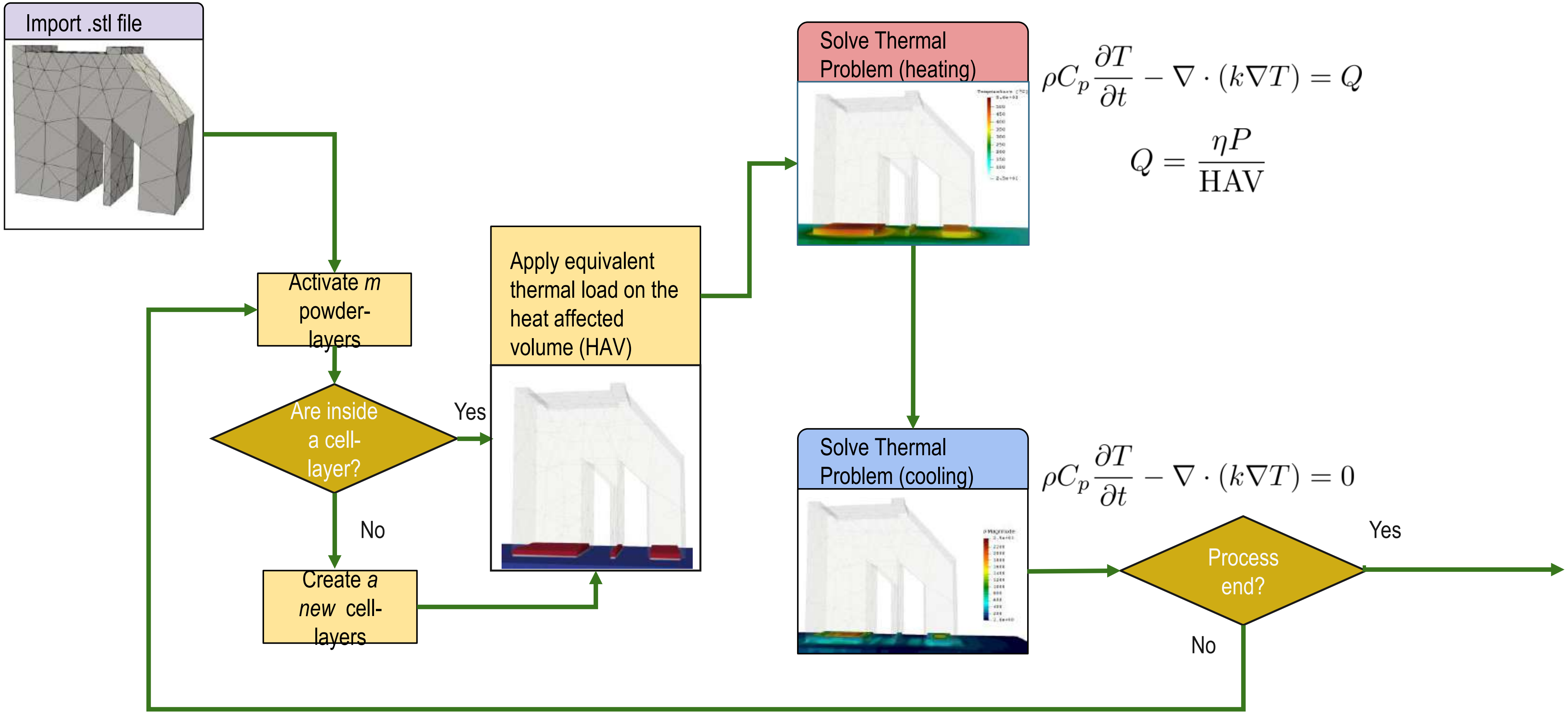


The cell-layer is not active

A first powder-layer is added to the physical domain and the cell-layer is activated

