Beyond Periodic Representation of Microstructural Geometry:

Geometry and numerics



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Motivation

Model of material microstructure: process generating individual realizations with spatial statistics corresponding to the investigated material [Liu and Shapiro, 2015]

(SE)PUC

- Lossless only for periodic materials
- Produces only one realization
- Artificial periodicity for SEPUC

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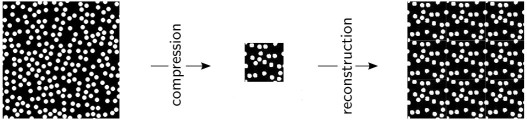

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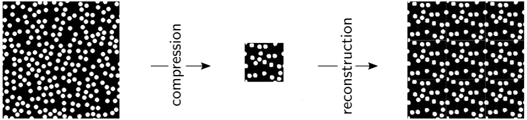
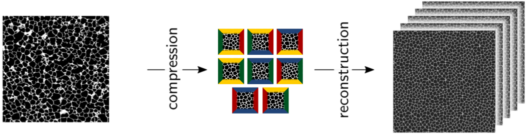


Wang tiles



- Lossless only for periodic materials
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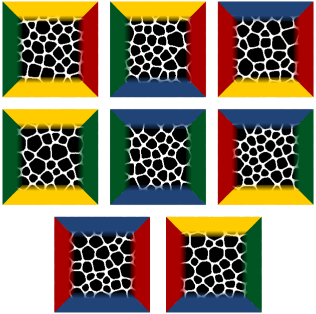
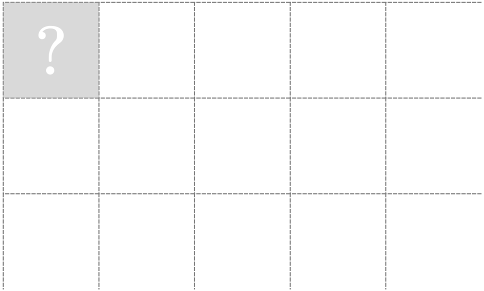
- Artificial periodicity for SEPUC

- **Modular** generalization of SEPUC
- Stochastic sequential algorithm
- Reduced geometrical model

Generating stochastic microstuctures





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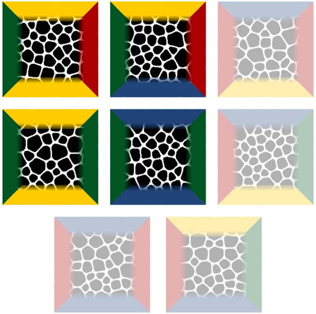

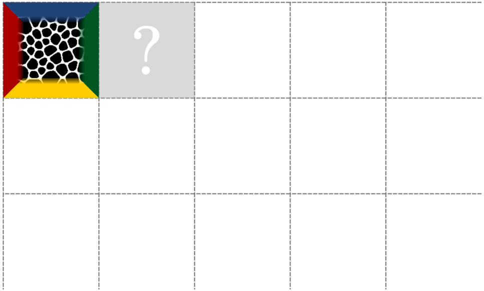

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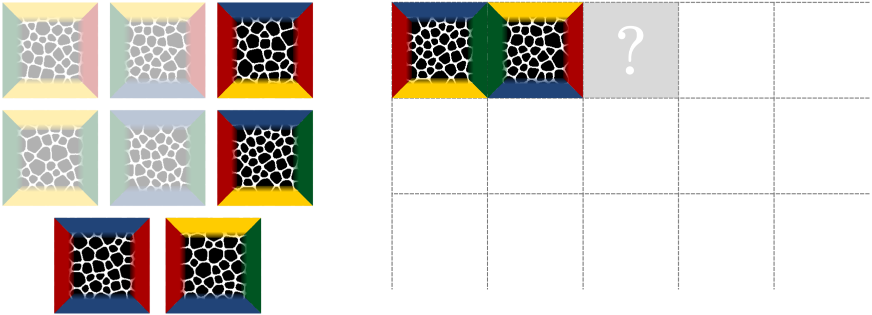

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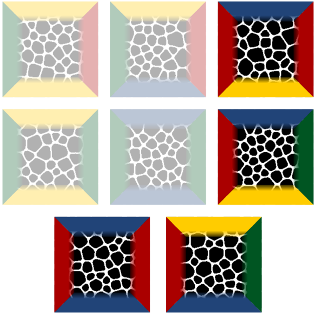

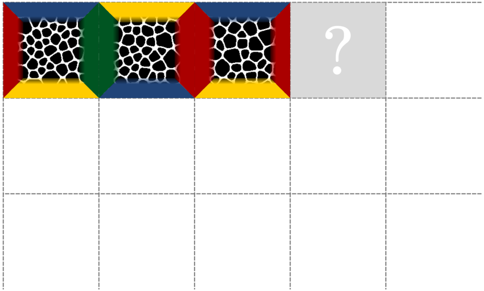

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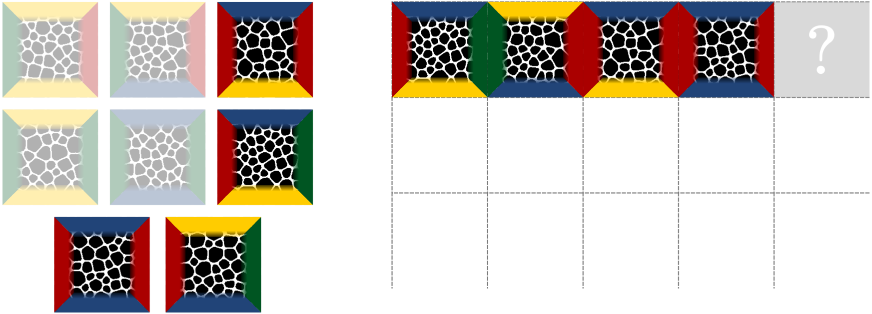

