COMPUTATIONAL METAMATERIAL DESIGN

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IMAL, CCT CONICET Santa Fe, 7/4/2017

OUTLINE

- Computational metamaterial design
- Microscale analysis
- Multiscale problem as a macroscopic one with inhomogeneous material
- Macroscopic thermo-mechanical response as a function of microstructure
- Material design as an optimization problem
- Applications:
  - Optimization of the mechanical response under thermal loads
  - Optimization of the thermal response using free material optimization (FMO)
  - Heat flux manipulation
    - Design of easy-to-make devices using discrete material optimization (DMO)
    - Design of easiest-to-make devices using topology optimization
- Advantages of computational metamaterial design
- Perspectives

METAMATERIAL DESIGN

- **MATERIAL DESIGN**: to modify the microstructure of the material in a macroscopic piece in order to obtain an optimal response of the piece

- **METAMATERIAL**: the so-designed material, usually having extraordinary **effective** properties:
  - optical or acoustical camouflage /invisibility
  - negative Poisson ratio
  - negative thermal conductivity, thermal camouflage, etc.

COMPUTATIONAL METAMATERIAL DESIGN

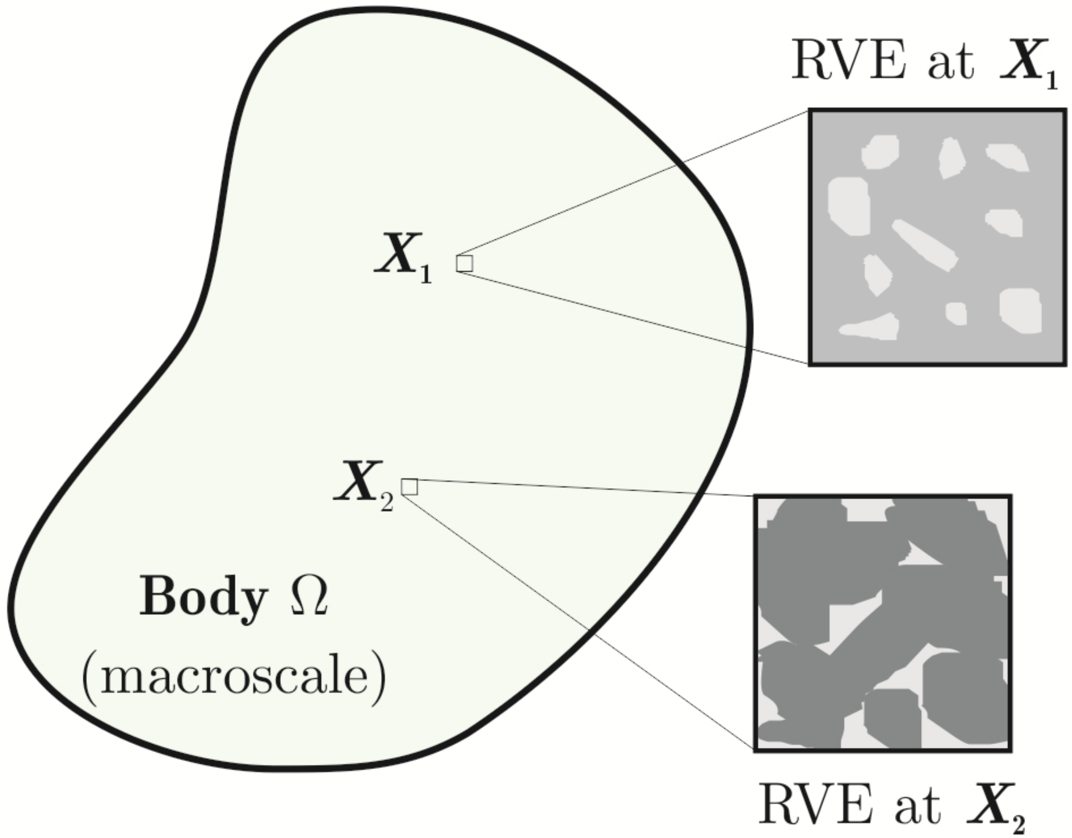
- **Computational Metamaterial Design (CMMD)** involves the computational solution of a series of multiscale problems for changing microstructure

until finding the optimal macroscopic response

MACROSCOPIC BODY WITH VARIABLE MICROSTRUCTURE

- Let the microstructure vary throughout the macroscopic domain, being sampled at a series of points $\boldsymbol{X}_\alpha$

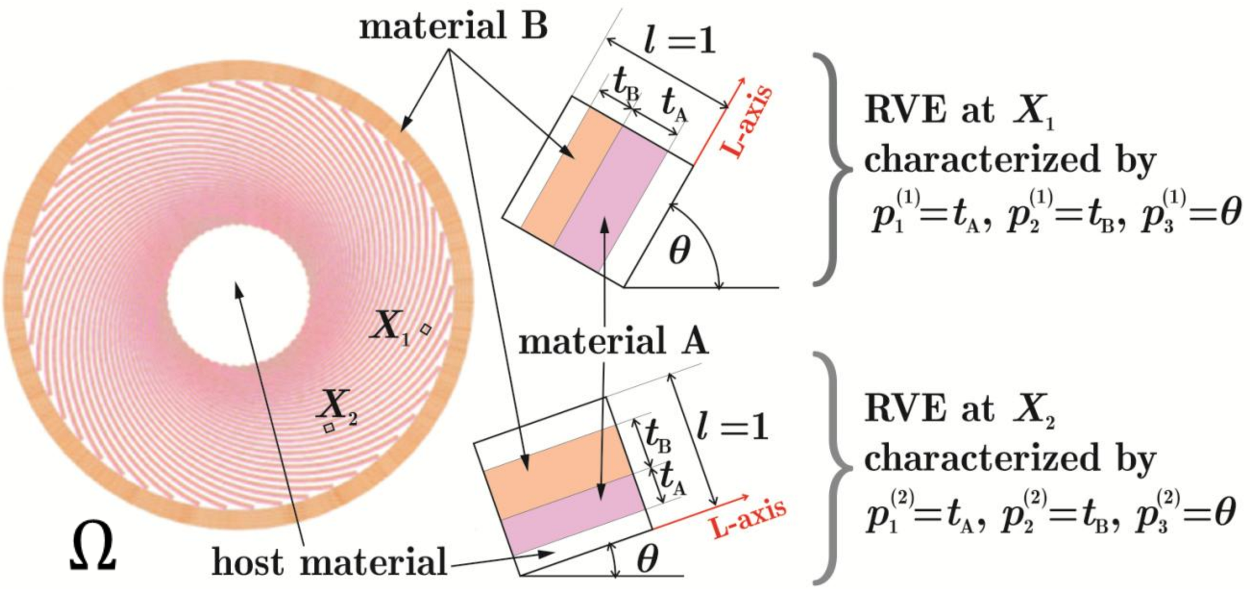
- Each $\boldsymbol{X}_\alpha$ has its own Representative Volume Element (RVE)



QUANTITATIVELY CHARACTERIZED MICROSTRUCTURE

- Let the RVE at any sampling point $\boldsymbol{X}_\alpha \in \Omega$ be characterized by a finite number of (micro)parameters $p_1^{(\alpha)}, p_2^{(\alpha)}, \ldots$

Ex.: Narayana & Sato's heat flux inverter (PRL 2012)

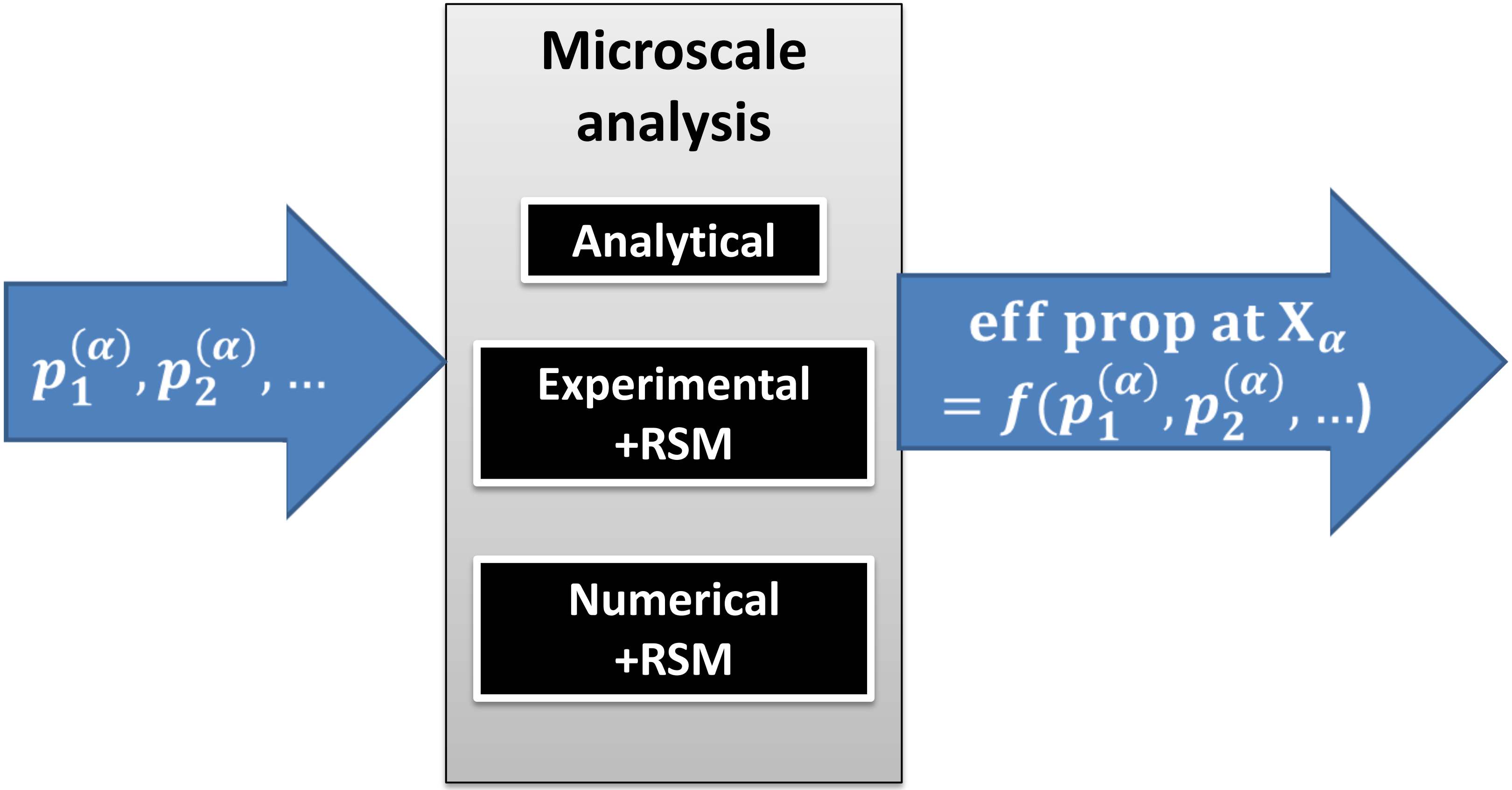


$\Rightarrow$ Effective properties at $\boldsymbol{X}_\alpha \in \Omega = f\,(p_1^{(\alpha)}, p_2^{(\alpha)}, \ldots)$

MICROSCALE ANALYSIS

MICROSCALE ANALYSIS

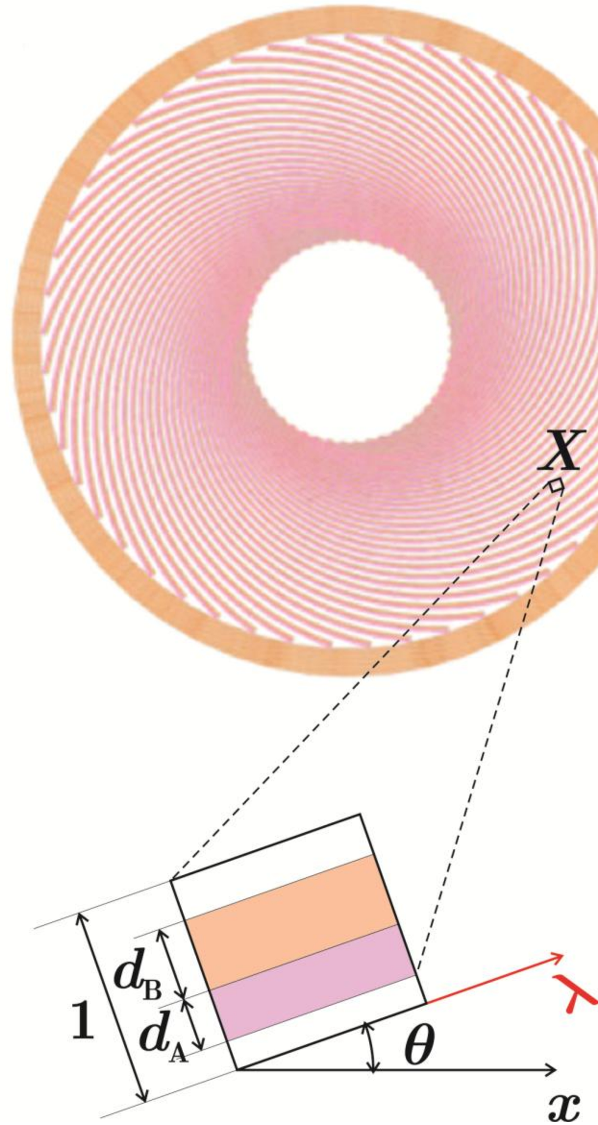
- **Goal:** determination of the effective properties as analytical functions of the microparameters



ANALYTICAL MICROSCALE ANALYSIS: LAMINATE

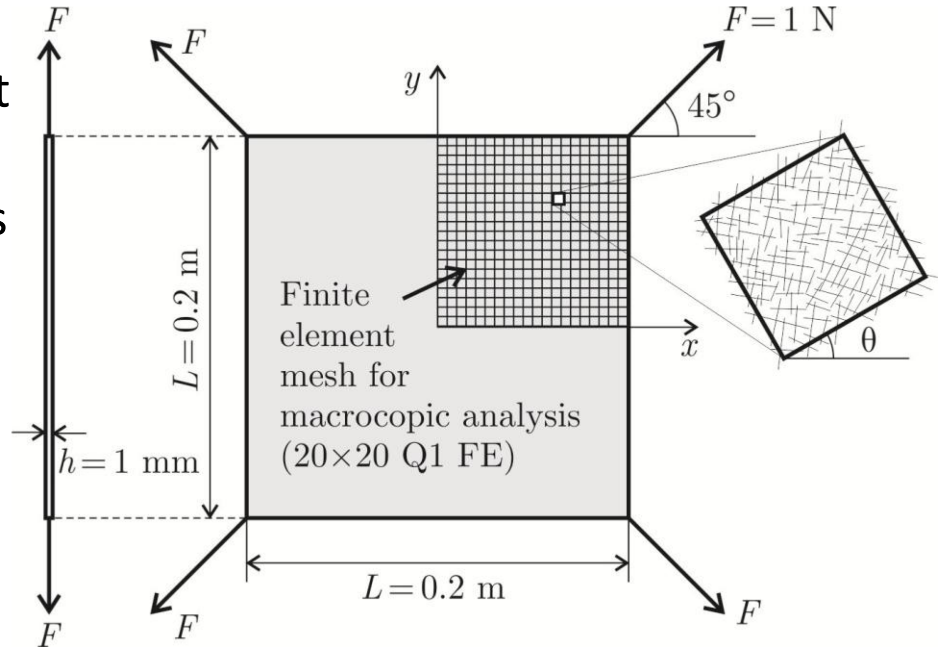
- Effective anisotropic conductivity

$$k_{\ldots} = \frac{d_A k_A + d_B k_B + d_C k_C}{}$$



EXPERIMENTAL+NUMERICAL MICROSCALE ANALYSIS: PAPER

- Using upscaling techniques, discrete element simulations and X-ray microtomography of the geometry of wood fibers and their bonds and the architecture of the fibrous network, **Marulier** (PhD thesis 2013) determined the **homogenized elastic moduli**:

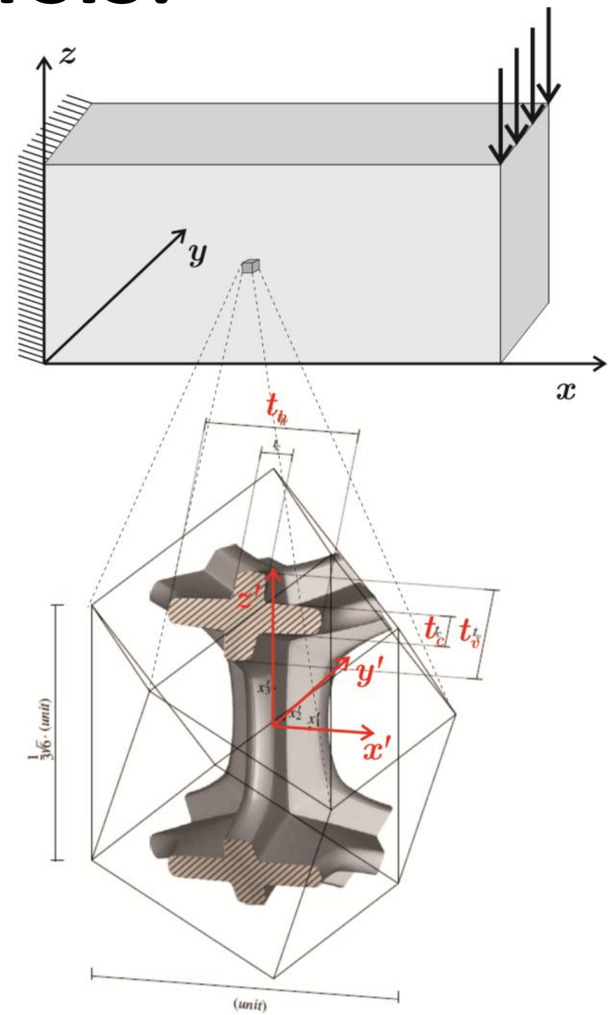


$$\boldsymbol{C}^{\text{orth}} = 1.14 \times 10^9 (\phi - 0{,}02)^2 \boldsymbol{A}(a)$$
$$\Longrightarrow \boldsymbol{C}_{xy} = \boldsymbol{\Theta}(\theta)\boldsymbol{C}^{\text{orth}}(\phi, a)[\boldsymbol{\Theta}(\theta)]^T$$