The entire domain embedded in the cell is now in the physical domain

Part-scale immersed thermal analysis



$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = Q$$

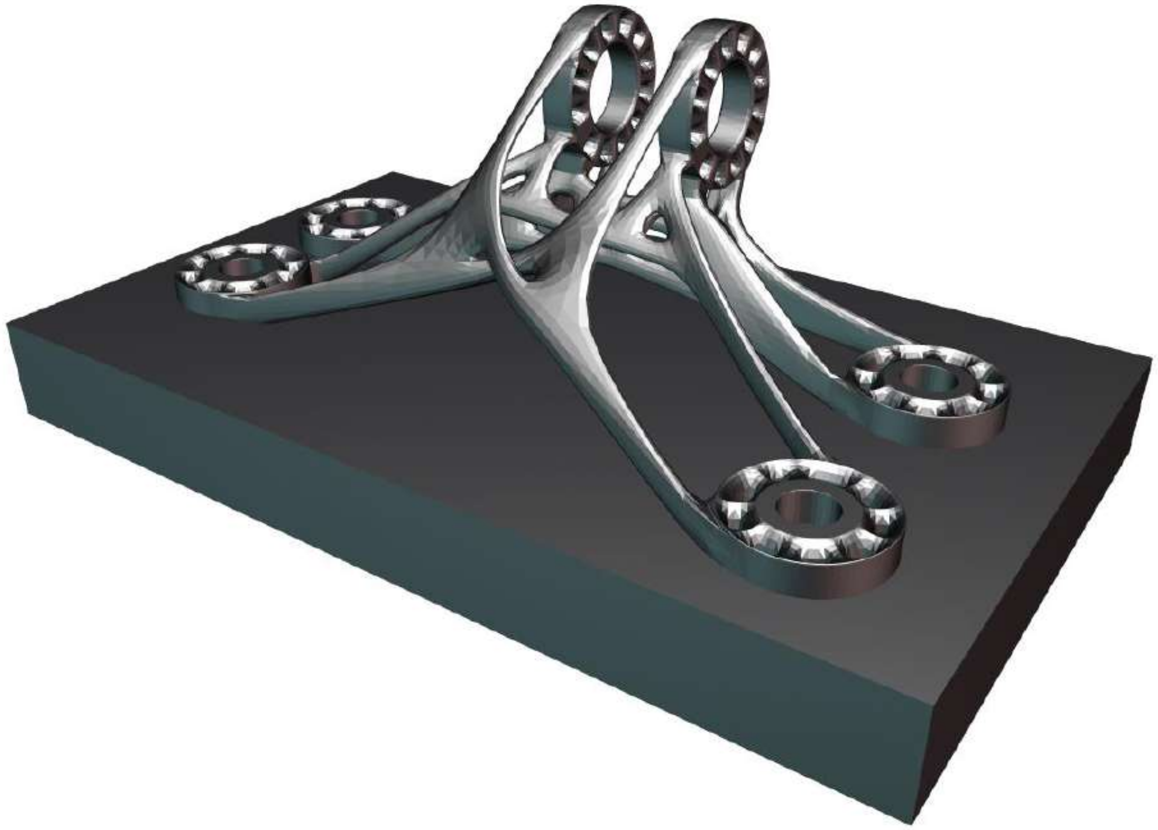
$$Q = \frac{\eta P}{\mathrm{HAV}}$$

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) = 0$$

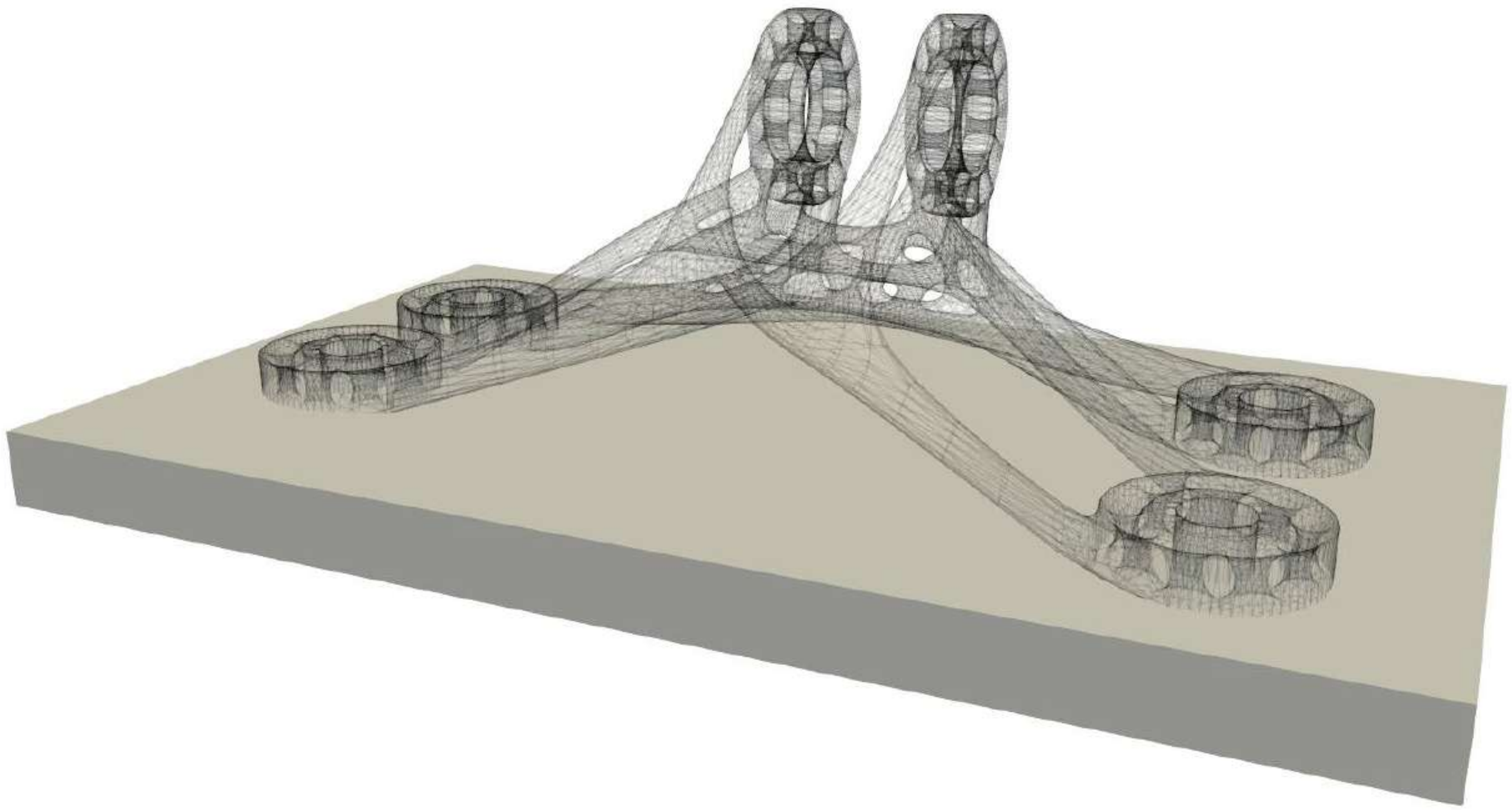
Carraturo M., Jomo J., Kollmannsberger S., Reali A., Auricchio,F. and Rank E. (*submitted*), Modeling and experimental validation of an immersed thermo-mechanical part-scale analysis for laser powder bed fusion processes. Additive Manufacturing.