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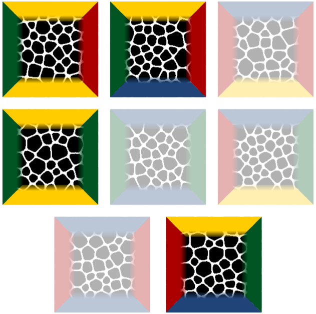

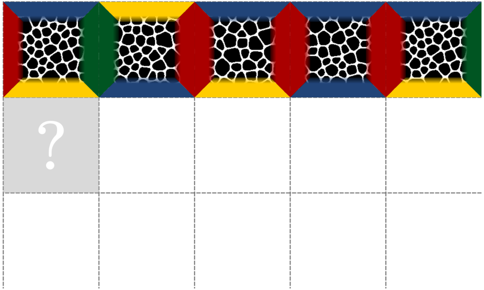

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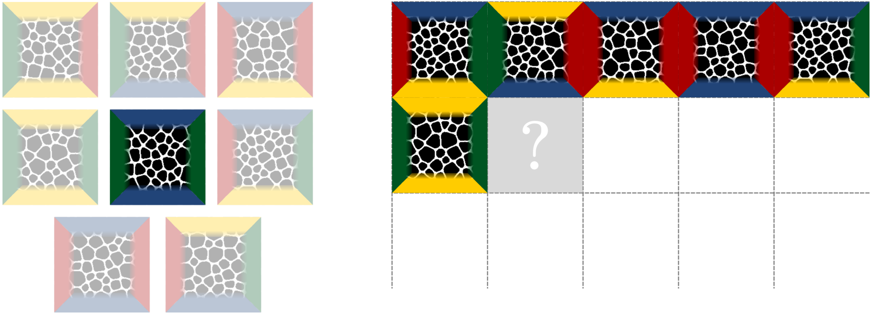

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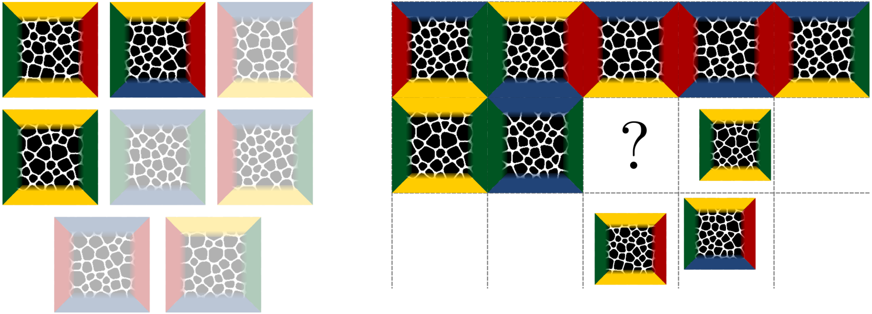

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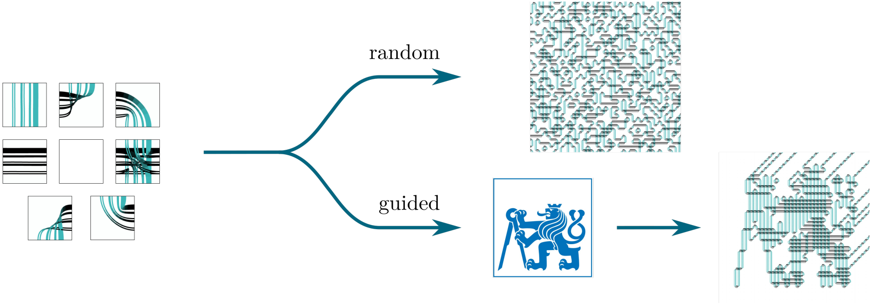

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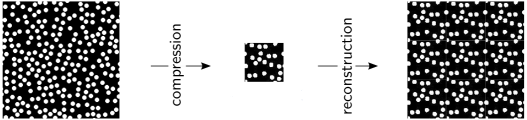

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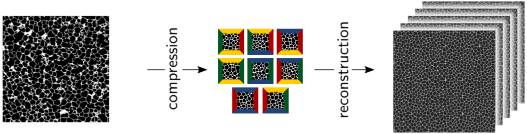

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Design of a compressed representation

