Master seminar Material and Topology optimization

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Organizational issues (time line)

- Introduction to topics: first week of semester
- Selection of topic via Stud-On
- Presentations of topics: January and February 2025
- Between: 14/10/2024 and **20/12/2024 at least one meeting with the supervisors!**

- … of course, more meetings can be scheduled on demand

Deliveries

- Handout
  - ~10 pages of Latex
  - First draft two weeks before presentation
  - Final version provided for the other the day before the presentation latest

- Presentation
  - ~60 minutes including discussion
  - Use latex or powerpoint for slides
  - Can be extended by white-/blackboard presentations

Master‘s thesis

- In summer semester
- potentially possible
- not necessarily but possibly based on seminar topics
- supervised by various members of our group depending on topic

Topics

- 10 topics will be briefly presented
- Typically a mix of theory and practice (programming involved!)
- Most of them extend contents of ISMO lecture
- Suggestion of “own“ topic still possible
  → requires accurate literature specification by students

Topics overview

Optimization solvers for MO/TO problems

1) The method of moving asymptotes (MMA): sequential programming, separability, Lagrange duality, implementation
2) MMA: convergence analysis

[MMA1, MMA2, MMA3]

Regularization of MO/TO problems

3) The density filter approach (idea, analysis, implementation in OCM or MMA method)

[REG1]

Topics overview

Material optimization extensions

4) Optimization with anisotropic materials: theory (existence, convergence), numerical realization
5) Material design: the homogenization method and inverse homogenization
6) The two-scale optimization approach for stiffness and buckling averse structures

[ANISO, HOM1,HOM2,BUCK]

MO with advanced state problems

7) MO in presence of cracks by Peridynamics model

[PERI1,PERI2]

Topics overview

Diverse

8) The feature mapping approach for TO/MO (concept and numerical realization, extensions)

[FM1,FM2]

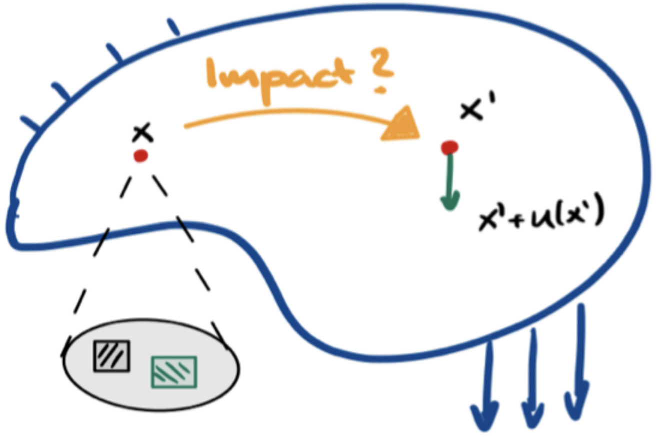
9) Porous materials: modelling of saturation through Young-Laplace-Algorithm and a PDE-based approach

[YL1]

10) Optimal on-ramp control for equilibrium measurements in analytical ultracentrifugation

[UC]

The Method of Moving Asymptotes



e. g. compliance: $J(\boldsymbol{D}) = u(\boldsymbol{D})^\top K(\boldsymbol{D}) u(\boldsymbol{D})$

$$= \sum_i u(\boldsymbol{D})^\top B_i^\top D_i B_i u(\boldsymbol{D})$$

non-separability solely through state …

mathematical motivation for separable model

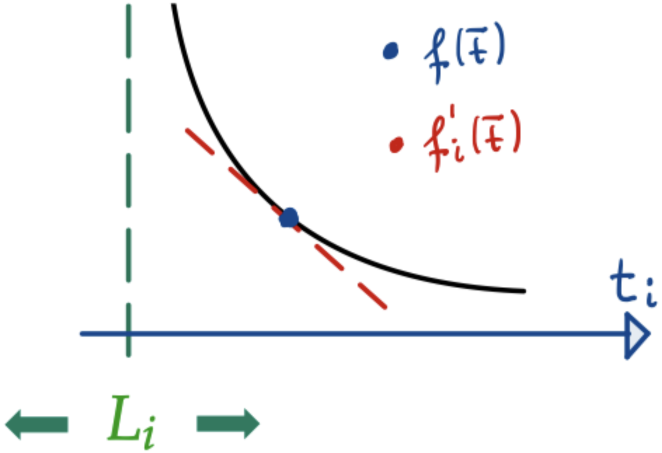
- $\widehat{f}(x) = \sum_i \widehat{f_i}(x_i) \;\rightarrow\; \min_x \sum_i \widehat{f_i}(x_i) \equiv \sum_i \min_{x_i} \widehat{f_i}(x_i)$
- solve *n* univariate problems (fully equivalent!)

White board illustration …

The Method of Moving Asymptotes

- Svanberg ('87, '95), Fleury ('86, '89, '94), to name only the pioneers …
- separable Ansatz (here simplified and for 'lower asymptotes' only):

$$f(t) \approx \widehat{f}(t) = C + \sum_i \frac{p_i}{t_i - L_i}$$



- C, p_i ($\sim f_i'(\bar{t})$, $i-$th partial derivative) chosen to match first order correctness
- L_i (asymptote) computed based on heuristics (e. g. Svanbverg, Zillober, …), 2nd order information (e. g. Duysinx, …), ...

MMA (topic 1: separable models and duality)

- distinguish box constraints and general inequality constraints; switch back to MO notation ...

$$\min_{\rho \in [\underline{\rho}, 1]^m} f(\rho), \quad \text{s.t. } g_j(\rho) \le 0, \; j = 1, 2, \ldots, n_g$$

- simplest approach: Lagrange function

$$L(\rho, \lambda) = f(\rho) + \sum_j \lambda_j g_j(\rho)$$

- use dual method based on Lagrange dualization
- assume separability, i. e. use separable $\widehat{f}$ and $\widehat{g}_j$ and form separable Lagrangian $\widehat{L}$ for those; then:

$$\min_{\rho \in [\underline{\rho}, 1]^m} \widehat{f}(\rho), \text{ s.t. } \widehat{g}(\rho) \le 0_{n_g} \iff \min_{\rho \in [\underline{\rho}, 1]^m} \max_{\lambda \ge 0_{n_g}} \widehat{L}(\rho, \lambda) \; (*)$$

- now dualize (switch min and max):

$$(*) \iff \max_{\lambda \ge 0_{n_g}} \underbrace{\min_{\rho \in [\underline{\rho}, 1]^m} \widehat{L}(\rho, \lambda)}_{:= d(\lambda) \text{ (dual function)}}$$

- evaluation of $d(\lambda)$ as before (exploiting separability!)