GE-bracket immersed thermal process analysis

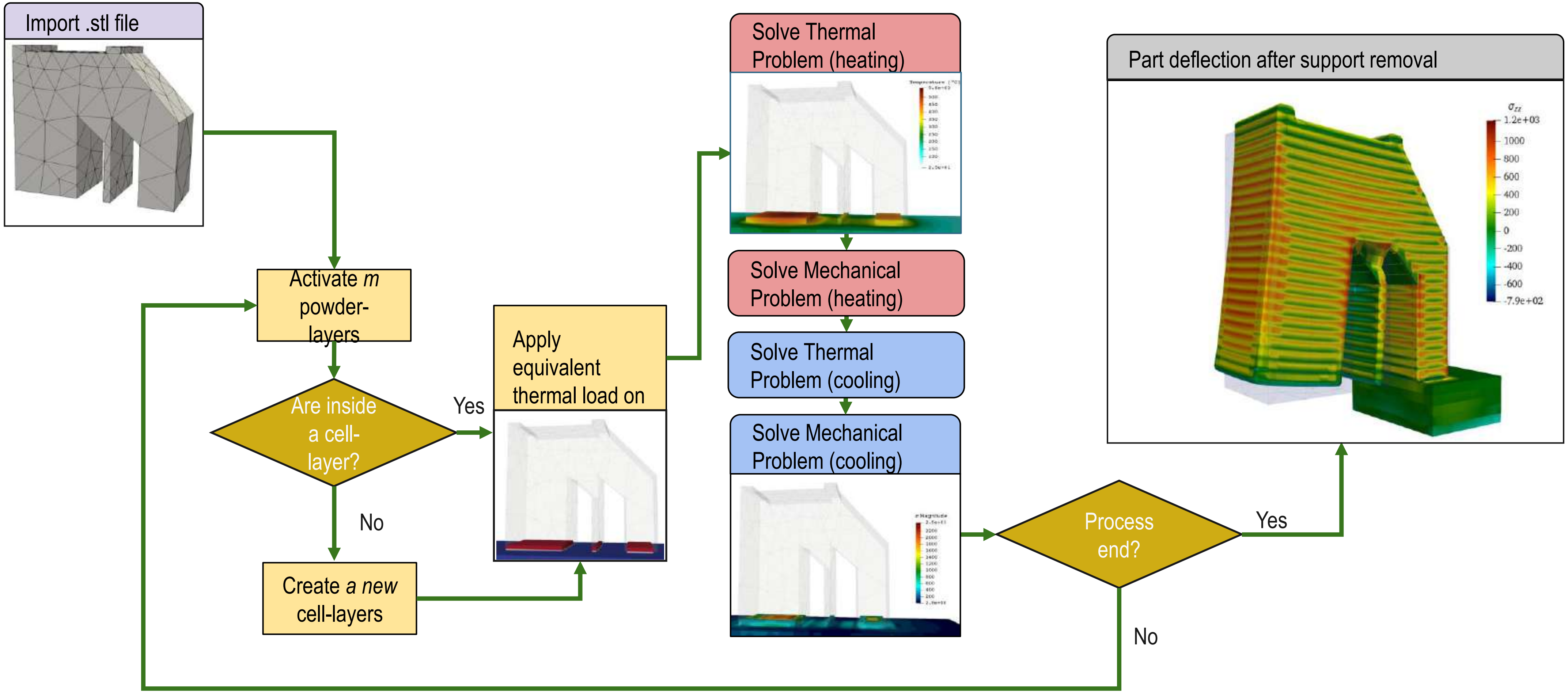
GE-bracket:
- Optimized AM component
- Material: Stainless steel 316L
- Dimensions: 48.5x80.0x28.5 mm^3
- # cells: 60x100x72
- # integration voxels/cell: 4x4x4
- # GPs/voxel: 8
- # powder-layer/cycle: 5
- Powder-layer thickness: 50 µm
- Number of time steps: 120



