Computational Homogenization and Multiscale Modeling

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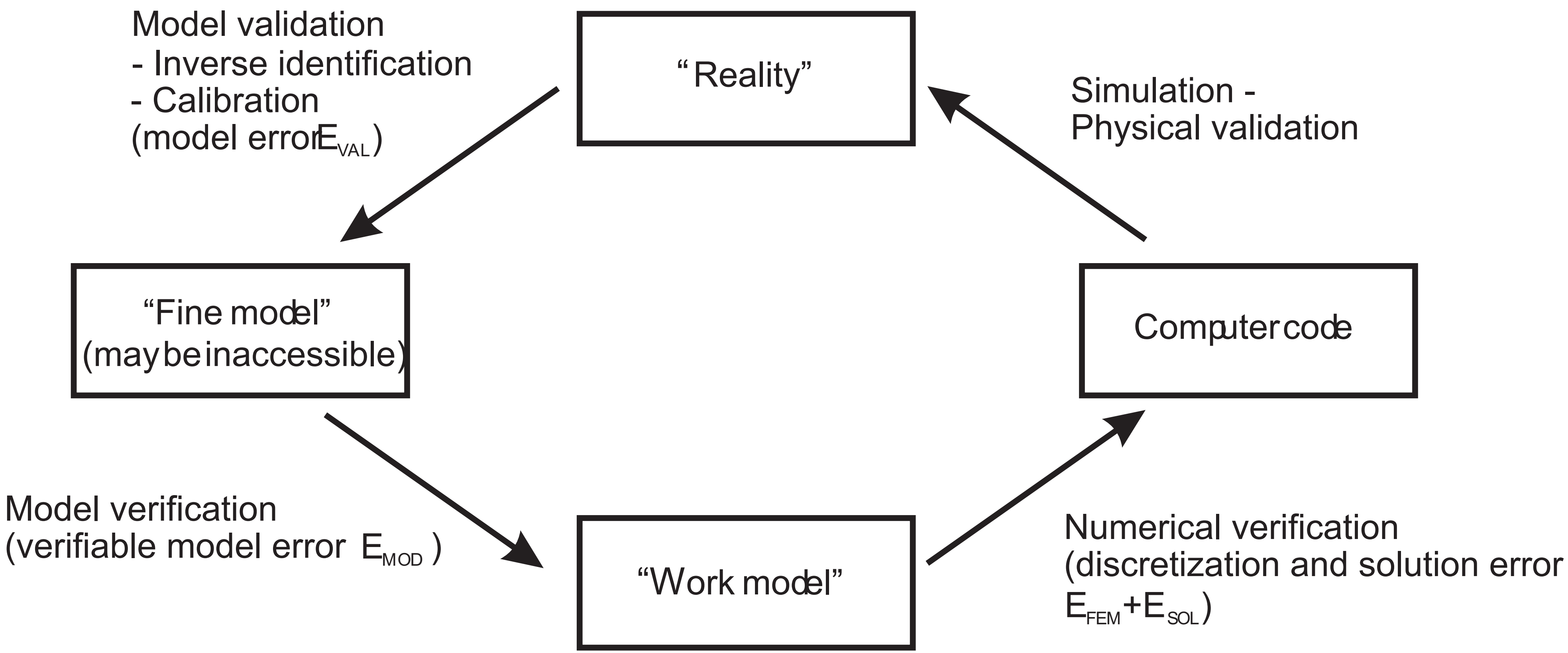
Lecture 3: Contents

- FE^2 with error estimation and adaptivity
  - Discretization and modeling errors
  - Error control for FE^2
  - Computational results for (simple) 2D model problems
  - Adaptive (seamless) bridging of scales
- Outlook - Selected research at Chalmers
  - Transient problems (Ph.D. student Su)
  - Permeability (Ph.D. student Sandström)
  - Powder metallurgy - Sintering (Ph.D. student Öhman)

Lecture 3 - Part I

FE^2 with error estimation and adaptivity

Modeling and Computation – Errors



Computational mechanics - Accuracy vs. cost

- Error control
  - What is the goal of the analysis and what is the accuracy?
- The optimization problem of adaptive analysis
  Obtain the required accuracy at minimum computational cost
  or
  Obtain maximum accuracy with available computational resources
- Different sources of errors
  Balance the accuracy (and required effort) in modeling and solution

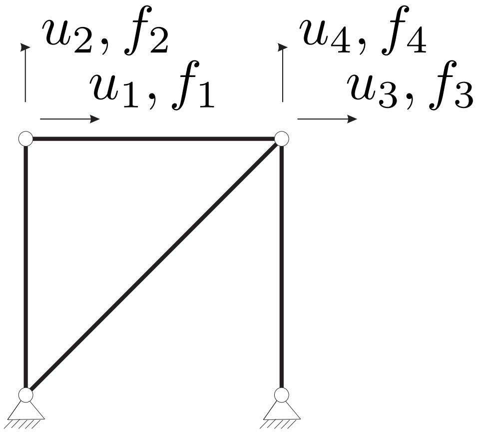
Error control

Are the equations solved right?

Are the right equations solved?

Goal oriented error control - The dual solution

Example structure



- Structural problem:

$$\underline{K}\,\underline{u} = \underline{f}$$

- Output of interest

$$Q = \underline{q}^{\mathrm{T}}\,\underline{u}$$

Study, e.g., elongation of the diagonal bar

$$Q = 1/\sqrt{2}\,u_3 + 1/\sqrt{2}\,u_4$$

- Dual problem (cf. influence/Green's functions)

$$\underline{K}^{\mathrm{T}}\,\underline{u}^* = \underline{q}$$

$$\Rightarrow Q = \underline{q}^{\mathrm{T}}\,\underline{u} = \underline{u}^{*\mathrm{T}}\underline{K}\,\underline{u} = \underline{u}^{*\mathrm{T}}\,\underline{f}$$

Goal oriented error control - Solution error

- Approximate solution to exact problem

$$\underline{K}\,\underline{u}_h \approx \underline{f} \quad \Rightarrow Q \approx Q_h = \underline{q}^{\mathrm{T}}\underline{u}_h$$

- Solution (discretization in FEM) error

$$E_h \stackrel{\mathrm{def}}{=} Q - Q_h = \underline{q}^{\mathrm{T}}\left(\underline{u} - \underline{u}_h\right) = \underline{u}^{*\mathrm{T}}\underline{K}\left(\underline{u} - \underline{u}_h\right) = \underline{u}^{*\mathrm{T}}\underline{r}_h$$

Computable residual

$$\underline{r}_h = \underline{K}\,\underline{u} - \underline{K}\,\underline{u}_h = \underline{f} - \underline{K}\,\underline{u}_h$$

- Adaptivity by controlling $\underline{r}_h$
- Issues in practice
  - Linearization of nonlinear problems
  - Approximate solution of $\underline{u}^*$ - Must be more accurate than the solution of $\underline{u}_h$

Goal oriented error control - Model error

- Exact solution to approximate problem

$$\underline{K}^m \, \underline{u}^m = \underline{f} \quad \Rightarrow Q \approx Q^m = \underline{q}^{\mathrm{T}} \underline{u}^m$$

- Model error

$$E^m \stackrel{\text{def}}{=} Q - Q^m = \underline{q}^{\mathrm{T}} \left(\underline{u} - \underline{u}^m \right) = \underline{u}^{*\mathrm{T}} \underline{K} \left(\underline{u} - \underline{u}^m \right) = \underline{u}^{*\mathrm{T}} \underline{r}^m$$

Computable residual

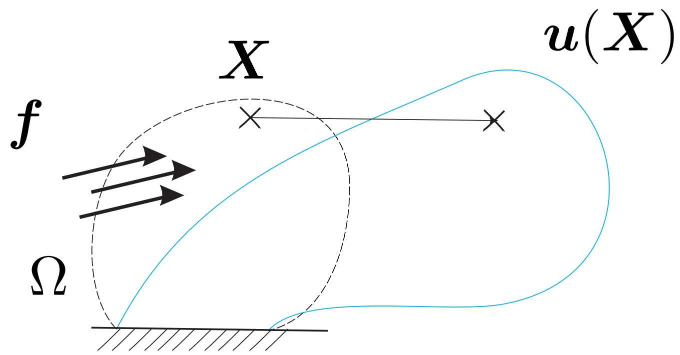
$$\underline{r}^m = \underline{K}\, \underline{u} - \underline{K}\, \underline{u}^m = \underline{f} - \underline{K}\, \underline{u}^m = \left(\underline{K}^m - \underline{K} \right) \underline{u}^m$$

- Adaptivity by controlling $\underline{r}^m$
- Issues in practice
  - Approximate solution of $\underline{u}^*$ - May be based on approximate model
  - Approximate evaluation of exact model, e.g. $\underline{K}$, for model residual - Must be more accurate than approximate model, e.g. $\underline{K}^m$

Prototype problem: Nonlinear elasticity

- Strong form: Solve for displacement field $\boldsymbol{u}(\boldsymbol{X})$ from

$$\begin{aligned} -\boldsymbol{P}\cdot\boldsymbol{\nabla} &= \boldsymbol{f} \quad \text{in } \Omega, \\ \boldsymbol{P} &= \boldsymbol{P}(\boldsymbol{F}), \\ \boldsymbol{F} &= \boldsymbol{I} + \boldsymbol{u}\otimes\boldsymbol{\nabla}, \\ + & \quad \text{Boundary conditions} \end{aligned}$$



- Weak form: Solve for displacements $\boldsymbol{u} \in \mathcal{U}$ s.t.

$$\int_\Omega \boldsymbol{P}\left(\boldsymbol{F}[\boldsymbol{u}]\right) : [\delta\boldsymbol{u}\otimes\boldsymbol{\nabla}]\,\mathrm{d}V = \int_\Omega \boldsymbol{f}\cdot\delta\boldsymbol{u}\,\mathrm{d}V, \quad \forall\delta\boldsymbol{u}\in\mathcal{U}^0$$

- Finite element formulation: Solve for displacements $\boldsymbol{u}_h \in \mathcal{U}_h \subset \mathcal{U}$ s.t.

$$\int_\Omega \boldsymbol{P}\left(\boldsymbol{F}[\boldsymbol{u}_h]\right) : [\delta\boldsymbol{u}\otimes\boldsymbol{\nabla}]\,\mathrm{d}V = \int_\Omega \boldsymbol{f}\cdot\delta\boldsymbol{u}\,\mathrm{d}V, \quad \forall\delta\boldsymbol{u}\in\mathcal{U}_h^0$$

Nonlinear elasticity - Error control

- Dual problem: Solve for displacements $\boldsymbol{u}^* \in \mathcal{U}^0$ s.t.

$$\int_\Omega [\boldsymbol{u}^* \otimes \boldsymbol{\nabla}] : \frac{\mathrm{d}\boldsymbol{P}}{\mathrm{d}\boldsymbol{F}} : [\delta \boldsymbol{u} \otimes \boldsymbol{\nabla}] \,\mathrm{d}V = \int_\Omega \boldsymbol{q} \cdot \delta \boldsymbol{u} \,\mathrm{d}V, \quad \forall \delta \boldsymbol{u} \in \mathcal{U}^0$$

  based on output of interest $Q(\boldsymbol{u}) = \int_\Omega \boldsymbol{q} \cdot \boldsymbol{u} \mathrm{d}V$

- Approximate model

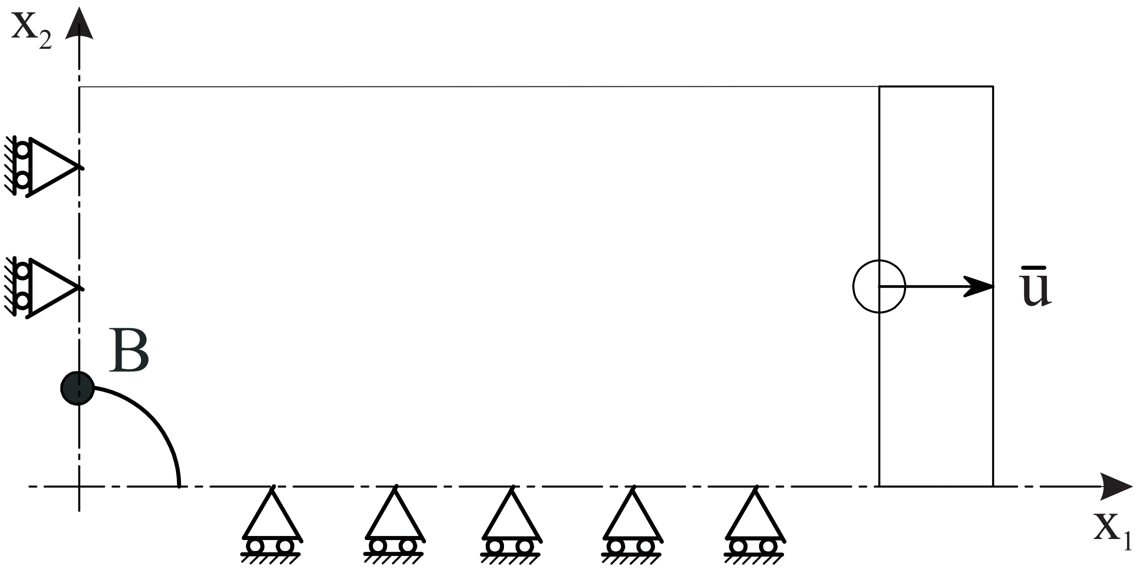
$$\boldsymbol{P}(\boldsymbol{F}) \approx \boldsymbol{P}^m(\boldsymbol{F})$$

- Error computation for approximation $\boldsymbol{u}_h^m$

$$E = \underbrace{\int_\Omega \boldsymbol{f} \cdot \boldsymbol{u}^* \,\mathrm{d}V - \int_\Omega \boldsymbol{P}^m \left(\boldsymbol{F}[\boldsymbol{u}_h^m]\right) : [\boldsymbol{u}^* \otimes \boldsymbol{\nabla}] \,\mathrm{d}V}_{\text{Discretization error}}$$

$$+ \underbrace{\int_\Omega \boldsymbol{P}^m \left(\boldsymbol{F}[\boldsymbol{u}_h^m]\right) : [\boldsymbol{u}^* \otimes \boldsymbol{\nabla}] \,\mathrm{d}V - \int_\Omega \boldsymbol{P} \left(\boldsymbol{F}[\boldsymbol{u}_h^m]\right) : [\boldsymbol{u}^* \otimes \boldsymbol{\nabla}] \,\mathrm{d}V}_{\text{Modeling error}}$$

Numerical example – Adaptive modeling

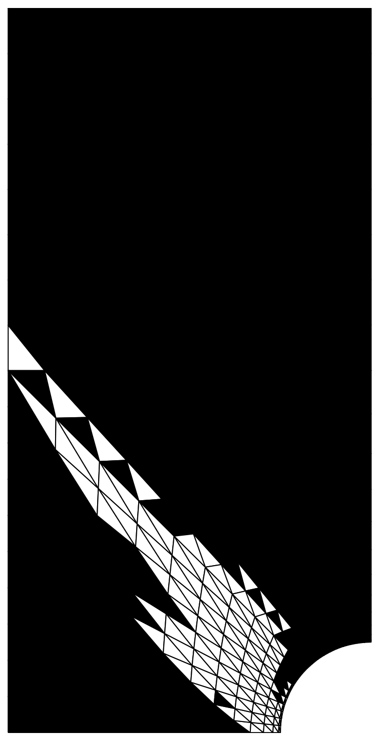


- "Exact" model: Elasto-plasticity
- "Approximate" model: Elasticity
- Error measure: Contraction of hole diameter $Q(\boldsymbol{u}) = -u_2|_{\boldsymbol{X}=\boldsymbol{X}_B}$
- **Note:** Only model error computed
  $\Rightarrow \quad \boldsymbol{u}_h^* \in \mathbb{V}_h$ considered ”exact”
- LARSSON, RUNESSON: *Comput.Meth.Appl.Mech.Eng.* (2004)