The Method of Moving Asymptotes

TOPIC 1 [MMA1, MMA2] :

- Separable approximation
- MMA approximation
- Dual algorithm
- Implementation and demonstration

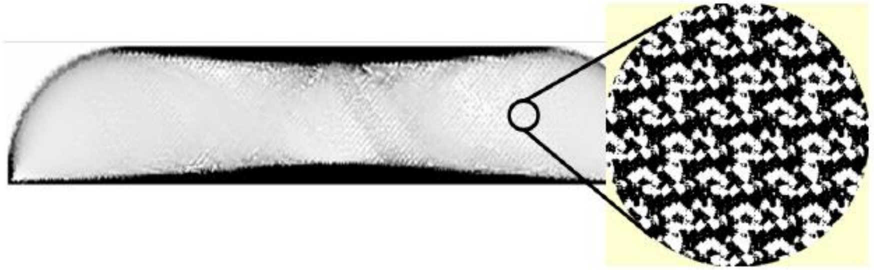
TOPIC 2 [MMA2, MMA3] :

- Outer algorithm (sequential separable approximation)
- Globalization
- Convergence Theory

Filter regularization (instead of Lipschitz-constraints)

- define neighborhood of element Ω_i; let ω_i be mid point of Ω_i

$$\mathcal{N}_i^R := \left\{ j \mid \|\omega_i - \omega_j\| \leq R \right\}$$



- sensitivity filtering (. . . heuristic!): use

$$\frac{\widetilde{\partial\Phi}}{\partial\rho_i} = \frac{\sum_{j\in\mathcal{N}_i} d_j\rho_j \frac{\partial\Phi}{\partial\rho_j}}{\sum_{j\in\mathcal{N}_i} d_j} \qquad (d_j = \max\{R - \|x_j - x_i\|, 0\})$$

instead of $\partial\Phi/\partial\rho_i = p\rho_i^{p-1} u^\top K_i u$ in OC scheme . . .

- mathematically more rigorous: density filtering $\tilde{\rho}_i = \frac{\sum_{j\in\mathcal{N}_i} d_j\rho_j}{\sum_{j\in\mathcal{N}_i} d_j} \qquad (d_j = R - \|x_j - x_i\|)$

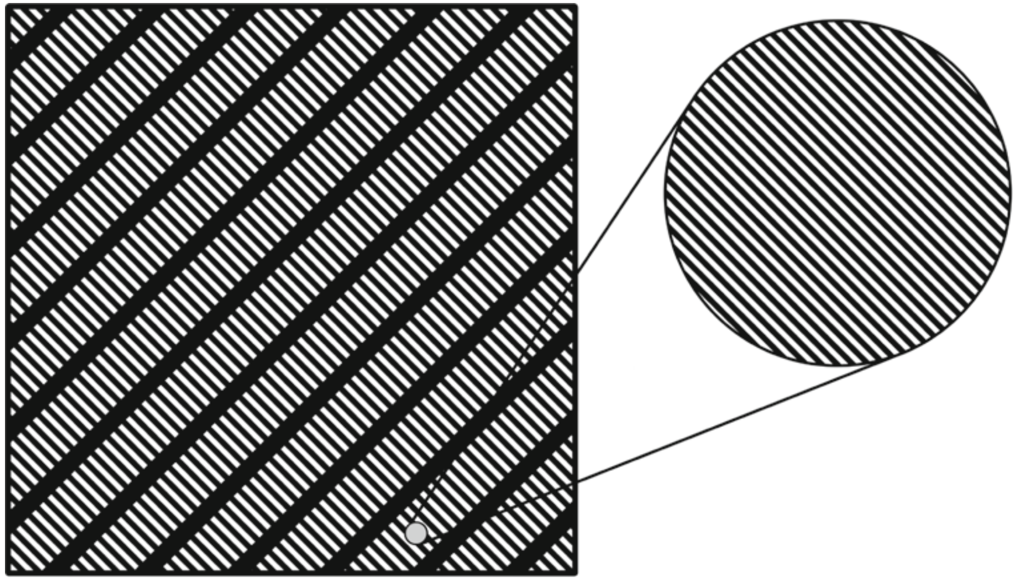
Filter regularization

TOPIC 3 [REG1] :

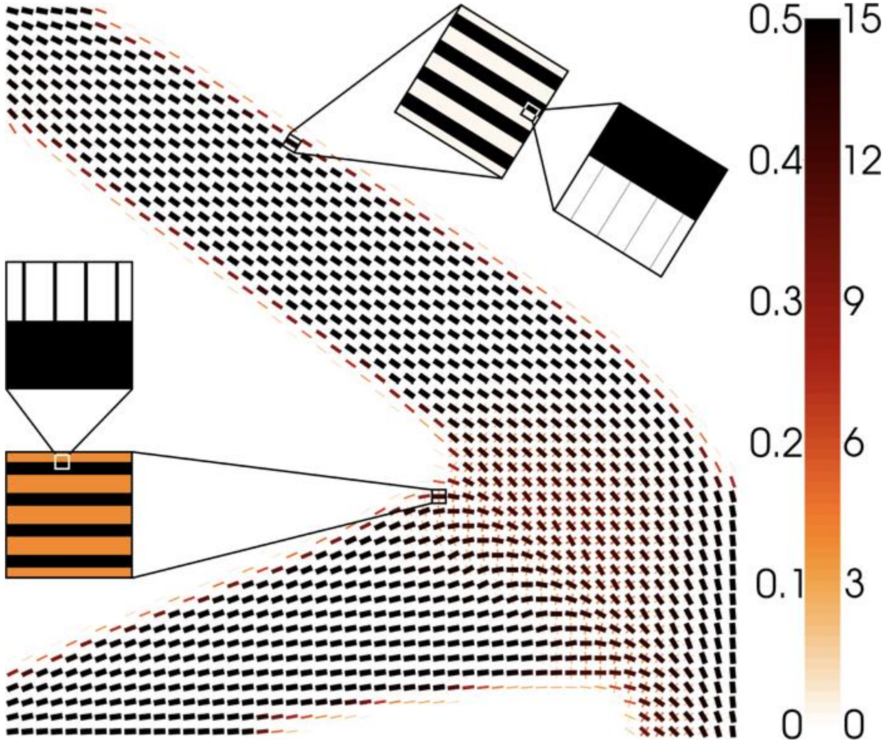
- Explanation of Filter concept
- Existence theory
- Discretization
- Implementation
  (e.g. via integration into OCM method, cf. Exercise 3 in ISMO)

Simultaneous topology and Material Optimization

Example: material with microstructure;
here: rank2-laminate



Questions: where to use material
... and if material is used, which one?