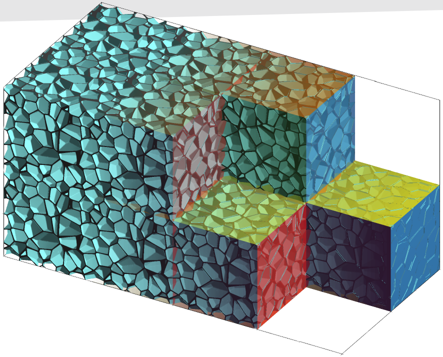
Requirements:
i) guarantee compatibility
ii) representativeness of a tiling

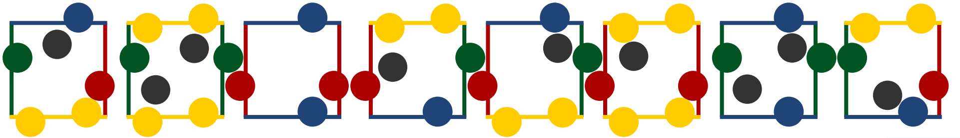
Design strategies:

i) Optimization approach [Novák et. al, PRE, 2012]
   - ✔ robust approach
   - ✘ critically slow

ii) Sample based design [Doškář et al., PRE, 2014]

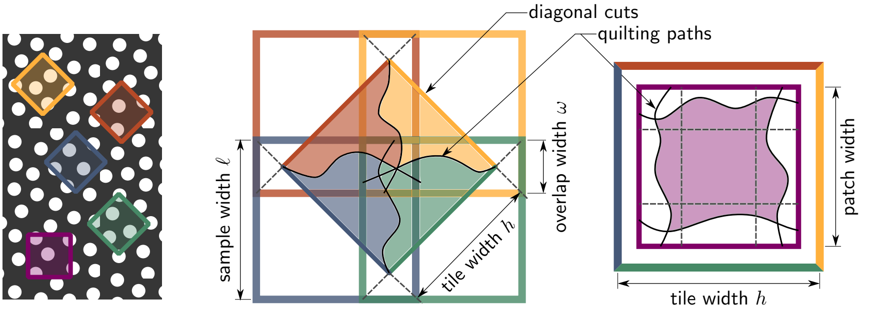
iii) Level-set based design [Doškář et al., CAD, 2020]





Sample based tile design

- Idea from computer graphics [Cohen et al., ACM Trans Graph, 2003]
- Supplemented with spatial statistics and patch enrichments

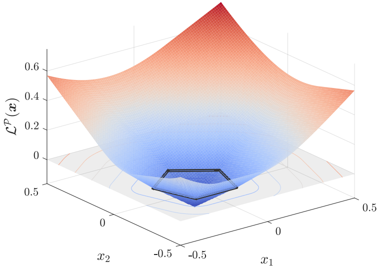


✔ efficient

✘ struggle with complex structures

Level-set based tile design (builds on [Sonon et al., CMAME, 2012])

- Implicit description of particle geometry via $\mathcal{L}^{\mathcal{P}}(\boldsymbol{x})$
- 2 steps method:
  - i) accelerated particle packing (RSA)
  - ii) morphing operations $\rightsquigarrow$ foam-like microstructures



✔ generates complex geometries

(✘ limited statistics control)

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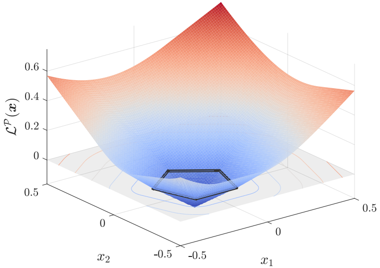

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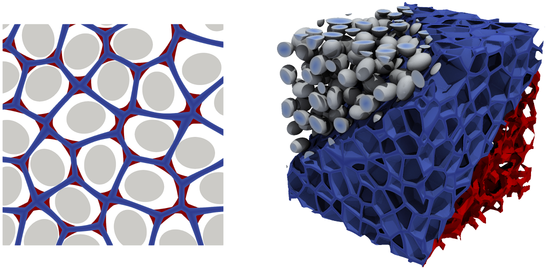

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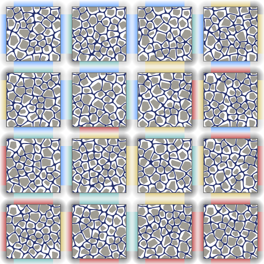

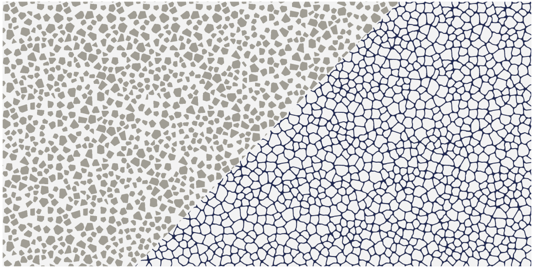

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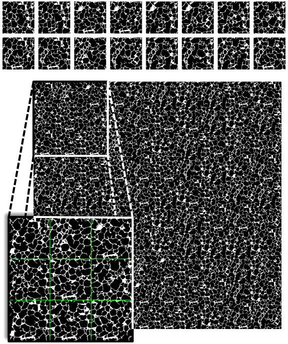
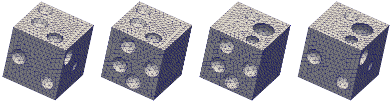
Reduction of spurious artefacts in synthesized system