GE-bracket immersed thermal process analysis

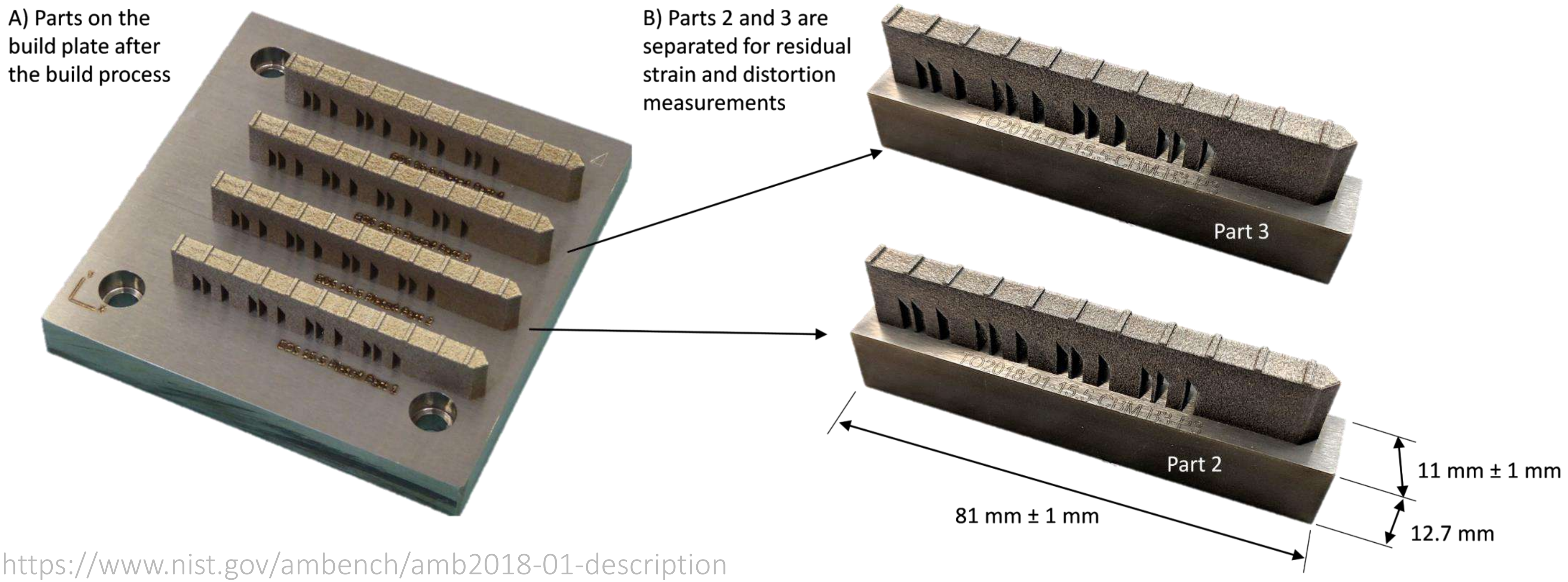


Growing domain thermo-mechanical problem solver



Experimental Validation

- ## Experimental setup

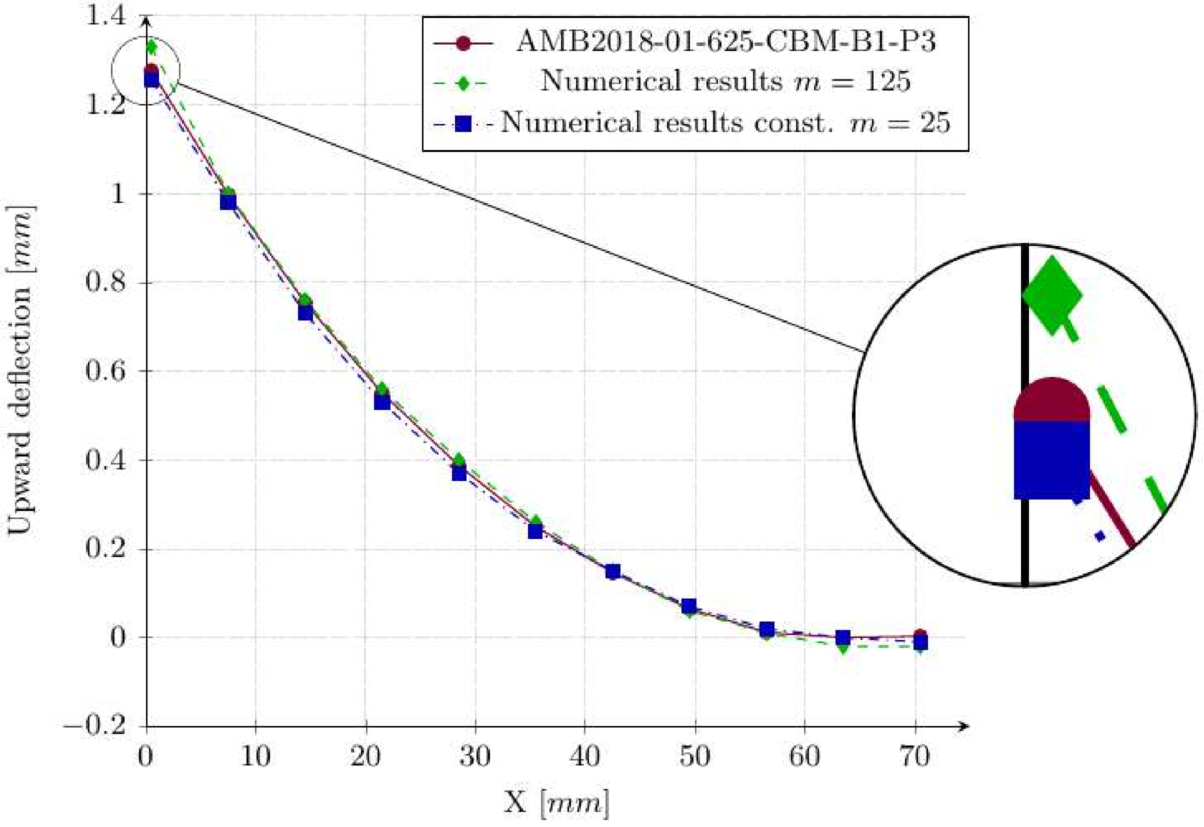


Source: https://www.nist.gov/ambench/amb2018-01-description

Experimental Validation

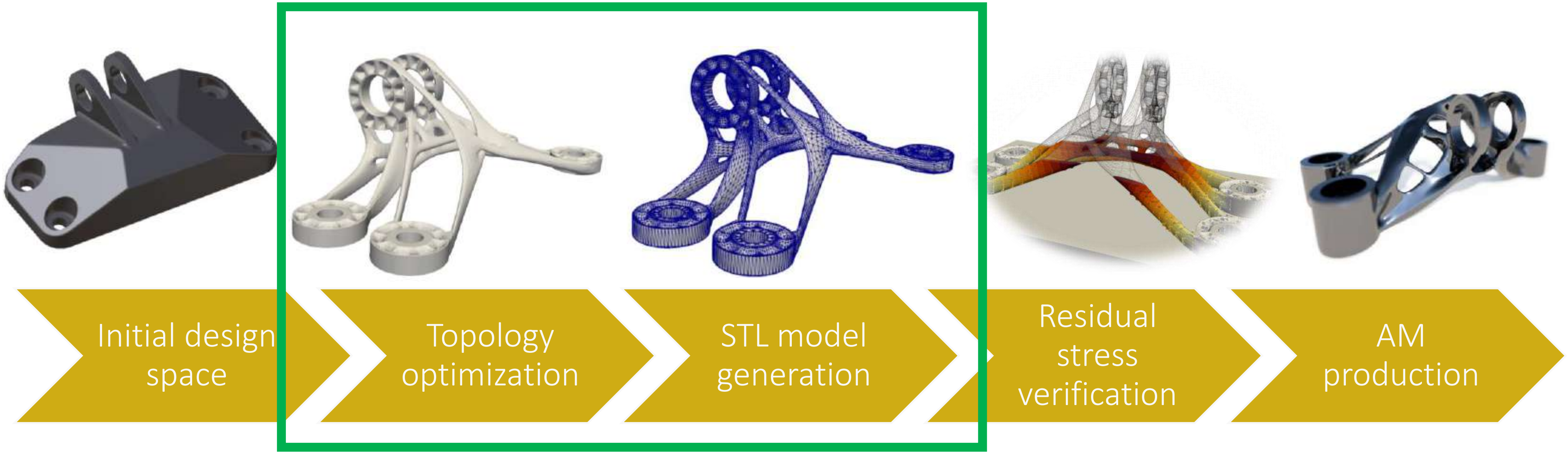
- Simulation vs. Experiment comparison

Max. deflection relative error < 5%
Data correlation ~ 99%



Functional Design for AM

- Multi-step design process driven by optimization, taking advantages from Additive Manufacturing but also knowing the limitations of the process.