Simultaneous topology and Material Optimization

TOPIC 4 [ANISO] :

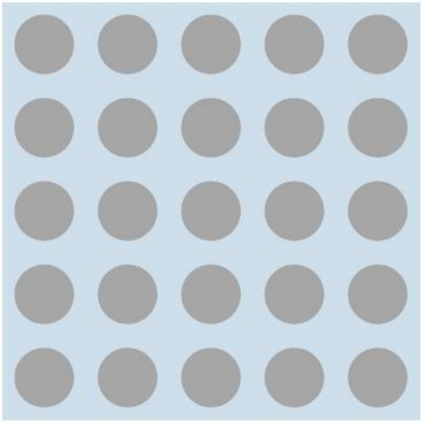
- TO/MO model
- Extension of existence & convergence theory
- Numerical approximation (rather standard!)
- Material parametrizations

Could be split into two 2 topics (theory, practice, ...)

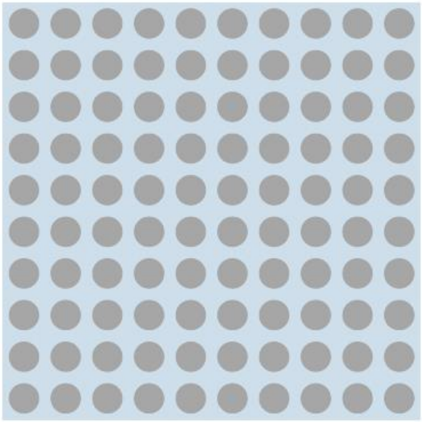
Inverse homogenization

How to define material with desired properties via ist microstructure?

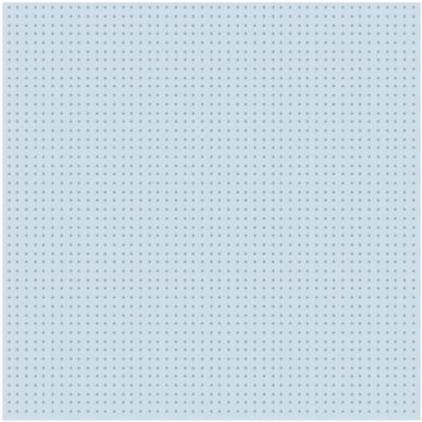
Homogenization procedure for periodic materials



$\varepsilon = 0.2$

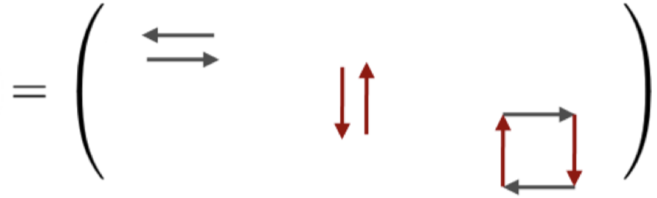


$\varepsilon = 0.1$



$\varepsilon \to 0$

$$E = \begin{pmatrix} E_{1111} & E_{1122} & \sqrt{2}E_{1112} \\ & E_{2222} & \sqrt{2}E_{2212} \\ \text{sym.} & & 2E_{1212} \end{pmatrix}$$



Numerical computation: solve state problem (elasticity) with periodic b.c. and specific right hand sides ...