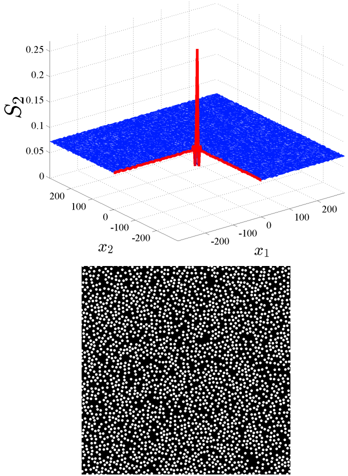
- efficient synthesis



including FE discretization



- periodicity reduction



Reference system

Reduction of spurious artefacts in synthesized system

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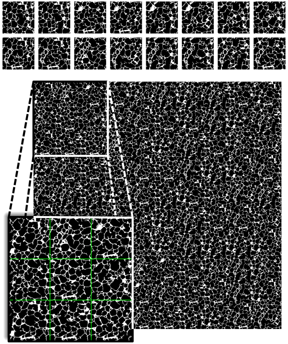

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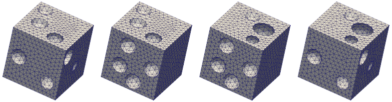

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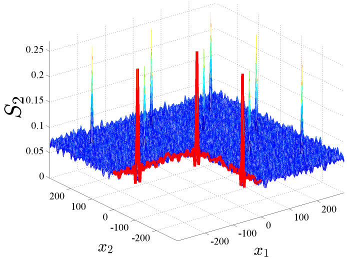

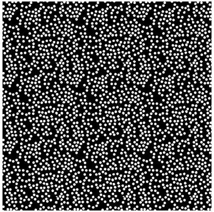

Set of 1 tile (PUC)

Reduction of spurious artefacts in synthesized system

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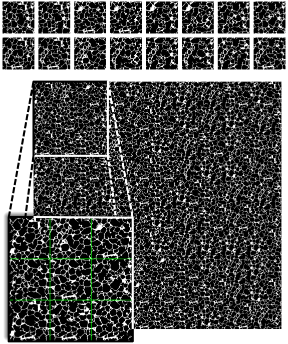

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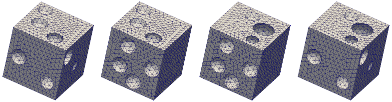

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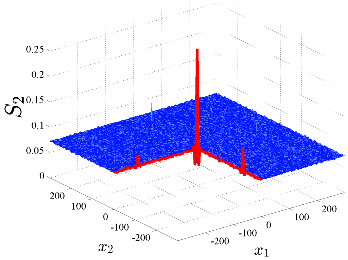
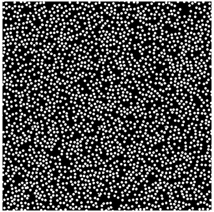
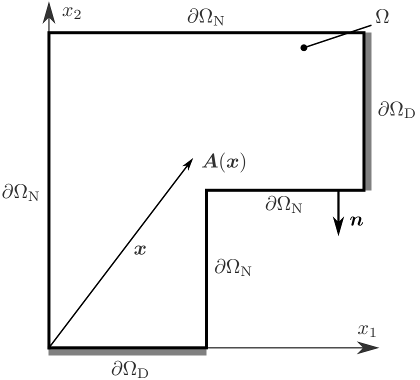




Set of 16 tiles

Numerics: problem formulation

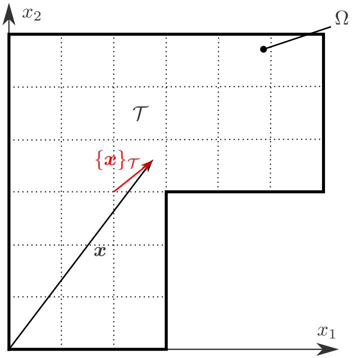


$$-\boldsymbol{\nabla} \cdot (\boldsymbol{A}(\boldsymbol{x})\boldsymbol{\nabla}\theta(\boldsymbol{x})) = f(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \Omega$$

$$\theta(\boldsymbol{x}) = \overline{\theta}(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \partial\Omega_D$$

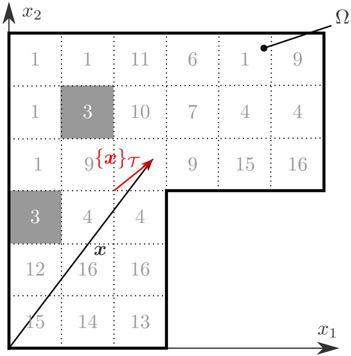
$$\boldsymbol{n}(\boldsymbol{x}) \cdot \boldsymbol{A}(\boldsymbol{x})\boldsymbol{\nabla}\theta(\boldsymbol{x}) = \overline{q}(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \in \partial\Omega_N$$