- ϕ: fiber content
- $\boldsymbol{A}(a)$: fiber orientation tensor (response surface from experiments), a: orientation intensity
- $\boldsymbol{\Theta}(\theta)$: serves to rotates from $\lambda\tau$ to xy, θ: angle between the x and λ

* Collaboration with S. Le Corre (LTN Nantes) and L. Orgéas (LCNRS Grenoble)

NUMERICAL MICROSCALE ANALYSIS: CANCELLOUS BONE



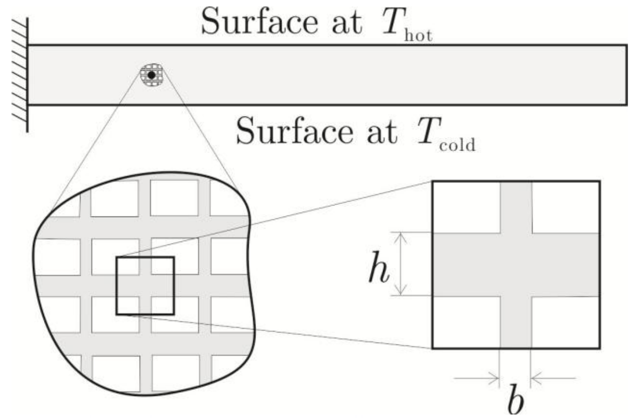
- Using FEM for a geometrically parameterized cell, Kowalczyk (2006) determined the **homogenized elastic moduli**:

$$C'_{ijkl} = f(t_c, t_v, t_h)$$
$$\Longrightarrow C_{ijkl} = R_{mi}R_{nj}R_{pk}R_{ql}C'_{mnpq}$$

– t_c, t_v, t_h : geometric parameters
– $\boldsymbol{R}(\psi_1, \psi_2, \psi_3)$: 3D rotation tensor

* Collaboration with A. Cisilino & L. Colabella (INTEMA)

NUMERICAL MICROSCALE ANALYSIS: SOLID WITH INCLUSIONS



- Using FEM on RVEs with variable b and h, we determined the effective thermomechanical properties

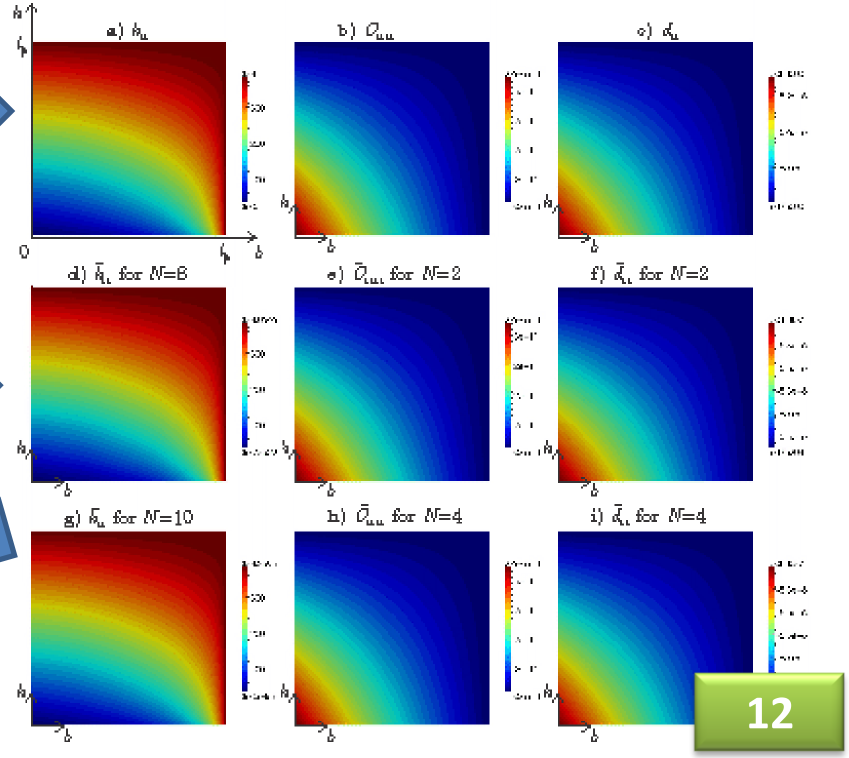
$$k_{ij} = k_{ij}(b,h)$$

$$C_{ijkl} = C_{ijkl}(b,h)$$

$$\frac{\partial \sigma_{ij}}{\partial T} = d_{ij}(b,h)$$

GRIDS FROM FEM PARAMETRIC ANALYSIS

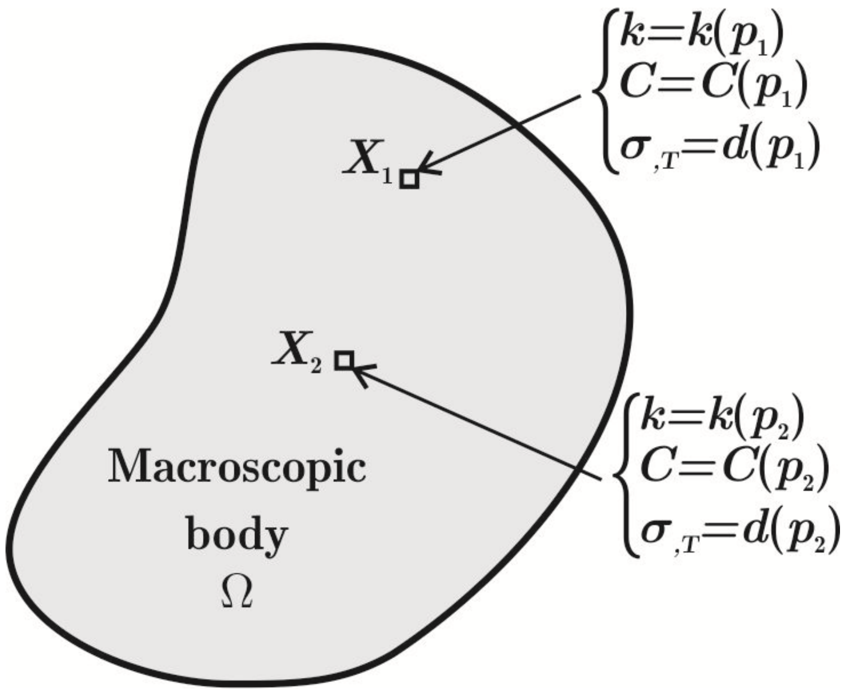
POLYNOMIAL RESPONSE SURFACES



* Fachinotti, Toro, Sánchez & Huespe, IJSS 2015

REDUCTION OF THE MULTISCALE PROBLEM

- Once you know the effective material properties as functions of the microparameters $\boldsymbol{p}$ from the microscale analysis, the multiscale problem becomes a **classic macroscopic problem with inhomogeneous material properties**



MACROSCOPIC THERMO-MECHANICAL RESPONSE AS A FUNCTION OF MICROSTRUCTURE

THERMOMECHANICAL RESPONSE AS A FUNCTION OF MICROSTRUCTURE

- Given the microstructure $\boldsymbol{P} = [\boldsymbol{p}_1, \boldsymbol{p}_2, \dots]$ througout Ω:
  1) solve the steady state FEM heat equation:

$$\int_\Omega \boldsymbol{B}^T \boldsymbol{k}(\boldsymbol{p}) \boldsymbol{B} \, dv \, \boldsymbol{T} + \int_{\partial\Omega_\mathrm{q}} \boldsymbol{N}^T q^{\mathrm{wall}} \, ds = \boldsymbol{0}$$

$$\Longrightarrow \boldsymbol{T} = \boldsymbol{T}(\boldsymbol{P})$$

  2) solve the FEM equilibrium equation:

$$\int_\Omega \boldsymbol{B}^T \boldsymbol{C}(\boldsymbol{p}) \boldsymbol{B} \, dv \, \boldsymbol{U} + \int_{\partial\Omega_\sigma} \boldsymbol{N}^T \boldsymbol{t}^{\mathrm{wall}} \, ds - \int_\Omega \boldsymbol{B}^T \boldsymbol{\sigma}_{,\boldsymbol{T}}(\boldsymbol{p}) \Delta T(\boldsymbol{P}) \, dv = \boldsymbol{0}$$

$$\Longrightarrow \boldsymbol{U} = \boldsymbol{U}(\boldsymbol{P})$$

- The macroscopic thermo-mechanical response is the function

$$\boxed{\mathcal{R} = f(\boldsymbol{U}(\boldsymbol{P}), \boldsymbol{T}(\boldsymbol{P}), \boldsymbol{P}) = \mathcal{R}(\boldsymbol{P})}$$

MATERIAL DESIGN AS AN OPTIMIZATION PROBLEM

- To design a material consists of finding the optimal set

$$\boldsymbol{P}^{\mathrm{opt}} = \left\{p_1^{(1)}, p_2^{(1)}, \dots, p_1^{(2)}, p_2^{(2)}, \dots\right\}^{\mathrm{opt}}$$

  that minimizes a given response function (describing the desired macroscopic task)

$$\mathcal{R}(\boldsymbol{P}^{\mathrm{opt}}) = \min_{\boldsymbol{P}} \mathcal{R}(\boldsymbol{P})$$

  subject to

$$a \leq P_i \leq b, c(\boldsymbol{P}) \leq 0, d(\boldsymbol{P}) = 0$$

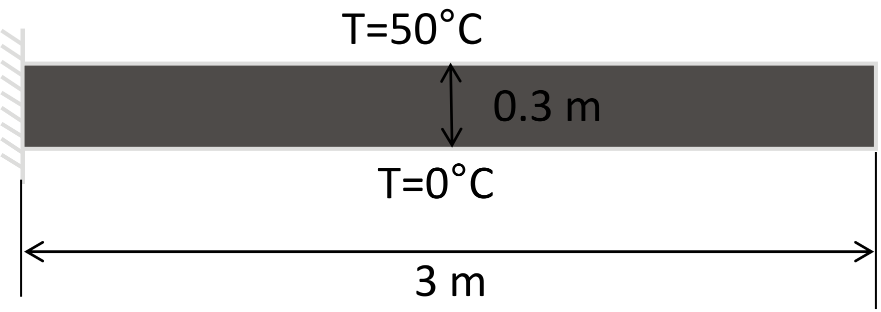
- This is generally a nonlinear constrained optimization problem with a large number of design variables

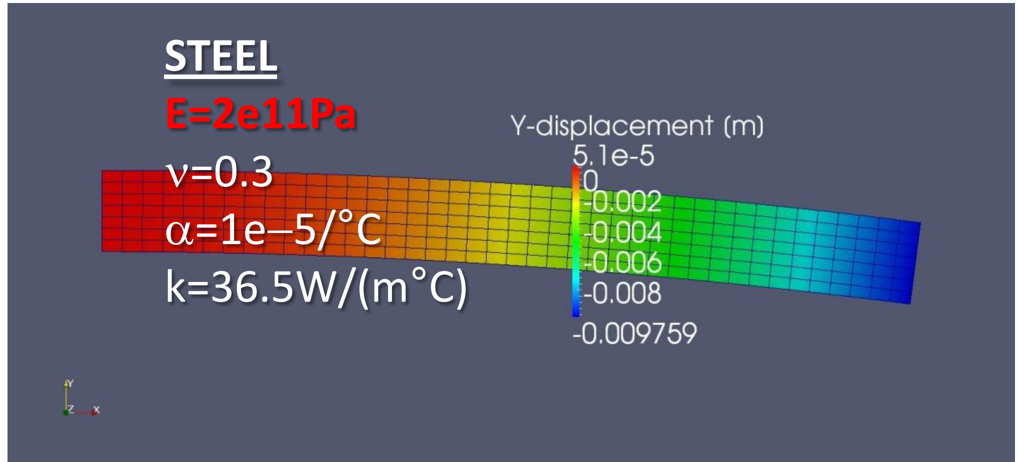
MATERIAL DESIGN FOR OPTIMAL MACROSCOPIC MECHANICAL RESPONSE UNDER THERMAL LOADS

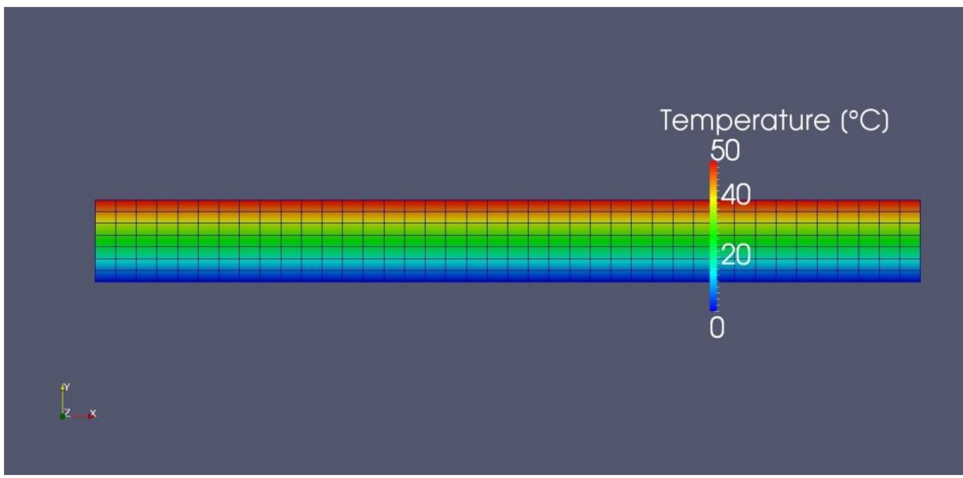
with

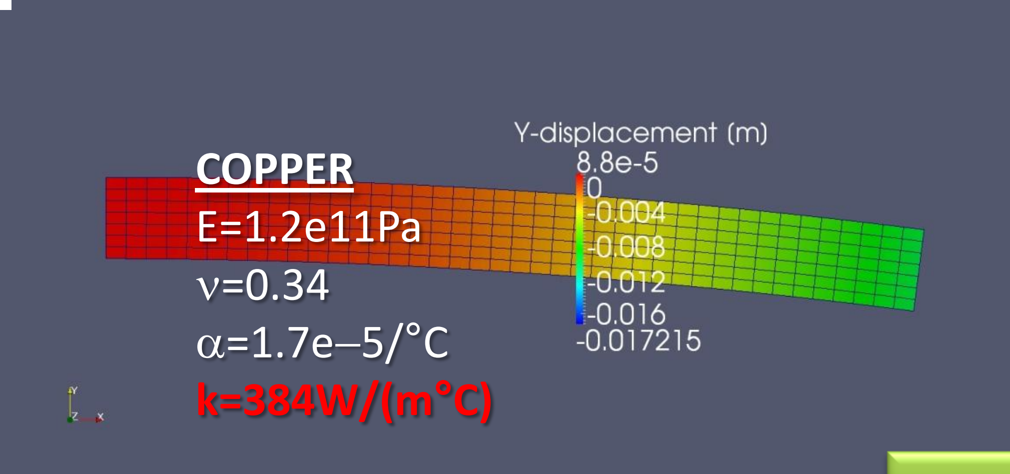
S. Toro, P. Sánchez & A. Huespe (CIMEC)