Inverse homogenization

$$\min_{\rho \in \mathbb{R}^{n_h}} \nu^H(C^H(\rho)) \text{ s. t.}$$

$$\sum_{r=1}^{n_h} |\Omega_r| \rho_r \leq \gamma$$

$$0 < \underline{\rho} \leq \rho_r \leq 1, \qquad r = 1, \ldots, n_h$$

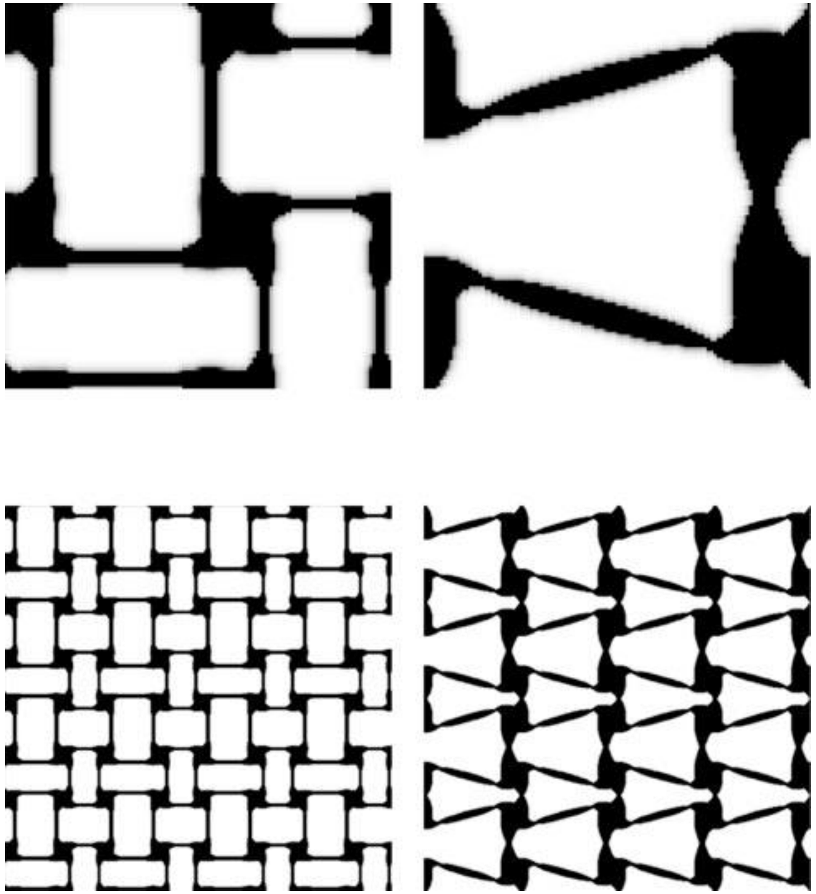
$$E^H(C^H(\rho)) \geq E_{\text{low}},$$

$$g^i_{\text{sym}}(C^H(\rho)) = 0, \qquad i = 1, \ldots, n_s,$$

$$|\rho_r - \rho_s| \leq ch, \qquad r \in \{1, \ldots, n_h\}, \; s \in N(r).$$

Computed by homogenization

Negative Poission‘s ratio material



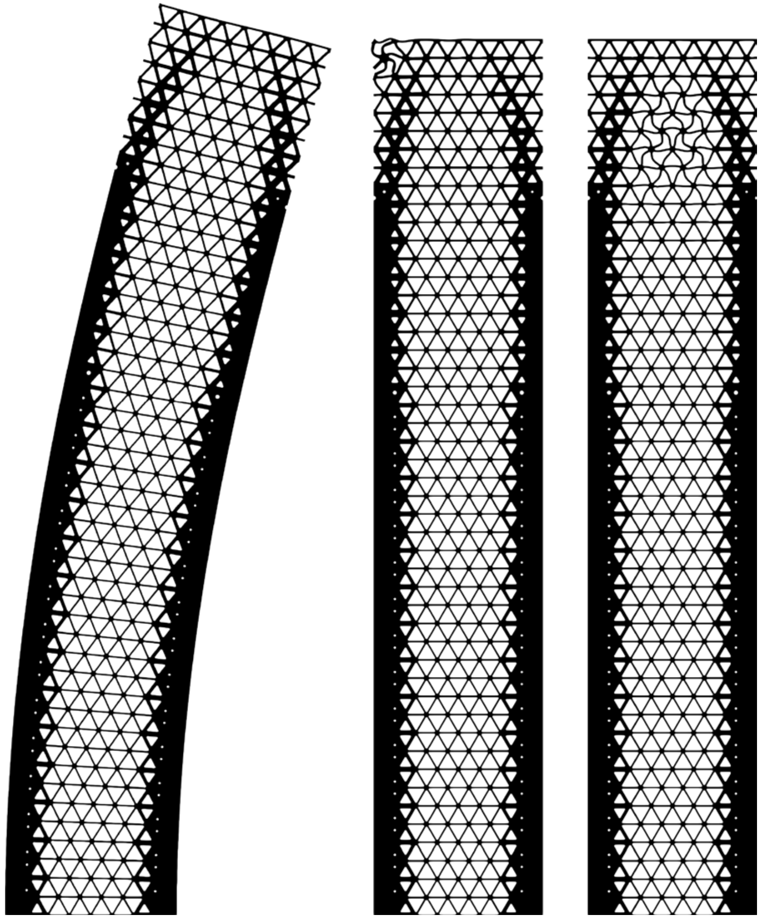
Inverse homogenization

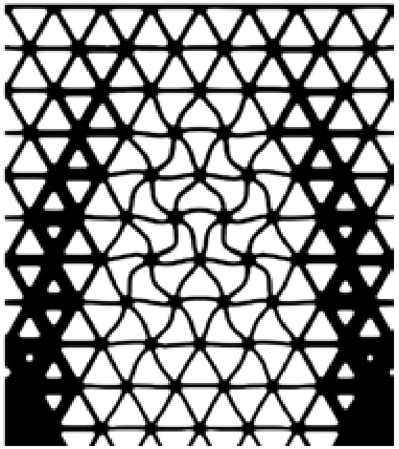
TOPIC 5 [HOM1, HOM2] :

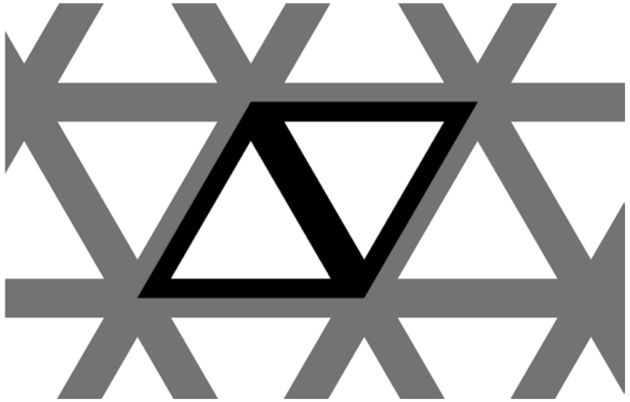
- Asymptotic homogenization (formal derivation of cell problem ...)
- The material design problem
- Existence, convergence ...
- Numerical realization and examples

Could be split into two 2 topics (theory, practice, ...)

Two-scale optimization and buckling







- Use parametrized microstructure (1 variable controls thickness of structure)
- Use homogenization approach to predict elastic properties and local buckling behaviour
- Integrate into macroscopic model

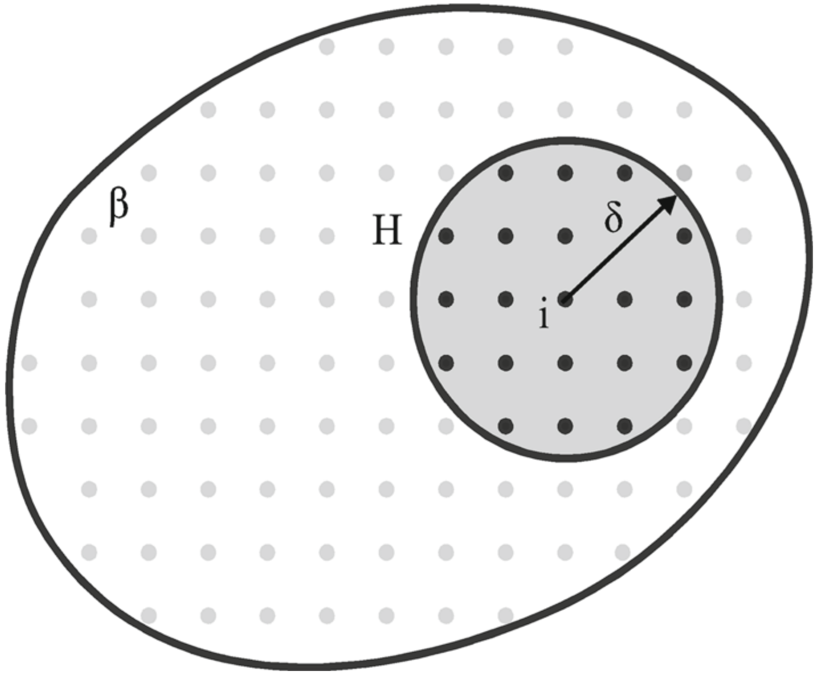
Two-scale optimization and buckling

TOPIC 6 [BUCK] :

- modelling of global buckling through eigenvalue problem
- Prediction of local properties (including local buckling) through homogenization approach
- Optional: own numerical realization (FE analysis for buckling non-trivial ...)
- examples

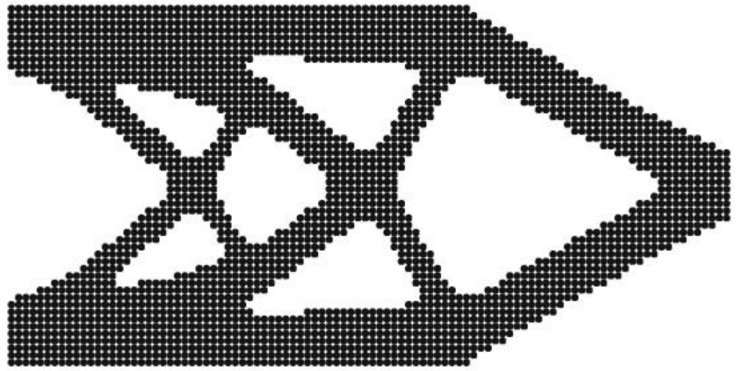
Could be split into two 2 topics (modelling, implementation, ...)