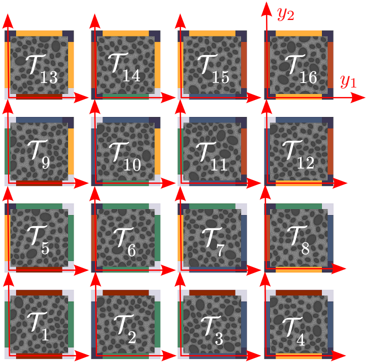
Numerics: problem formulation



$$\boldsymbol{A}(\boldsymbol{x}) =$$

Numerics: problem formulation





$$\boldsymbol{A}(\boldsymbol{x}) = \sum_{t=1}^{n_t} \chi_t(\boldsymbol{x}) \boldsymbol{A}_t\left(\{\boldsymbol{x}\}_\mathcal{T}\right) \quad \text{for } \boldsymbol{x} \in \Omega, \quad \boldsymbol{y} = \{\boldsymbol{x}\}_\mathcal{T} \in \mathcal{T}$$

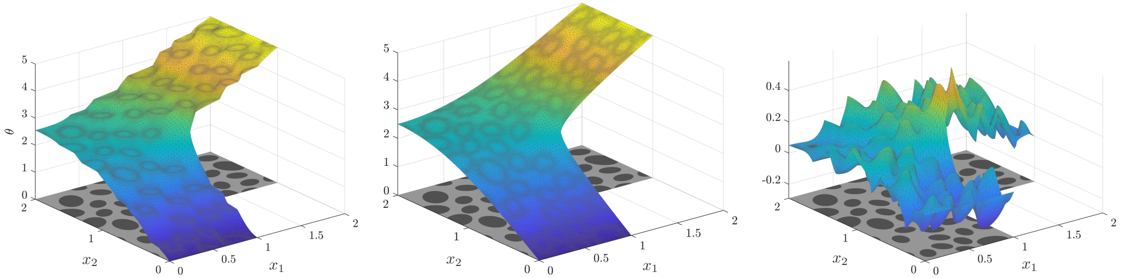
H. Wang, *Bell Syst Tech J* **40**, 1 (1961)

Numerics: problem formulation

- ✘ Fully resolved local fields
- ✘ Non-separated lengthscales ($\ell_{\mathcal{T}} \not\ll \ell_{\Omega}$)
- ✘ Exploits modularity and adjacency rules of Wang tiles

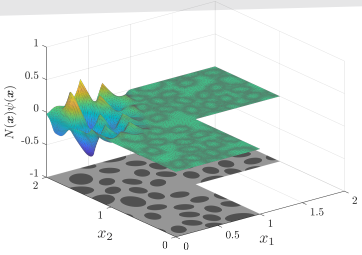
1. Multigrid/Domain decomposition approaches
2. Heterogeneous/Multiscale finite element methods and relatives
3. Partition of unity/Generalized finite element methods
    - Matache, A. M., Babuška, I., & Schwab, C. (2000). Generalized p-FEM in homogenization. *Numerische Mathematik*, 86(2), 319–375.
    - Matache, A. M., & Schwab, C. (2002). Two-scale FEM for homogenization problems. *ESAIM: Mathematical Modelling and Numerical Analysis*, 36(4), 537–572.
    - Fish, J., & Yuan, Z. (2005). Multiscale enrichment based on partition of unity. *International Journal for Numerical Methods in Engineering*, 62(10), 1341–1359.
    - Fish, J., & Yuan, Z. (2007). Multiscale enrichment based on partition of unity for nonperiodic fields and nonlinear problems. *Computational Mechanics*, 40(2), 249–259.

Microstructure-informed Partition-of-Unity schemes



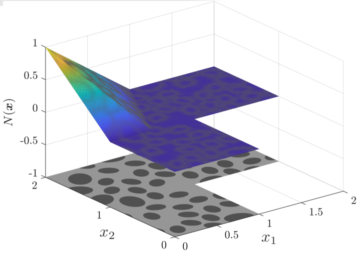
total solution = homogeneous part (standard FE) + fluctuation part (tile-based)

Microstructure-informed Partition-of-Unity schemes



PU enrichment

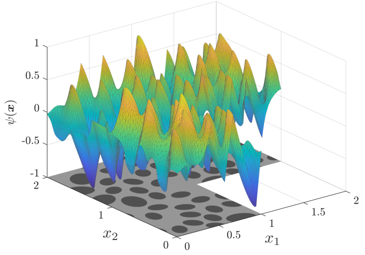
=



shape function

(standard/coarse FE)

×



fluctuation

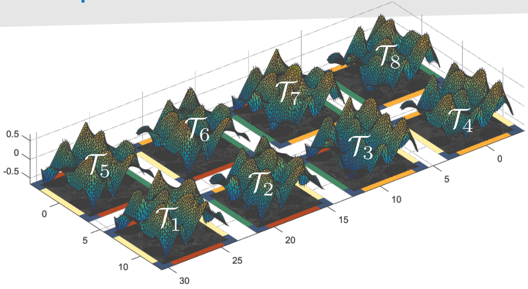
(tile-based)

- Partition-of-unity ansatz

$$\theta(\boldsymbol{x}) \approx \sum_{i=1}^{n} N_i^c(\boldsymbol{x}) \left[u_i + \sum_{j=1}^{m} \psi^j \left(\{\boldsymbol{x}\}_{\mathcal{T}} \right) \alpha_i^j \right] \quad \text{for } \boldsymbol{x} \in \Omega$$

J. M. Melenk, I. Babuška, *Comput Method Appl M* **139**, 289 (1996); I. Babuška, J. M. Melenk, *Int J Numer Meth Eng* **40**, 727 (1997); . . .