THERMAL DEFLECTION OF A CANTILEVER PLATE





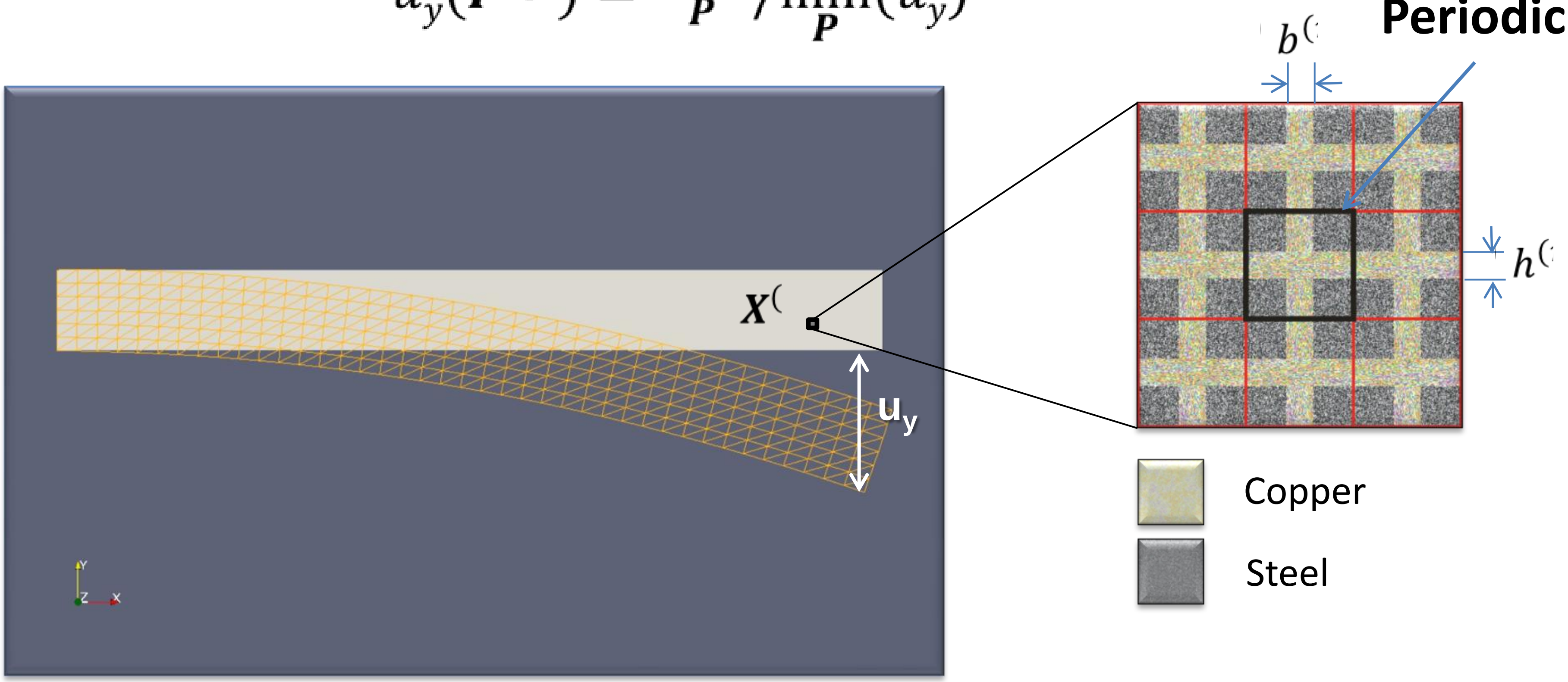




OPTIMIZING THE COMPLIANCE/STIFFNESS

- The maximal/minimal compliance problem consists of finding $\boldsymbol{P}^{\mathrm{opt}} = \left[b^{(1)}, h^{(1)}, b^{(2)}, h^{(2)}, \ldots\right]^{\mathrm{opt}}$ such that

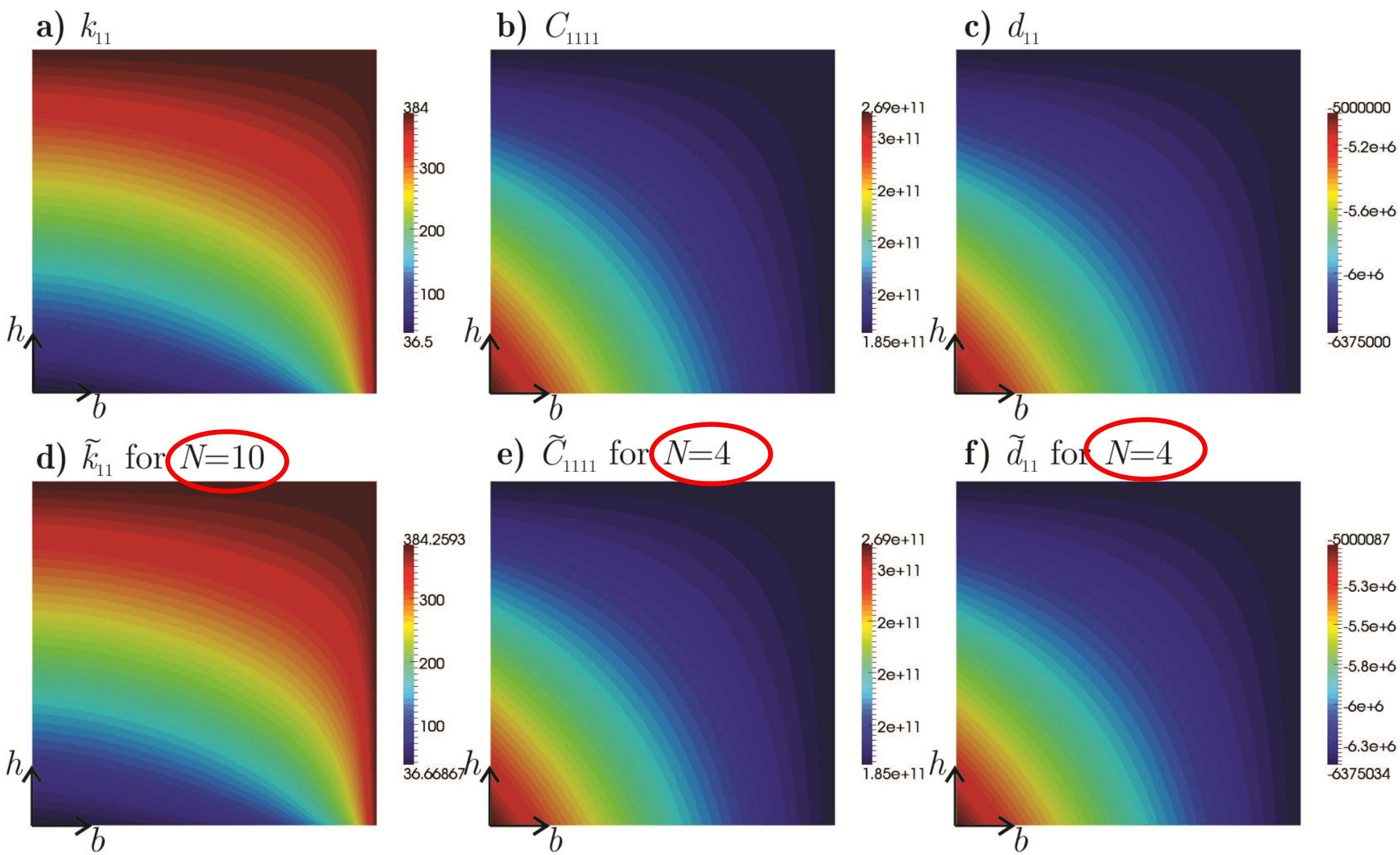
$$u_y(\boldsymbol{P}^{\mathrm{opt}}) = \max_{\boldsymbol{P}}/\min_{\boldsymbol{P}}(u_y)$$