MO in presence of cracks by Peridynamics model



Coontinuum model replaced by peridynamics model:

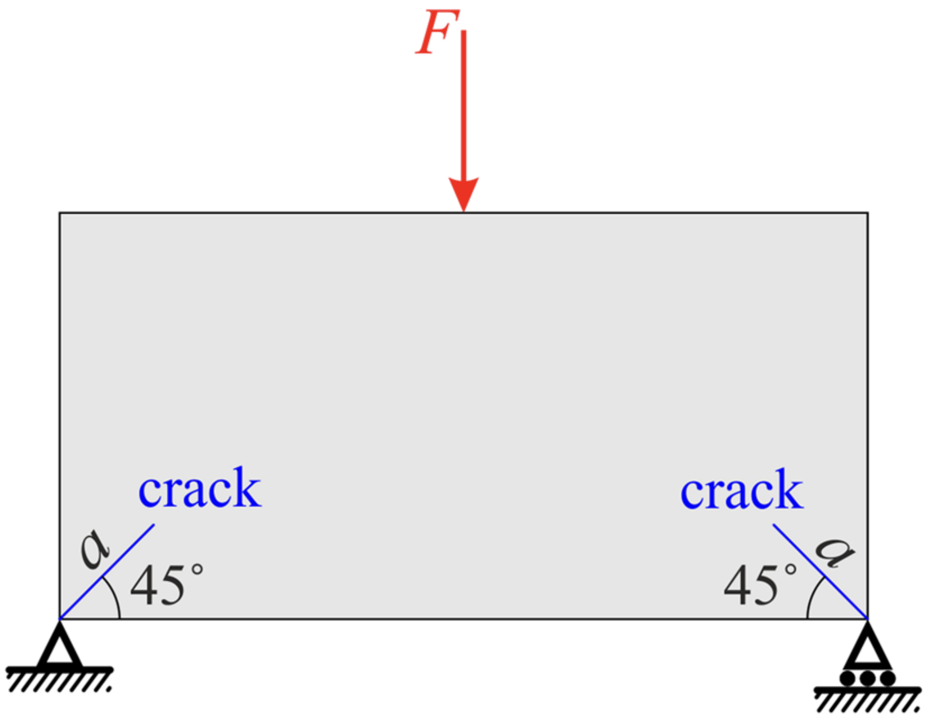
material properties computed from potentials
along connections through bonds in finite horizon



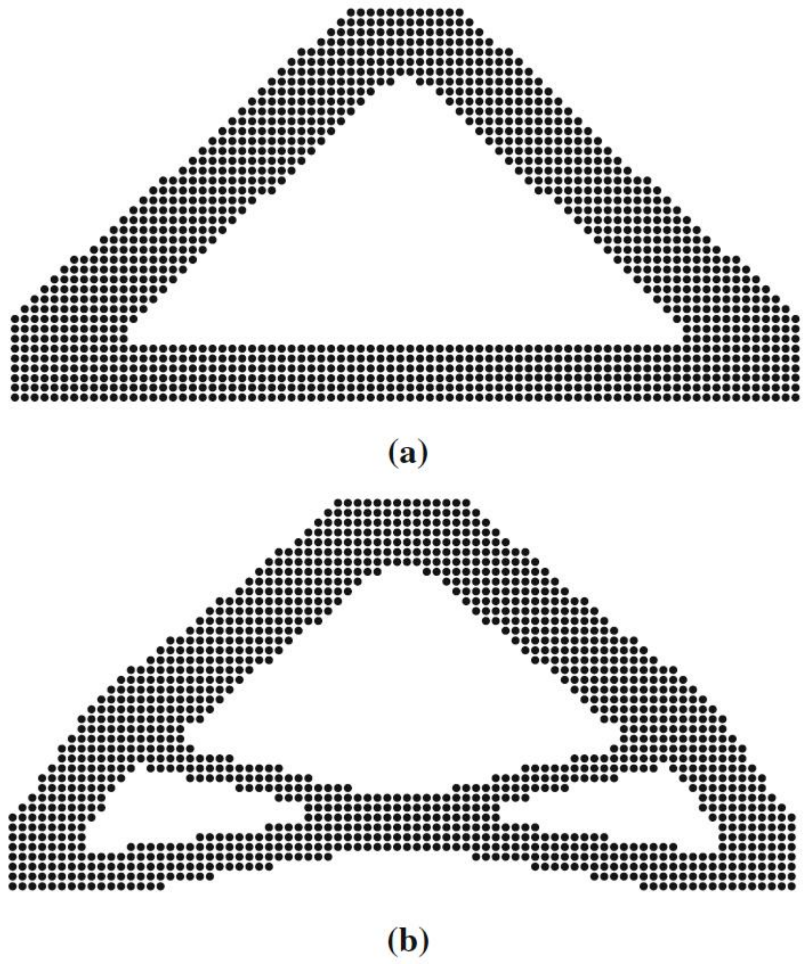
(c) PD 100×50

(d) FEM 100×50

MO in presence of cracks by Peridynamics model



(Pre-)crack modelling through “missing bonds“



Topology with and w/o crack …

MO in presence of cracks by Peridynamics model

TOPIC 7 [PERI1,PERI2] :

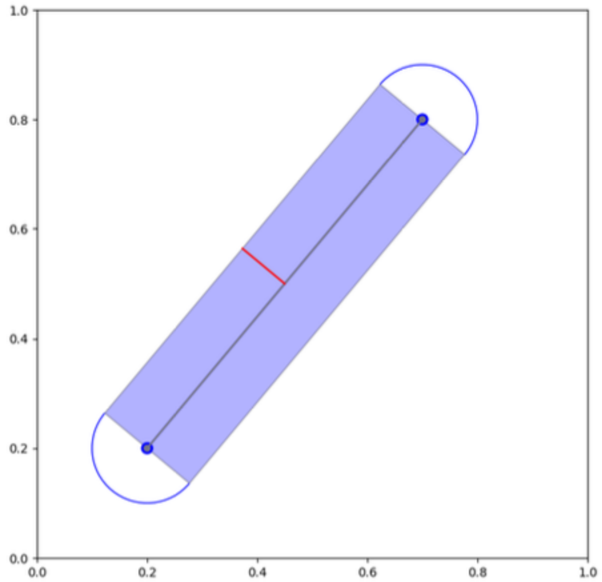
- Derivation of PD model for elasticity
- Implementation of PD model
- Experiments

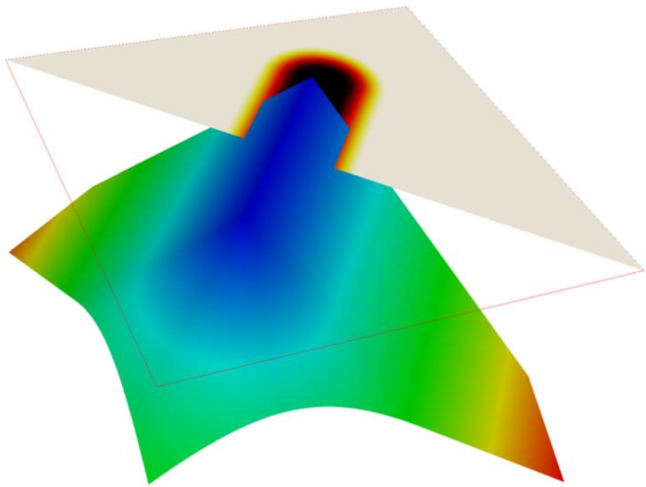
In addition, theory topics could be identified ...