Phase-field topology optimization

Objective

Minimize the Lagrangian functional such that the admissibility conditions are fulfilled:

$$\min\ \mathcal{L}(\mathbf{u}, \mathbf{p}, \varphi, \chi, \lambda_\varphi, \lambda_\chi) = \mathcal{J}^\varepsilon(\mathbf{u}, \varphi, \chi) + \lambda_\varphi \mathcal{M}_\varphi + \lambda_\chi \mathcal{M}_\chi + \mathcal{S}(\mathbf{p}, \varphi, \chi)$$

$$D_\phi \mathcal{L}(\bar{\varphi}, \bar{\chi}, \bar{\mathbf{u}}, \bar{\mathbf{p}}, \bar{\lambda}_\varphi, \bar{\lambda}_\chi)\,(\varphi - \bar{\varphi}) \geq 0 \quad \forall \varphi \in \Phi_{ad}$$
$$D_\chi \mathcal{L}(\bar{\varphi}, \bar{\chi}, \bar{\mathbf{u}}, \bar{\mathbf{p}}, \bar{\lambda}_\varphi, \bar{\lambda}_\chi)\,(\chi - \bar{\chi}) \geq 0 \quad \forall \chi \in \Xi_{ad}$$

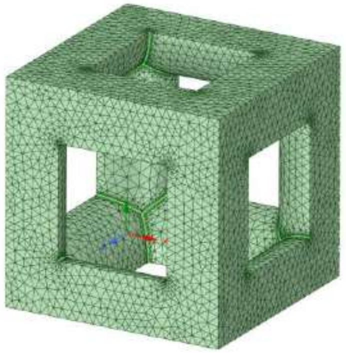
$$\Phi_{ad} := \{\varphi \in H^1(\Omega)\ :\ 0 \leq \varphi \leq 1 \quad \text{a.e. in } \Omega\}$$
$$\Xi_{ad} := \{\chi \in H^1(\Omega)\ :\ 0 \leq \chi \leq \phi \quad \text{a.e. in } \Omega\}$$

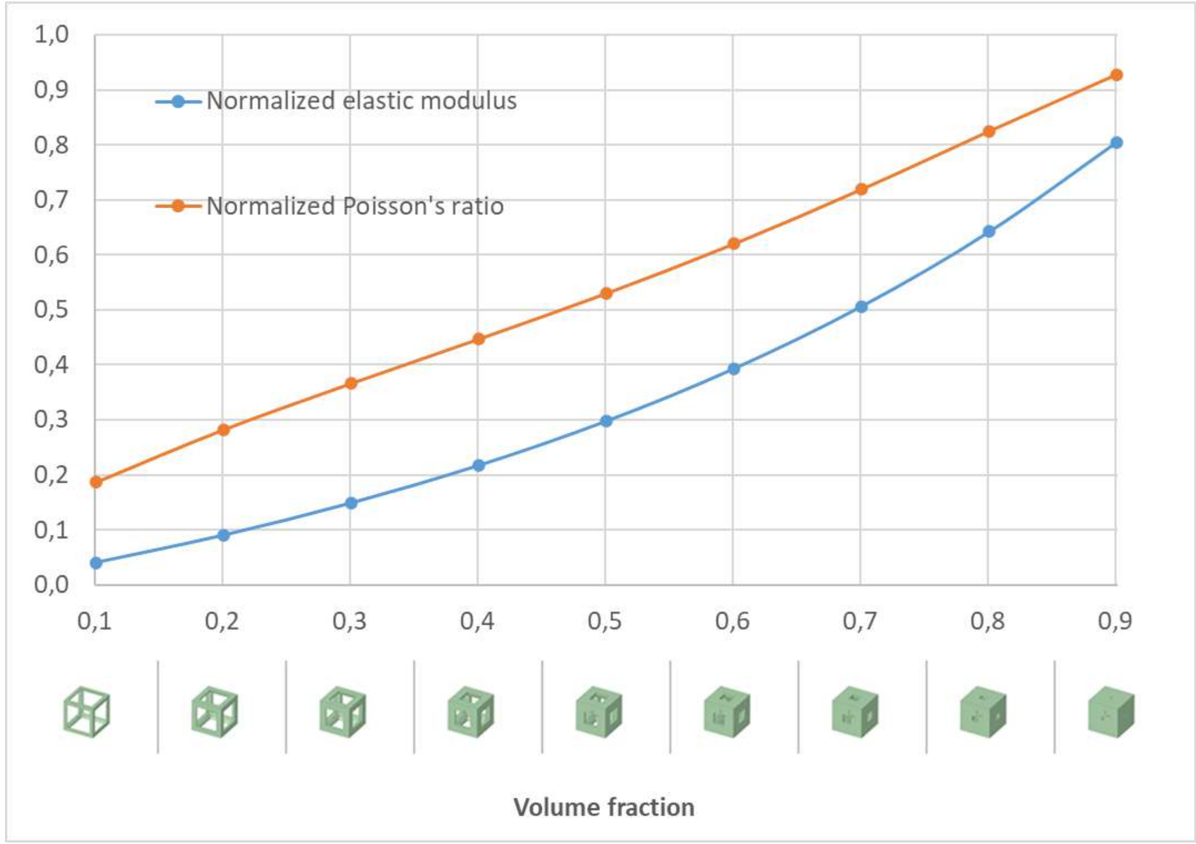
Auricchio F., Carraturo M., Bonetti E., Hömberg D., Reali A. and Rocca,E. (*submitted*). A phase-field based graded-material topology optimization with stress constraint. *M3AS*.