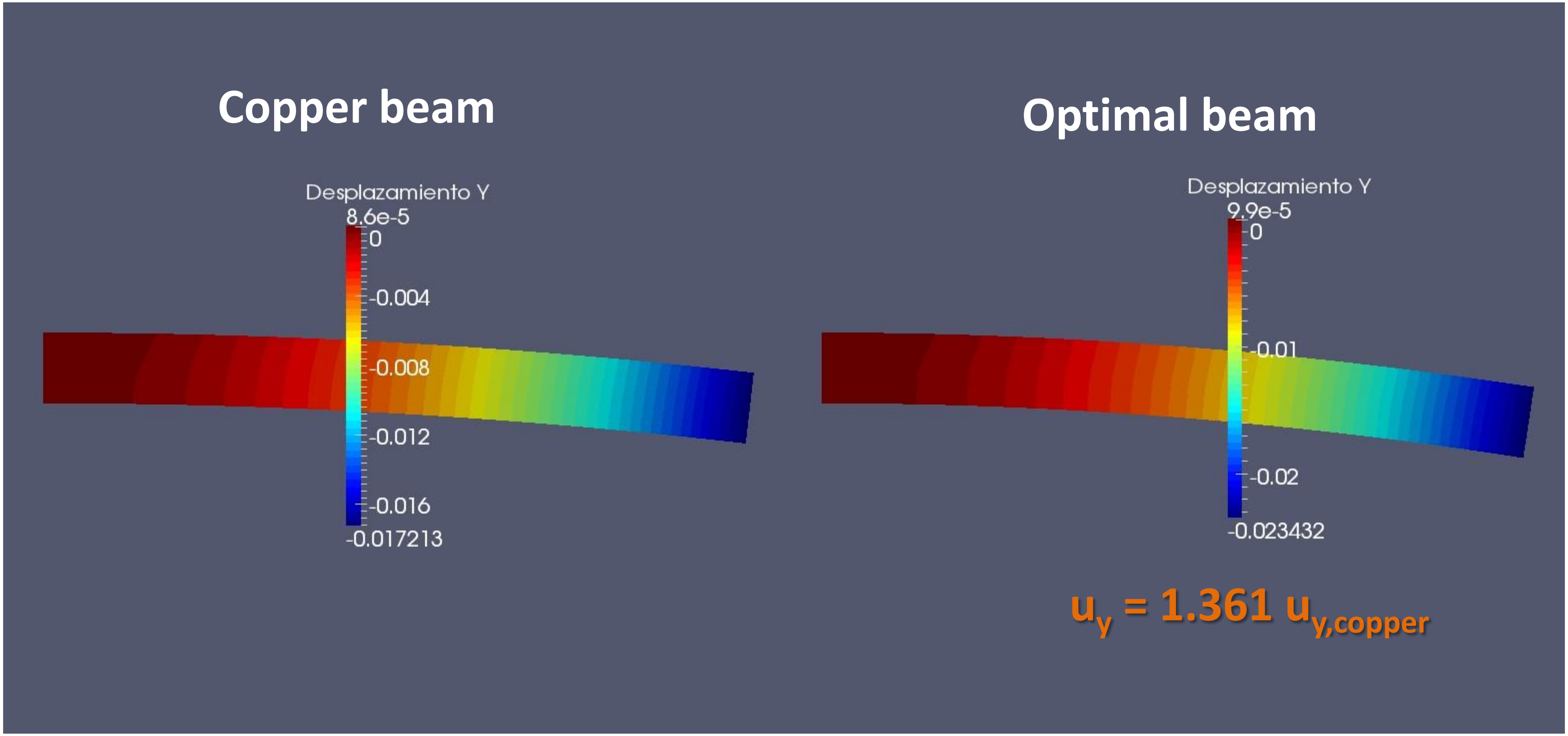
EFFECTIVE PROPERTIES AS FUNCTIONS OF MICROSTRUCTURE

Grids from FEM microscale analysis

Polynomial response surfaces

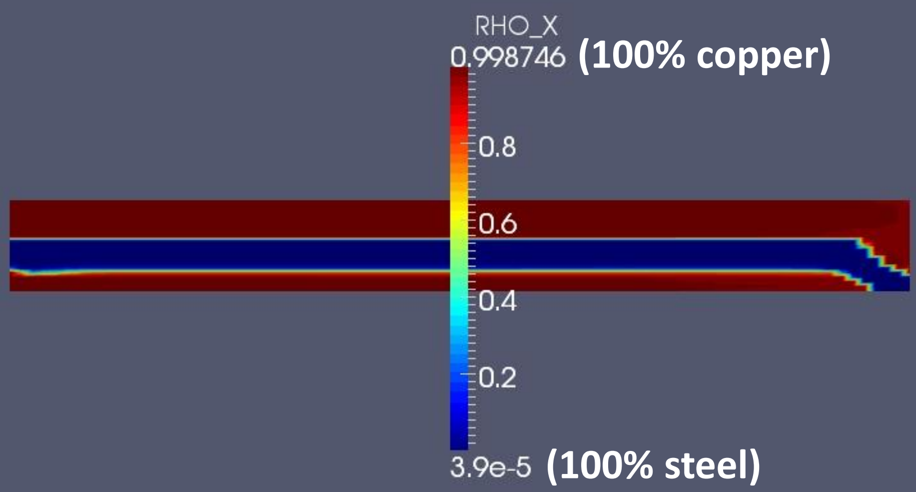


MAXIMAL COMPLIANCE: VERTICAL DISPLACEMENTS

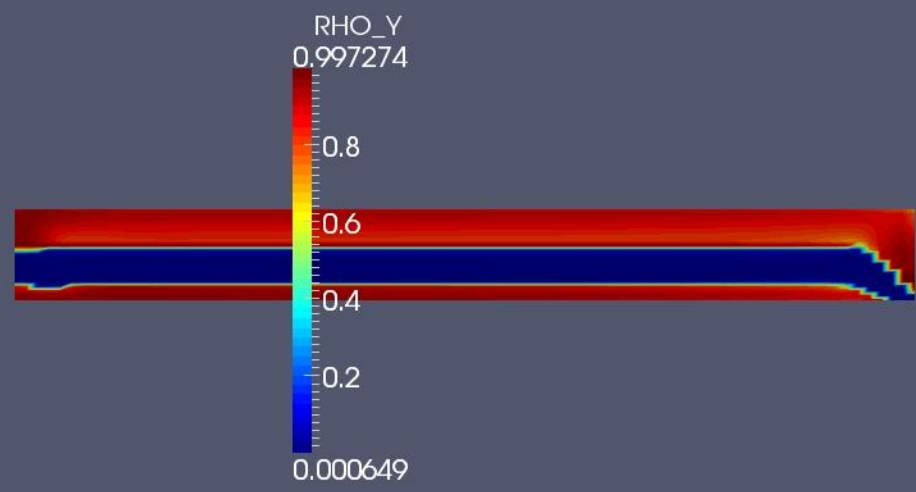


MAXIMAL COMPLIANCE:
OPTIMAL MATERIAL DISTRIBUTION

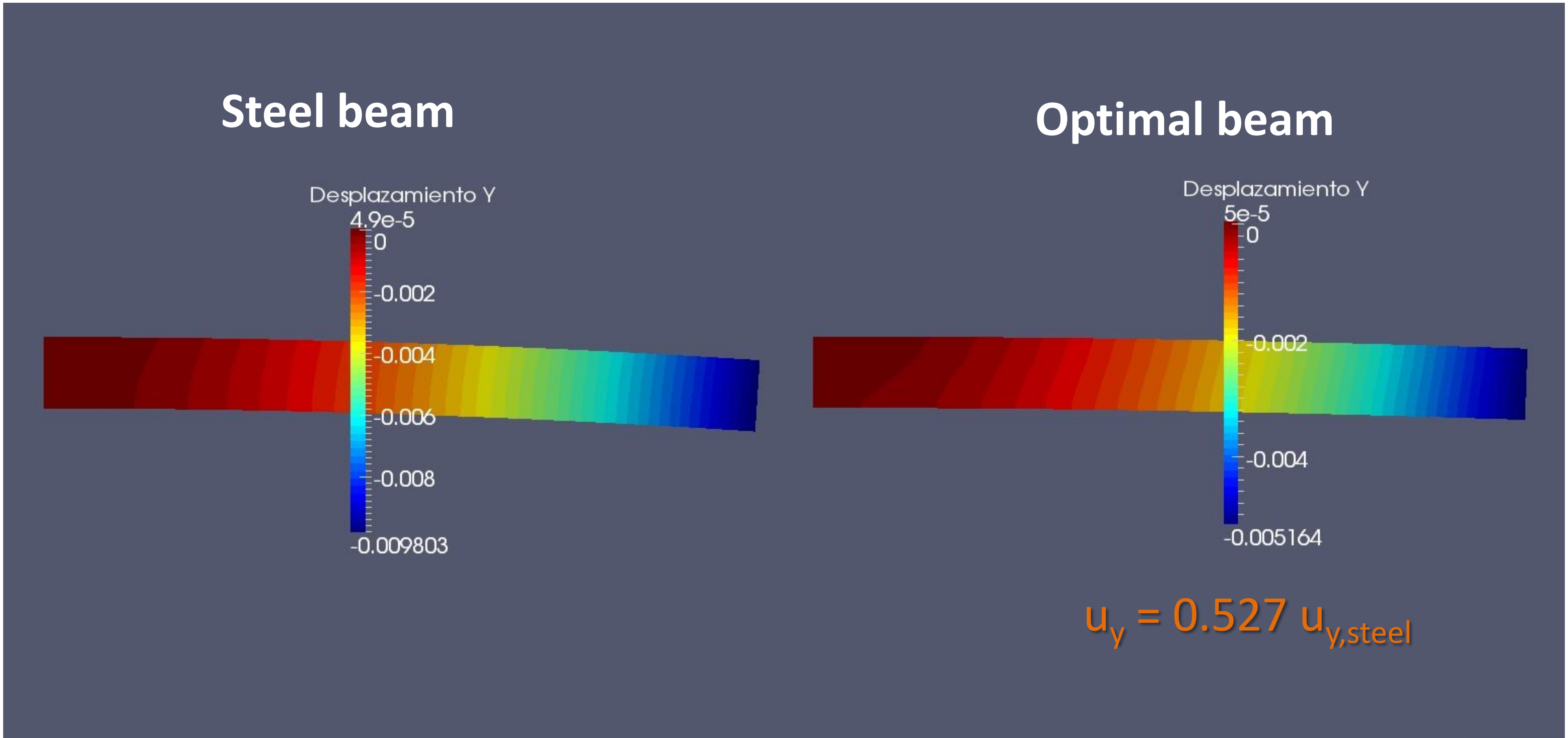
Thickness of the vertical layers



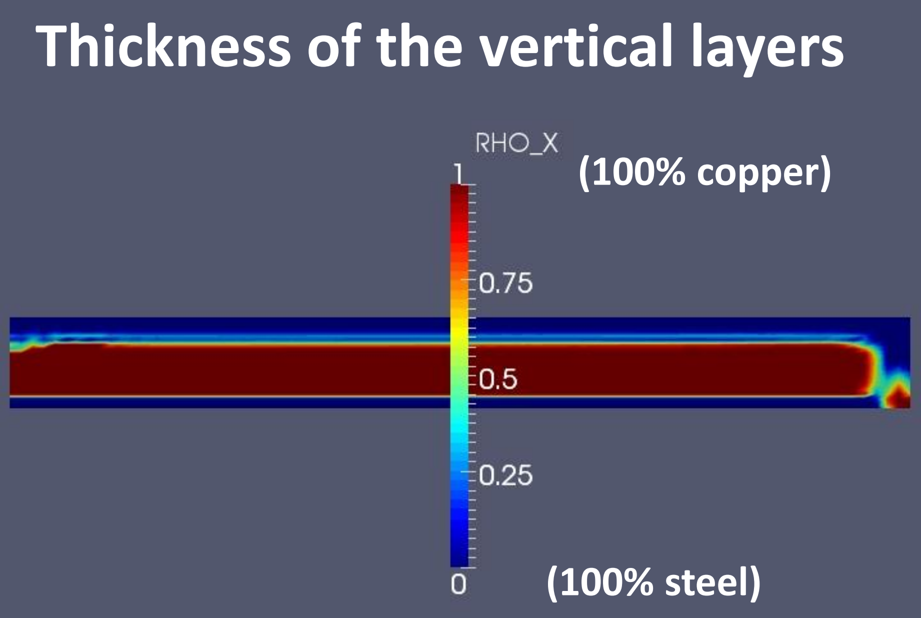
Thickness of the horizontal layers

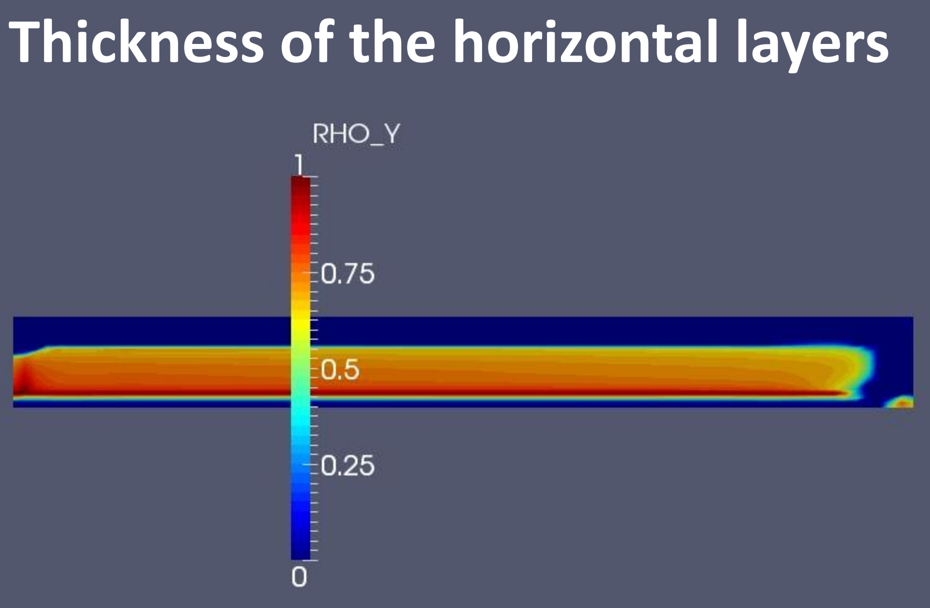


MINIMAL COMPLIANCE: VERTICAL DISPLACEMENTS



MINIMAL COMPLIANCE:
OPTIMAL MATERIAL DISTRIBUTION





MATERIAL DESIGN FOR OPTIMAL MACROSCOPIC THERMAL RESPONSE USING FREE MATERIAL OPTIMIZATION (FMO)

with S. Giusti (GIDMA)

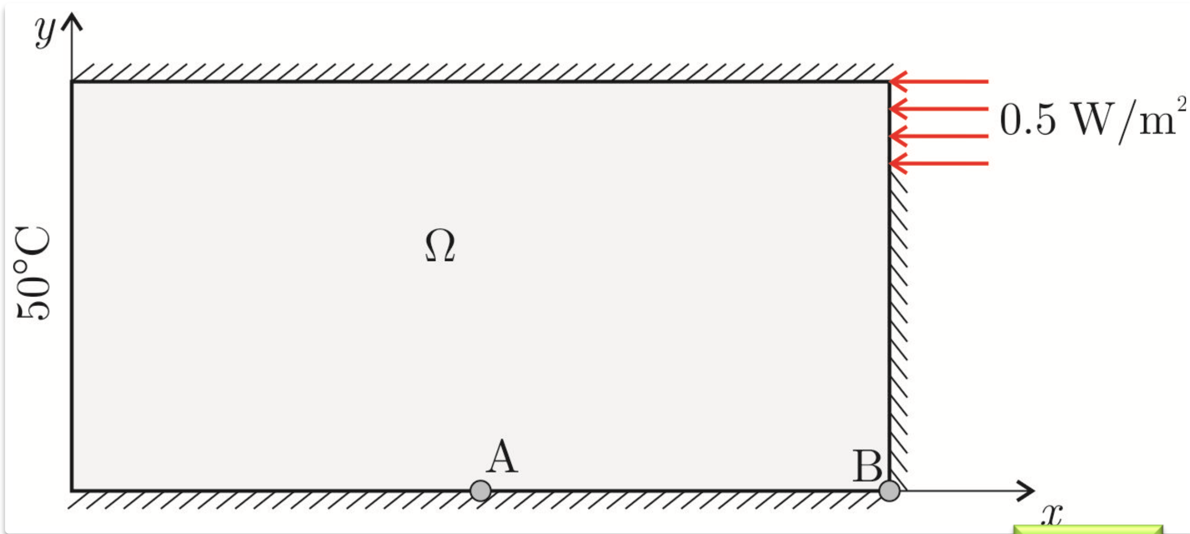
FREE MATERIAL OPTIMIZATION OF THE THERMAL RESPONSE

- **FREE MATERIAL OPTIMIZATION (FMO):** the design variables are the effective properties themselves
- For $\boldsymbol{P} = \left[k_{xx}^{(1)}, k_{yy}^{(1)}, k_{xx}^{(2)}, k_{yy}^{(2)}, \ldots\right]$ (with $k_{xx}^{(n)}, k_{yy}^{(n)}$, and $k_{xy}^{(n)} = 0$ being the effective conductivities at node n), let us find

$$\boldsymbol{P}^{\text{opt}} = \arg\min_{\boldsymbol{P}} \sum_{i \in \overline{AB}} (T_i(\boldsymbol{P}) - 200°\text{C})^2$$