Homogenization-inspired fluctuation fields



$$\boldsymbol{H} = [1; 0]$$

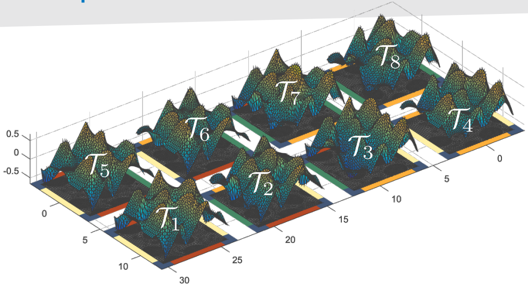
$$-\boldsymbol{\nabla} \cdot \left(\boldsymbol{A}_t(\boldsymbol{y}) \boldsymbol{\nabla} \left(\boldsymbol{H} \cdot \boldsymbol{y} + \psi_t^{\boldsymbol{H}}(\boldsymbol{y})\right)\right) = 0 \quad \text{for } \boldsymbol{y} \in \mathcal{T}, \, t = 1, 2, \ldots, n_\mathrm{t}$$

- Continuity across matching edges
- Uniqueness:

$$\sum_{t=1}^{n_\mathrm{t}} \int_{\mathcal{T}_t} \psi_t^{\boldsymbol{H}}(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y} = 0$$

e.g., V. Kouznetsova, W. A. Brekelmans, F. P. Baaijens, *Comp Mech* **27**, 37 (2001)

Homogenization-inspired fluctuation fields



$\boldsymbol{H} = [1; 0]$

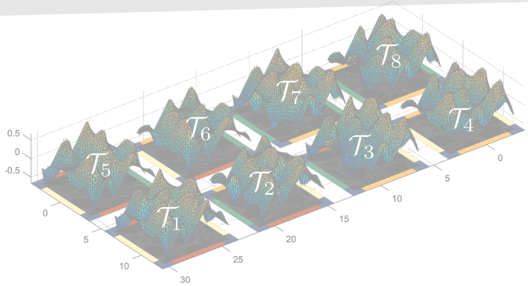
- Consistency
  1. Tile-wise Dirichlet boundary conditions: $\psi_t^{\boldsymbol{H}}(\boldsymbol{y}) = 0$ for $\boldsymbol{y} \in \partial\mathcal{T}$, $t = 1, \ldots, n_{\mathrm{t}}$
  2. Tile-wise zero gradient:

$$\int_{\partial\mathcal{T}} \psi_t^{\boldsymbol{H}}(\boldsymbol{y})\boldsymbol{n}(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \boldsymbol{0} \text{ for } t = 1, \ldots, n_{\mathrm{t}}$$

  3. Set-wise zero gradient:

$$\sum_{t=1}^{n_{\mathrm{t}}} \int_{\partial\mathcal{T}} \psi_t^{\boldsymbol{H}}(\boldsymbol{y})\boldsymbol{n}(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} = \boldsymbol{0}$$

Homogenization-inspired fluctuation fields



- Second-order homogenization

$$-\nabla \cdot \left(A_t(y) \nabla \left(H \cdot y + \frac{1}{2} y \cdot G \cdot y + \psi_t^{H,G}(y) \right) \right) = 0 \quad \text{for } y \in \mathcal{T},\ t = 1, 2, \ldots, n_t$$

- Continuity across matching edges
- Uniqueness + consistency

V. Kouznetsova, M. G. Geers, W. A. Brekelmans, *Int J Numer Meth Eng* **54**, 1235 (2002)

Online solution strategy

- Two levels of FE discretization:

  $\mathcal{V}^c$ Coarse domain discretization
  $\rightsquigarrow$ defines N_i^c

  $\mathcal{V}^f$ Assembled tile-based fine discretization
  $\rightsquigarrow$ $\mathsf{Ku} = \mathsf{f}$ (DNS) + ψ_t^j lives here

- Partition of unity ansatz

$$\theta(\boldsymbol{x}) \approx \sum_{i=1}^{n} N_i^c(\boldsymbol{x}) \left[u_i + \sum_{j=1}^{m} \psi^j \left(\{\boldsymbol{x}\}_{\mathcal{T}} \right) \alpha_i^j \right] \quad \text{for } \boldsymbol{x} \in \Omega$$

$\rightsquigarrow$ interpolation $\mathsf{u} \approx \mathsf{Qa}$ with coarse DOFs $\mathsf{a} = \left[u_i ; \alpha_i^j \right]_{i,j=1}^{n,m}$