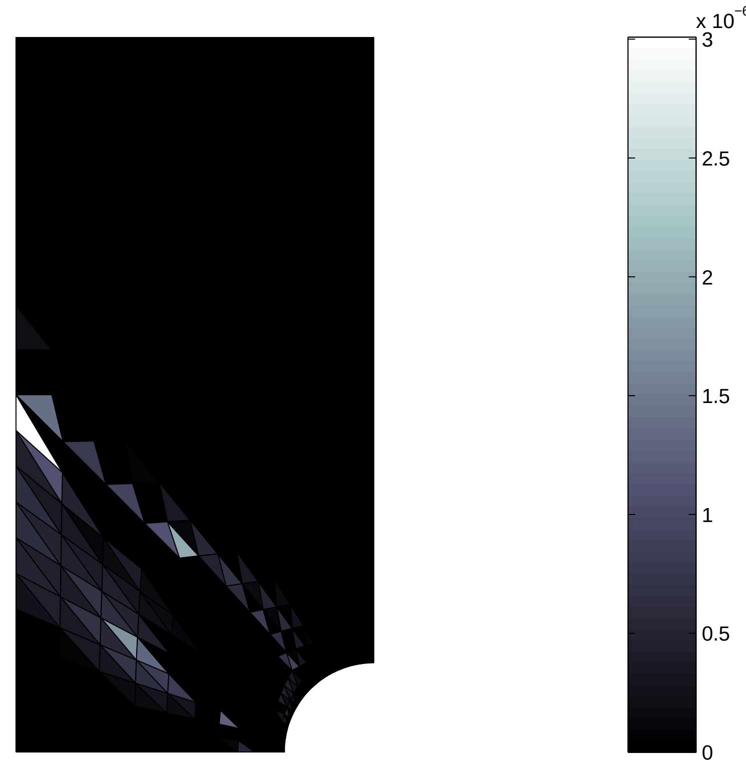
Model adaptivity – Coarse tolerance

$$TOL = 10\%$$

Model resolution



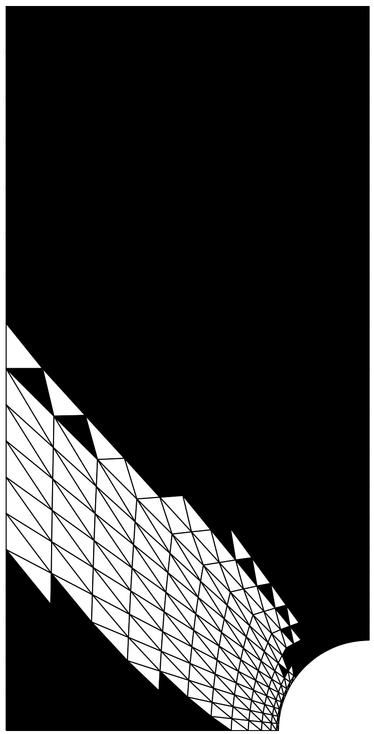
Error distribution



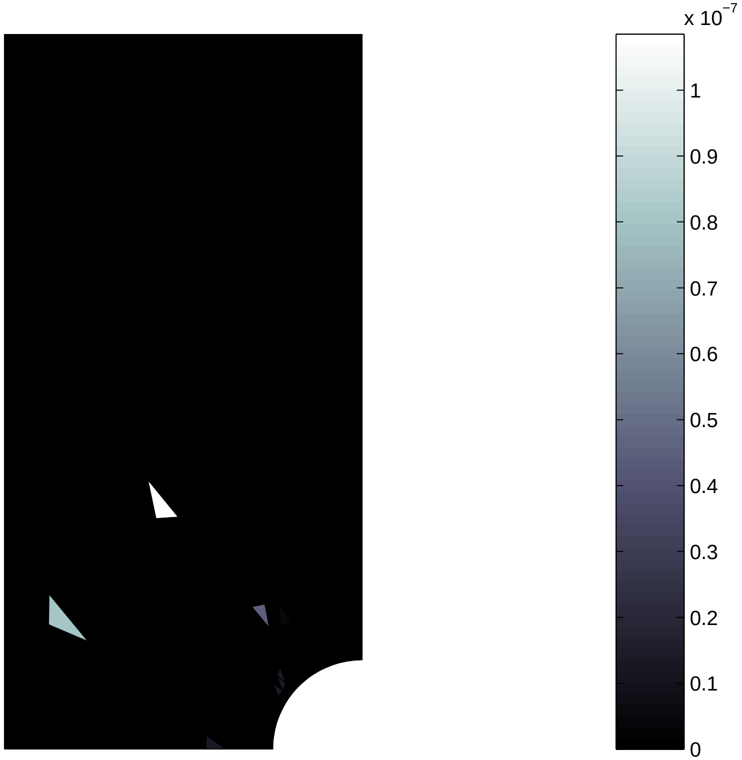
Model adaptivity – Fine tolerance

$$TOL = 1\%$$

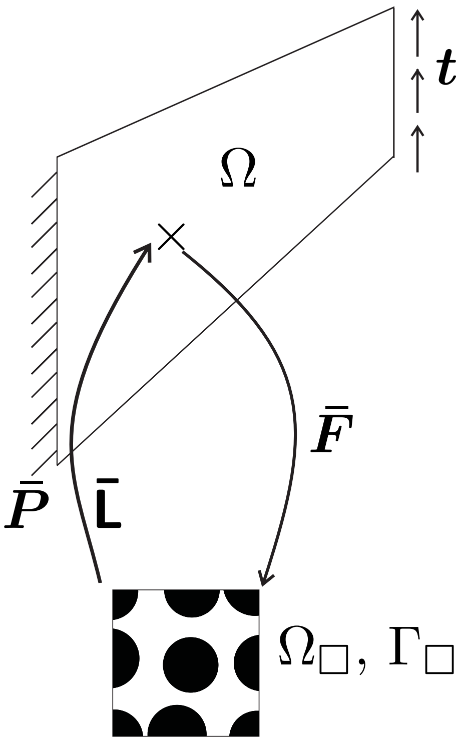
Model resolution



Error distribution



Classical (first order) homogenization



Macro-scale (equilibrium): $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$

$$\bar{a}\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}\} = \bar{l}\{\delta\bar{\boldsymbol{u}}\}, \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0$$

$$\to \bar{\boldsymbol{H}} \; (= \bar{\boldsymbol{F}} - \boldsymbol{I})$$

"Typical subscale problem" for Representative Volume Element (RVE): For given $\bar{\boldsymbol{H}}$, find $\boldsymbol{u} \in \mathbb{U}_\square(\bar{\boldsymbol{H}})$

$$"a_\square(\boldsymbol{u}; \delta\boldsymbol{u}) = l_\square(\delta\boldsymbol{u})", \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_\square^0$$

$$\to \bar{\boldsymbol{P}}, \bar{\mathsf{L}} \quad [\mathrm{d}\bar{\boldsymbol{P}} = \bar{\mathsf{L}} : \mathrm{d}\bar{\boldsymbol{F}} \text{ algorithmic relation}]$$

- Remarks
  - Basis for FE^2 method, iterative solution involving macro- and subscales
  - $\{\bullet\}$ implicit function (via homogenization)
  - Functions in $\bar{\mathbb{U}}$ smoother than $\mathbb{U}_\square(\bar{\boldsymbol{H}})$

Macroscale model and discretization errors

- ”Fine” model: Exact solution $\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}$ solves

$$\bar{a}\{\bar{\boldsymbol{u}}; \delta\bar{\boldsymbol{u}}\} = \bar{l}\{\delta\bar{\boldsymbol{u}}\} \quad \forall \delta\bar{\boldsymbol{u}} \in \bar{\mathbb{U}}^0$$

- ”Work” model ($q =$ hierarchical model parameter): FE-solution $\bar{\boldsymbol{u}}_{Hq} \in \bar{\mathbb{U}}_H \subset \bar{\mathbb{U}}$ solves

$$\bar{a}_{(q)}\{\bar{\boldsymbol{u}}_{Hq}; \delta\bar{\boldsymbol{u}}_H\} = \bar{l}\{\delta\bar{\boldsymbol{u}}_H\} \quad \forall \delta\bar{\boldsymbol{u}}_H \in \bar{\mathbb{U}}_H^0 \subset \bar{\mathbb{U}}^0$$

- Error measure $E\{\bar{\boldsymbol{u}}; \bar{\boldsymbol{u}}_{Hq}\} = Q\{\bar{\boldsymbol{u}}\} - Q_{(q)}\{\bar{\boldsymbol{u}}_{Hq}\}$
- Exact error representation using dual solution $\bar{\boldsymbol{u}}^* \in \bar{\mathbb{U}}^0$

$$E\{\bar{\boldsymbol{u}}, \bar{\boldsymbol{u}}_{Hq}\} = \underbrace{R_{\mathrm{FEM}}\{\bar{\boldsymbol{u}}_{Hq}; \bar{\boldsymbol{u}}^* - \bar{\boldsymbol{\rho}}_H\}}_{E_{\mathrm{FEM}}} + \underbrace{R_{\mathrm{MOD}}\{\bar{\boldsymbol{u}}_{Hq}; \bar{\boldsymbol{u}}^*\}}_{E_{\mathrm{MOD}}}, \quad \forall \bar{\boldsymbol{\rho}}_H \in \mathbb{U}_H^0$$

Macroscale model and discretization errors

- Discretization and model residuals

$$R_{\mathrm{FEM}}\{\bar{\boldsymbol{u}}_{Hq};\delta\bar{\boldsymbol{u}}\} = \bar{l}\{\delta\bar{\boldsymbol{u}}\} - \int_{\Omega} \bar{\boldsymbol{P}}_{(q)}\{\bar{\boldsymbol{u}}_{Hq}\} : \bar{\boldsymbol{H}}[\delta\bar{\boldsymbol{u}}]\,\mathrm{d}\Omega$$

$$R_{\mathrm{MOD}}\{\bar{\boldsymbol{u}}_{Hq};\delta\bar{\boldsymbol{u}}\} = -\int_{\Omega} \left[\bar{\boldsymbol{P}}\{\bar{\boldsymbol{u}}_{Hq}\} - \bar{\boldsymbol{P}}_{(q)}\{\bar{\boldsymbol{u}}_{Hq}\}\right] : \bar{\boldsymbol{H}}[\delta\bar{\boldsymbol{u}}]\,\mathrm{d}\Omega$$

- **Remarks**
  - R_{FEM} captures macroscale discretization error
  - R_{MOD} captures macroscale error due to inexact computation of subscale stresses: $\bar{\boldsymbol{P}}\{\bar{\boldsymbol{u}}\} - \bar{\boldsymbol{P}}_{(q)}\{\bar{\boldsymbol{u}}\}$ macroscale stress error
  - $\bar{\boldsymbol{P}}_{(q)}$ computable for given subscale "model", $\bar{\boldsymbol{P}}$ normally inaccessible $\leadsto$ need for approximation, i.e. ”best possible accessible model”, $\bar{\boldsymbol{P}}_{(q^+)}$, $q^+ \gg q$
  - Hierarchical model parameter $q(\boldsymbol{X},t) \in [q_{\mathrm{coarse}}, q_{\mathrm{fine}}]$ in $\Omega \times I$, q_{fine} may be inaccessible!! E.g. $L_{\square} = L_{\mathrm{RVE}} = \infty$
  - Adaptive choice of (balanced) discretization and model errors fulfills accuracy requirement

Sources of macroscale model errors

- Inadequate constitutive models for subscale constituents
- Inexact prolongation conditions (variational framework, boundary conditions) of Representative Volume Element, RVE
- Finite size of RVE, (should rather be denoted Subscale Volume Element for $L_{\square} < \infty$)
- FE-discretization of subscale problem – (Adaptive FE)^2
- Neglecting subscale transient character
- **Remark**: Exact solution still based on complete scale separation within the chosen framework of model-based homogenization. Error due to scale-mixing is *not* (and cannot be) included in this framework!

Transfer of error across the scales

- Verifiable errors: Model, discretization, numerical solution, etc

  Scale 0 (macroscale)
  model error, discretization error

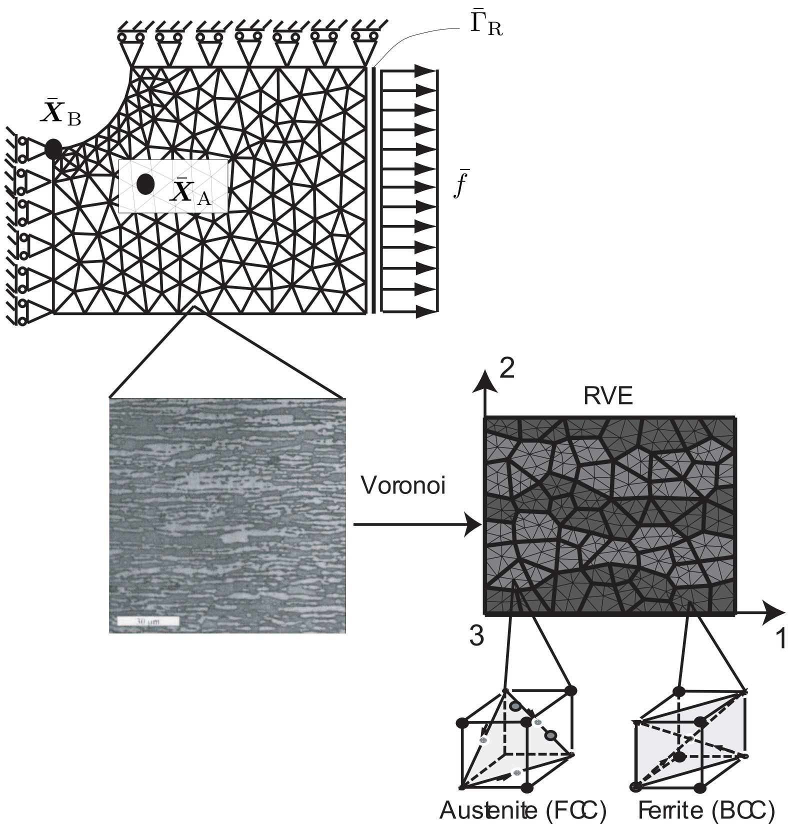
  $\upuparrows$
  Subscale 1
  model error , discretization error

  $\upuparrows$
  Subscale 2
  model error, discretization error

  $\upuparrows$
  . . .

- **Remark**: All errors on a given subscale appear as model error on the nearest coarser scale

Example: Membrane of Duplex Stainless Steel



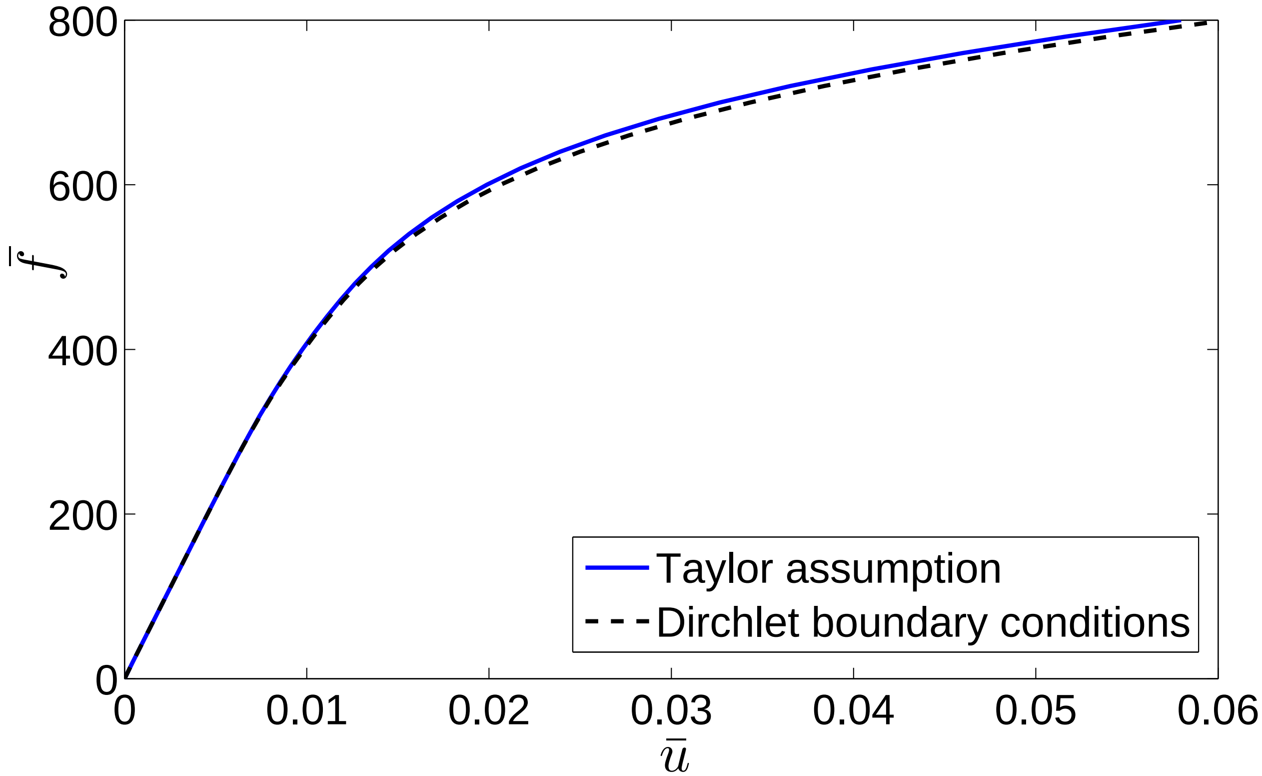
- Macro-scale plane stress, $\bar{P}_{33} = 0$
- Crystal plasticity in each phase
- Only model error considered
- Subscale modeling: Prolongation conditions
  - Dirichlet boundary conditions: accurate - expensive ($q = 1$)
  - Voigt (=Taylor) approximation: approximate - low cost ($q = 0$)
- $Q = \bar{u}_2(\bar{\boldsymbol{X}}_B)$ diameter contraction

- Material parameter values for two phases of SAF 2507 DSS

	λ [GPa]	G [GPa]	q	ξ	h_0 [MPa]	h_∞ [MPa]	τ_y [MPa]	n	t_* [s]
austenite	71	106	1.40	188	3680	0	164	1	small
ferrite	71	106	1.61	148	768	0	321	1	small

Macroscale response (non-adaptive)

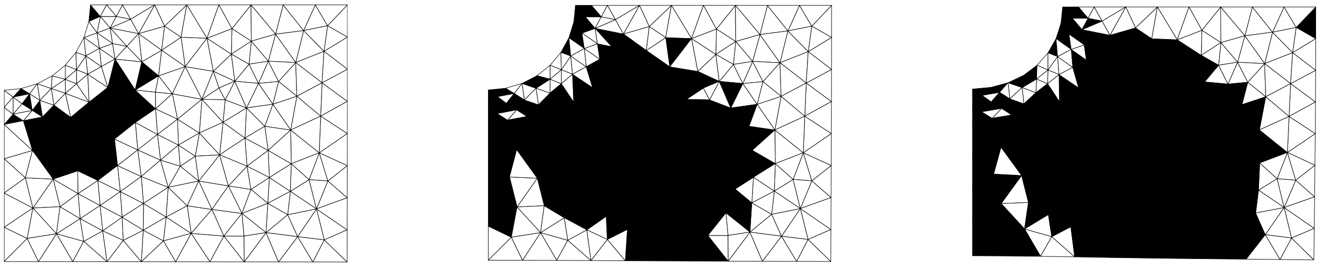
- Global load-displacement response for DSS-membrane



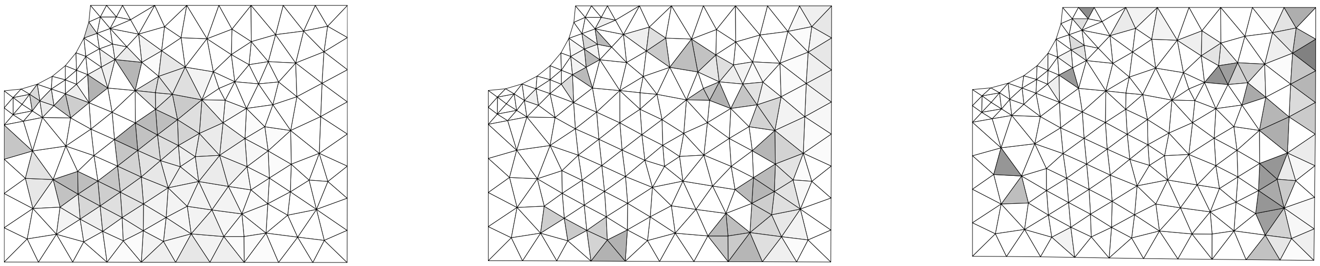
- Only one single realization of RVE in each macroscale GP
- **Note:** Global response is quite insensitive. Would the Taylor model (fluctuation field omitted) suffice?