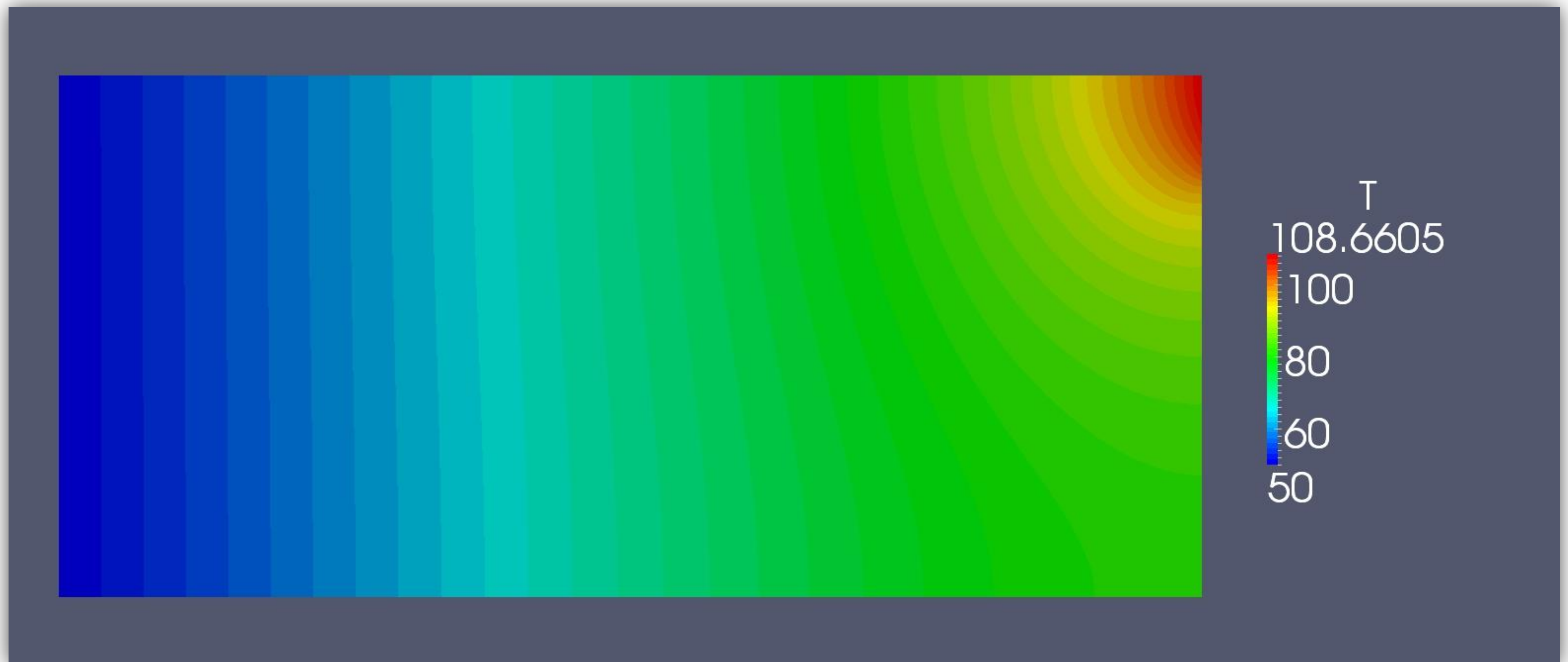
subject to

$$0.001 \leq k_{xx}^{(n)}, k_{yy}^{(n)} \leq 1$$

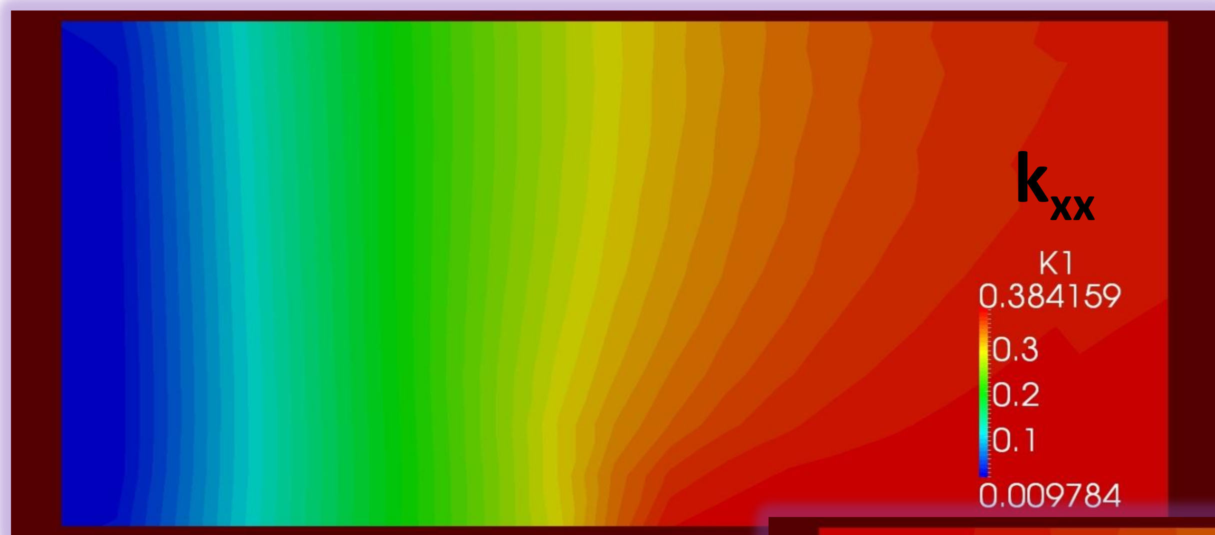


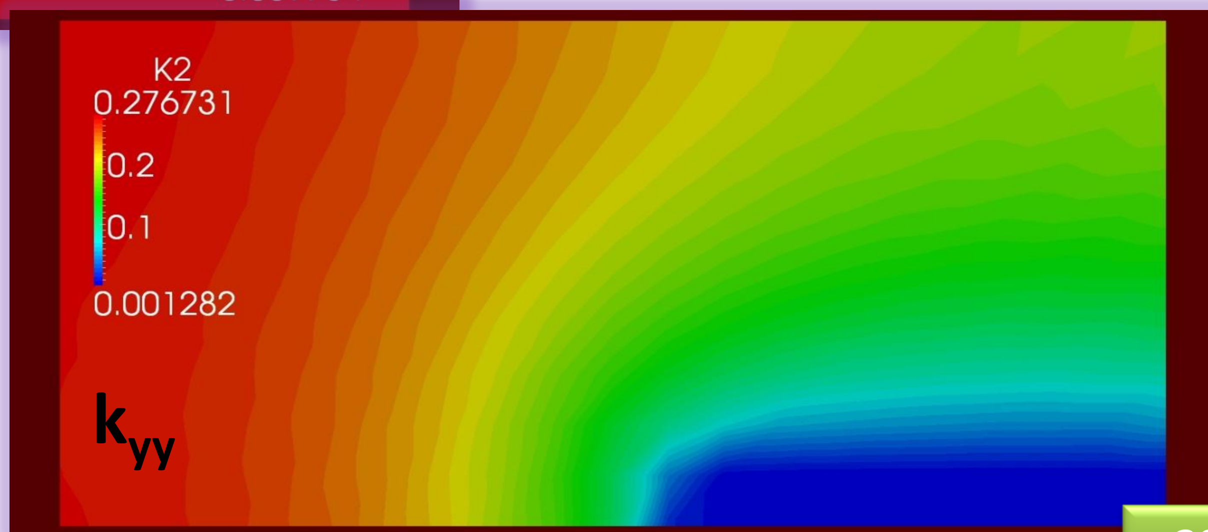
INITIAL TEMPERATURE DISTRIBUTION

Initial guess: $k_{xx} = k_{yy} = 0.5$

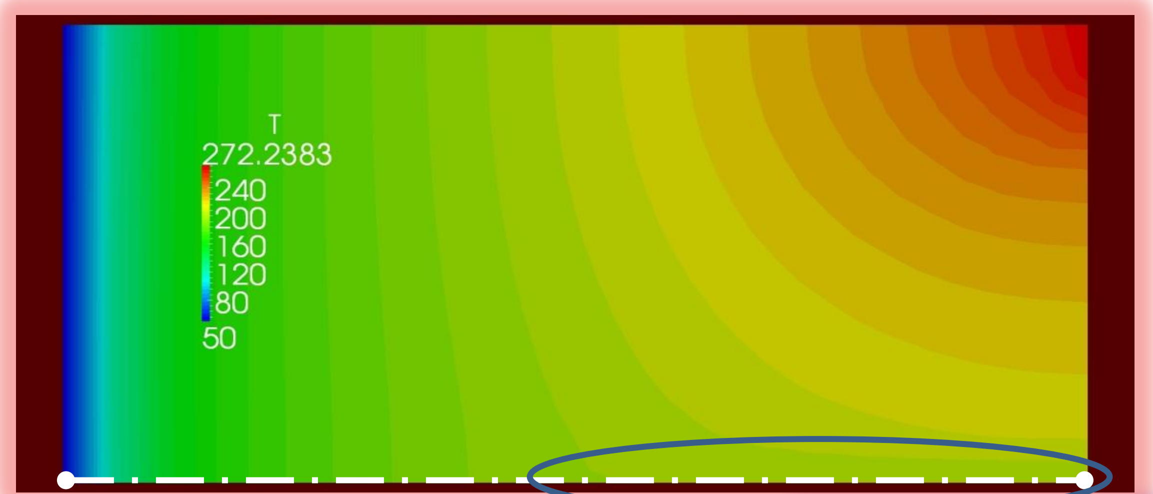


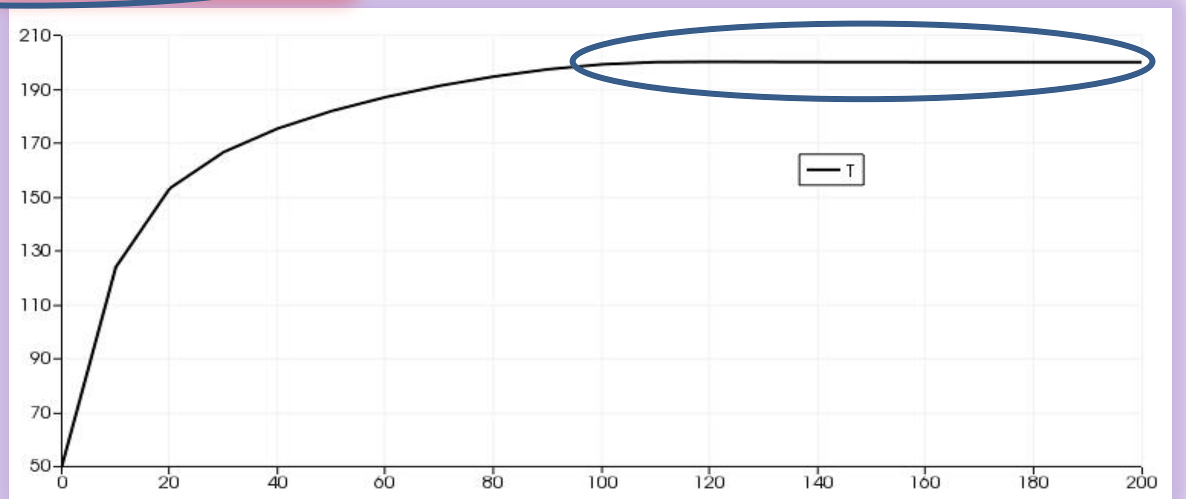
OPTIMAL DISTRIBUTIONS OF CONDUCTIVITIES





TEMPERATURE FOR THE OPTIMAL SOLUTION



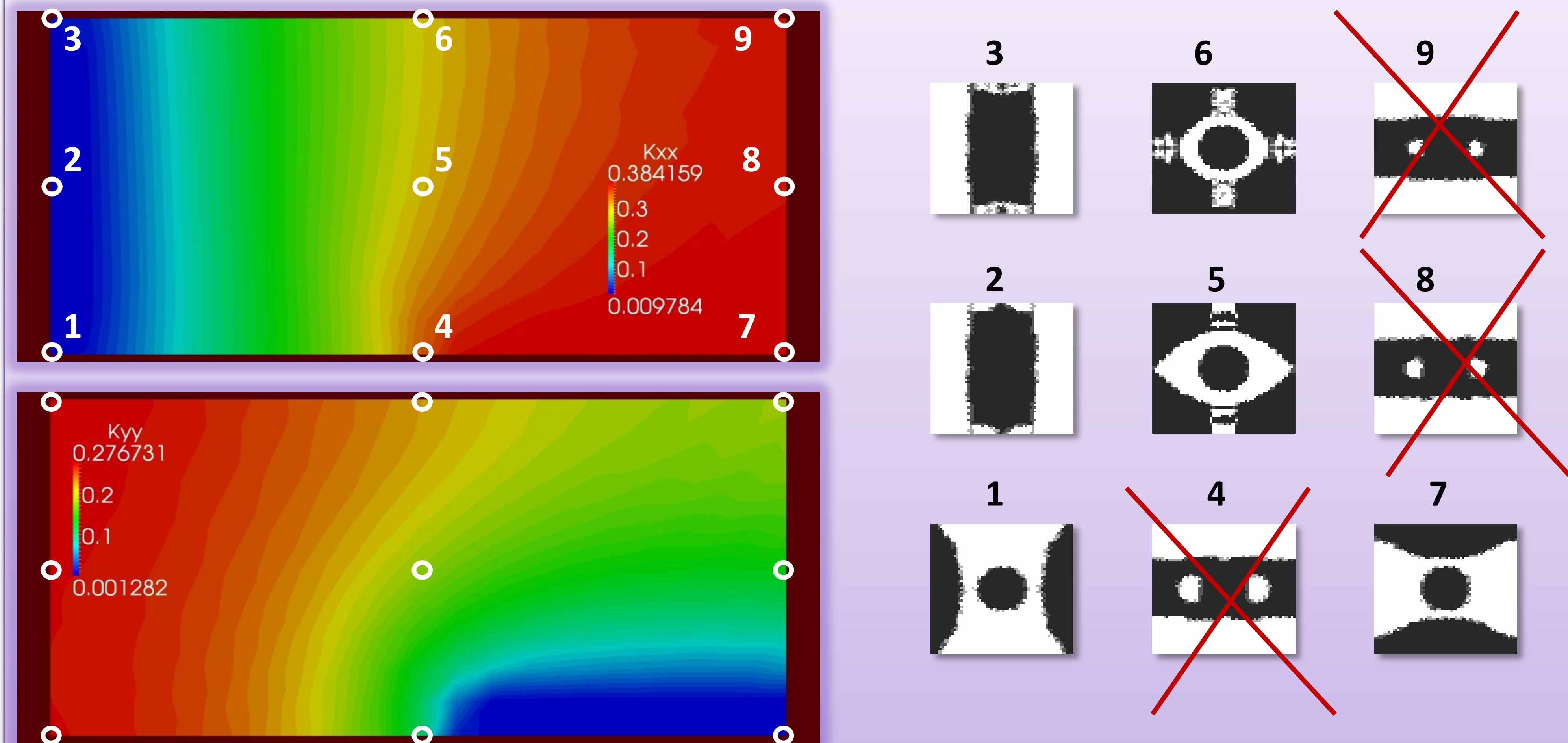


DETERMINATION OF THE MICROSTRUCTURE

- Knowing the optimal macroscopic k_{xx} and k_{yy} at a point of the mesh, a **topology optimization** problem is solved to determine the microstructure we need to achieve such k_{xx} and k_{yy}

- Topology optimization using the **topology derivative** approach

TOPOLOGY OPTIMIZATION AT THE MICROSCALE

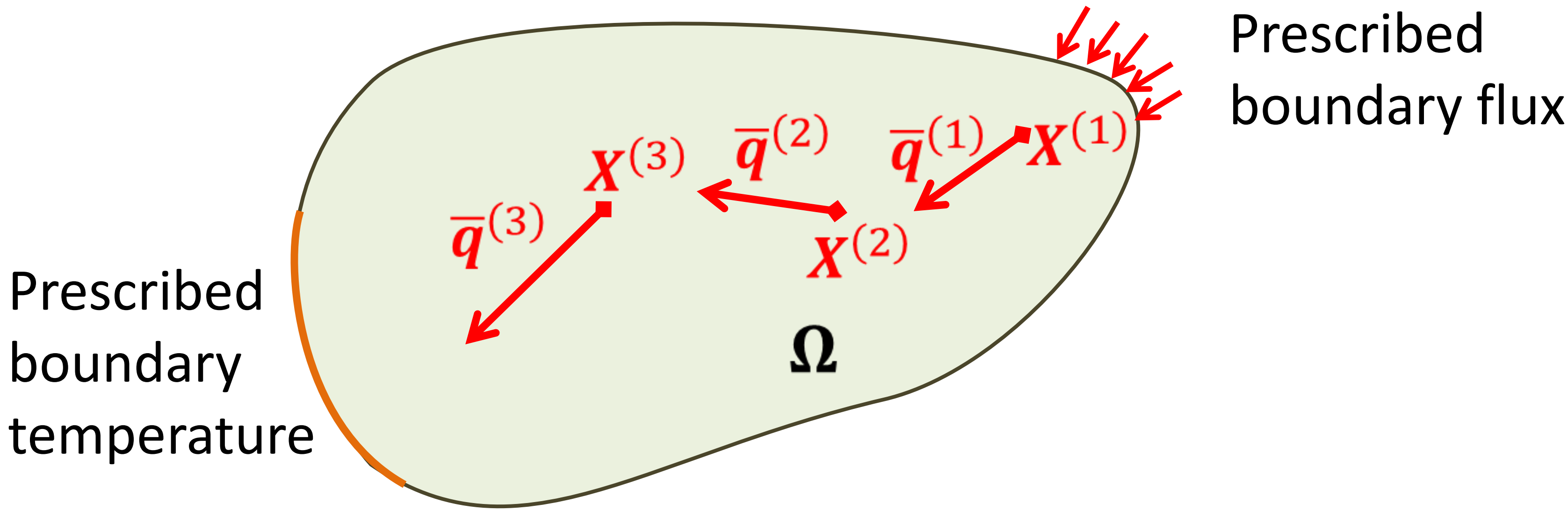


COMPUTATIONAL METAMATERIAL DESIGN FOR HEAT FLUX MANIPULATION

with

I. Peralta, A. Ciarbonetti (CIMEC)

MANIPULATING THE HEAT FLUX



- Given $\overline{\boldsymbol{q}}^{(q)}$ as the desired heat flux at $\boldsymbol{X}^{(q)}$, $q = 1,2,\dots,N_q$, you have to find $\boldsymbol{P}$ such that

$$[-\boldsymbol{k}(\boldsymbol{p})\mathrm{grad}\, T(\boldsymbol{P})]_{\boldsymbol{X}^{(q)}} = \overline{\boldsymbol{q}}^{(q)} \qquad \text{for } i = 1,2,\dots,N_q$$

HEAT FLUX MANIPULATION AS AN OPTIMIZATION PROBLEM

- In order to perform the given task as well as possible, let us solve the nonlinear optimization problem

$$\min_{\text{feasible } \boldsymbol{P}} \underbrace{\frac{1}{N_q} \sum_{q=1}^{N_q} \left\| [-\boldsymbol{k}(\boldsymbol{p}) \operatorname{grad} T(\boldsymbol{P})]_{\boldsymbol{X}^{(q)}} - \overline{\boldsymbol{q}}^{(q)} \right\|^2}_{\mathrm{MSE}(\boldsymbol{P})}$$

  subject to constraints accounting for, *at least*, the feasibility of the microstructure.

☹ Maybe, $\mathrm{MSE}(\boldsymbol{P}) \neq 0$ for all feasible $\boldsymbol{P}$

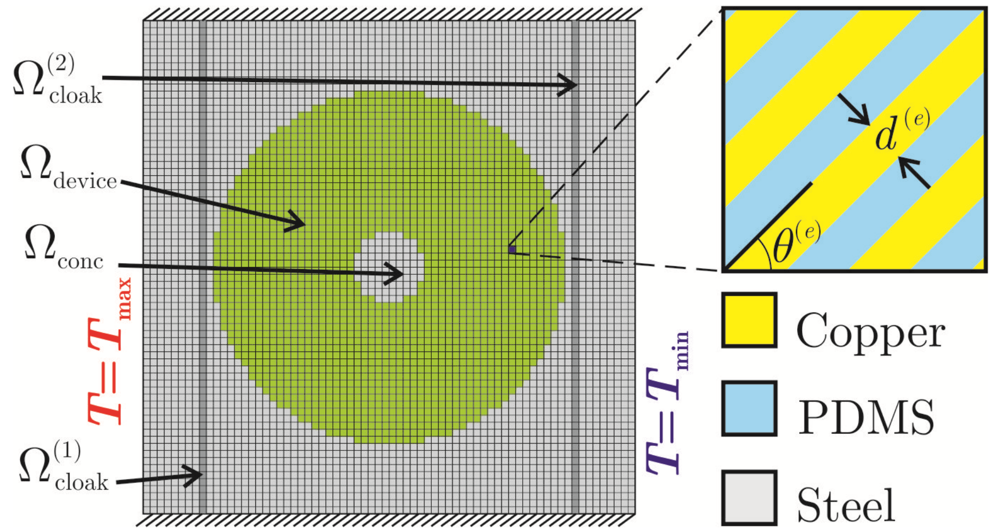
☺ We'll find the "optimal" feasible $\boldsymbol{P}$

DESIGN OF A HEAT FLUX CONCENTRATION AND CLOAKING DEVICE

- To find $\boldsymbol{P}^{\text{opt}} = [d^{(1)}, \theta^{(1)}, \dots, d^{(N)}, \theta^{(N)}]^{\text{opt}}$ ($N = 1896$ is the # elems in Ω_{device}) such that

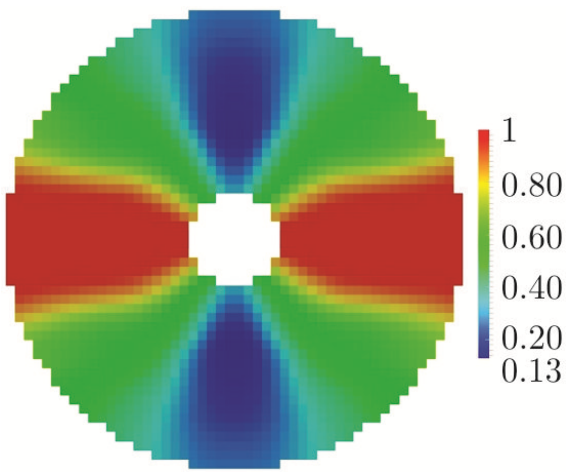
$$\boldsymbol{P}^{\text{opt}} = \arg\min_{\boldsymbol{P}} \frac{1}{N_q} \Sigma_q \left\| [-\boldsymbol{k}(\boldsymbol{p}) \text{grad}\, T(\boldsymbol{P})]_{\boldsymbol{X}^{(q)}} - \overline{\boldsymbol{q}}^{(q)} \right\|^2$$