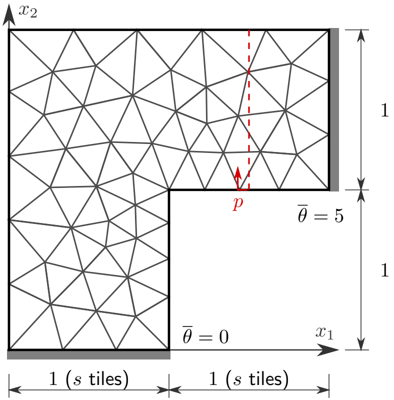
- Posed as ROM

$$\mathsf{Q}^\mathsf{T}\mathsf{KQa} = \mathsf{Q}^\mathsf{T}\mathsf{f}\,,$$

✔ Straightforward integration (potential for hyper-reduction)
✔ Simplifies imposing Dirichlet BC
✔ Enables switching to fine discretization locally

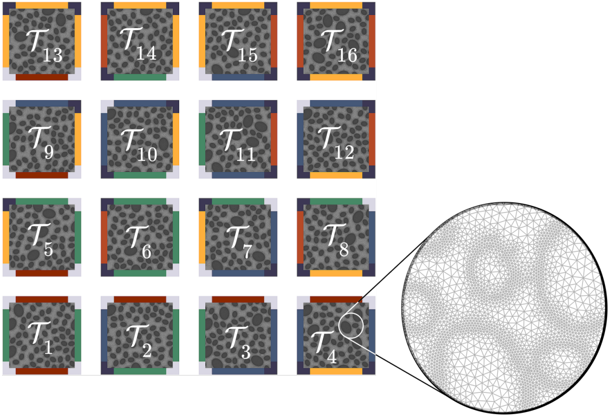
Example

- Example setup



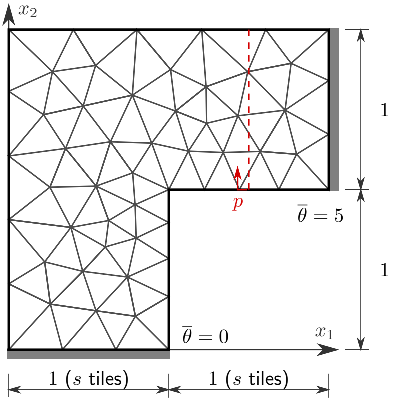
- Linear isotropic material
- 1 : 100 contrast in phase properties

- Tile set



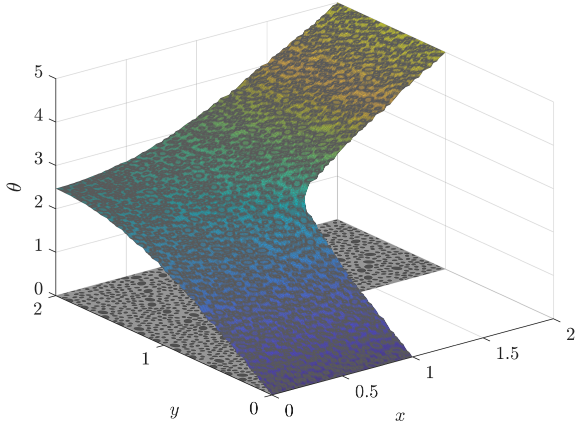
Example

- Example setup



  - Linear isotropic material
  - 1 : 100 contrast in phase properties

- DNS solution (for $s = 5$)



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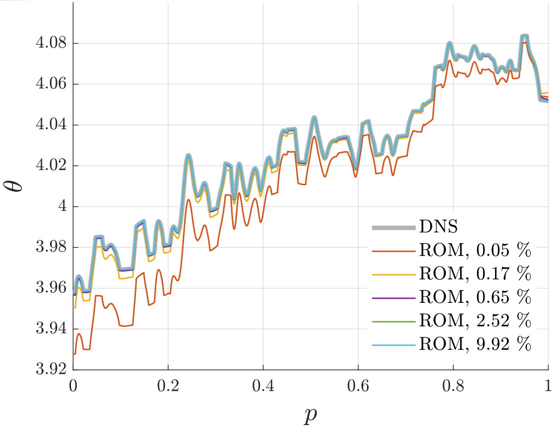
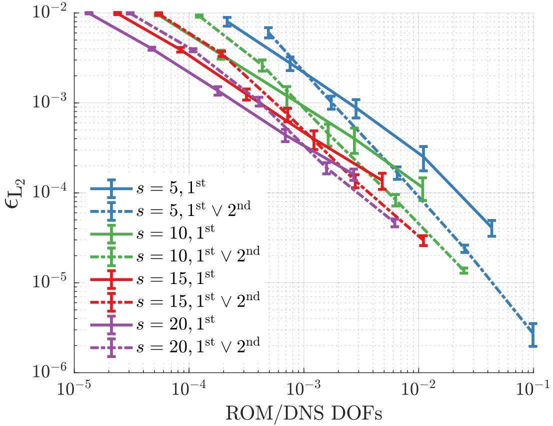
Local and global errors