Adaptive subscale Dirichlet-Taylor

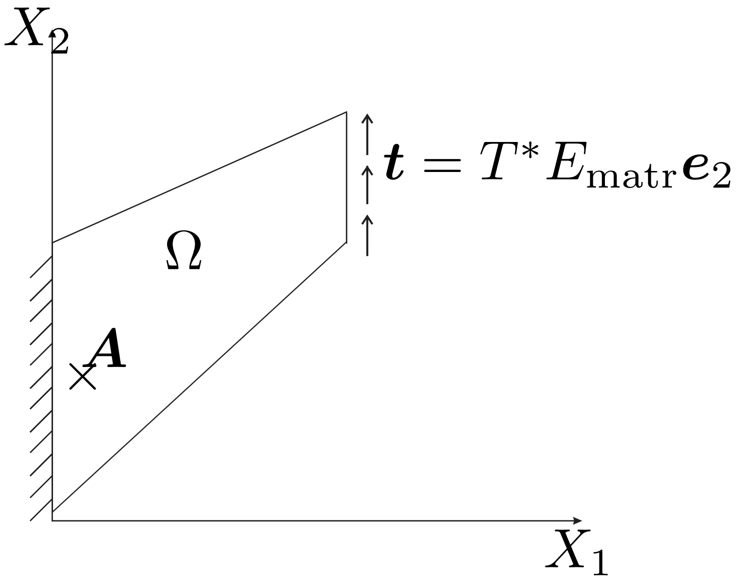
- Adaptive results for TOL$\approx 10^{-4}$ at completed loading (40 load incr). Assumed at most linear error growth. **Note:** Very small tolerance!
  - Model distribution (dark=Dirichlet) after 20, 30 and 40 load increments (left to right)

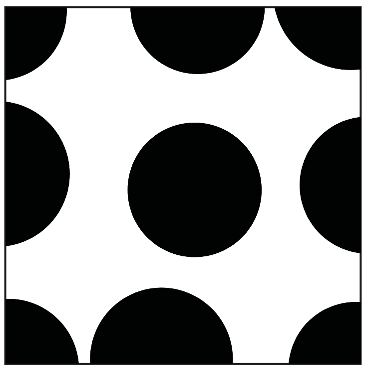


  - Distribution of error (dark=high) generated during 20th, 30th and 40th load increment (left to right)



Example: Meso-macro-scale modeling



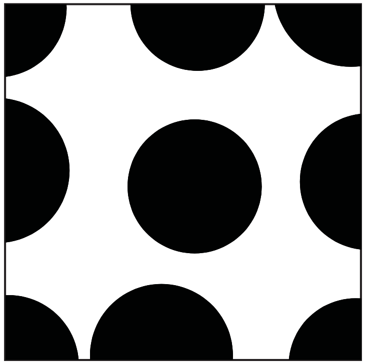


- Macro-scale problem
  - Ramp loading in time, $T^* = 0.01\, t/t_*, \quad t/t_* \in (0, 4)$
  - Goal function: $Q(\boldsymbol{u}) \overset{\mathrm{def}}{=} H_{11}[\boldsymbol{u}]|_{\bar{\boldsymbol{X}}_{\mathrm{A}}}$
  - Aim: Model error $\approx$ Macro-scale discretization error
- Meso-scale problem
  - Random realization (perturbation of particle size and lattice) of composite for particle volume fraction.

Subscale: Adaptive constitutive modeling

- Elasto-plastic matrix

$$E_{\rm matr},\ \nu_{\rm matr} = 0.3$$
$$\sigma_{\rm y} = 0.01\, E_{\rm matr} \text{ (von Mises)}$$
$$H = 0.2\, E_{\rm matr},\ r = 0.5 \text{ (mixed hardening)}$$
$$t_* \text{ (Perzyna visco-plasticity)}$$



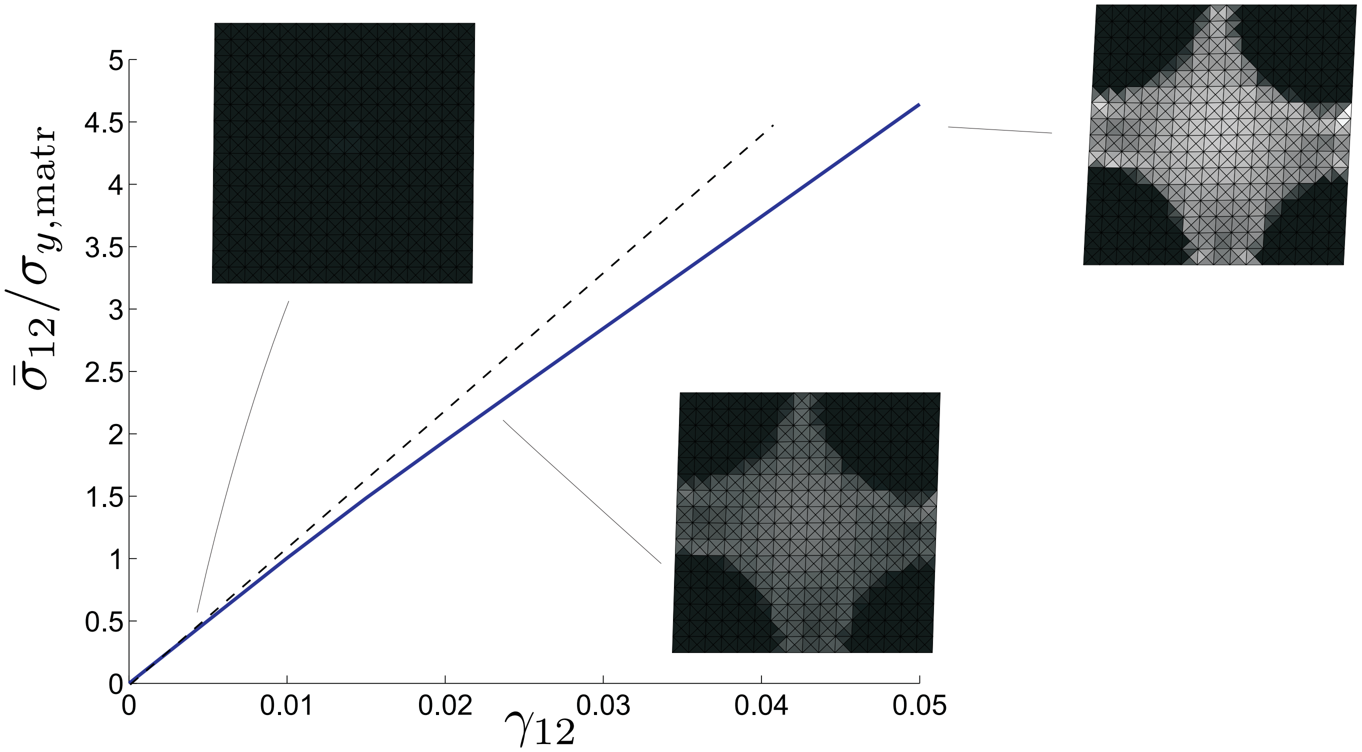
- Elastic grains

$$E_{\rm part} = 5\, E_{\rm matr},\ \nu_{\rm part} = 0.3$$

- Model hierarchy
  - $q = q_{\rm fine} = 1$: Elasto-plastic matrix $\rightsquigarrow$ Meso-macro-scale model
  - $q = 0$: Linear elastic matrix $\rightsquigarrow$ A priori homogenized macro-model

Meso-scale Example: Simple shear test

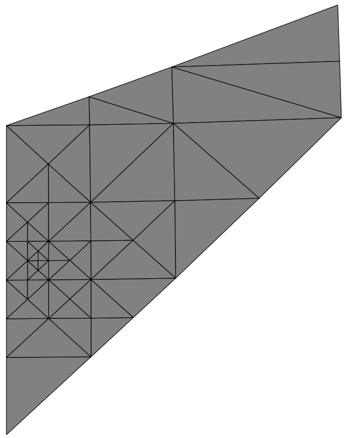
- Elasto-plastic composite
  - Elasto-plastic matrix
  - Elastic particles
- Macroscopic simple shear test (of RVE)
  Effective plastic strain: 0 (black) – $\sim 2.5\%$ (white)



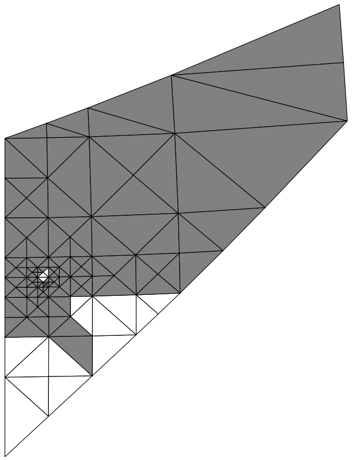
Constitutive modeling – Adaptive results

- Adaptive error control
- Total (spatial) error $\tilde{E}_{\mathrm{rel}} \approx 5\%$ within each time-step
- Aim: Model error ≈ Macro-scale discretization error

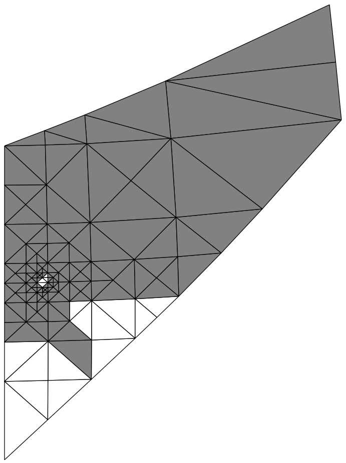
Adapted mesh and model, $t/t_* = 1$



Adapted mesh and model, $t/t_* = 2$

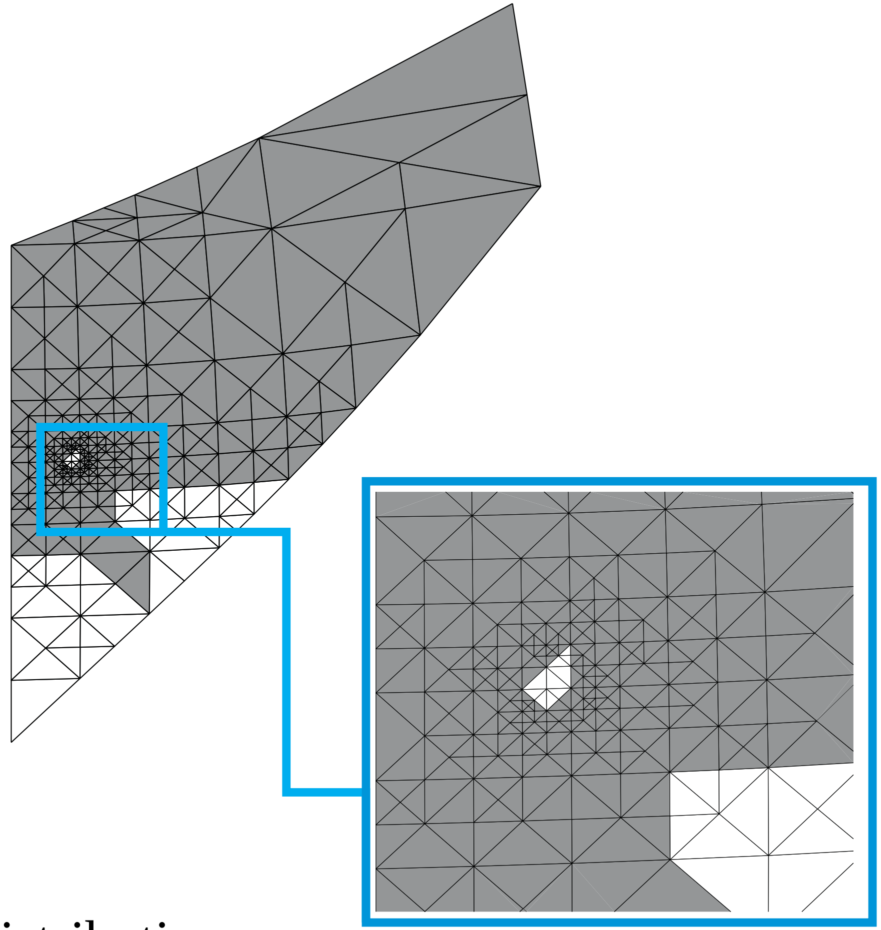


Adapted mesh and model, $t/t_* = 3$



- Adapted model distribution
  - $q = 0$: Elastic matrix (dark)
  - $q = 1$: Elasto-plastic matrix (light)

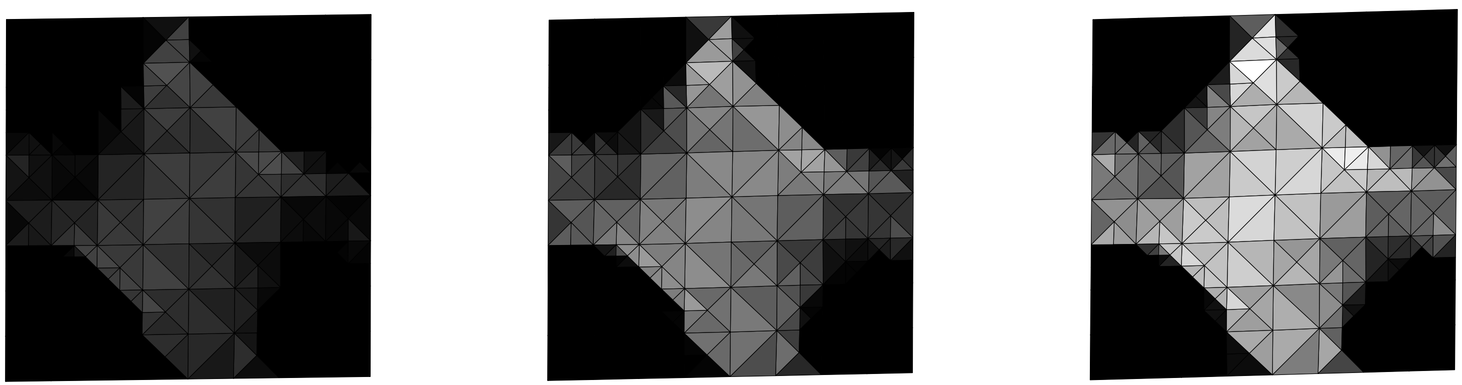
- Final adapted mesh and model, $t/t_* = 4$



- Adapted model distribution
  - $q = 0$: Elastic matrix (dark) – $q = 1$: Elasto-plastic matrix (light)

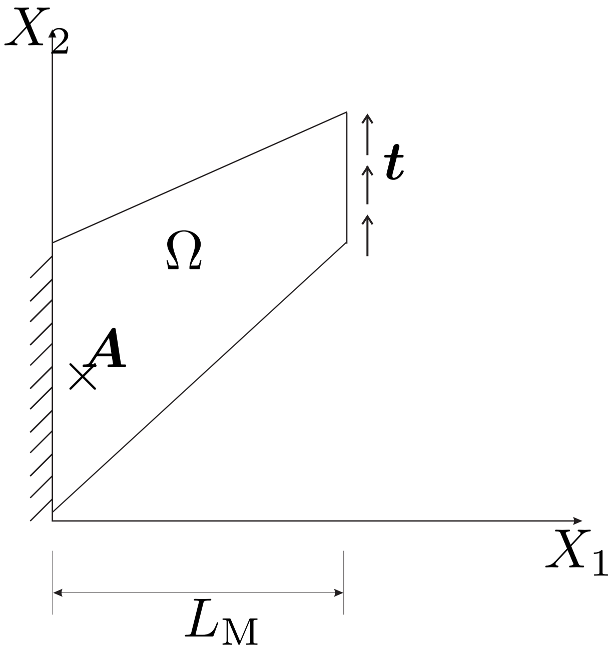
- Example of actual deformed elasto-plastic RVE

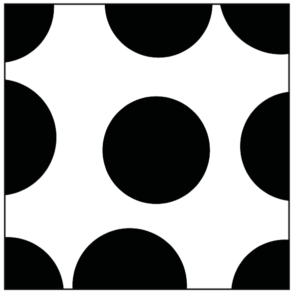
$t/t_* = 2$ $t/t_* = 3$ $t/t_* = 4$ (final)



- Effective plastic strain 0 (black) – $\sim 3.8\%$(white)

Example: Particle composite





- Macro-scale plane strain, $\bar{H}_{33} = 0$
- Nonlinear elastic phases
- Dirichlet b.c. on RVE
- Discretization and model errors considered
- Subscale modeling: FE-discretization, resolved with discrete set of tolerances w.r.t error in macroscale stress components
  - $TOL_\mathrm{sub}(q) = 10^{-(q+1)/2}$, $q = \{1, 2, \ldots\}$

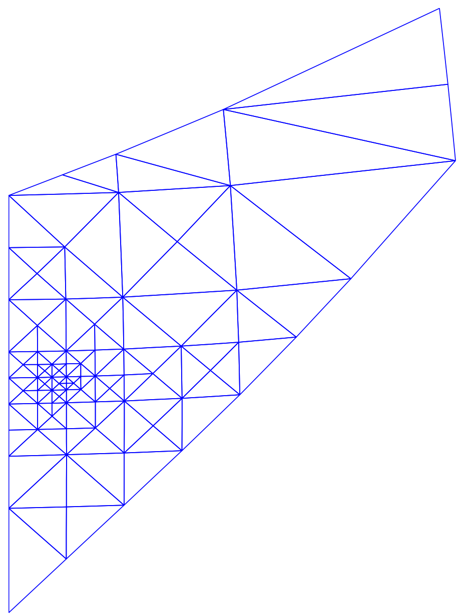
- Material parameter values for two phases

	K [GPa]	G [GPa]
matrix	20	10
particles	300	100

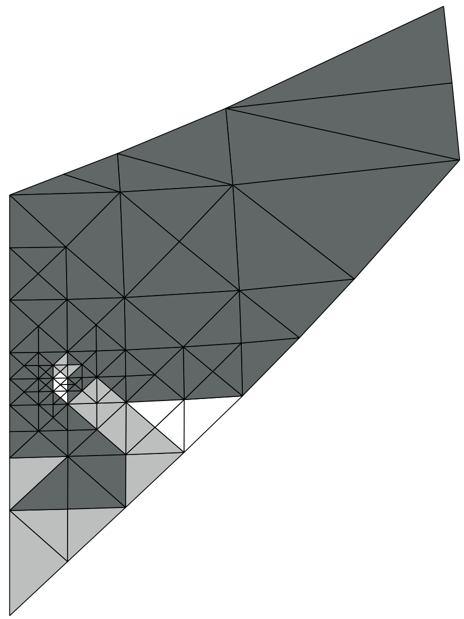
Adaptive discretization of RVE (FE^2)