subject to the box constraints

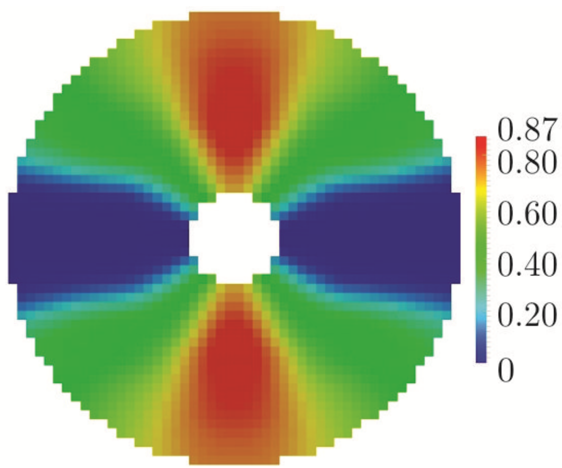


HEAT FLUX CONCENTRATION AND CLOAKING: OPTIMAL METAMATERIAL DISTRIBUTION

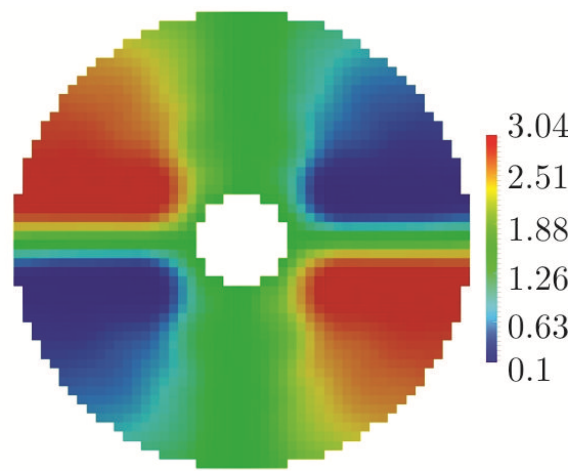
Fraction of copper



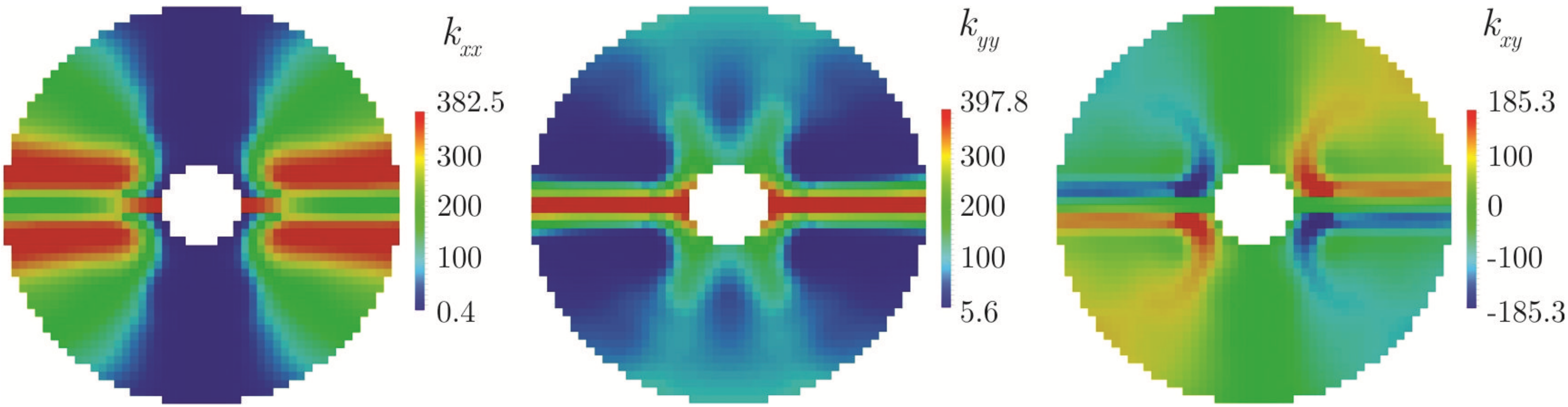
Fraction of PDMS



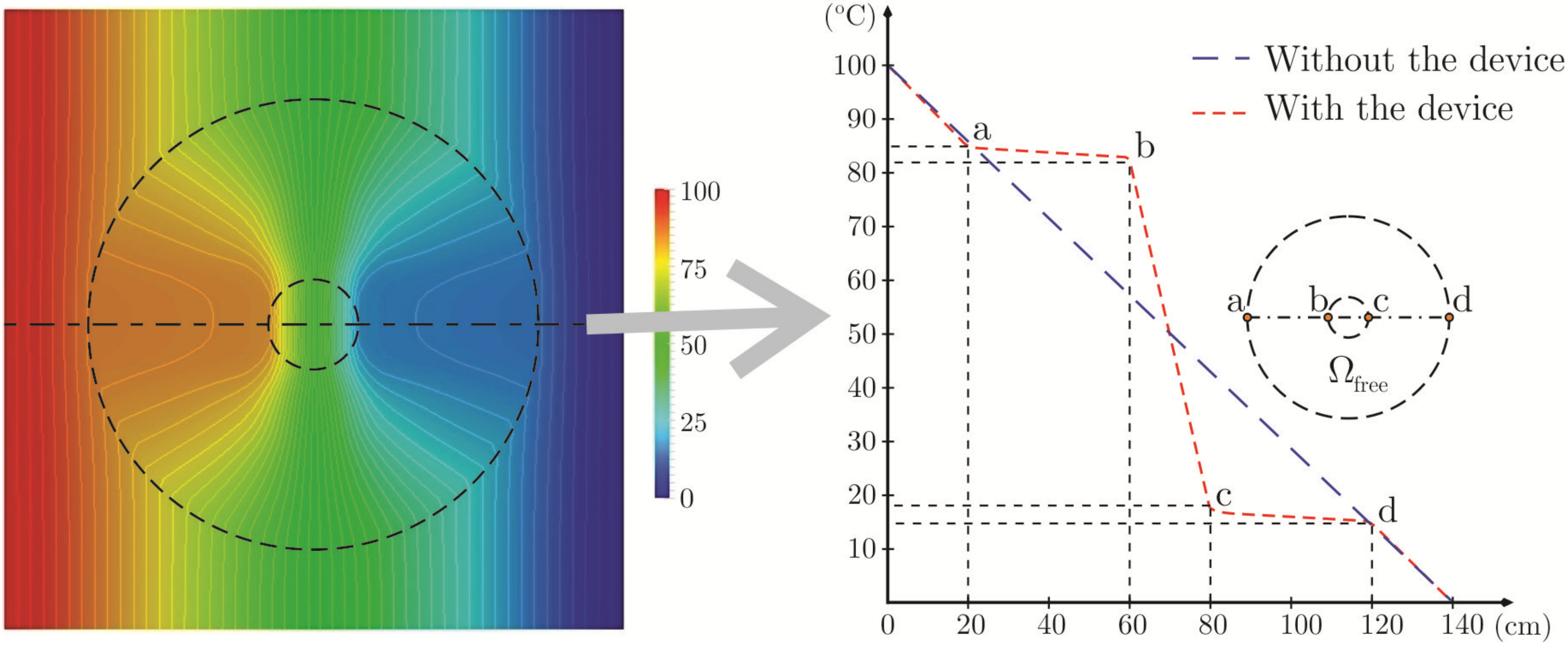
Orientation



HEAT FLUX CONCENTRATION AND CLOAKING: OPTIMAL CONDUCTIVITY DISTRIBUTION



HEAT FLUX CONCENTRATION AND CLOAKING: OPTIMAL TEMPERATURE DISTRIBUTION



* Peralta, Fachinotti & Ciarbonetti, Scientific Reports 2017 (http://www.nature.com/articles/srep40591)

EASY-TO-MAKE HEAT FLUX MANIPULATING DEVICES USING DISCRETE MATERIAL OPTIMIZATION (DMO)

with

I. Peralta, A. Ciarbonetti (CIMEC)

MULTIPHASE TOPOLOGY OPTIMIZATION

- The material at the element $\Omega^{(e)}$ is either one of M predefined, candidate materials with conductivities $\boldsymbol{k}_1, \boldsymbol{k}_2, \dots, \boldsymbol{k}_M$
- Each material maybe a **metamaterial** itself
- The design variables for $\Omega^{(e)}$ are the fractions $f_m^{(e)}$ of each material $m = 1,2, \dots, M$
- The conductivity at $\Omega^{(e)}$ is defined by the mixture law

$$\boldsymbol{k}^{(e)} = f_1^{(e)}\boldsymbol{k}_1 + f_2^{(e)}\boldsymbol{k}_2 + \cdots + f_M^{(e)}\boldsymbol{k}_M$$

- We must use an optimization algorithm driving to optimal solutions with $f_m^{(e)} \approx 1$ or $f_m^{(e)} \approx 0$

DISCRETE MATERIAL OPTIMIZATION

- Using the **Discrete Material Optimization (DMO)** approach proposed by Stegmann & Lund (IJNME 2005), we define:

$$f_m^{(e)} = \frac{f_m^*(\boldsymbol{p}^{(e)})}{\sum_i f_i^*(\boldsymbol{p}^{(e)})} = f_m(\boldsymbol{p}^{(e)})$$

$$\text{with } f_m^*(\boldsymbol{p}^{(e)}) = \left(\rho_i^{(e)}\right)^p \prod_{j=1, j\neq i}^{M} \left[1 - \left(\rho_i^{(e)}\right)^p\right]$$

- The design variables for $\Omega^{(e)}$ are $p^{(e)} = [\rho_1^{(e)}, \rho_2^{(e)}, \dots, \rho_M^{(e)}]$

  $\rho_i^{(e)}$: artificial density of material m at $\Omega^{(e)}$, like in Topology Optimization
- $p \geq 3$, like in SIMP for Topology Optimization
- This definition strongly forces $\rho_{j\neq i}^{(e)} \to 0$ when $\rho_i^{(e)} \to 1$
- It doesn't need a constraint (one per finite element!) to make $\sum_i f_i^{(e)} = 1$

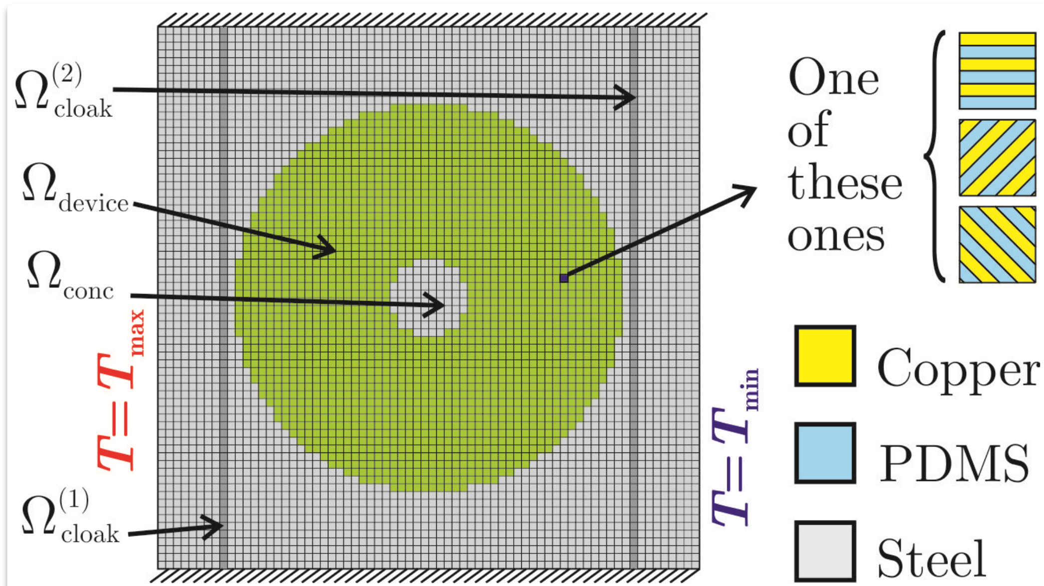
DESIGN OF A HEAT FLUX CONCENTRATION AND CLOAKING DEVICE USING DMO

- To find $\boldsymbol{P}^{\mathrm{opt}} = [\rho_1^{(1)}, \rho_2^{(1)}, \rho_3^{(1)}, \dots, \rho_1^{(1896)}, \rho_2^{(1896)}, \ \rho_3^{(1896)}]^{\mathrm{opt}}$ such that

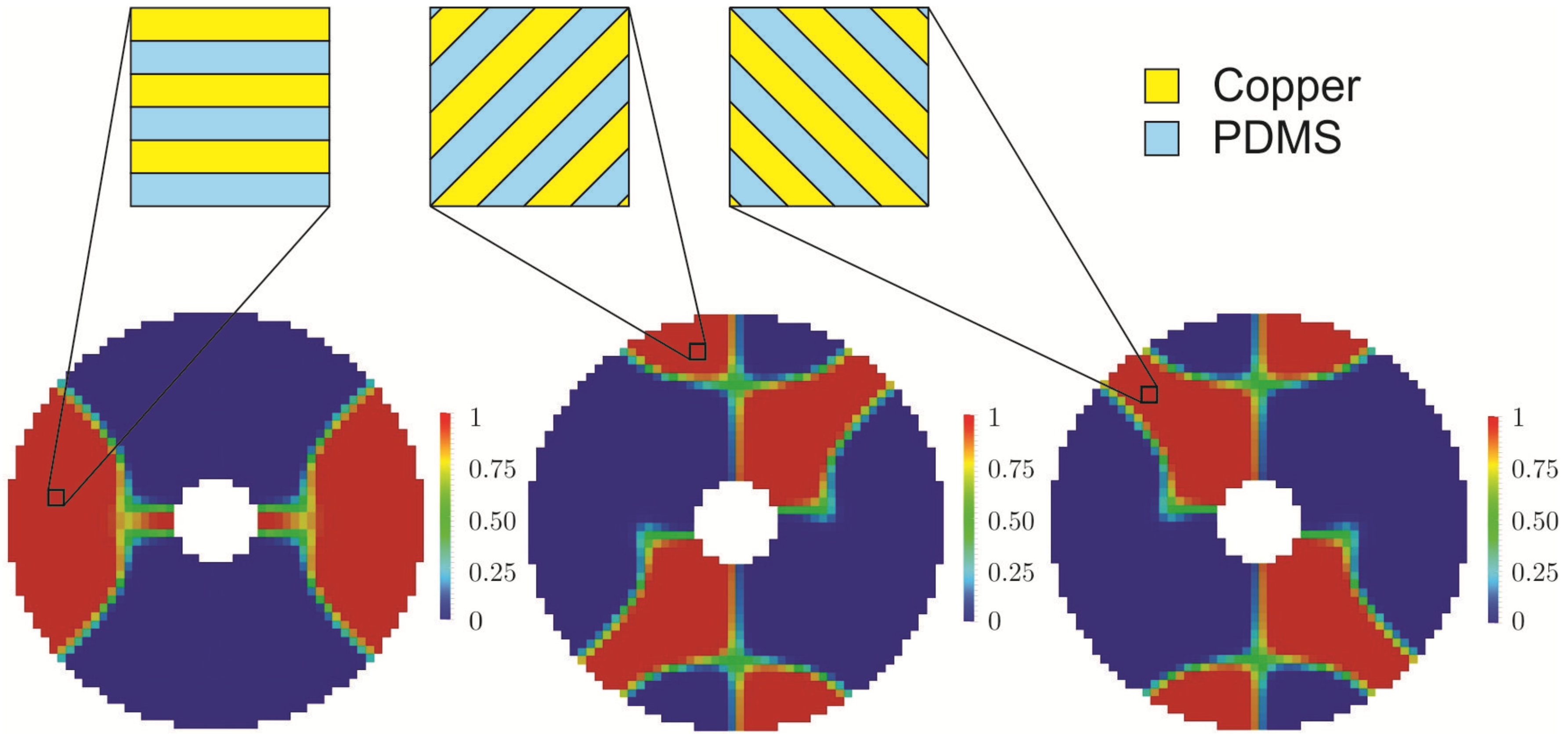
$$\boldsymbol{P}^{\mathrm{opt}} = \arg\min_{\boldsymbol{P}} \frac{1}{N_q} \sum_q \left\| \left[-\boldsymbol{k}(\boldsymbol{p}) \operatorname{grad} T(\boldsymbol{P}) \right]_{\boldsymbol{X}^{(q)}} - \overline{\boldsymbol{q}}^{(q)} \right\|^2$$

subject to the box constraints

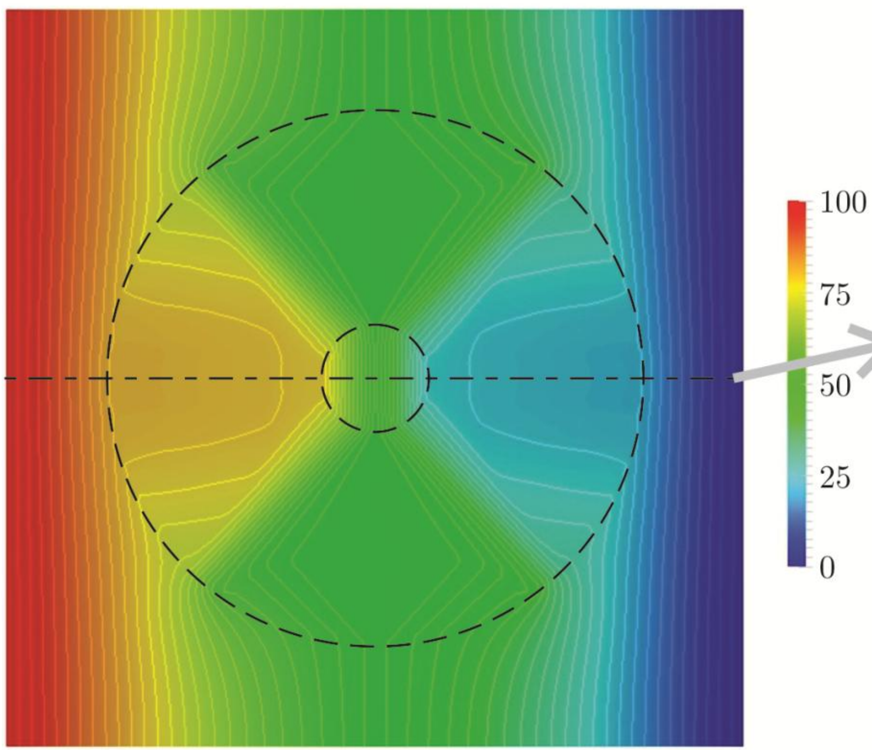
$0 \leq P \leq 1$

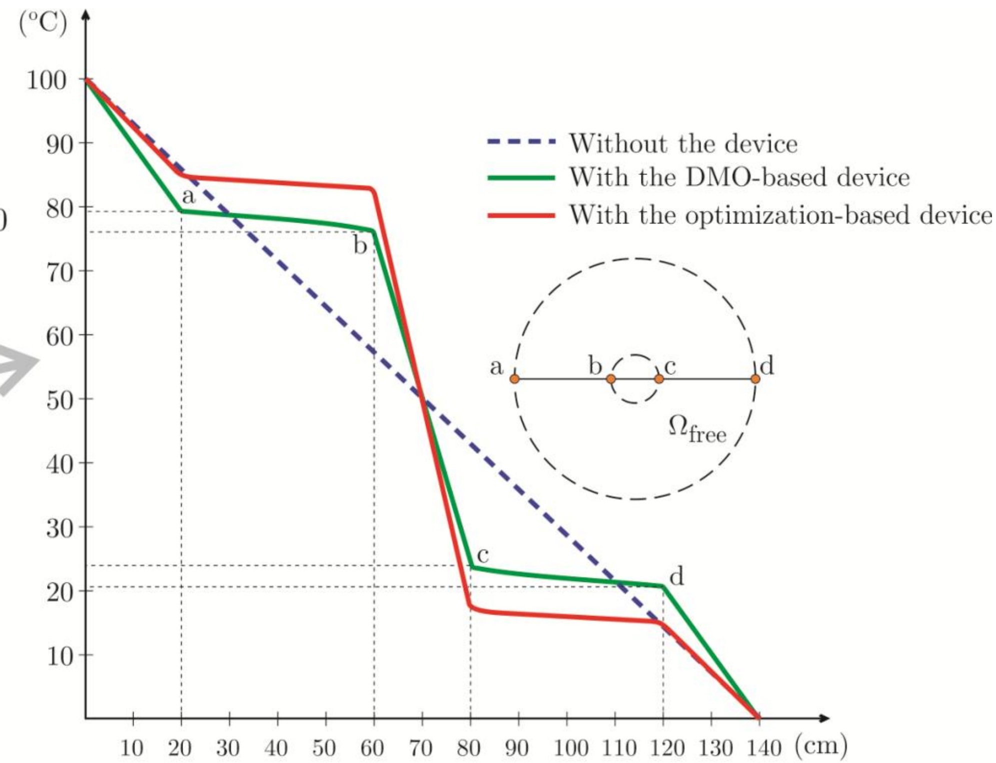


HEAT FLUX CONCENTRATION AND CLOAKING USING DMO: OPTIMAL METAMATERIAL DISTRIBUTION



HEAT FLUX CONCENTRATION AND CLOAKING USING DMO: OPTIMAL TEMPERATURE DISTRIBUTION





EASIEST-TO-MAKE HEAT FLUX MANIPULATING DEVICES USING TOPOLOGY OPTIMIZATION

with

A. Ciarbonetti, I. Peralta (CIMEC),

I. Rintoul (INTEC)

TOPOLOGY OPTIMIZATION

- The material at the element $\Omega^{(e)}$ is either one of two predefined, candidate materials with conductivities $\boldsymbol{k}_1, \boldsymbol{k}_2$
- Each material is isotropic
- There is only one design variable for $\Omega^{(e)}$: the artificial density $\rho^{(e)}$ of material 1
- The conductivity at $\Omega^{(e)}$ is defined using **SIMP (Solid Isotropic Material with Penalization)**

$$\boldsymbol{k}^{(e)} = \left(\rho^{(e)}\right)^p \boldsymbol{k}_1 + \left[1 - \left(\rho^{(e)}\right)^p\right] \boldsymbol{k}_2$$