- 50 microstructure realizations, uniform refinement

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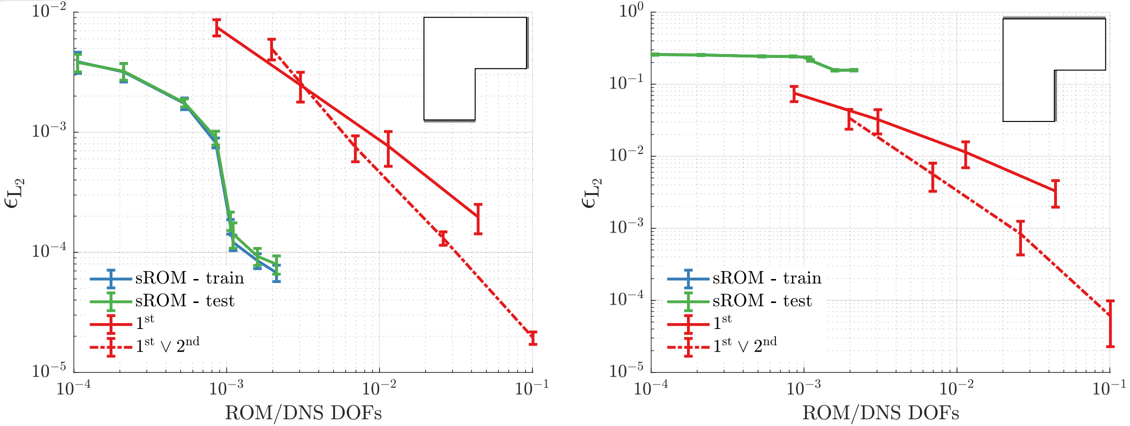
Comparison with snapshot-based reduced-order models



- $10,000$ microstructure realizations ($s = 4$); SVD decomposition

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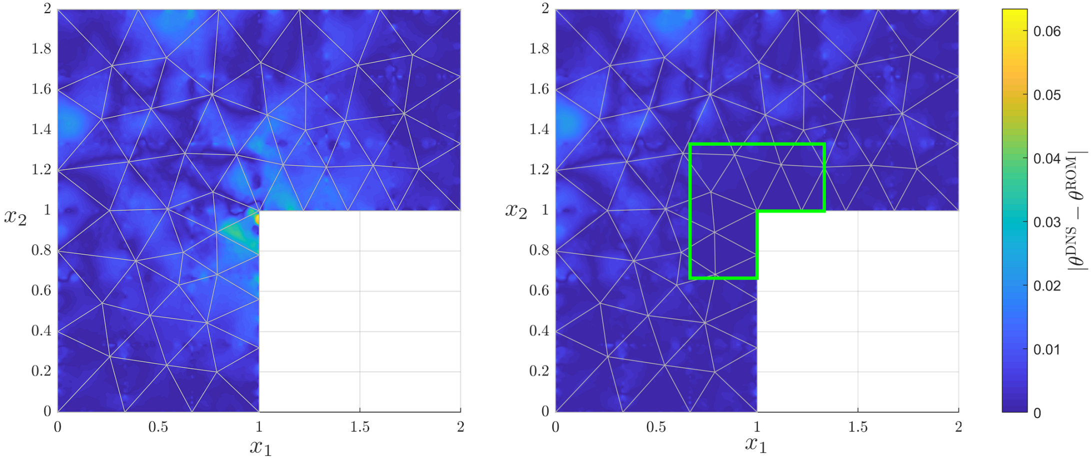
Local refinement ($s = 4$)



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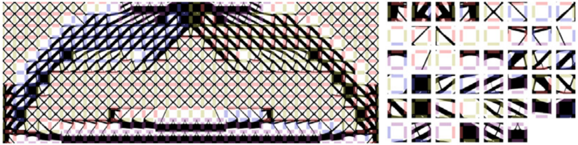
Summary

- Wang tiles as natural extension of (SE)PUC/reduced geometrical model of a microstructure
  - Instant stochastic microstructural samples
  - Suppressed periodicity
  - Convenient framework for simulations with tunable randomness
- Wang tiles combined with Partition of unity method enable
  - Accurate analysis of local fields in non-periodic heterogeneous media (with fewer DOFs)
  - Generic enrichment functions pre-computed off-line
  - Seamless transition to the full model

Extensions:

- Modular-topology optimization
- Robotic and self- assembly



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M. Doškář, J. Novák, J. Zeman, Aperiodic compression and reconstruction of real-world material systems based on Wang tiles, Physical Review E 90 (6) (2014) 062118, arXiv:1406.7812.

M. Doškář, J. Novák, A jigsaw puzzle framework for homogenization of high porosity foams, *Computers & Structures* 166 (2016) 33–41, arXiv:1507.08521.

M. Doškář, J. Zeman, D. Jarušková, J. Novák, Wang tiling aided statistical determination of the Representative Volume Element size of random heterogeneous materials, *European Journal of Mechanics - A/Solids* 70 (2018) 280–295, arXiv:1709.05926.

M. Doškář, J. Zeman, D. Rypl, J. Novák, Level-set based design of Wang tiles for modelling complex microstructures, *Computer-Aided Design* 123 (2020) 102827, arXiv:1904.07657.

M. Doškář, J. Zeman, P. Krysl, J. Novák, Microstructure-informed reduced modes synthesized with Wang tiles and the Generalized Finite Element Method, *Computational Mechanics* 68 (2) (2021) 233–253, arXiv:2010.02690.

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