Homogenization

- Asymptotic homogenization using Ansys

RVE + periodic BCs

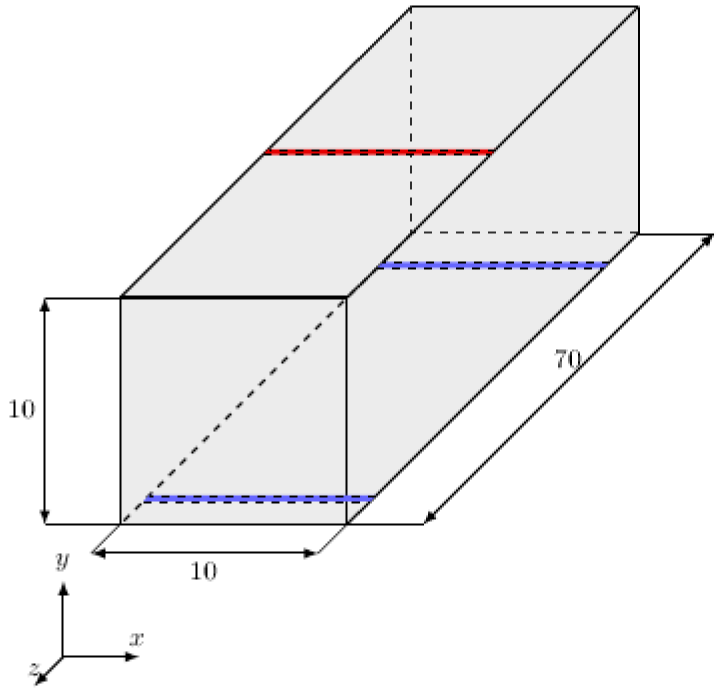


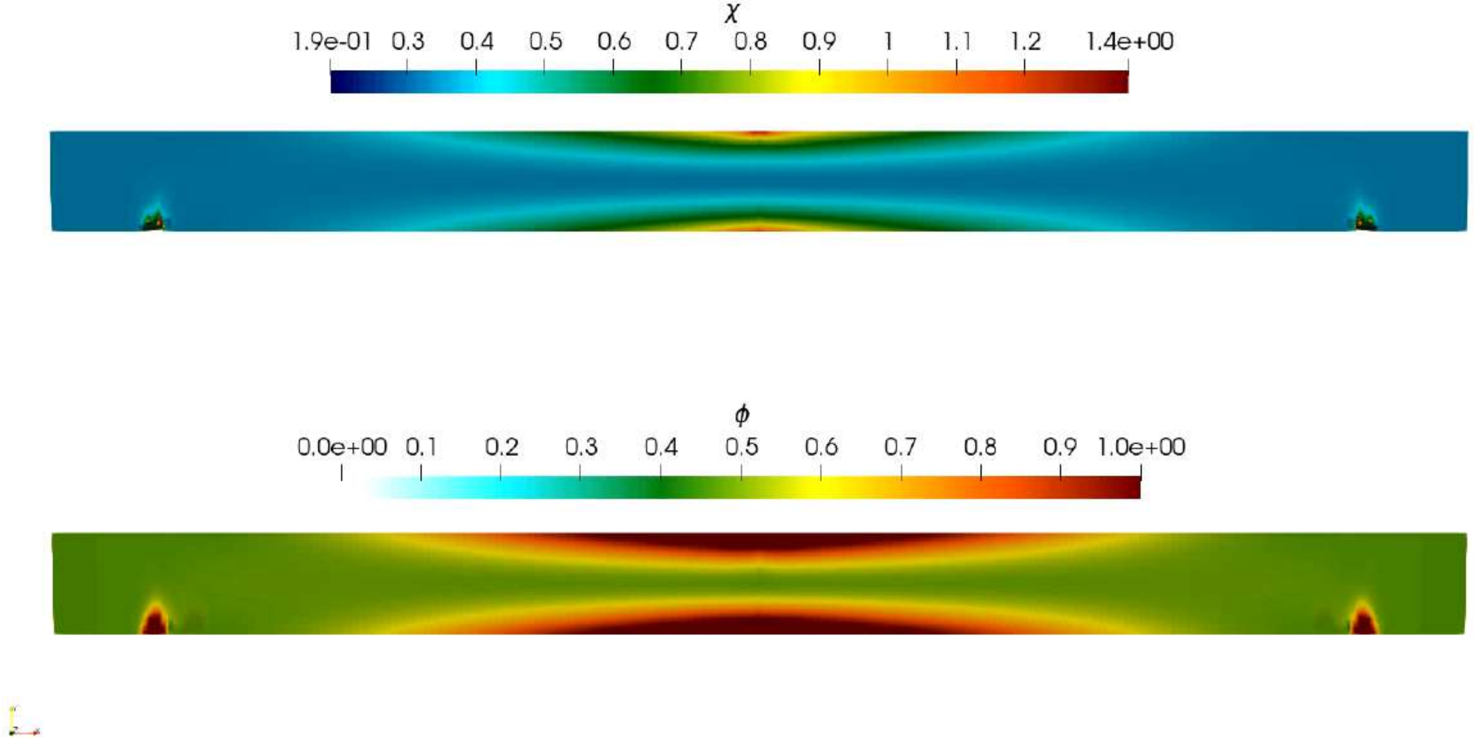


Homogenized elasticity tensor as a function of volume fraction

Topology Optimization

- Phase-field based topology optimization of MBB-beam problem





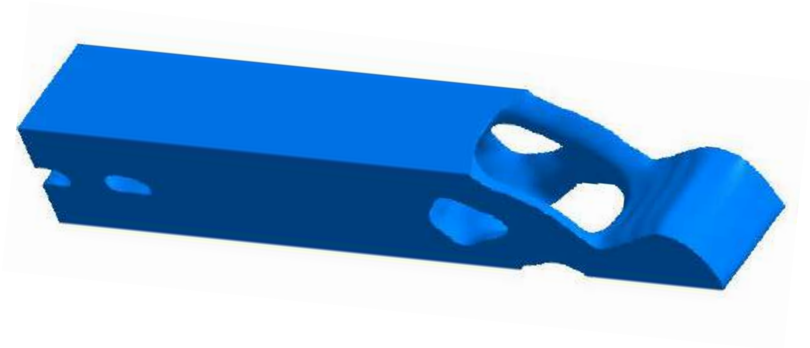
3D virtual model reconstruction

WOLFRAM
MATHEMATICA 12
Version: 12.0.0.0

1. Slicing of the 3D results
2. Generation of a grid, where each cell corresponds to a lattice cell
3. Assign the corresponding average χ value to each cell
4. Generate the void CAD model in each cell
5. Generate the bulk material CAD model
6. Assemble the slices and smooth out the bordes
7. Subtract the voids to the bulk model
8. 3D virtual model ready to be printed

3D virtual model reconstruction

Phi field



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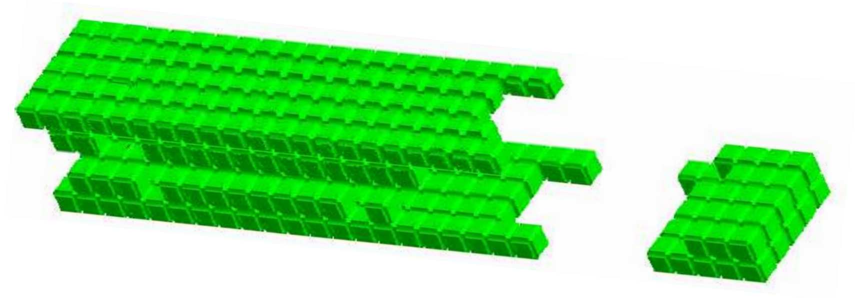
Chi field



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