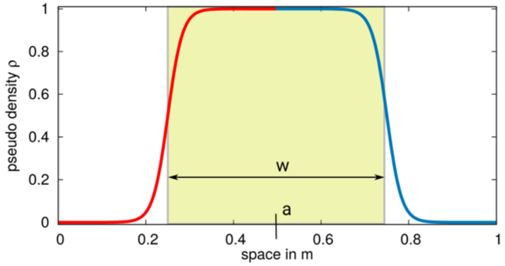
The feature-mapping approach for TO/MO

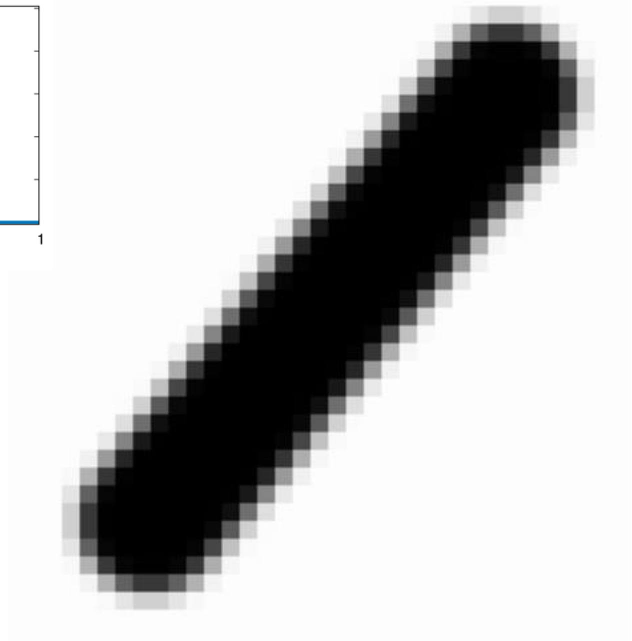
Mapping of high order geometries (circles, bars, …) to element wise pseudo density field: object → signed distance → boundary function → integration of pseudo density → FEM

- math. programming for arbitrary functions/ geometries/ physics



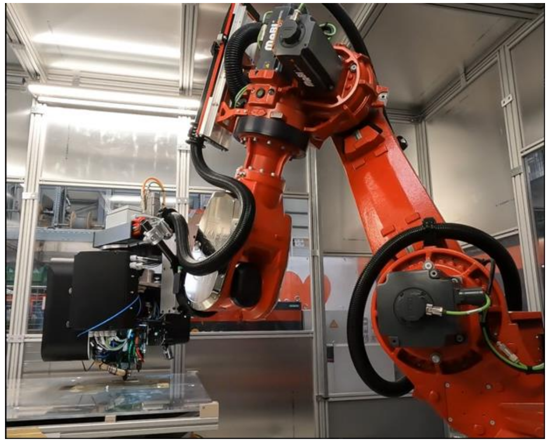


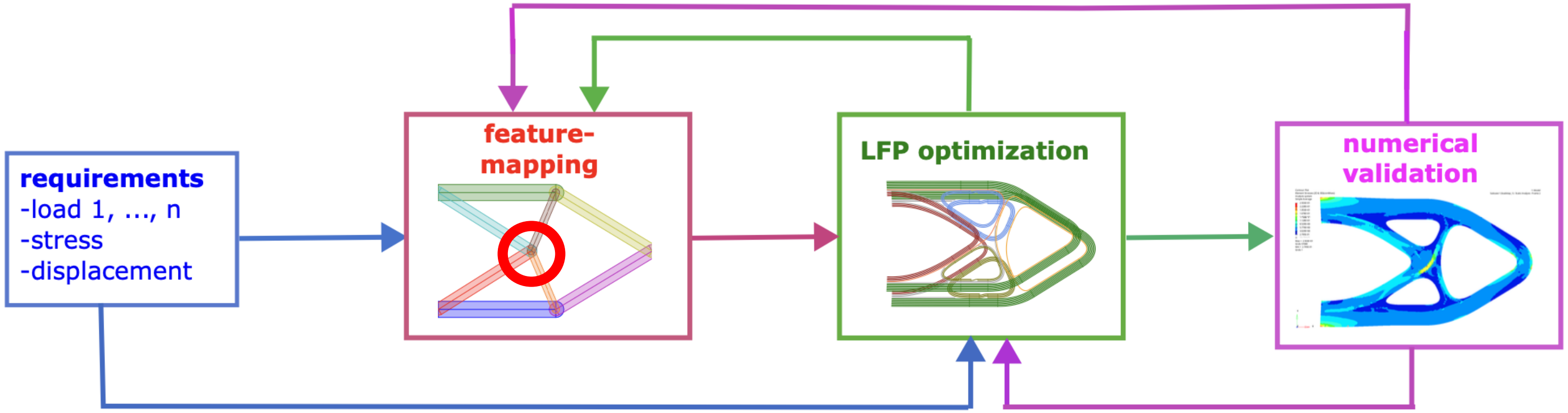


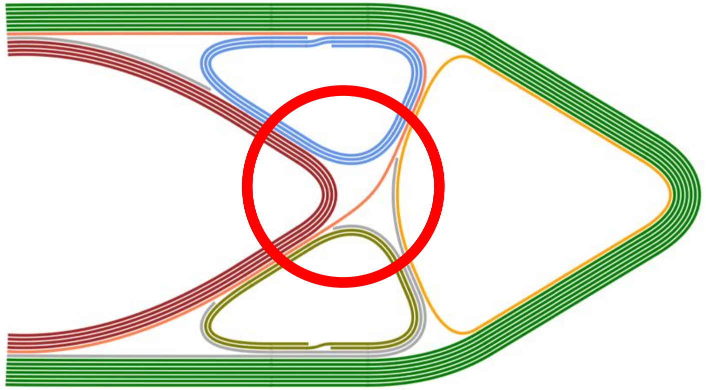


The feature-mapping approach for TO/MO

Possible Master‘s thesis: Modeling multi-layer continuous carbon fiber-reinforced printing in a feature-mapping material model.