- Adaptive computation $\rightsquigarrow$ Total relative error $\tilde{E}_{\text{rel}} \approx 5.8\%$ (after 6 macroscale refinements)

Adapted macroscale mesh



Adapted model distribution $q \in [1, 3]$ (dark – light)

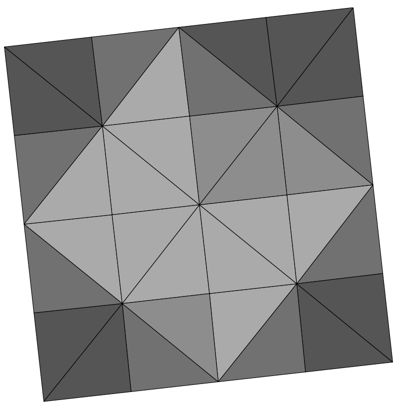


- **Note**: Only one single realization of RVE in each macroscale GP

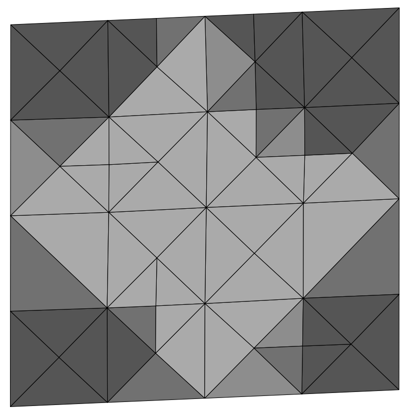
Adaptive discretization of RVE (FE^2)

- Snapshots of deformed RVE's for actual values of macroscale $\bar{\boldsymbol{F}}$ and subscale error tolerance level q

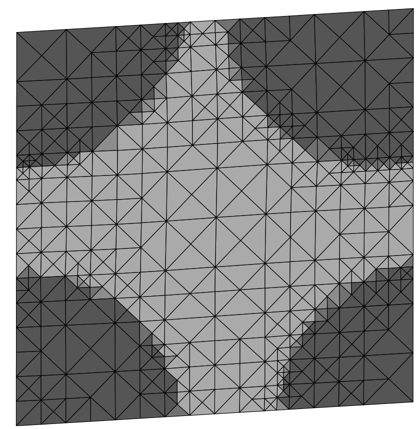
$q = 1$
$TOL_{\text{sub}} = 10\%$



$q = 2$
$TOL_{\text{sub}} = 3.2\%$

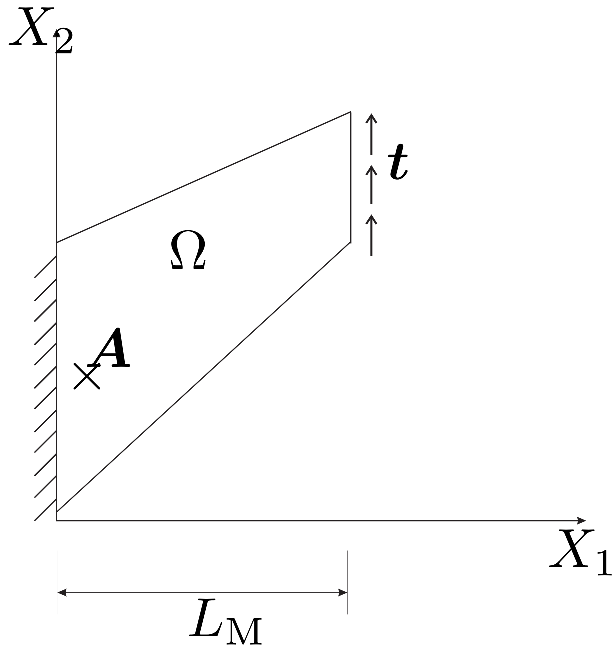


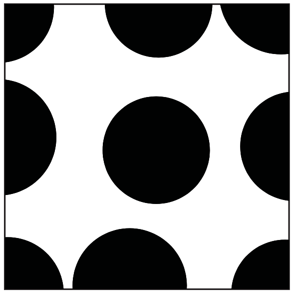
$q = 3$
$TOL_{\text{sub}} = 1\%$



- **Note**: Enhanced (automatic) subscale resolution for reduced tolerance, TOL_{sub}, on subscale discretization error

Example: Particle composite



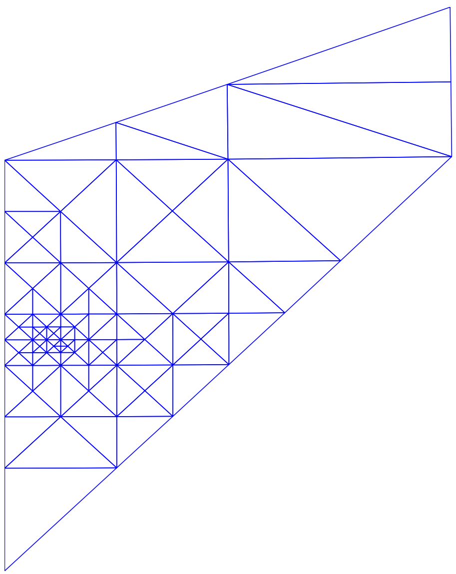


- Macro-scale plane strain, $\bar{H}_{33} = 0$
- Nonlinear elastic phases
- Dirichlet b.c. on RVE
- Fixed tolerance ($TOL_{\mathrm{sub}} = 5\%$) for RVE discretization w.r.t. error in macro-scale stress components $\rightsquigarrow$ adaptive subscale meshes (unique for each RVE)
- Discretization and model errors considered
- Subscale modeling: Size of RVE
  - $L_{\square} = q\times$ lattice size, $q = \{1, 2, \ldots\}$

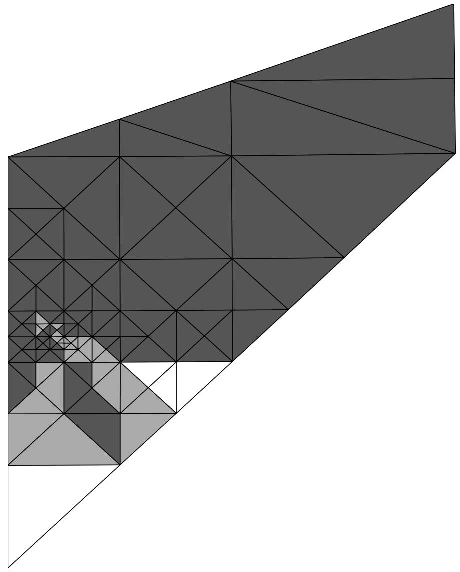
Adaptive size of RVE (FE^2)

- Adaptive computation $\rightsquigarrow$ Total relative error $\tilde{E}_{\text{rel}} \approx 4.1\%$ (after 5 refinements)

Adapted mesh

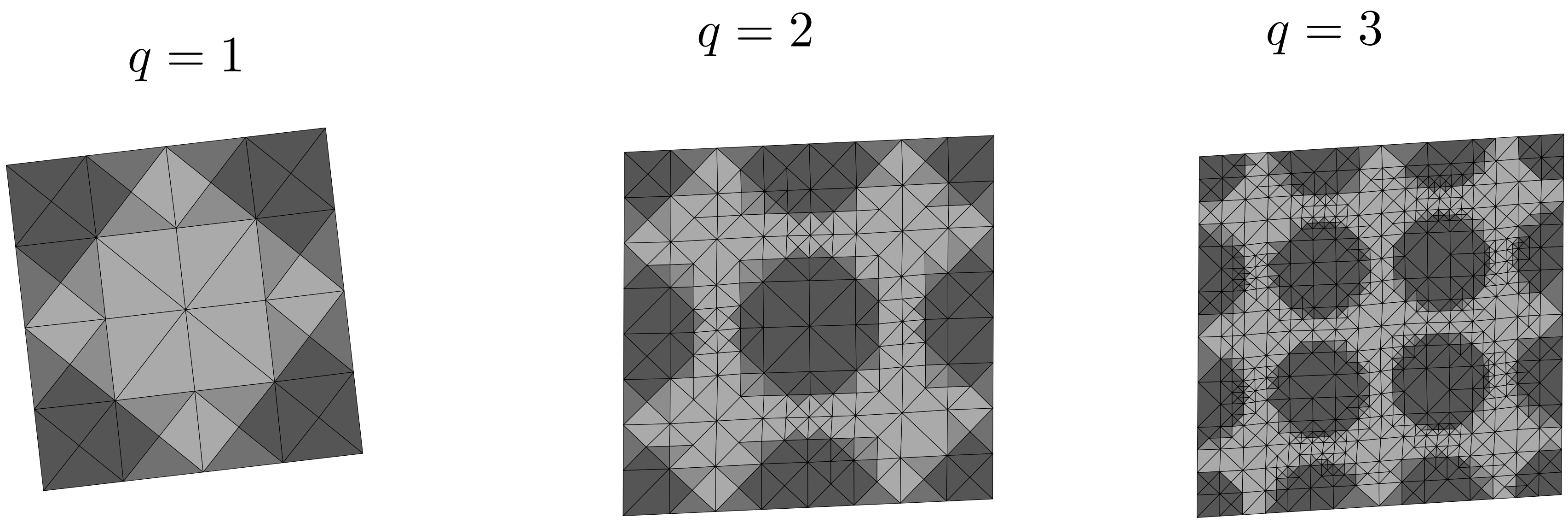


Adapted model distribution $q \in [1,3]$ (dark – light)



Adaptive size of RVE (FE^2)

- Snapshots of deformed QVE's for actual values of macroscale $\bar{\boldsymbol{F}}$ (deformation magnified) and subscale error tolerance level q



- Remarks:
  - Small macro-deformations (although possibly large RBM, which contribute to $\bar{\boldsymbol{F}}$) $\rightsquigarrow$ Small-size QVE
  - Small-size QVE $\rightsquigarrow$ Near-homogeneous sub-scale deformations for Dirichlet B.C. ($\sim$ Taylor assumption) $\rightsquigarrow$ Coarse sub-scale mesh for given tolerance

Two-scale modeling - ”The basic dilemma”

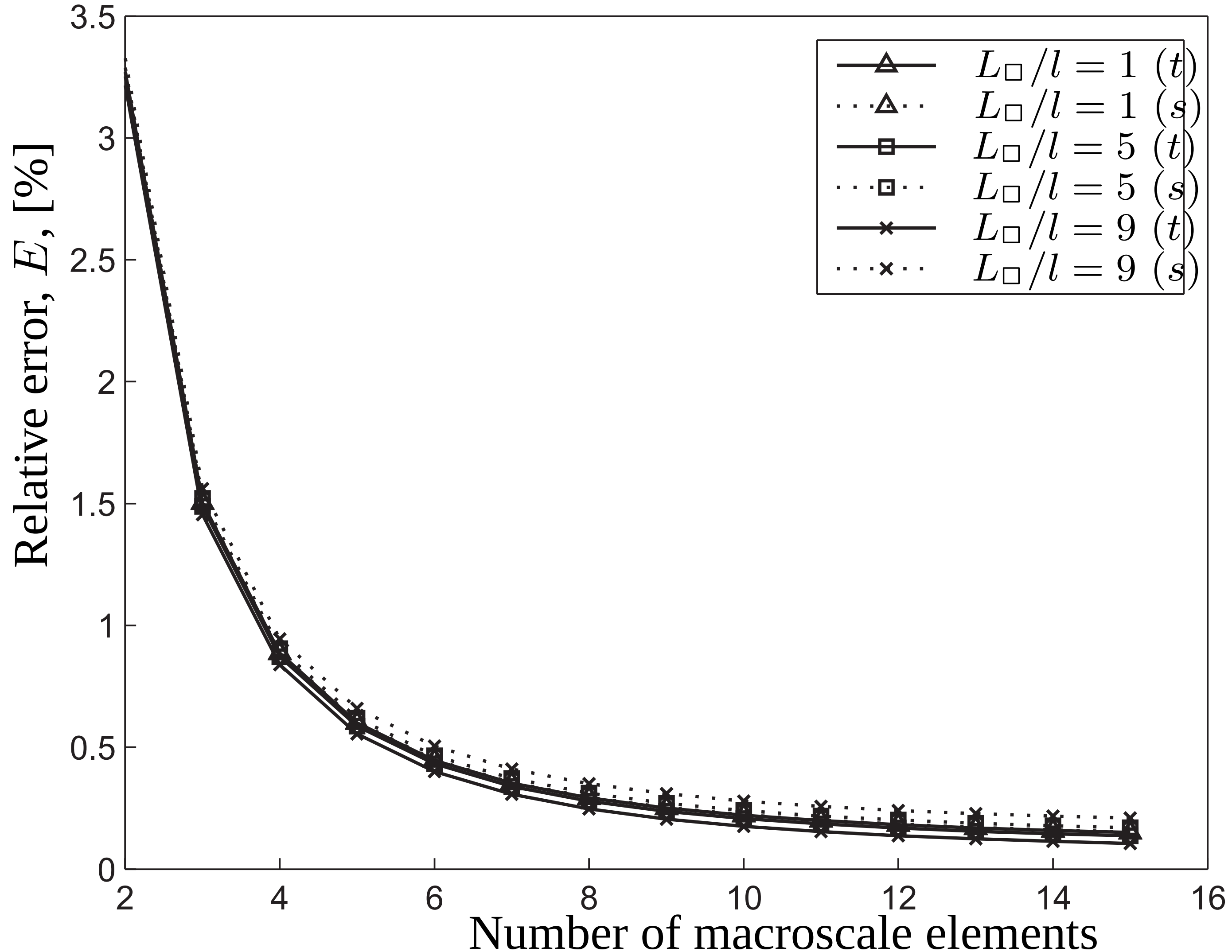
- Mixing/separation of scales: Two extreme cases
  1. Adopt (1st order) homogenization everywhere (complete scale separation) – inexpensive
     Note: Communication via macro- and subscales entirely via homogenized quantities, e.g. strains and stresses
  2. Resolve fine scale evereywhere in the space/time domain (complete scale mixing), "overkill" solution – expensive
- Need to account for scale-mixing depends on
  - Physical phenomena resulting in smooth or non-smooth fields, e.g. localized damage and deformations is stress problems
  - Required level of accuracy in desired output (quantity of interest): Local (subscale) or global (macroscale)

Example of scalemixing – Transient problems

- Transient RVE-problem
  $\rightsquigarrow$ Size-effect (Physical & Numerical)
  0^{th} and 1^{st} order derivatives in space
- Stationary RVE-problem (Exact for the limit $L_\square \rightarrow 0$)
  $\rightsquigarrow$ Complete scale separation
  cf. ÖZDEMIR ET AL. (2008), TEMIZER & WRIGGERS (2010)
- Investigation of error for 1D heat flow example
  - Macroscale problem of size L
  - Harmonic variation of heat capacity and conductivity with wavelength l
  - FE^2-solutions with different RVE-sizes, $L_\square$, and different macro-scale discretizations

Homogenization of transient problems

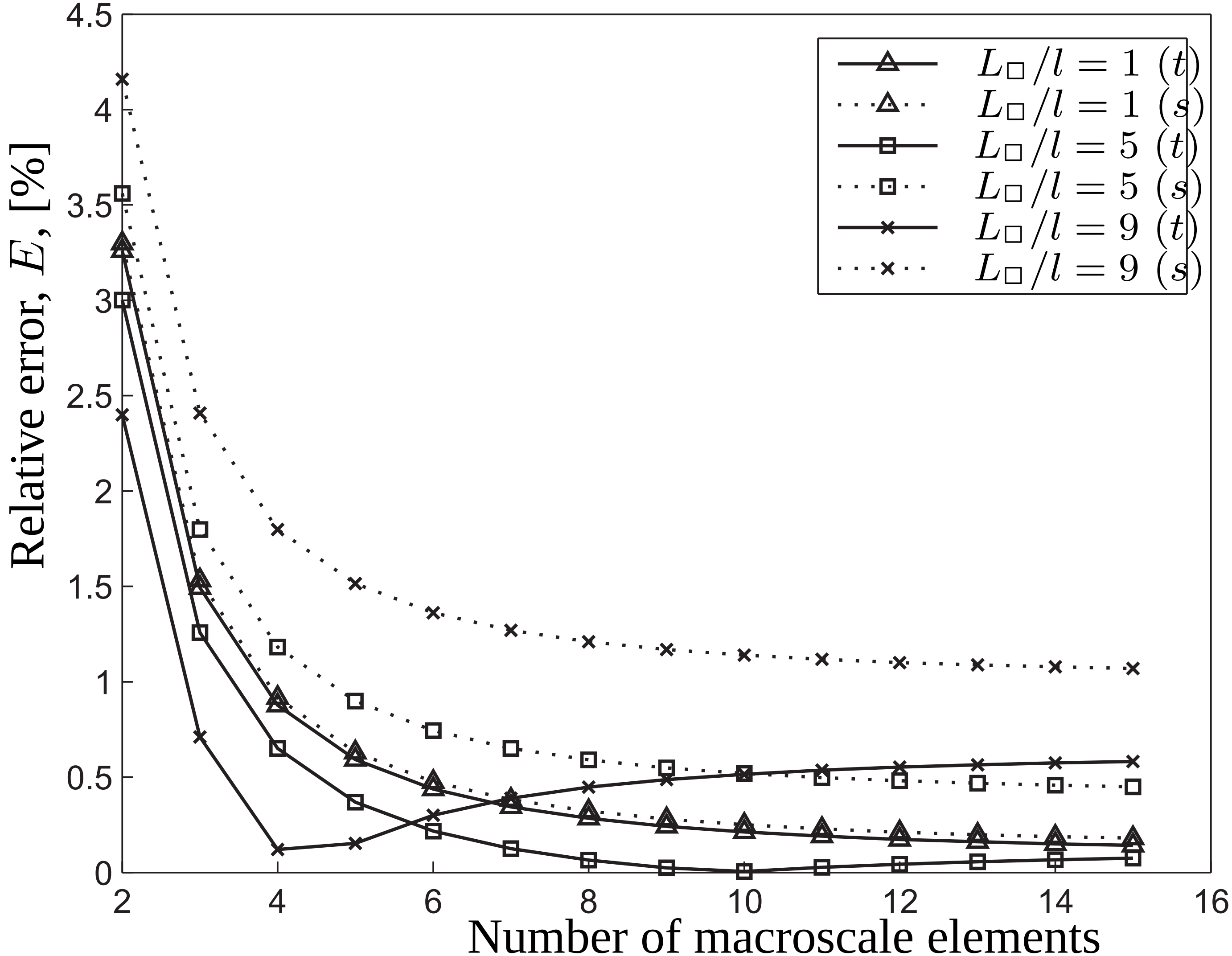
- Large scale separation ($L/l = 100$)