- *A priori*, using $p \geq 3$, $\rho^{(e)} \rightarrow 0$ or $\rho^{(e)} \rightarrow 1$ for the optimal solution

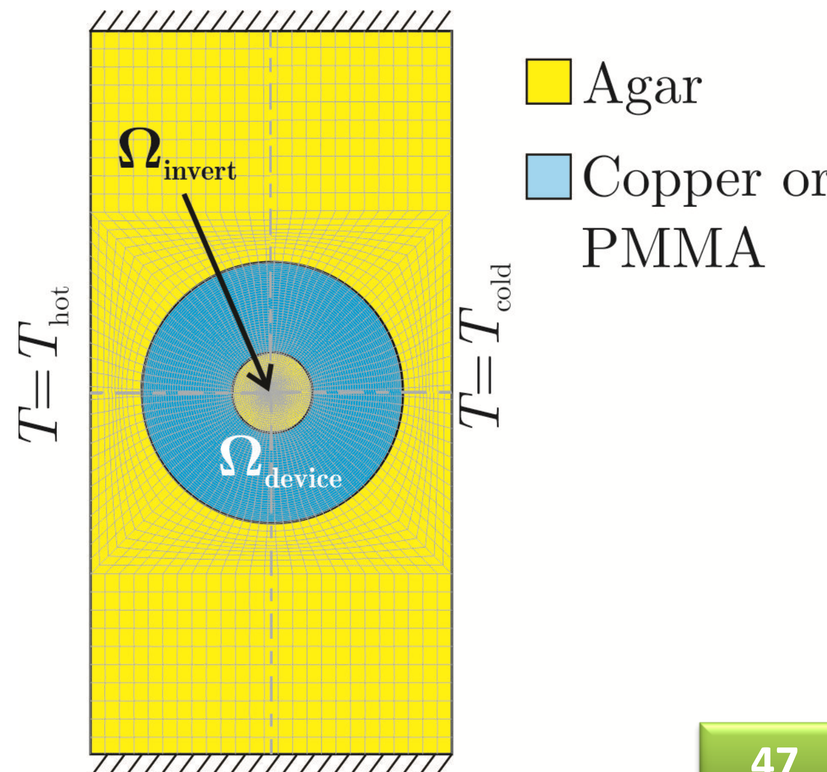
DESIGN OF HEAT FLUX INVERTER USING TOPOLOGICAL OPTIMIZATION

- To find $\boldsymbol{P}^{\text{opt}} = [\rho^{(1)}, \dots, \rho^{(4000)}]^{\text{opt}}$ such that

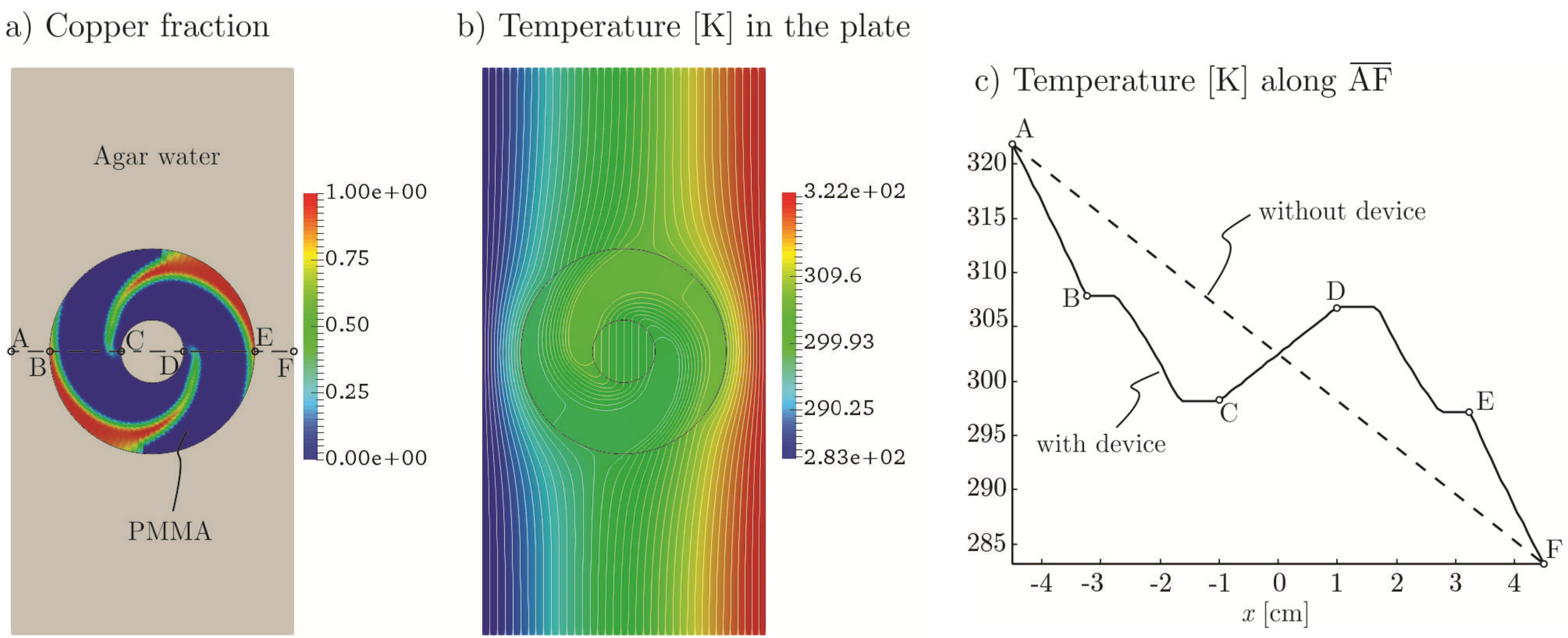
$$\boldsymbol{P}^{opt} = \arg\min_{\boldsymbol{P}} \frac{1}{N_q} \sum_q \left\| [-\boldsymbol{k}(\boldsymbol{p}) \operatorname{grad} T(\boldsymbol{P})]_{\boldsymbol{X}^{(q)}} - \overline{\boldsymbol{q}}^{(q)} \right\|^2$$

subject to the box constraints

$$0 \leq \rho^{(e)} \leq 1$$

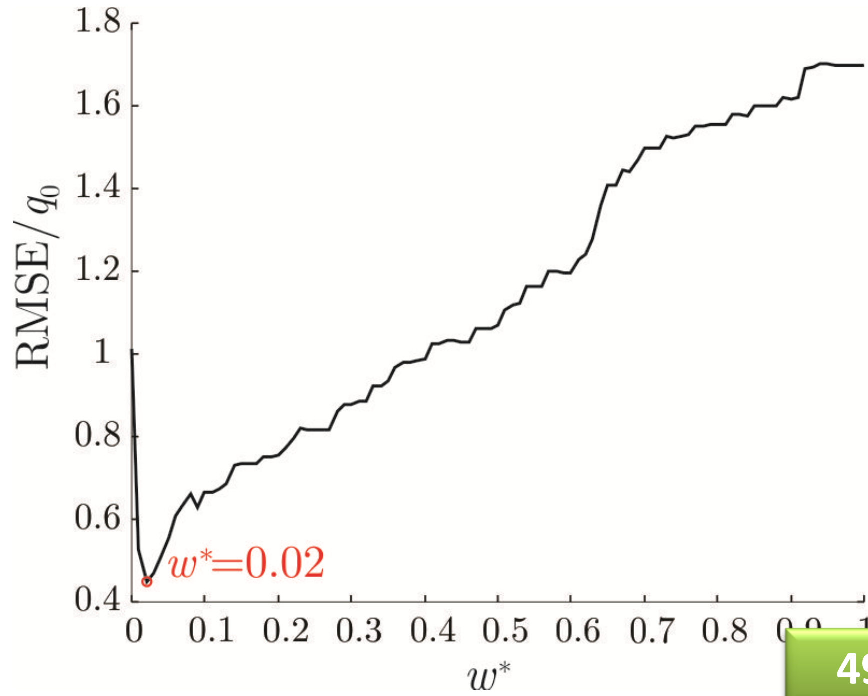


HEAT FLUX INVERTER: TOPOLOGY OPTIMIZATION SOLUTION

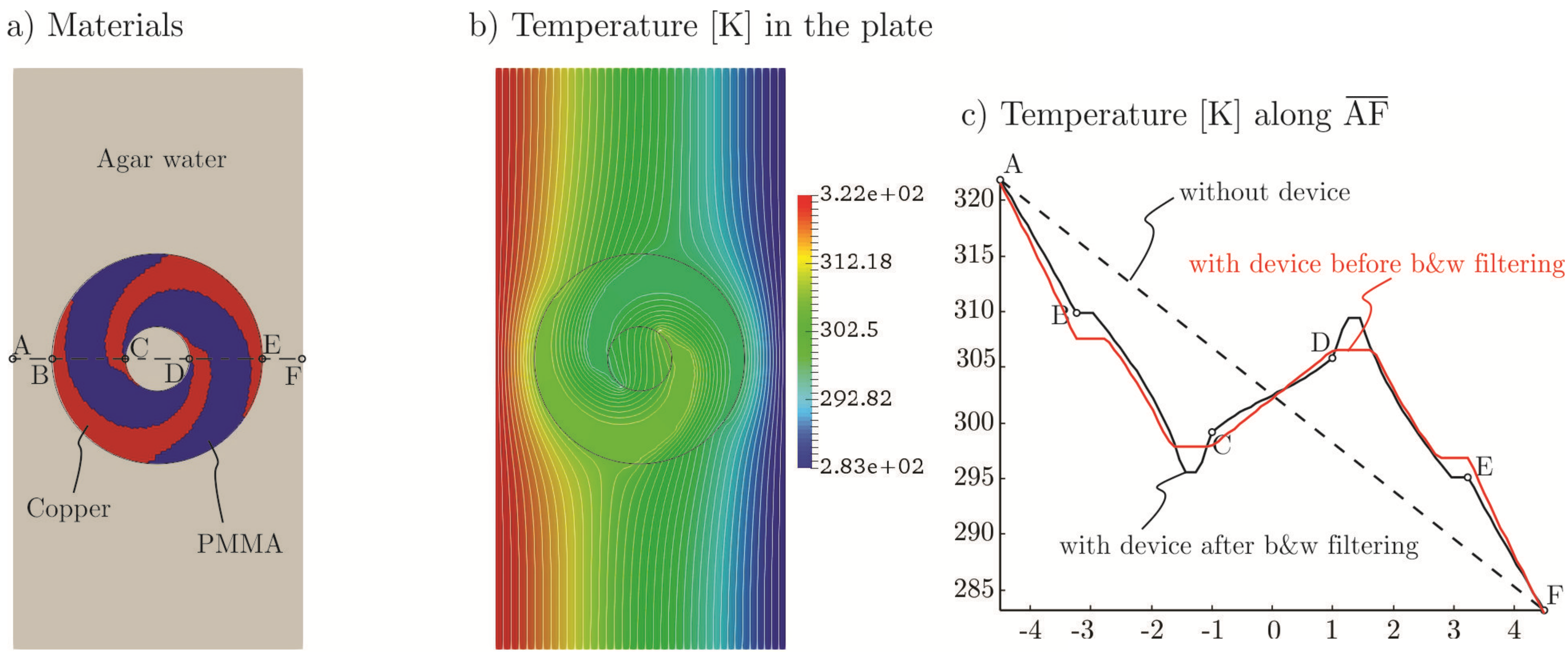


HEAT FLUX INVERTER: BLACK AND WHITE FILTERING

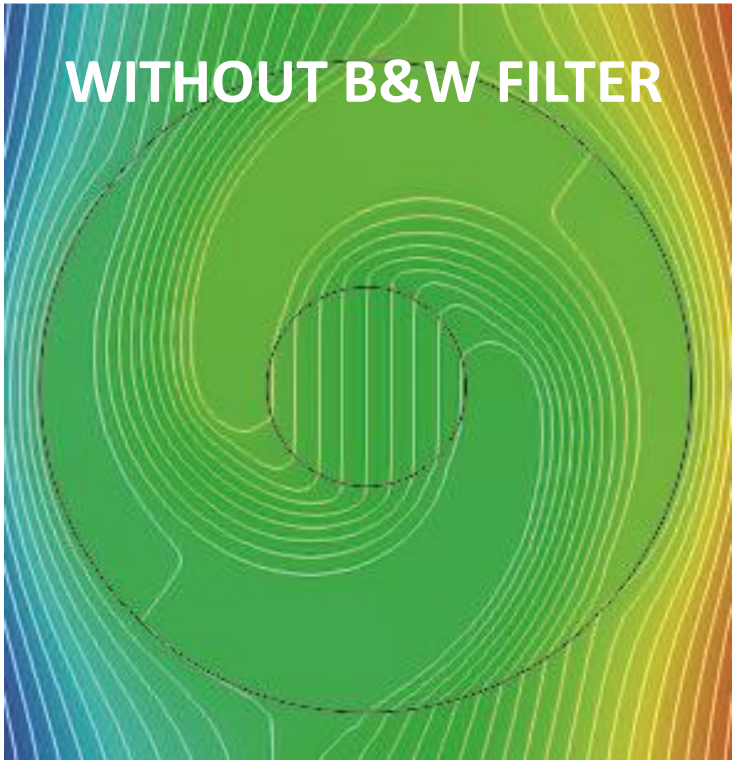
- For manufacturability, regions with intermediate material fractions ("grey zones") must be avoided
- Black and white filters (Sigmund 2007) serve to this end
- Here, a simple *a posteriori* b&w filter is preferred: material fraction greater than w^* is taken to 1; otherwise, it is taken to 0

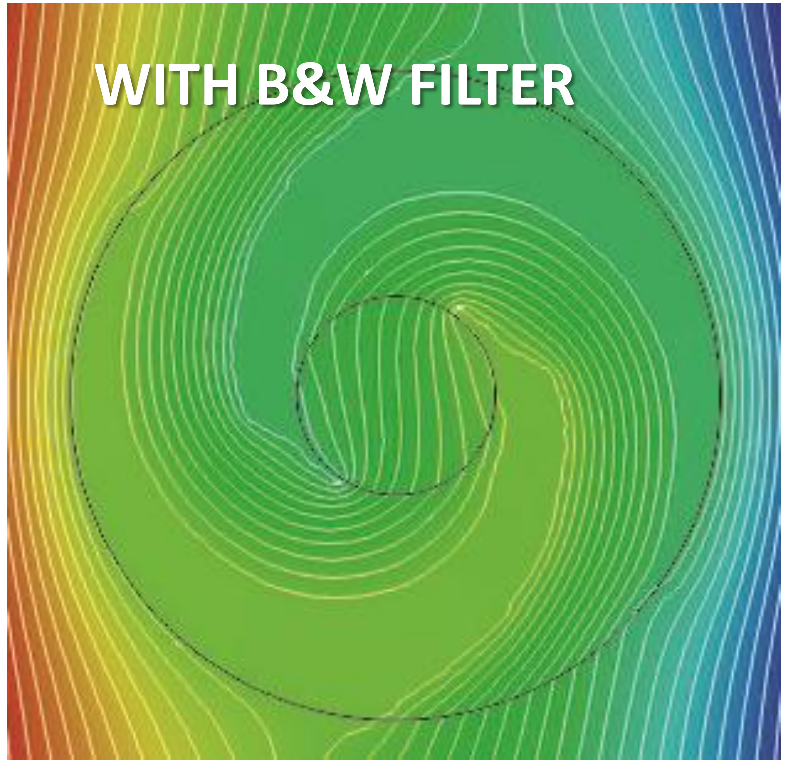


HEAT FLUX INVERTER:
TOPOLOGY OPTIMIZATION SOLUTION
+ BLACK AND WHITE FILTERING



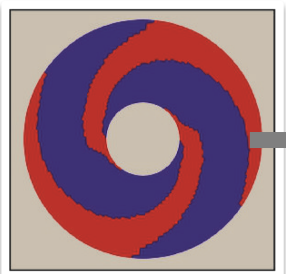
HEAT FLUX INVERTER: TOPOLOGY OPTIMIZATION WITH AND WITHOUT BLACK AND WHITE FILTERING