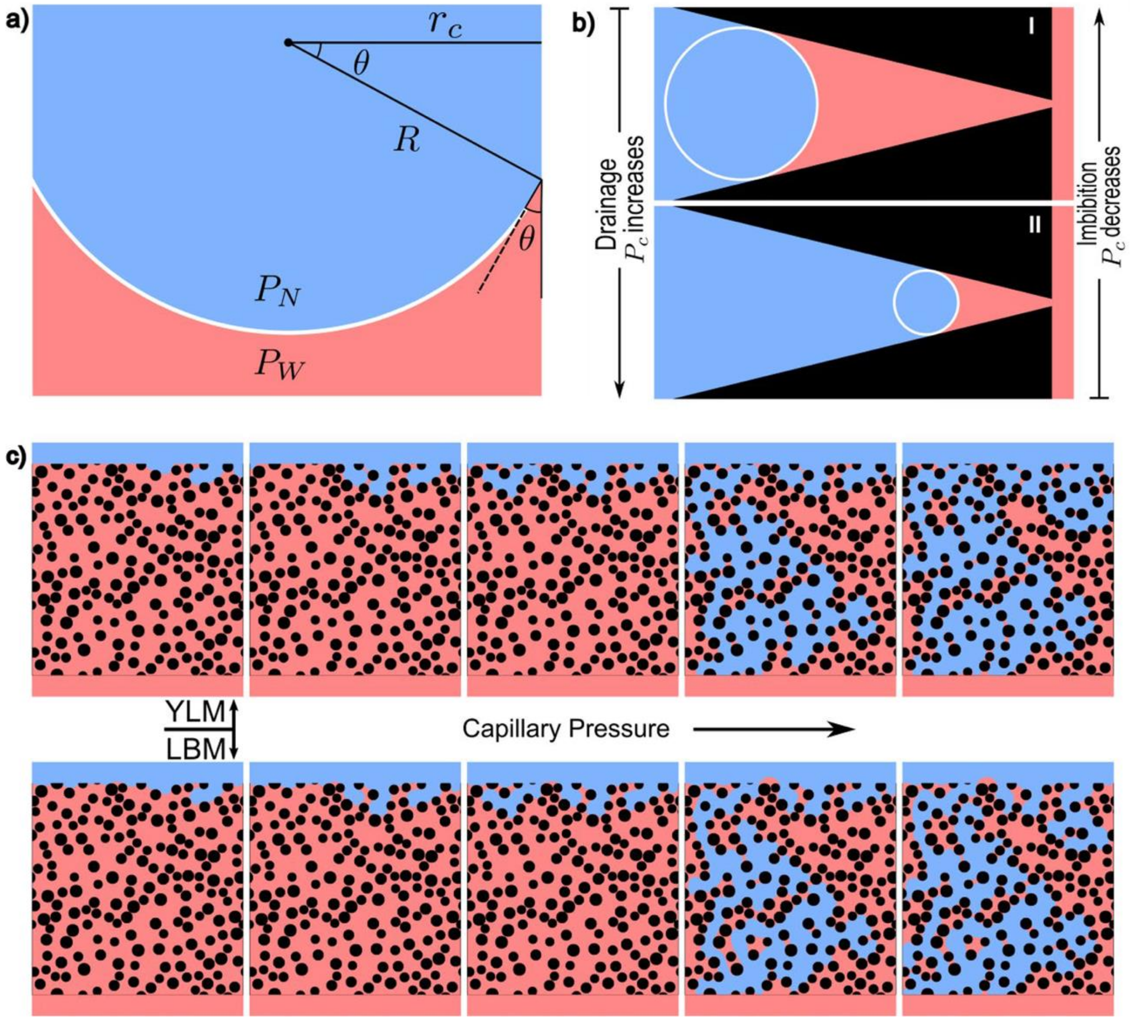


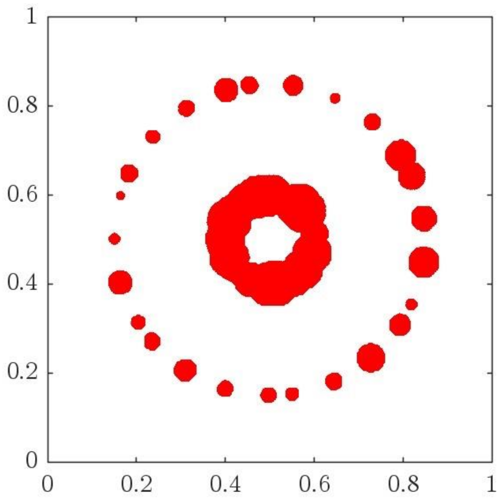


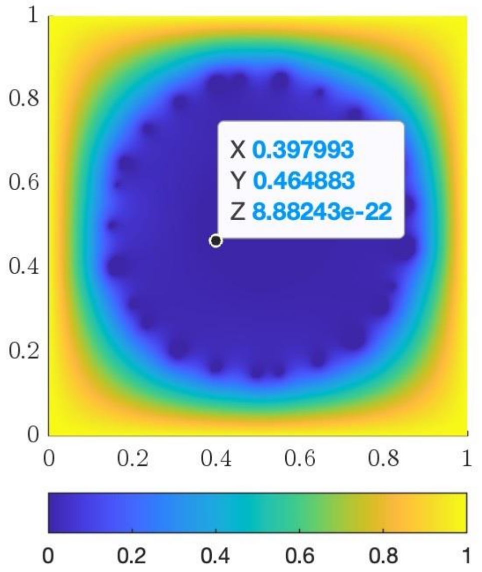


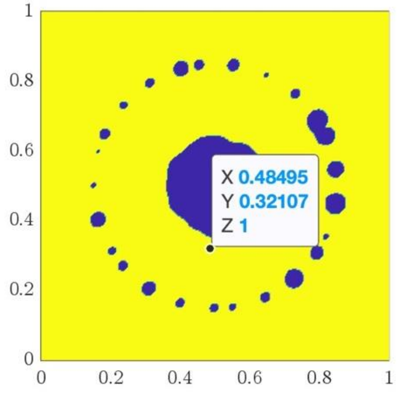
- layered fiber pattern optimization finds manufacturable realization for 3D printing of continuous carbon fiber-reinforced filament
- large discrepance model vs. realization
- model „realization“ within structural optimization, e.g. junction

Porous materials: modelling of saturation through Young-Laplace-Algorithm and a PDE-based approach