- Converging results

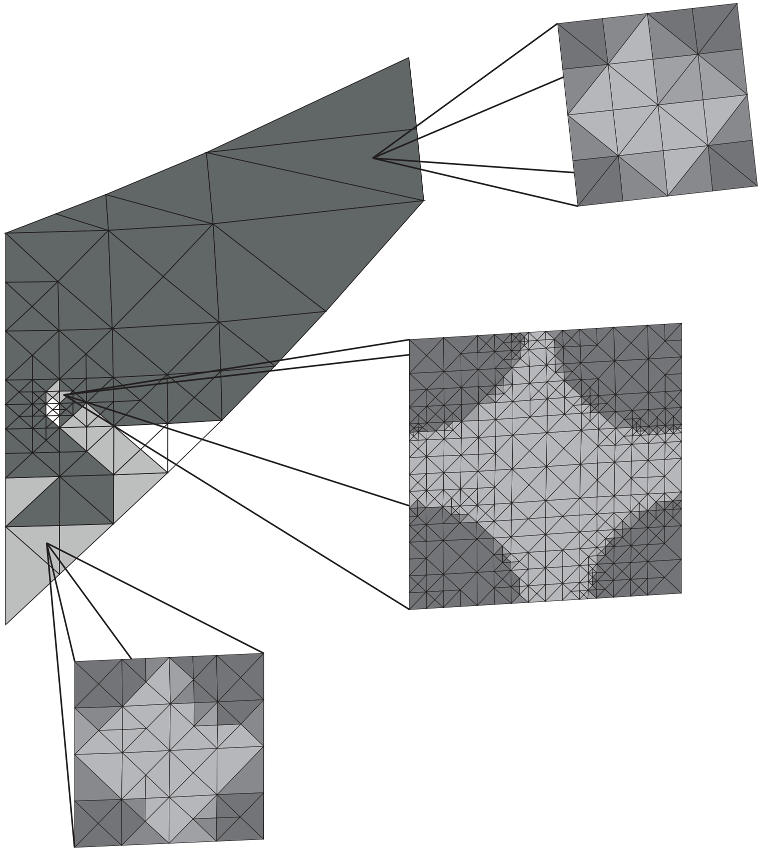
Homogenization of transient problems

- Small scale separation ($L/l = 25$)



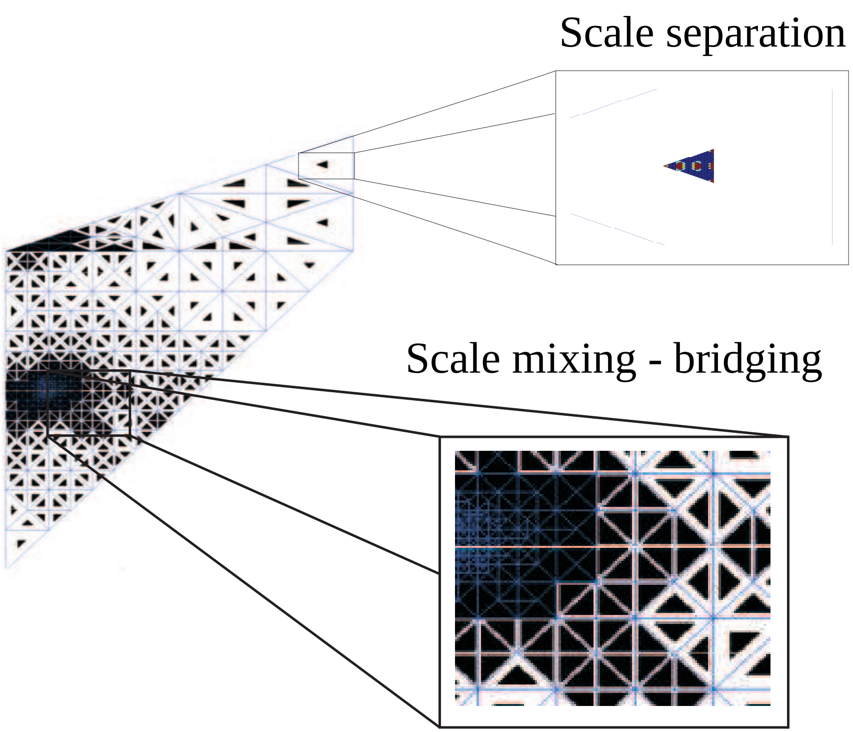
- Optimal RVE-size meshdependent!

"Model-based" homogenization



- A priori assumed separation of scales
- Order of homogenization (1st, 2nd, etc) part of modeling
- Homogenization on RVE's in quadrature points
- Prolongation condition, i.e. how to impose $\bar{\boldsymbol{F}}$ on the subscale (defining the RVE-problem), is part of modeling
- No possibility for "built-in" scale-bridging

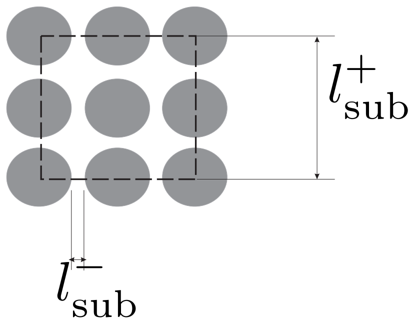
”Discretization-based” homogenization



- No a priori assumed homogenization on RVE’s
- Order of homogenization (1st, 2nd, etc) determined by macroscale FE-approximation (no model assumption)
- Variationally consistent "nonlocal homogenization" on QVE=Quadrature Volume Element (in case of sufficient scale separation)
- Possibility for adaptive FE^2
- Admits adaptive (seamless) bridging of scales

Micro-inhomogeneity - Characteristics

- Characteristic dimensions of substructure
  Note: Periodic lattice structure shown for illustration only



- Resolution length of subscale (e.g. fraction of lattice size with presumed homogeneous material properties): l^-_{sub}
- Size of QVE (Quadrature Volume Element): l^+_{sub}
- **Remark**: Aim for $l^+_{\mathrm{sub}} \approx l_{\mathrm{RVE}}$ = size of RVE (Representative Volume Element)

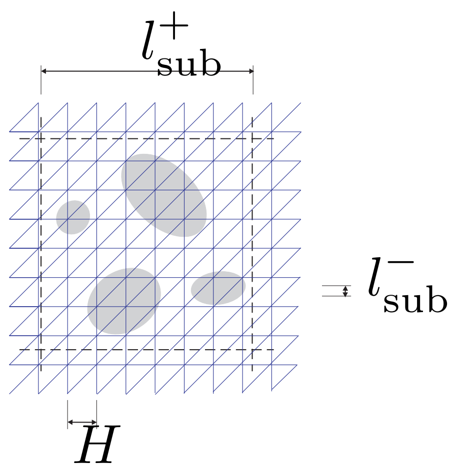
- **Remark**: $l^+_{\mathrm{sub}}, l^-_{\mathrm{sub}}$ obtained as the result of *analysis* of the properties of the substructure: Topology and size of lattice structure (in case of ordered structure), volume fraction of particles, statistical properties, etc. They are not physical lengths *per se* but are rather model assumptions and should be chosen adaptively!

Discretization-based scale-bridging

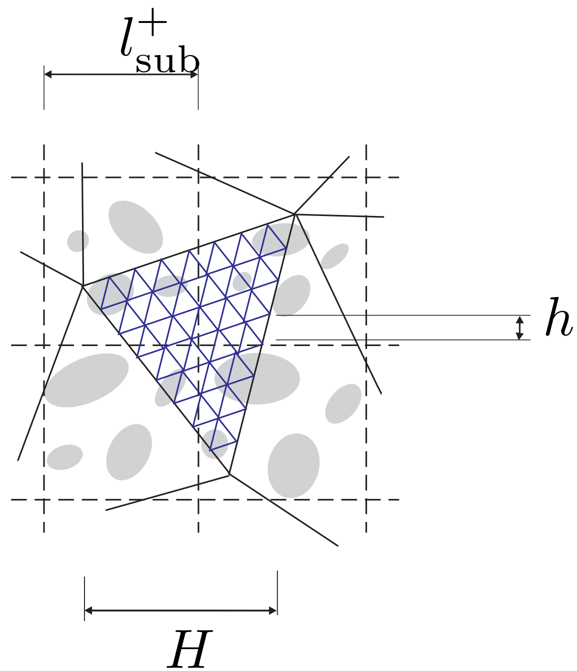
- Model resolution defined by macroscale FE-mesh diameter H
- Scale-bridging levels in present framework relevant to
  - No scale separation (level I)
  - Partial scale separation (level II)
  - (Near-)complete separation (level III)
- The *adaptively* chosen value of H determines the appropriate modeling level!
  $\Rightarrow$ Not quite (but close to) seamless algorithm

Scale-bridging levels

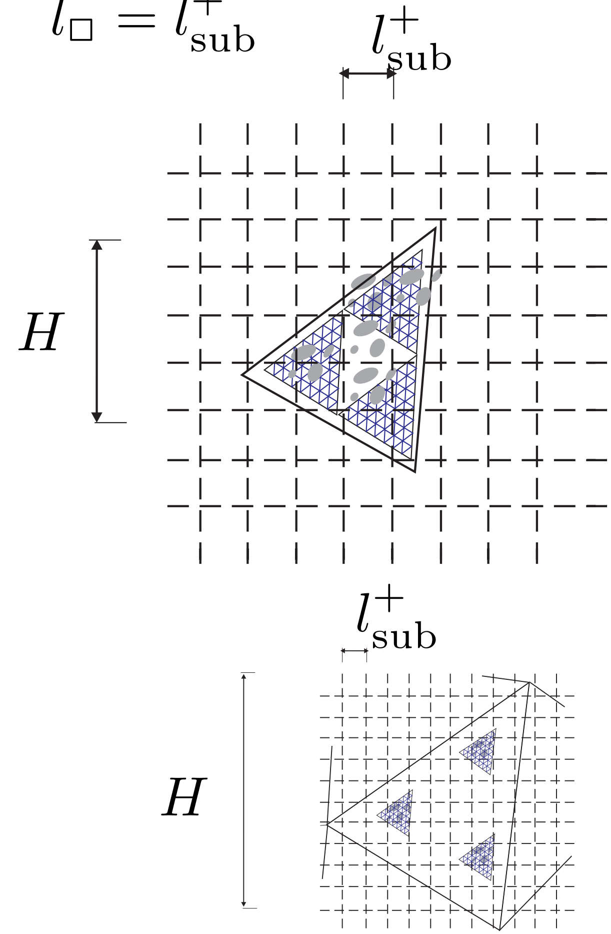
Level I.
$H_{\max} < l_{\text{sub}}^{-}$,
no subscale problem



Level II.
$H_{\max} > l_{\text{sub}}^{-}$, $H_{\min} < l_{\text{sub}}^{+}$,
$l_{\square} = H$



Level III.
$H_{\min} > l_{\text{sub}}^{+}$,
$l_{\square} = l_{\text{sub}}^{+}$



- Level II: cf. Variational Multiscale Method, HUGHES (1995), MÅLQVIST & M. LARSON (2006), . . .

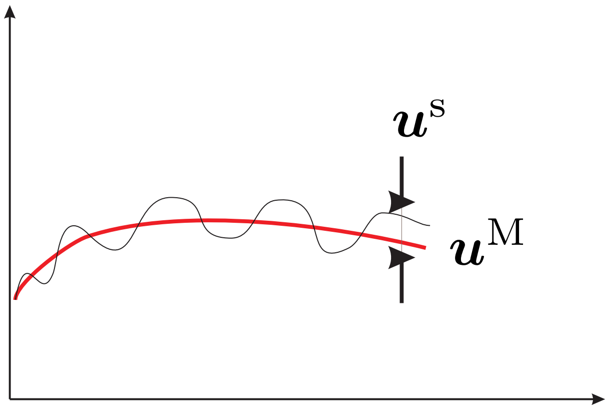
Macro-subscale coupling and homogenization

- (De)coupling of coarse and fine scales

Given $\boldsymbol{u}^{\rm M}$, $\exists$ prolongation $\tilde{\boldsymbol{u}}^{\rm s}\{\boldsymbol{u}^{\rm M}\}$ s.t.

$$\boldsymbol{u} = \tilde{\boldsymbol{u}}\{\boldsymbol{u}^{\rm M}\} \stackrel{\rm def}{=} \boldsymbol{u}^{\rm M} + \tilde{\boldsymbol{u}}^{\rm s}\{\boldsymbol{u}^{\rm M}\}$$

$$\boldsymbol{u}^{\rm M} \to \boldsymbol{u} \;\Rightarrow\; \tilde{\boldsymbol{u}}^{\rm s} \to \boldsymbol{0}$$



$$\boldsymbol{u}^{\rm M} \quad = \quad \text{"coarse scale" - macroscale solution}$$
$$\tilde{\boldsymbol{u}}^{\rm s}\{\boldsymbol{u}^{\rm M}\} \quad = \quad \text{"fine scale" - subscale solution (fluctuation field)}$$

- Condition for $\boldsymbol{u}^{\rm M}$ to act as "homogenizer": Satisfaction of Hill-Mandel macro-homogeneity condition
  - Model-based homogenization: A priori assumption on the variation of $\boldsymbol{u}^{\rm M}$ within RVE's
  - Discretization-based homogenization: FE-approximation for $\boldsymbol{u}^{\rm M} \to \boldsymbol{u}^{\rm M}_H$ within QVE = Quadrature Volume Element

Discretization-based homogenization

- Subscale problem on QVE: Given macroscale FE-solution $\boldsymbol{u}_H^{\mathrm{M}} \mapsto$ subscale prolongation $\tilde{\boldsymbol{u}}^{\mathrm{s}}\{\boldsymbol{u}_H^{\mathrm{M}}\}$ (may be incomputable) replaced by $\tilde{\boldsymbol{u}}^{\mathrm{s}}_{(q)}\{\boldsymbol{u}_H^{\mathrm{M}}\}$ (always computable)
  - q represents hierarchical level of subscale model and defines "work model" Example: Local tolerance: $tol = 10^{-q/2}$
- Subscale "Dirichlet problem" on QVE: For given $\boldsymbol{u}_H^{\mathrm{M}}$, find subscale solution $\tilde{\boldsymbol{u}}^{\mathrm{s}} \in \mathbb{U}_\square = \mathbb{U}_\square^0$, $\tilde{\boldsymbol{u}}^{\mathrm{s}} = \boldsymbol{0}$ on $\Gamma_\square$, s.t.

$$R_\square(\delta\boldsymbol{u}^{\mathrm{s}}) \stackrel{\mathrm{def}}{=} l_\square(\delta\boldsymbol{u}^{\mathrm{s}}) - a_\square(\boldsymbol{u}_H^{\mathrm{M}} + \tilde{\boldsymbol{u}}^{\mathrm{s}}; \delta\boldsymbol{u}^{\mathrm{s}}) = 0 \quad \forall \delta\boldsymbol{u}^{\mathrm{s}} \in \mathbb{U}_\square$$

$$a_\square(\boldsymbol{u};\delta\boldsymbol{u}) \stackrel{\mathrm{def}}{=} \langle \boldsymbol{P}(\boldsymbol{F}) : \boldsymbol{G}[\delta\boldsymbol{u}]\rangle_\square, \quad \langle\bullet\rangle_\square \stackrel{\mathrm{def}}{=} \frac{1}{|\Omega_\square|}\int_{\Omega_\square} \bullet \,\mathrm{d}V, \quad \boldsymbol{G}[\boldsymbol{u}] \stackrel{\mathrm{def}}{=} \boldsymbol{u}\otimes\boldsymbol{\nabla}$$

- **Remark**: Variational framework may be extended to accomodate discont. $\boldsymbol{u}^{\mathrm{s}}$ on $\Gamma_\square$, eg. weakly periodic variational framework [future work]

Discretization-based homogenization

- Macroscale FE-problem for work model: Solve for $\boldsymbol{u}_H^{\mathrm{M}} \in \mathbb{U}_H^{\mathrm{M}}$ that satisfies:

$$R^{(q)}\{\boldsymbol{u}_H^{\mathrm{M}}; \delta\boldsymbol{u}_H^{\mathrm{M}}\} \stackrel{\text{def}}{=} l(\delta\boldsymbol{u}_H^{\mathrm{M}}) - a^{(q)}\{\boldsymbol{u}_H^{\mathrm{M}}; \delta\boldsymbol{u}_H^{\mathrm{M}}\} = 0 \quad \forall \delta\boldsymbol{u}_H^{\mathrm{M}} \in \mathbb{U}_H^{\mathrm{M},0}$$

$$a^{(q)}\{\boldsymbol{u}_H^{\mathrm{M}}; \delta\boldsymbol{u}^{\mathrm{M}}\} \stackrel{\text{def}}{=} \int_\Omega a_\square^{(q)}\{\boldsymbol{u}_H^{\mathrm{M}}; \delta\boldsymbol{u}^{\mathrm{M}}\}\,\mathrm{d}V = \int_\Omega \left\langle \boldsymbol{P}^{(q)}\{\boldsymbol{u}_H^{\mathrm{M}}\} : \boldsymbol{G}[\delta\boldsymbol{u}^{\mathrm{M}}] \right\rangle_\square \mathrm{d}V$$

$$\boldsymbol{P}^{(q)}\{\boldsymbol{u}_H^{\mathrm{M}}\} \stackrel{\text{def}}{=} \boldsymbol{P}(\boldsymbol{G}[\tilde{\boldsymbol{u}}_{Hq}\{\boldsymbol{u}_H^{\mathrm{M}}\}])$$

$$\tilde{\boldsymbol{u}}_{Hq}\{\boldsymbol{u}_H^{\mathrm{M}}\} \stackrel{\text{def}}{=} \boldsymbol{u}_H^{\mathrm{M}} + \tilde{\boldsymbol{u}}_{(q)}^{\mathrm{s}}\{\boldsymbol{u}_H^{\mathrm{M}}\}$$

Discretization-based homogenization

- Macroscale quadrature for FE-solution $\tilde{\boldsymbol{u}}_{Hq}\{\boldsymbol{u}_H^{\mathrm{M}}\} \stackrel{\mathrm{def}}{=} \boldsymbol{u}_H^{\mathrm{M}} + \tilde{\boldsymbol{u}}_{(q)}^{\mathrm{s}}\{\boldsymbol{u}_H^{\mathrm{M}}\}$ of "work model"

$$a(\tilde{\boldsymbol{u}}_{Hq}; \delta\boldsymbol{u}_H^{\mathrm{M}}) = \int_\Omega a_\square^{(q)}\{\boldsymbol{u}_H^{\mathrm{M}}; \delta\boldsymbol{u}_H^{\mathrm{M}}\}\mathrm{d}V \approx \sum_{i=1}^{NQVE} W_i\, a_{\square,i}^{(q)}\{\boldsymbol{u}_H^{\mathrm{M}}; \delta\boldsymbol{u}_H^{\mathrm{M}}\}$$

$W_i =$ quadrature weights

- "Homogenization" on a QVE does not introduce a macroscale error *per se*; however, **quadrature does**!