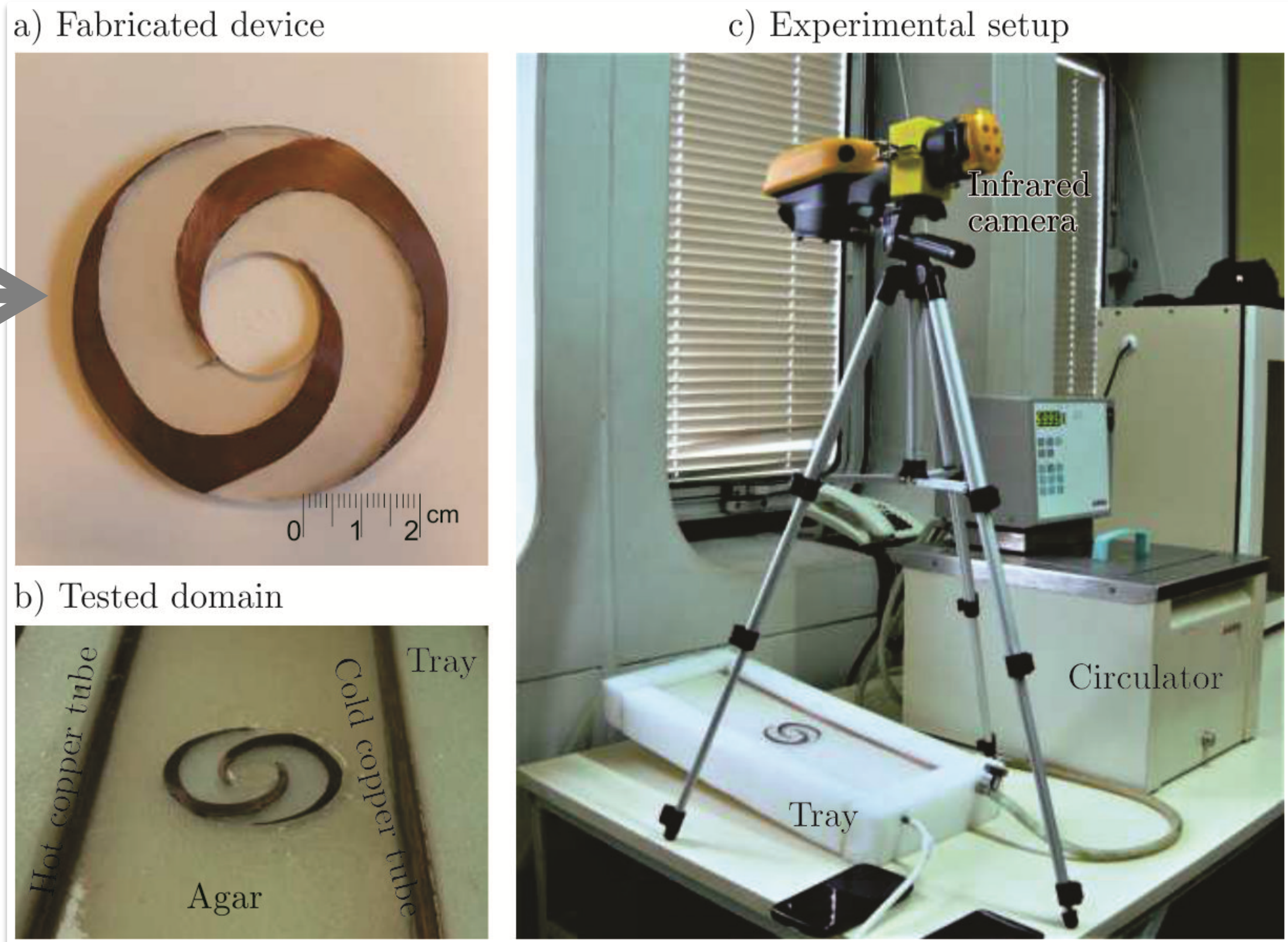




HEAT FLUX INVERTER: EXPERIMENTAL VALIDATION

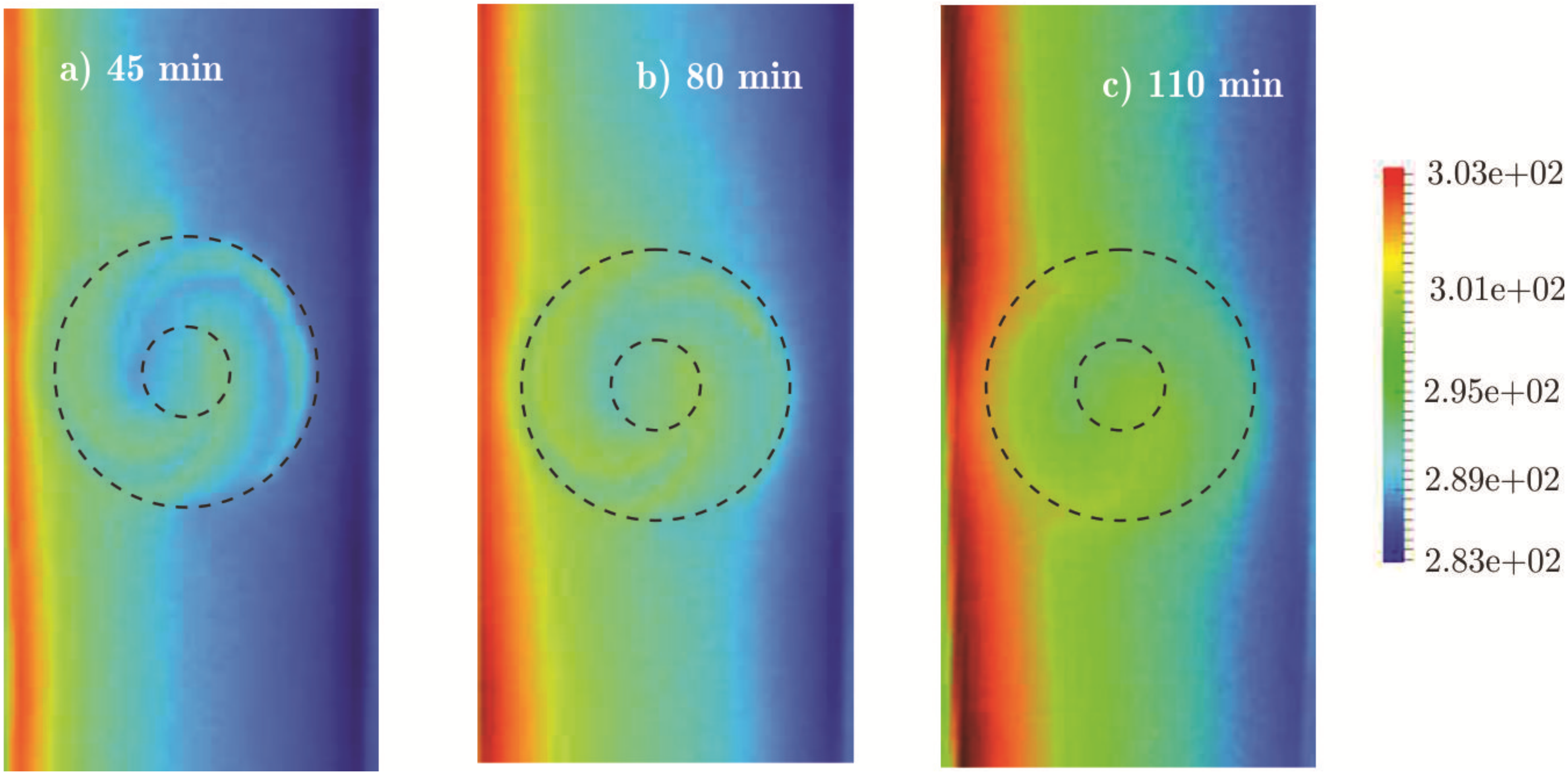
Computationally designed device



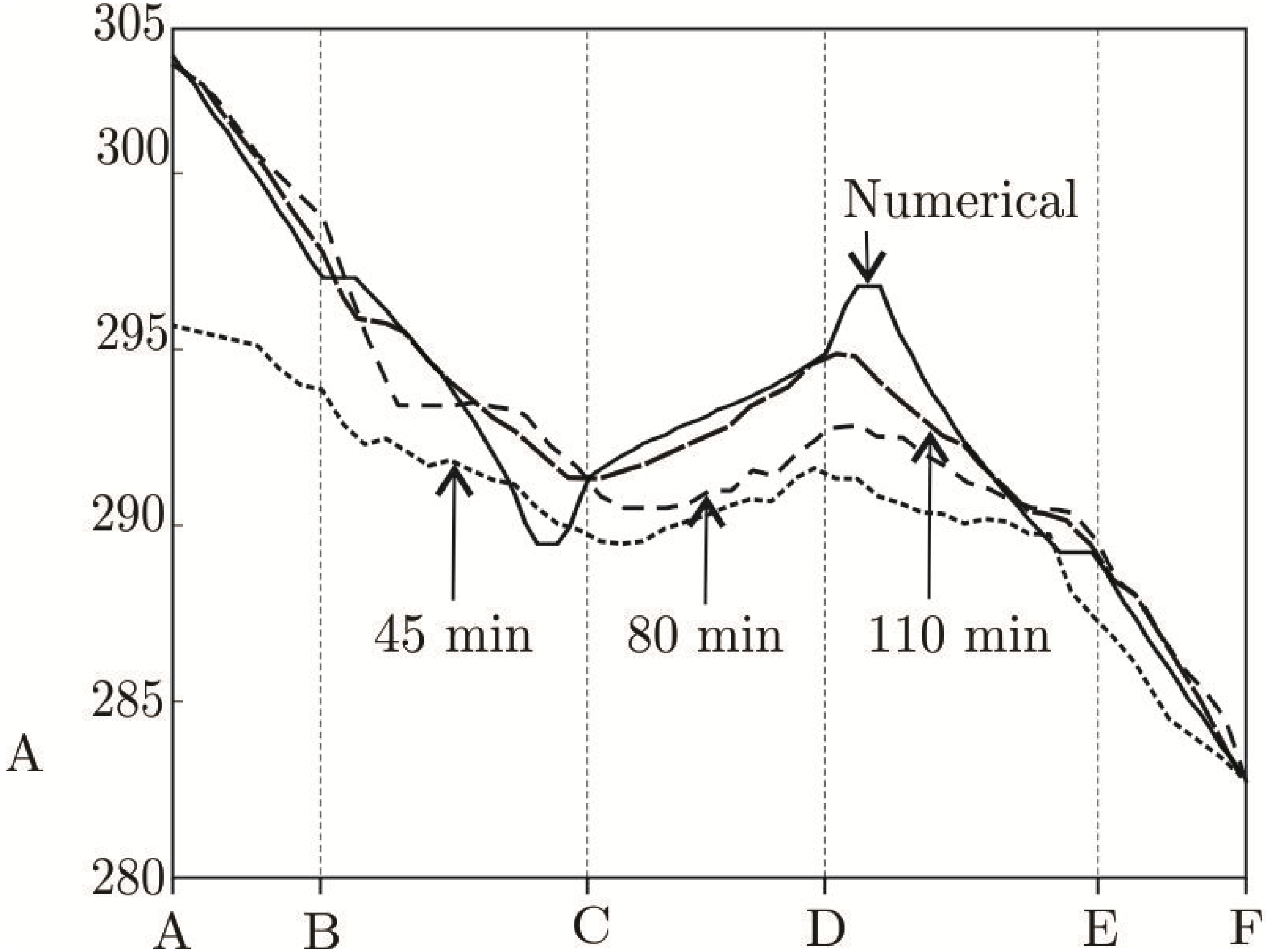


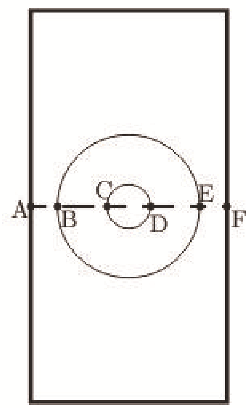
HEAT FLUX INVERTER: EXPERIMENTAL VALIDATION

Temperature evolution during the experiment [K]



HEAT FLUX INVERTER: EXPERIMENTAL VALIDATION

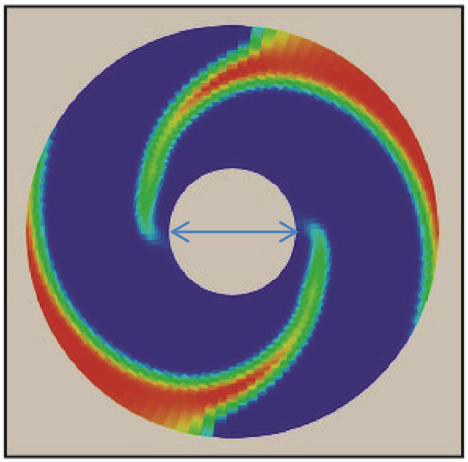




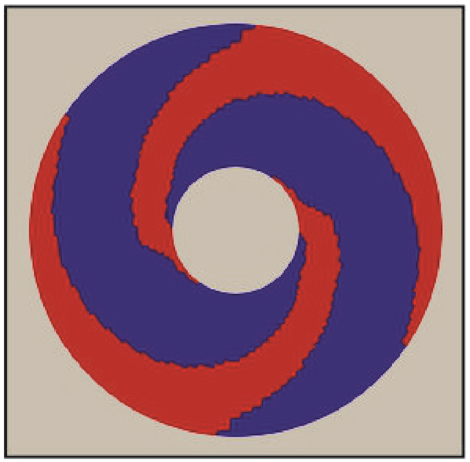
HEAT FLUX INVERTER: COMPARISON WITH NARAYANA AND SATO´S INVERTER

- Accomplishment of the inversion task

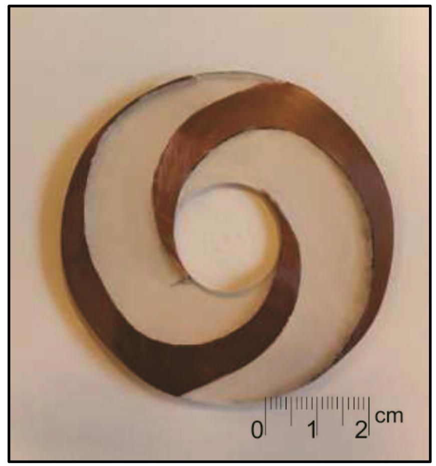
$$q_{\text{invert}} = -k_{\text{agar}} \frac{T_D - T_C}{|CD|} = -\alpha q_0$$



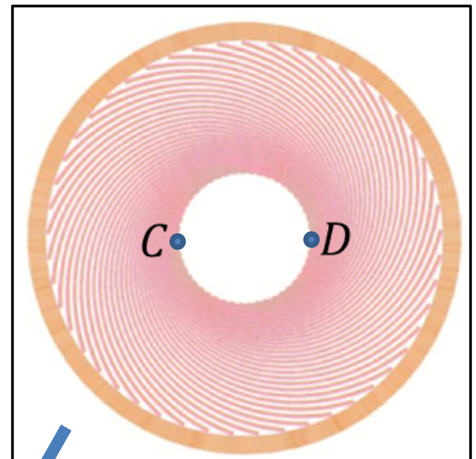
$\alpha = 0.997$



$\alpha = 0.778$



$\alpha = 0.774$



$\alpha = 0.395$

S. Narayana & Y. Sato, “Heat Flux Manipulation with Engineered Thermal Materials”, Physical Review Letters 2012

HEAT FLUX INVERTER: COMPARISON WITH NARAYANA AND SATO´S INVERTER

- Narayana and Sato’s device, designed using the **transformation-based** aproach inherited from electromagnetism, has 96 PMMA-copper laminate arms to invert the flux coming from every where
  - The current device, designed using the **optimization-based** approach, has 2 copper arms to invert the given heat flux
- Narayana and Sato’s device also performs cloaking as a collateral effect of its transformation-based design
  - The current device doesn’t perform cloaking (it was not required)

  $\Rightarrow$ better accomplishment of the inversion task

ADVANTAGES OF THE OPTIMIZATION-BASED DESIGN

- The optimization-based design (OBD) gives you the material distribution (inducing an adequate conductivity distribution) to accomplish a given task
  - The transformation-based design (TBD) gives you a required anisotropic conductivity field, and then you have to manage to achieve it
- OBD can be applied to arbitrary tasks, geometries and boundary conditions
  - TBD has not been (can't be?) applied to arbitrary tasks, geometries and boundary conditions
- OBD gives you the optimal device to accomplish the given task
  - TBD gives you the device to accomplish the given task + cloaking

  $\Rightarrow$ overdimensioning

  $\Rightarrow$ poorer accomplishment of the given task

PERSPECTIVES

- Robustness
  - instabilities
  - grey zones
  - convergence
- 3D
- Applications
  - Isolation: to deviate the heat flux from the zones where it is undesired, to drive it to somewhere where it maybe useful
  - Optimization of Austempered Ductile Iron (with B. Tourn)
    - Mechanical properties depend on the thermal history
    - Topology and heat treatment optimization to make a macroscopic piece have a given mechanical response
  - Metamaterials for wind turbine blades (with A. Albanesi)
- Fabrication, patents

ACKNOWLEDGEMENTS

- European Research Council under the Seventh Framework Program
  - ERC Grant Agreement n. 320815 “COMP-DES-MAT: Advanced Tools for Computational Design of Engineering Materials”, leaded by X. Oliver (CIMNE-UPC)

- Council for Scientific and Technical Research of Argentina (CONICET)
  - Research project PIP 2012-2014 GI-1105: “Computational Simulation of Multiphysics Problems. Application to Metal Solidification and Micro-Electro-Mechanical Devices”

- You, for your attention