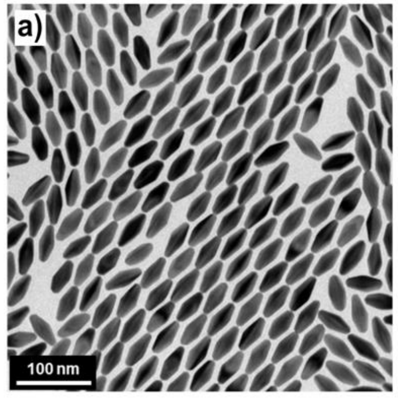


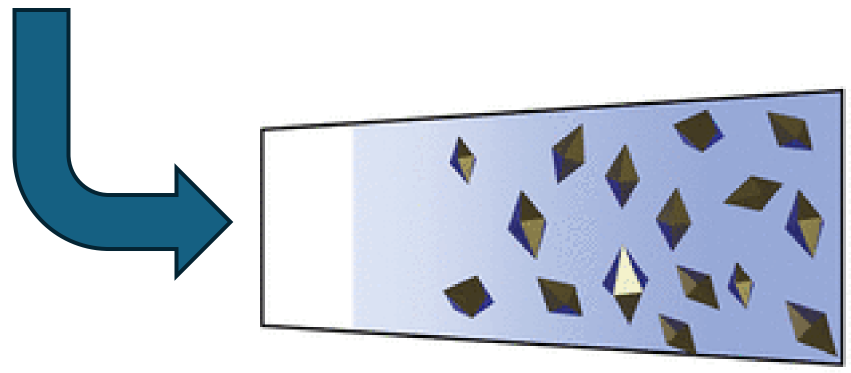
Porous materials: modelling of saturation through Young-Laplace-Algorithm and a PDE-based approach

TOPIC 9 [YL] :

- Modelling of staturation in porous medium via YL-equation
- Implementation of stabdard algorithm
- Implementation of PDE based approach (e.g. through static heat equation with high contrast materials)
- Experiments, Comparisons

Optimal on-ramp control for equilibrium measurements in analytical ultracentrifugation





e.g. 30.000 rpm

Optimal on-ramp control for equilibrium measurements in analytical ultracentrifugation

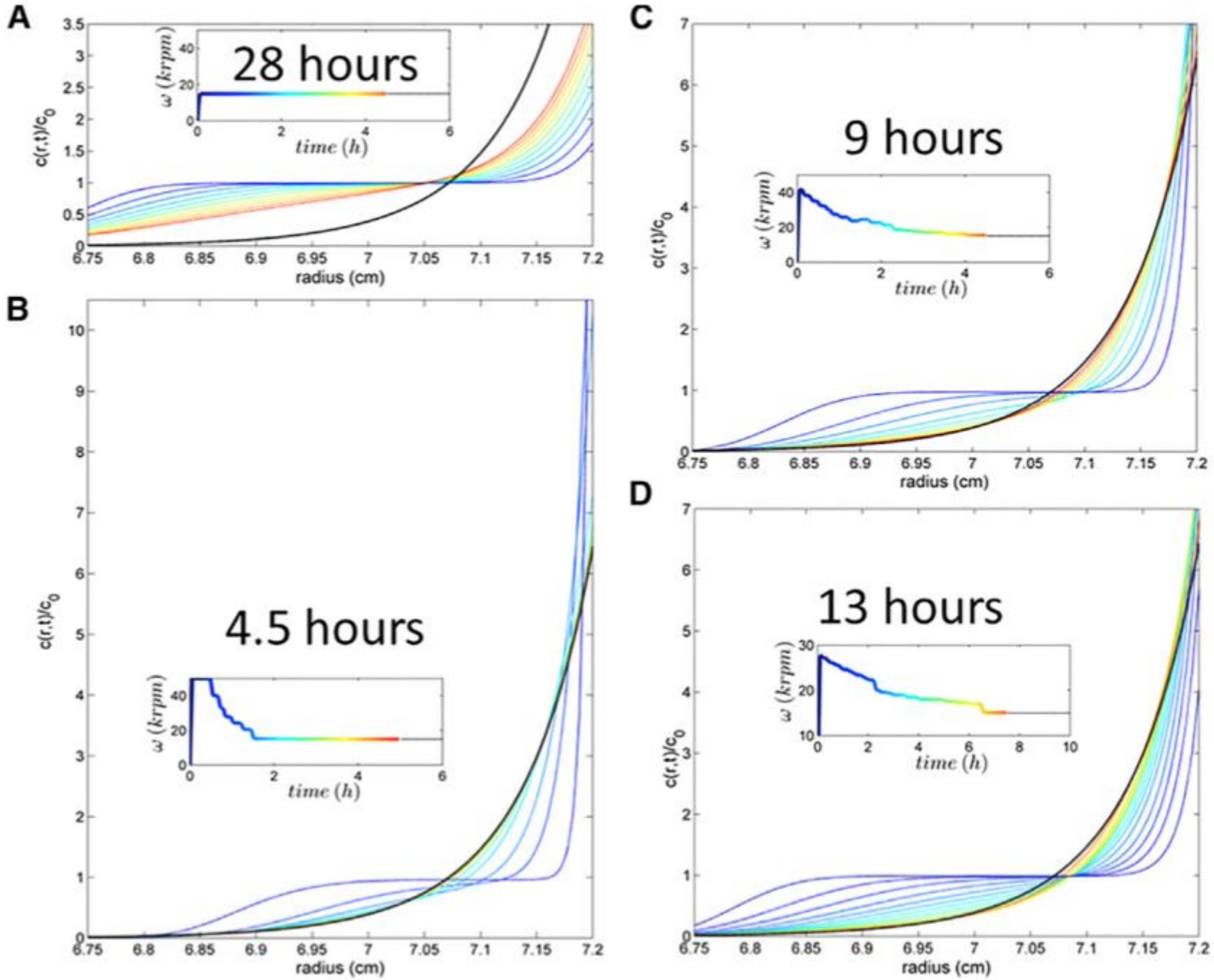
$$\partial_t c(r,t) + \boldsymbol{\omega}(t)^2 s r^{-1} \partial_r \left(c(r,t) r^2\right) = D r^{-1} \partial_r (\partial_r c(r,t) r)$$
$$c(r,0) = c_0$$

on $[r_0, r_1] \times [0, T]$

Find $\mathbf{T > 0}$ minimal and $\boldsymbol{\omega} \in \boldsymbol{\Omega}$ s.t.

$$c(r,T) = c_{eq}(r) \qquad \forall r$$

Optimal on-ramp control for eq. meas. in AUC



Potential topics for master‘s thesis

- Follow up of MMA topics
  - sequential separable programming using sparse grids
  - almost exact separable models through topological derivatives
- Two-scale optimization: continuation of buckling topic (exact treatment of local buckling)
- Inverse homogenization: nonlinear homogenization and progressive materials
- Porous materials: optimal design of porous materials with desired permeabiliy and saturation curves

Potential topics for master‘s thesis (II)

- Peridynamics
  - Crack propagation ...
- Shape mappings
  - Fiber interpretation approach
  - ...
- Optimal on-ramp control for equilibrium measurements in analytical ultracentrifugation (direct continuation of seminar topic)
- Your own suggestions …