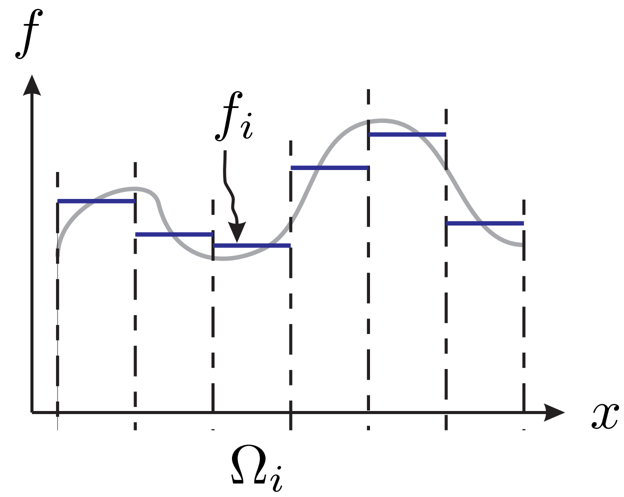
A trivial observation ....

$\mathcal{I} \stackrel{\mathrm{def}}{=} \int_\Omega f(x)\,\mathrm{d}x$

"Homogenization": $f_i \stackrel{\mathrm{def}}{=} \frac{1}{|\Omega_i|}\int_{\Omega_i} f\,\mathrm{d}x$

Define $\tilde{f}(x) = f_i$ if $x \in \Omega_i$

$\Rightarrow \int_\Omega \tilde{f}(x)\,\mathrm{d}x = \mathcal{I}$!!!



Discretization-based homogenization: Evaluation

- "Homogenization property" for macroscale FE-approximation $\boldsymbol{u}_H^{\mathrm{M}}$ of polynomial order p:

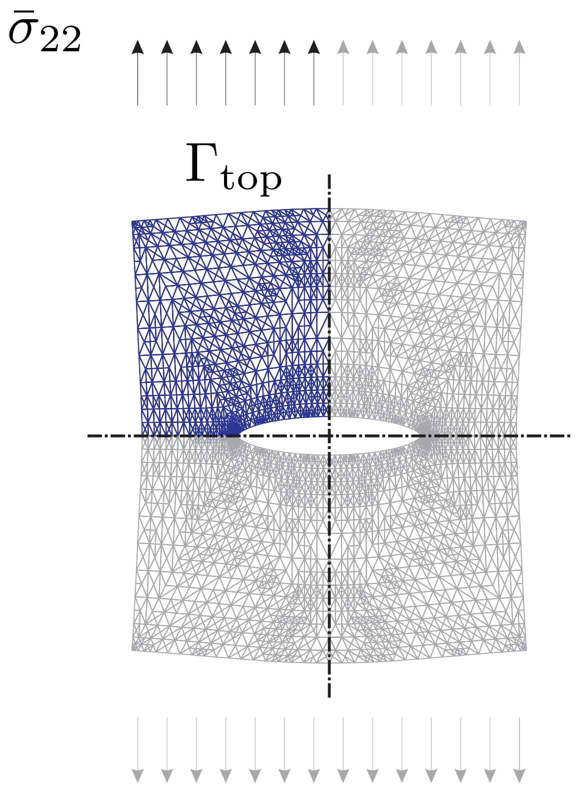
$$\langle \boldsymbol{P} : \boldsymbol{G}[\delta \boldsymbol{u}_H^{\mathrm{M}}] \rangle_\square = \bar{\boldsymbol{P}}^{(1)} : \delta \bar{\boldsymbol{H}}^{(1)} + \bar{\boldsymbol{P}}^{(2)} : \delta \bar{\boldsymbol{H}}^{(2)} + \ldots + \bar{\boldsymbol{P}}^{(p)} : \delta \bar{\boldsymbol{H}}^{(p)}$$

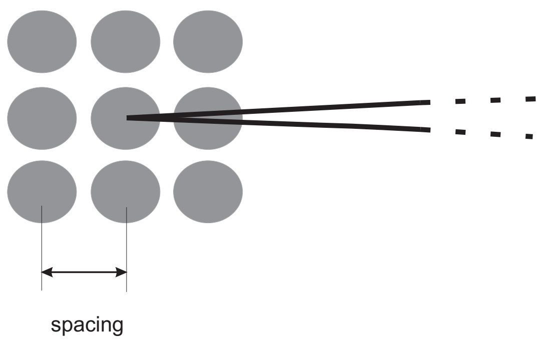
$$\bar{\boldsymbol{P}}^{(k)} \stackrel{\mathrm{def}}{=} \langle \boldsymbol{P} \otimes \underbrace{[\boldsymbol{X} - \bar{\boldsymbol{X}}] \otimes [\boldsymbol{X} - \bar{\boldsymbol{X}}] \otimes \ldots \otimes [\boldsymbol{X} - \bar{\boldsymbol{X}}]}_{k-1} \rangle_\square$$

$$\delta \bar{\boldsymbol{H}}^{(k)} \stackrel{\mathrm{def}}{=} (\boldsymbol{G}[\delta \boldsymbol{u}_H^{\mathrm{M}}] \otimes \underbrace{\boldsymbol{\nabla} \otimes \boldsymbol{\nabla} \otimes \ldots \otimes \boldsymbol{\nabla}}_{k-1})(\bar{\boldsymbol{X}})$$

- **Remark**: $\bar{\boldsymbol{P}}^{(k)}$, $\bar{\boldsymbol{H}}^{(k)}$ live in "the discrete world"
- **Remark**: 1st order homogenization obtained for $p = 1$: only classical volume average $\bar{\boldsymbol{P}}^{(1)}$ remains

Example: Stationary macro-crack

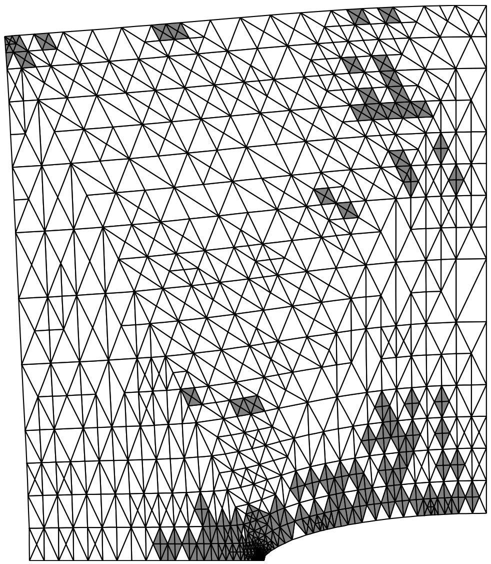


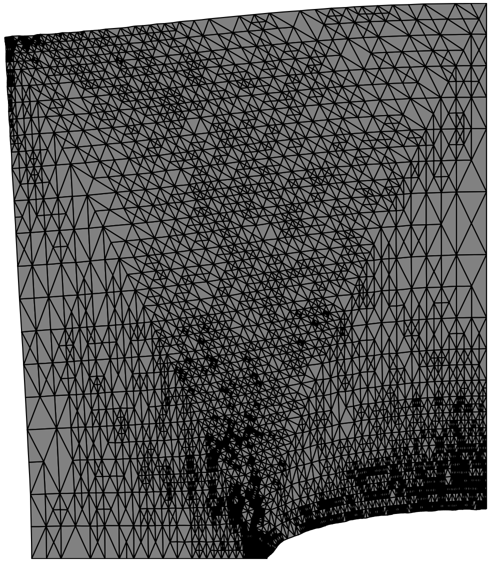


- Sub-scale problem characterization
  - Stiff elastic particles, G_P, $K_\text{P} = 10G_\text{P}$
  - Elastic-plastic matrix, $G_\text{M} = G_\text{P}/10$, $K_\text{M} = K_\text{P}/10$, $\sigma_{\text{Y},\text{M}} = G_\text{M}/10$
- Adaptive control of average displacement $Q = \frac{1}{|\Gamma_\text{top}|}\int_{\Gamma_\text{top}} u_2 \mathrm{d}A$

Results: Stationary macro-crack

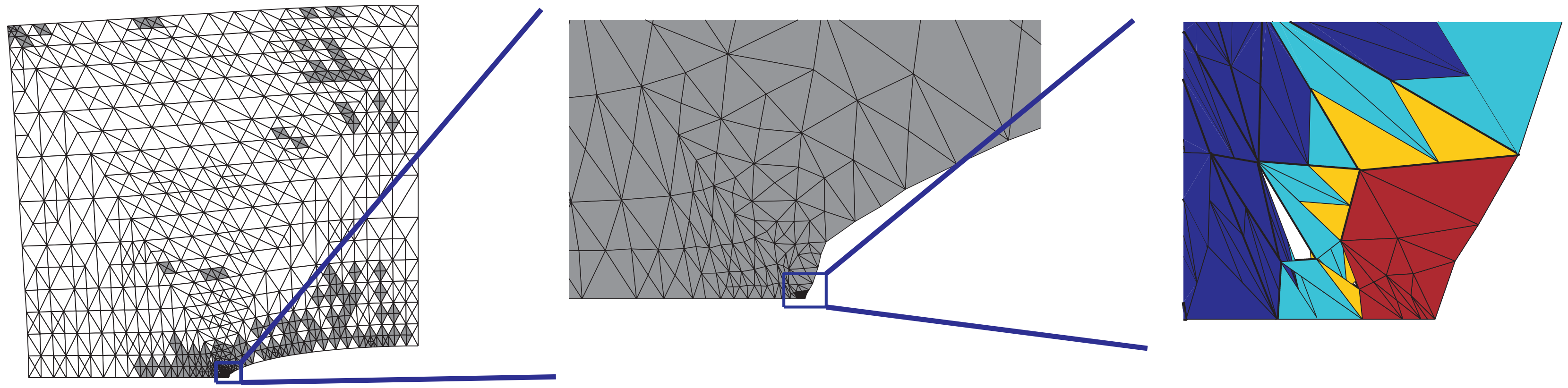
- Large scale separation, $d/L_{\mathrm{MAC}} = 1/100$, adaptive algorithm aiming for $TOL = 2\%$
- Small scale separation, $d/L_{\mathrm{MAC}} = 1/10$, adaptive algorithm aiming for $TOL = 20\%$ **Note:** Substructure not yet well resolved!



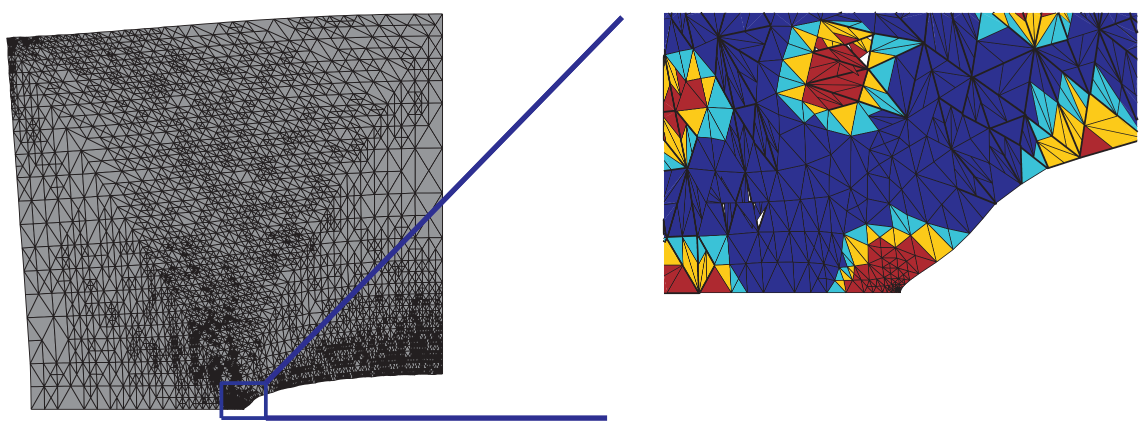


black: level I (full resolution),
grey: level II (special case of VMS),
white: level III (homogenization)

- Large scale separation - "multiscale closeup"



- Small scale separation - "multiscale closeup": **Note**: still large error, substructure not yet well resolved!



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Selected references, cont'd

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Lecture 3 - Part II

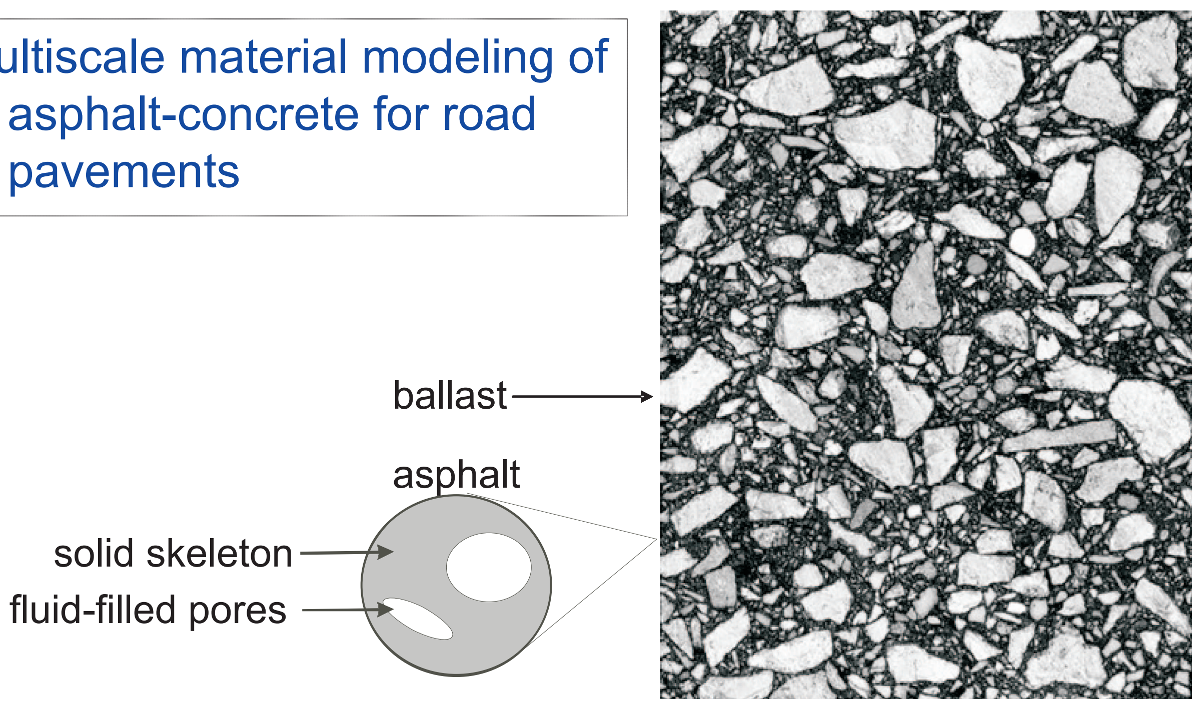
Outlook - Selected research at Chalmers

Consolidation in porous granular media

Su, Larsson, Runesson

- Multiscale modeling of porous fine-grained granular material with pore-fluid, such as asphalt concrete (sand/bitumen mixture with embedded stones)
- Micro-inhomogeneity: particles in matrix
- **Note**: Intrinsically time-dependent (seepage)

Multiscale material modeling of asphalt-concrete for road pavements



Quasi-static consolidation problem

- Balance equations for subscale porous medium (mixture) subjected to quasistatic loading

$$
\begin{aligned}
-\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{\nabla} - \hat{\varrho}\boldsymbol{g} &= \mathbf{0} \text{ in } \Omega \times [0, T), \quad \text{momentum balance} \\
\mathrm{d}_t \Phi + \hat{\boldsymbol{w}} \cdot \boldsymbol{\nabla} &= 0 \text{ in } \Omega \times [0, T), \quad \text{mass balance of pore fluid}
\end{aligned}
$$

- Storage function

$$
\Phi = \phi \left[1 + \frac{u - u_0}{K^{\mathrm{F}}} \right] + \epsilon_{\mathrm{vol}}, \quad \epsilon_{\mathrm{vol}} \overset{\mathrm{def}}{=} \boldsymbol{u} \cdot \boldsymbol{\nabla}
$$

- Bulk stress, effective stress: $\hat{\boldsymbol{\sigma}} = \boldsymbol{\sigma}' - u\boldsymbol{I}$
- Hooke's law for solid skeleton: $\boldsymbol{\sigma}' = \boldsymbol{\sigma}'_0 + 2G\boldsymbol{\epsilon}_{\mathrm{dev}} + K\epsilon_{\mathrm{vol}}\boldsymbol{I}$
- Nonlinear Darcy's law for seepage: $\hat{\boldsymbol{w}} = -k(u, \boldsymbol{\nabla}u) \left[\boldsymbol{\nabla}u - \varrho^{\mathrm{F}}\boldsymbol{g} \right]$
- **Remark:** $\hat{\boldsymbol{\sigma}}_0 =$ initial equilibrium stress, $u_0 =$ non-flow pore pressure $[\boldsymbol{\nabla}u_0 = \varrho^{\mathrm{F}}\boldsymbol{g}]$. Henceforth: Set $\hat{\boldsymbol{\sigma}}_0 = \mathbf{0}$, $u_0 = 0$ without loss of generality

Decoupled theory – Pore pressure equation

- Decoupled theory: $\epsilon_{\rm vol} = K^{-1}[u + \hat{\sigma}_{\rm m}] \overset{\text{approx}}{\rightarrow} K^{-1}[u + \hat{\sigma}^*_{\rm m}]$
  cf. CHRISTIAN AND BOEHMER, ASCE J. Eng. Mech., 1970
- *Approximate* "total mean stress" $\hat{\sigma}^*_{\rm m}$ computed *a priori*. Assumptions:
  - Assume undrained condition in each micro-constituent (matrix, particles) $\leadsto$ "undrained macroscale elastic moduli" $\bar{G}^*$, $\bar{K}^*$
  - Total stress analysis $\rightarrow$ equilibrium stress $\hat{\boldsymbol{\sigma}}^* \rightarrow \hat{\sigma}^*_{\rm m}$
- "Decoupled storage function"

$$\Phi(u) = \phi + \left[\frac{1}{K} + \frac{\phi}{K^{\rm F}}\right] u + \frac{1}{K}\hat{\sigma}^*_{\rm m}$$

- **Remark**: Computation of undrained macroscale moduli based on the assumptions:
  - homogeneous stress $\hat{\sigma}^*_{\rm m}$ within each RVE
  - homogeneous elastic moduli within each micro-constituent

Decoupled consolidation problem

- Space/time variational format: Find $u(\boldsymbol{x}, t) \in \mathbb{U}$ s. t.

$$R(u; \delta u) = L(\delta u) - A(u; \delta u) \quad \forall \delta u \in \mathbb{U}^0$$

$$A(u; \delta u) \stackrel{\text{def}}{=} \int_0^T (\,\mathrm{d}_t \Phi, \delta u)\,\mathrm{d}t + \int_0^T a(u; \delta u)\,\mathrm{d}t + (\Phi(u|_{t=0^+}), \delta u|_{t=0^+})$$

$$L(\delta u) \stackrel{\text{def}}{=} \int_0^T l(\delta u)\,\mathrm{d}t + (\Phi_0, \delta u|_{t=0^+})$$

with

$$a(u; \delta u) \stackrel{\text{def}}{=} -\int_\Omega \hat{\boldsymbol{w}} \cdot \boldsymbol{\nabla}(\delta u)\,\mathrm{d}V, \quad l(\delta u) \stackrel{\text{def}}{=} -\int_{\Gamma_\mathrm{N}} q_\mathrm{p}\,\delta u\,\mathrm{d}S$$

- FE-discretized macroscale and subscale problems (on RVE's) in space/time: p.w. quadratic in space, p.w. constant in time from dG(0) (problem has strongly dissipative character)
- **Remark**: A priori restriction to algorithmic format $\rightsquigarrow$ No possibility to control time error (only spatial error)

Nested Multiscale Method – FE^2

- Macroscale FE-problem on space-time slab $\Omega \times I_n$ for $n = 1, 2, \ldots$ using dG(0): Find ${}^n\bar{u} \in \bar{\mathbb{U}}$ s.t.

$$\begin{aligned}\bar{R}\{{}^n\bar{u}; \delta\bar{u}\} \quad &= \quad \left[\int_{I_n} \bar{l}(\delta u)\,\mathrm{d}t + \Delta t\left(\bar{\hat{\boldsymbol{w}}}\{{}^n\bar{u}, \bar{\boldsymbol{\nabla}}{}^n\bar{u}\}, \bar{\boldsymbol{\nabla}}\delta\bar{u}\right)\right] \\ &\quad - \left(\left[\bar{\Phi}\{{}^n\bar{u}, \bar{\boldsymbol{\nabla}}{}^n\bar{u}\} - {}^{n-1}\bar{\Phi}\right], \delta\bar{u}\right) - \left(\left[\bar{\bar{\boldsymbol{\Phi}}}\{{}^n\bar{u}, \bar{\boldsymbol{\nabla}}{}^n\bar{u}\} - {}^{n-1}\bar{\bar{\boldsymbol{\Phi}}}\right], \bar{\boldsymbol{\nabla}}\delta\bar{u}\right) \\ &= \quad 0, \quad \forall \delta\bar{u} \in \bar{\mathbb{U}}^0.\end{aligned}$$

- Homogenized quantities:

$$\bar{\hat{\boldsymbol{w}}}\{\bar{u}, \bar{\boldsymbol{\xi}}\} = \langle \hat{\boldsymbol{w}}(u, \boldsymbol{\xi})\rangle_\square\,, \quad \bar{\Phi}\{\bar{u}, \bar{\boldsymbol{\xi}}\} = \langle \Phi(u)\rangle_\square$$

$$\bar{\bar{\boldsymbol{\Phi}}}\{\bar{u}, \bar{\boldsymbol{\xi}}\} \stackrel{\text{def}}{=} \langle \Phi(u)\left[\boldsymbol{x} - \bar{\boldsymbol{x}}\right]\rangle_\square$$

- **Remark:** "Quasi-separation" of scales inherent in "2nd order storage function" $\bar{\bar{\boldsymbol{\Phi}}}\{\bar{u}, \bar{\boldsymbol{\xi}}\}$, cf. KOUZNETSOVA ET AL. (2002)
- **Remark:** $\bar{\bar{\boldsymbol{\Phi}}}\{\bar{u}, \bar{\boldsymbol{\xi}}\} \to \boldsymbol{0}$ when $l_{\text{RVE}} \to 0$

Nested Multiscale Method – FE^2

- SVE-problem: Dirichlet b.c. for pressure ${}^{n}u$.
- Subscale FE-problem on space-time slabs $\Omega_\Box \times I_n$ for $n = 1, 2, \ldots$ using dG(0):
  For given ${}^{n}u^{\mathrm{M}}(\bar{\boldsymbol{x}}; \boldsymbol{x}, t)$, find ${}^{n}u^{\mathrm{s}} \in \mathbb{U}^0_\Box$ s. t.

$$
\begin{aligned}
R_\Box({}^{n}u^{\mathrm{M}} + {}^{n}u^{\mathrm{s}}; \delta u^{\mathrm{s}}) &= \int_{I_n} l_\Box(\delta u^{\mathrm{s}})\,\mathrm{d}t - \Delta t\, a_\Box({}^{n}u^{\mathrm{M}} + {}^{n}u^{\mathrm{s}}; \delta u^{\mathrm{s}}) \\
&\quad - \left\langle \left[\Phi({}^{n}u^{\mathrm{M}} + {}^{n}u^{\mathrm{s}}) - {}^{n-1}\Phi\right] \delta u \right\rangle_\Box \\
&= 0, \quad \forall \delta u^{\mathrm{s}} \in \mathbb{U}^0_\Box
\end{aligned}
$$

$$
a_\Box(u; \delta u) \stackrel{\mathrm{def}}{=} -\langle \hat{\boldsymbol{w}} \cdot \boldsymbol{\nabla} \delta u \rangle_\Box\,, \quad l_\Box(\delta u) = 0
$$

- **Remark**: For the coupled problem it is possible to choose different prolongation conditions for different fields

Macroscale algorithmic tangent operators

- Linearization of macroscale problem for each space-time slab $\rightsquigarrow$ bilinear but generally *non-symmetric* form

$$
\begin{aligned}
\bar{R}'\{\bullet;\delta\bar{u},\,\mathrm{d}\bar{u}\} \quad = \quad & -\int_\Omega \delta\bar{u}\bar{C}\,\mathrm{d}\bar{u}\,\mathrm{d}V - \int_\Omega \delta\bar{u}\bar{\boldsymbol{B}}\cdot\bar{\boldsymbol{\nabla}}(\,\mathrm{d}\bar{u})\,\mathrm{d}V \\
& + \int_\Omega \bar{\boldsymbol{\nabla}}(\delta\bar{u})\cdot\left[\Delta t\,\bar{\boldsymbol{Y}} - \bar{\bar{\boldsymbol{C}}}\right]\,\mathrm{d}\bar{u}\,\mathrm{d}V \\
& - \int_\Omega \bar{\boldsymbol{\nabla}}(\delta\bar{u})\cdot\left[\Delta t\,\bar{\boldsymbol{K}} + \bar{\bar{\boldsymbol{B}}}\right]\cdot\bar{\boldsymbol{\nabla}}(\,\mathrm{d}\bar{u})\,\mathrm{d}V
\end{aligned}
$$

- Macroscale tangent operators defined by

$$
\begin{aligned}
\mathrm{d}\bar{\hat{\boldsymbol{w}}} &= \bar{\boldsymbol{Y}}\,\mathrm{d}\bar{u} - \bar{\boldsymbol{K}}\cdot\,\mathrm{d}\bar{\boldsymbol{\xi}} \\
\mathrm{d}\bar{\Phi} &= \bar{C}\,\mathrm{d}\bar{u} + \bar{\boldsymbol{B}}\cdot\,\mathrm{d}\bar{\boldsymbol{\xi}} \\
\mathrm{d}\bar{\bar{\boldsymbol{\Phi}}} &= \bar{\bar{\boldsymbol{C}}}\,\mathrm{d}\bar{u} + \bar{\bar{\boldsymbol{B}}}\cdot\,\mathrm{d}\bar{\boldsymbol{\xi}}
\end{aligned}
$$

- **Note:** $\bar{\bar{\boldsymbol{B}}}$ 3rd order tensor

Macroscale algorithmic tangent operators

- Algorithmic tangent operators $\bar{C}, \bar{\boldsymbol{Y}}, \bar{\boldsymbol{B}}, \bar{\bar{\boldsymbol{C}}}, \bar{\boldsymbol{K}}, \bar{\bar{\boldsymbol{B}}}$ computed via sensitivity fields $\hat{u}^{\mathrm{s}}_{\bar{\mathrm{u}}}, \hat{u}^{\mathrm{s}(j)}_{\bar{\xi}} \in \mathbb{U}^0_{\square}$ on RVE .

  Example:

$$(\bar{\boldsymbol{K}})_{ij} = \langle(\boldsymbol{K})_{ij}\rangle_{\square} + \left\langle(\boldsymbol{K}\cdot\boldsymbol{\nabla}\hat{u}^{\mathrm{s}(j)}_{\bar{\xi}})_i\right\rangle_{\square} - \underbrace{\langle(\boldsymbol{Y})_i[x_j - \bar{x}_j]\rangle_{\square}}_{\text{"2nd order"}} - \left\langle(\boldsymbol{Y})_i\hat{u}^{\mathrm{s}(j)}_{\bar{\xi}}\right\rangle_{\square}$$

$$\boldsymbol{Y} \overset{\text{def}}{=} \frac{\partial\hat{\boldsymbol{w}}}{\partial u}, \; \boldsymbol{K} \overset{\text{def}}{=} -\frac{\partial\hat{\boldsymbol{w}}}{\partial(\boldsymbol{\nabla}u)}$$

- Definition of sensitivities in terms of *ansatz* for $\mathrm{d}u^{\mathrm{s}}$ related to differential changes of $\bar{u}$ and $\bar{\xi}_j \overset{\text{def}}{=} (\bar{\boldsymbol{\nabla}}\bar{u})_j$:

$$\mathrm{d}u^{\mathrm{s}}(\boldsymbol{x}) = \hat{u}^{\mathrm{s}}_{\bar{\mathrm{u}}}(\boldsymbol{x})\,\mathrm{d}\bar{u} + \sum_{i=1}^{NDIM} \hat{u}^{\mathrm{s}(i)}_{\bar{\xi}}(\boldsymbol{x})\,\mathrm{d}\bar{\xi}_i$$

Macroscale algorithmic tangent operators

- Sensitivity fields are solutions of tangent problems on RVE's:

  (i) Solve for $\hat{u}^{\rm s}_{\bar{\rm u}} \stackrel{\rm def}{=} {}^n\hat{u}^{\rm s}_{\bar{\rm u}} \in \mathbb{U}^0_\square$ from

$$\langle \Phi' \delta u^{\rm s}\, \hat{u}^{\rm s}_{\bar{\rm u}} \rangle_\square - \Delta t \,\langle \boldsymbol{\nabla}[\delta u^{\rm s}] \cdot \boldsymbol{Y} \hat{u}^{\rm s}_{\bar{\rm u}} \rangle_\square + \Delta t \,\langle \boldsymbol{\nabla}[\delta u^{\rm s}] \cdot \boldsymbol{K} \cdot \boldsymbol{\nabla}[\hat{u}^{\rm s}_{\bar{\rm u}}] \rangle_\square$$
$$= - \langle \Phi' \delta u^{\rm s} \rangle_\square + \Delta t \,\langle \boldsymbol{\nabla}[\delta u^{\rm s}] \cdot \boldsymbol{Y} \rangle_\square \,,$$
$$\forall \delta u^{\rm s} \in \mathbb{U}^0_\square .$$

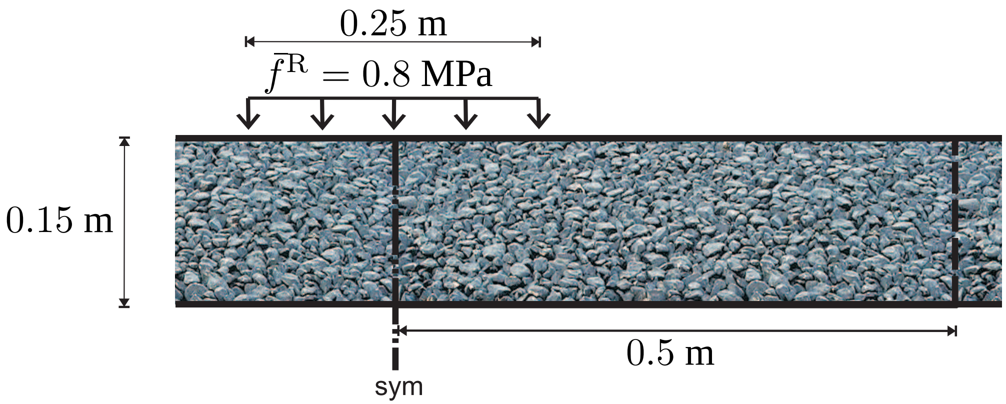
  (ii) Solve for $\hat{u}^{{\rm s}(i)}_{\bar{\xi}} \stackrel{\rm def}{=} {}^n\hat{u}^{{\rm s}(i)}_{\bar{\xi}} \in \mathbb{U}^0_\square, i = 1, 2, \ldots, NDIM$, from

$$\left\langle \Phi' \delta u^{\rm s}\, \hat{u}^{{\rm s}(i)}_{\bar{\xi}} \right\rangle_\square - \Delta t \left\langle \boldsymbol{\nabla}[\delta u^{\rm s}] \cdot \boldsymbol{Y} \hat{u}^{{\rm s}(i)}_{\bar{\xi}} \right\rangle_\square + \Delta t \left\langle \boldsymbol{\nabla}[\delta u^{\rm s}] \cdot \boldsymbol{K} \cdot \boldsymbol{\nabla}[\hat{u}^{{\rm s}(i)}_{\bar{\xi}}] \right\rangle_\square$$
$$= - \langle \Phi' \delta u^{\rm s} [x_i - \bar{x}_i] \rangle_\square + \Delta t \,\langle \boldsymbol{\nabla}[\delta u^{\rm s}] \cdot \boldsymbol{Y}\, [x_i - \bar{x}_i] \rangle_\square - \Delta t \,\langle \boldsymbol{\nabla}[\delta u^{\rm s}] \cdot \boldsymbol{K} \cdot \boldsymbol{e}_i] \rangle_\square$$
$$\forall \delta u^{\rm s} \in \mathbb{U}^0_\square .$$

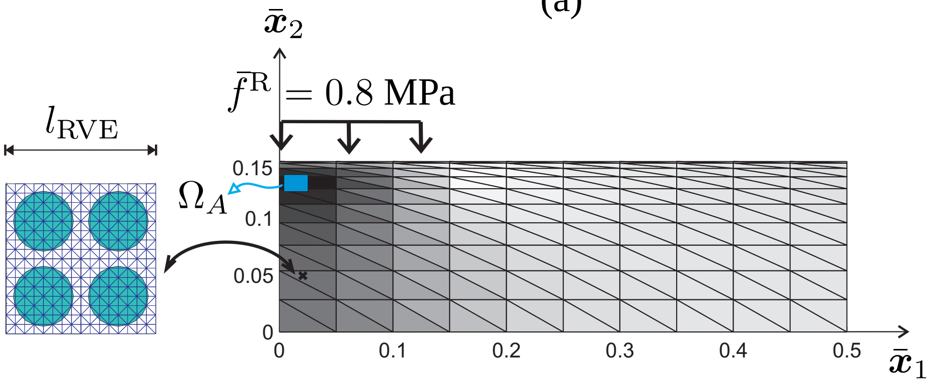
- **Remark:** $\hat{u}^{\rm s}_{\bar{\rm u}} = 0$ for stationary problems

Consolidation of pavement layer – coupled model

- Plane consolidation of symmetrically loaded (semi-infinite) layer of asphalt-concrete. RVE consisting of 2 × 2 unit cells. Dirichlet b.c. adopted.



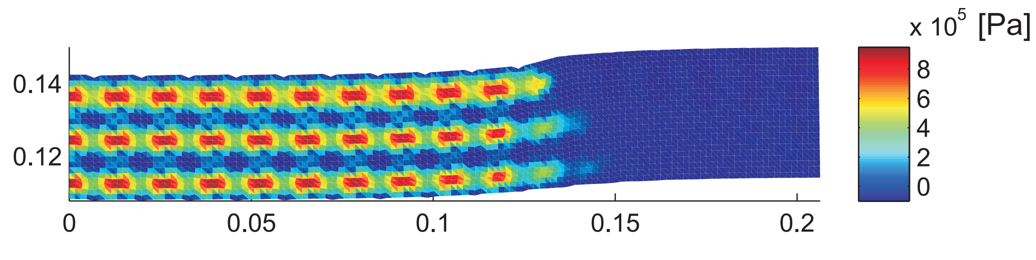
(a)



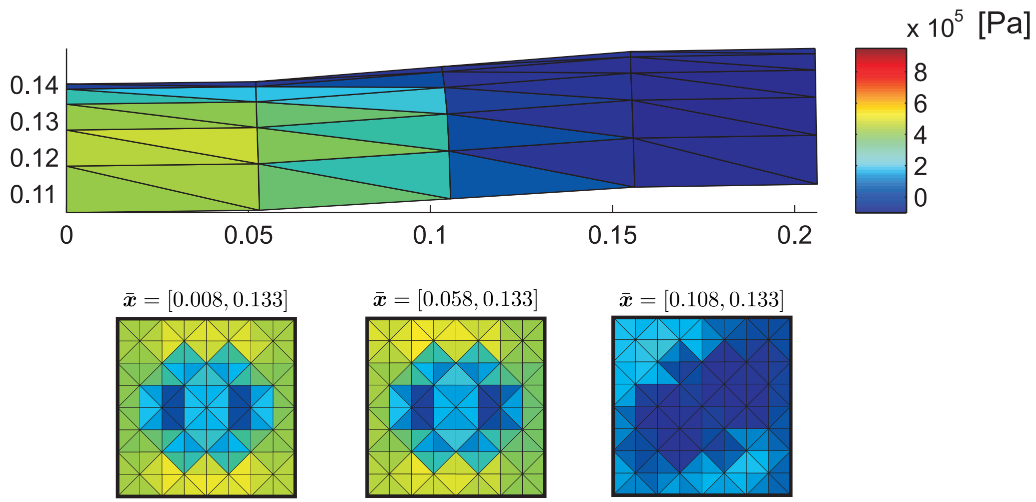
(b)

FE^2 algorithm: Results

- Pore pressure field on top of deformed mesh after 0.0001 sec. (a) Single-scale analysis. (b) Multiscale analysis: macroscale solution and RVE- solutions at three different macroscale quadrature points.



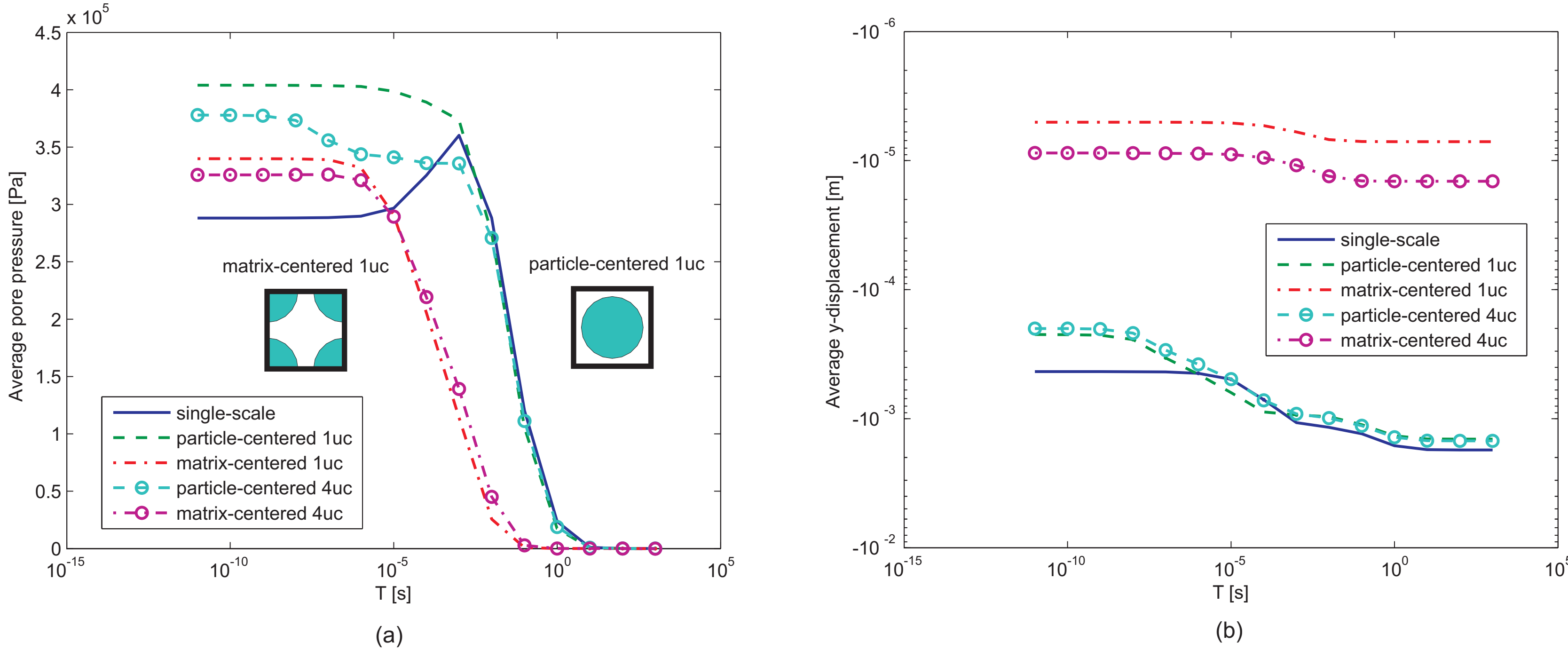
(a)



(b)

FE^2 algorithm: Results, cont'd

- Comparison of different particle distributions inside RVE: one particle in the center (particle-centered topology) vs. 4 quarters of a particle in the corners of a unit cell (matrix-centered topology). (a) Average pore pressure in the selected region Ω_A. (b) Average **v**ertical (x_2-) displacement the selected region Ω_A.



Computational homogenization of porous media

Sandström, Larsson, Johansson, Runesson

- Up-scaling and computational homogenization of flow in porous media coupled to solid skeleton deformation
  $\rightsquigarrow$ Improved modeling for
  - deformation-dependent permeability
  - gas-fluid mixtures
  - ...
- Initial analysis: Homogenization of porous media flow (rigid solid)
  - Macroscale: Darcy-type flow

$$\bar{\boldsymbol{q}} \cdot \bar{\boldsymbol{\nabla}} = 0$$

where $\bar{\boldsymbol{q}}$ is seepage

  - Subscale: incompressible Stoke's flow

$$\begin{aligned} -\left[\boldsymbol{\sigma}^{\mathrm{v}}(\boldsymbol{v} \otimes \boldsymbol{\nabla}) - p\boldsymbol{I}\right] \cdot \boldsymbol{\nabla} &= \boldsymbol{0} \\ \boldsymbol{v} \cdot \boldsymbol{\nabla} &= 0 \end{aligned}$$

$\boldsymbol{v}$ velocity
p pressure and $\boldsymbol{\sigma}^{\mathrm{v}}$ viscous stress

Macroscale permeability

- Prolongation: Ensure prescribed macroscale pressure gradient $\bar{\boldsymbol{\xi}}$
- Homogenization $\rightsquigarrow$ $\bar{\boldsymbol{q}} = \bar{n}\langle \boldsymbol{v} \rangle_\square$
  n porosity
- Consider Linear Stokes' law, i.e.

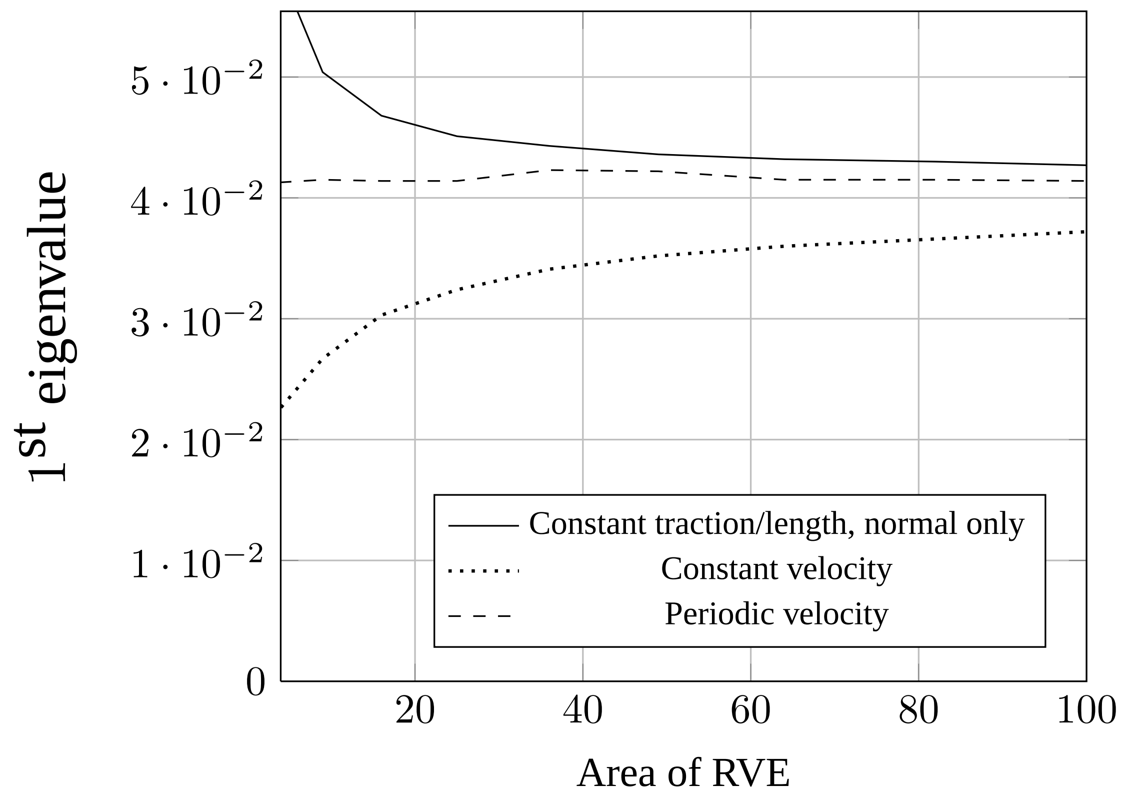
$$\boldsymbol{\sigma}^{\mathrm{v}} = 2\mu\left[\boldsymbol{v} \otimes \boldsymbol{\nabla}\right]^{\mathrm{sym}}$$

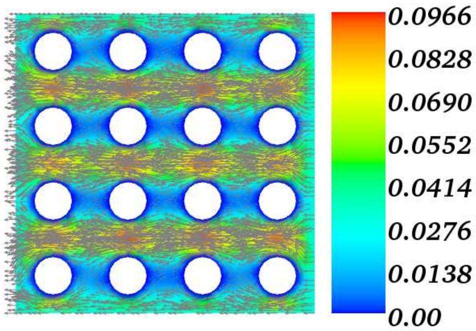
- Macroscale constitutive relation for seepage velocity (flux) $\bar{\boldsymbol{q}}$ in terms of pressure gradient $\bar{\boldsymbol{\xi}} \stackrel{\mathrm{def}}{=} \bar{\boldsymbol{\nabla}}\bar{p}$:

$$\bar{\boldsymbol{q}} = -\bar{\boldsymbol{K}} \cdot \bar{\boldsymbol{\xi}}$$

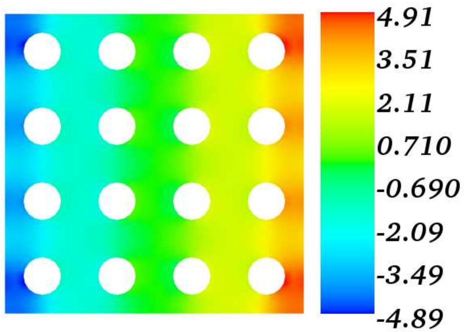
Dirichlet conditions on $\boldsymbol{v}$

Prescribed $\boldsymbol{\nabla}\tilde{p} = [1 \;\; 0]^T$





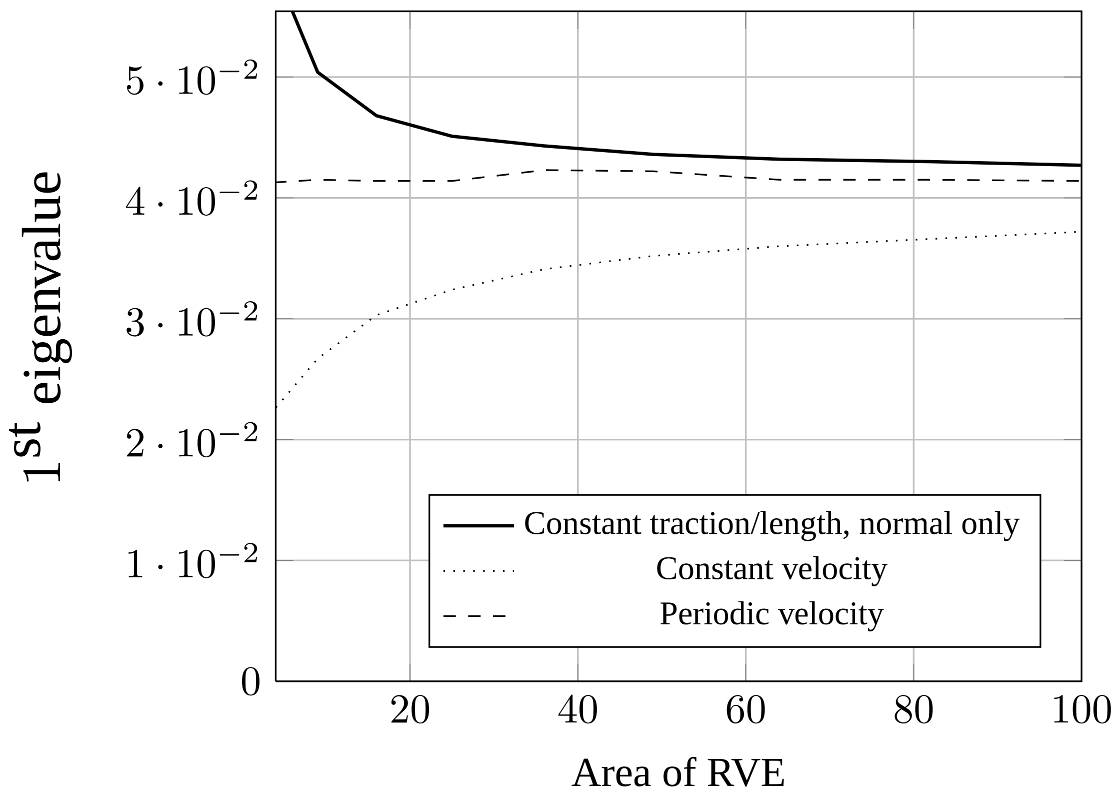
Velocity field

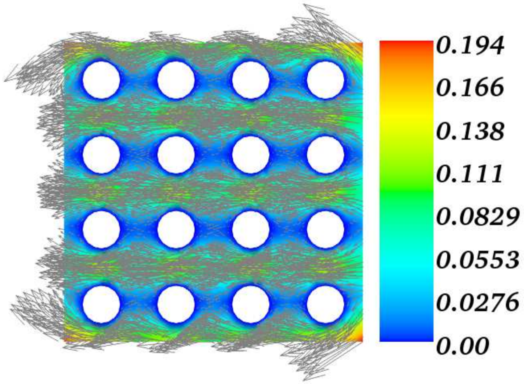


Pressure field

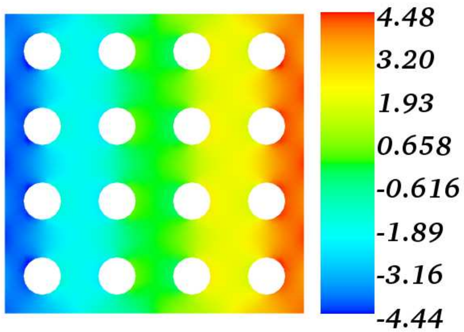
Neumann conditions on t^{v}

Prescribed $\nabla\tilde{p} = [1 \;\; 0]^T$





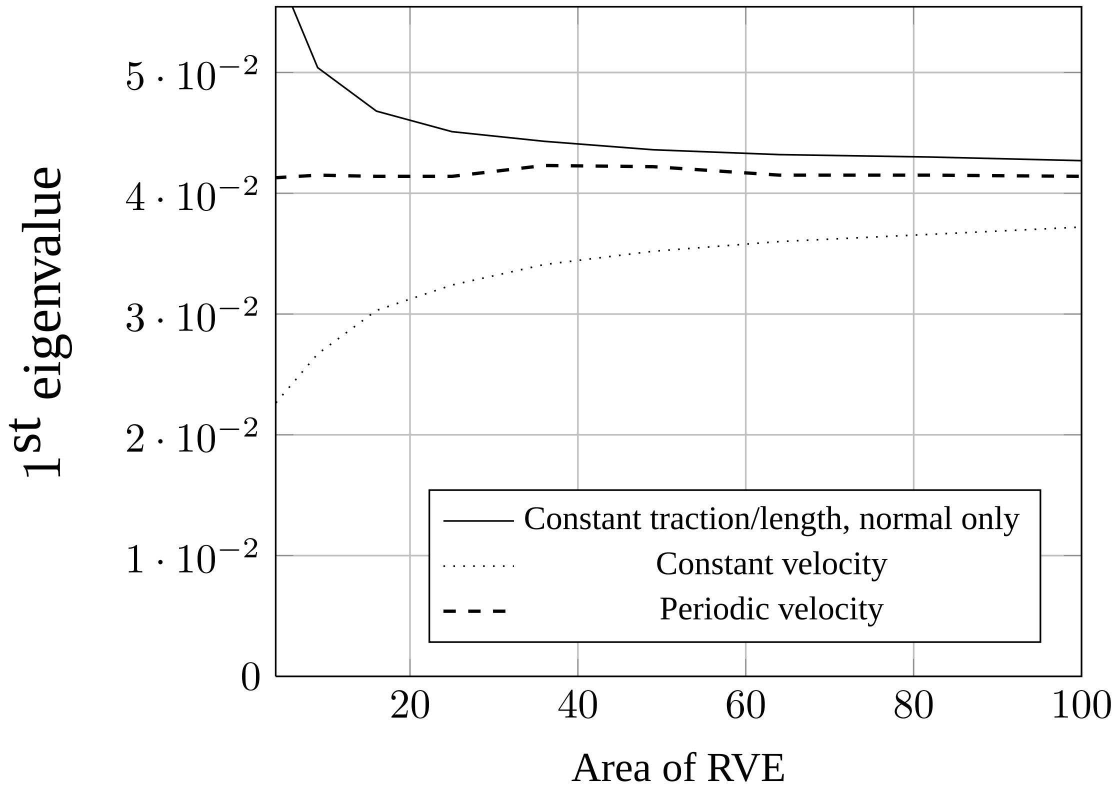
Velocity field

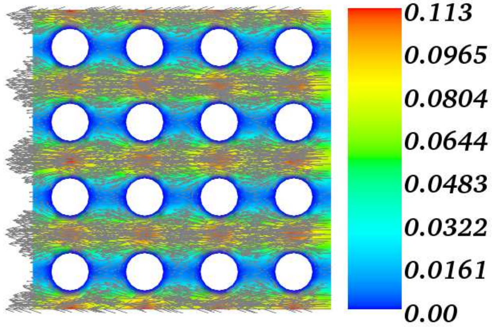


Pressure field

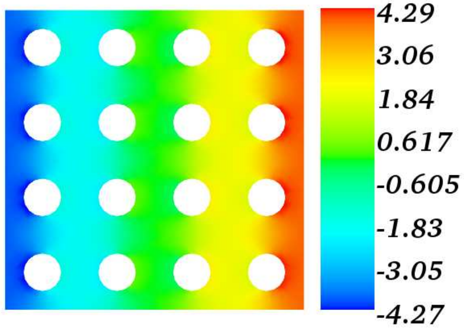
Periodic conditions

Prescribed $\boldsymbol{\nabla}\tilde{p} = [1 \;\; 0]^T$





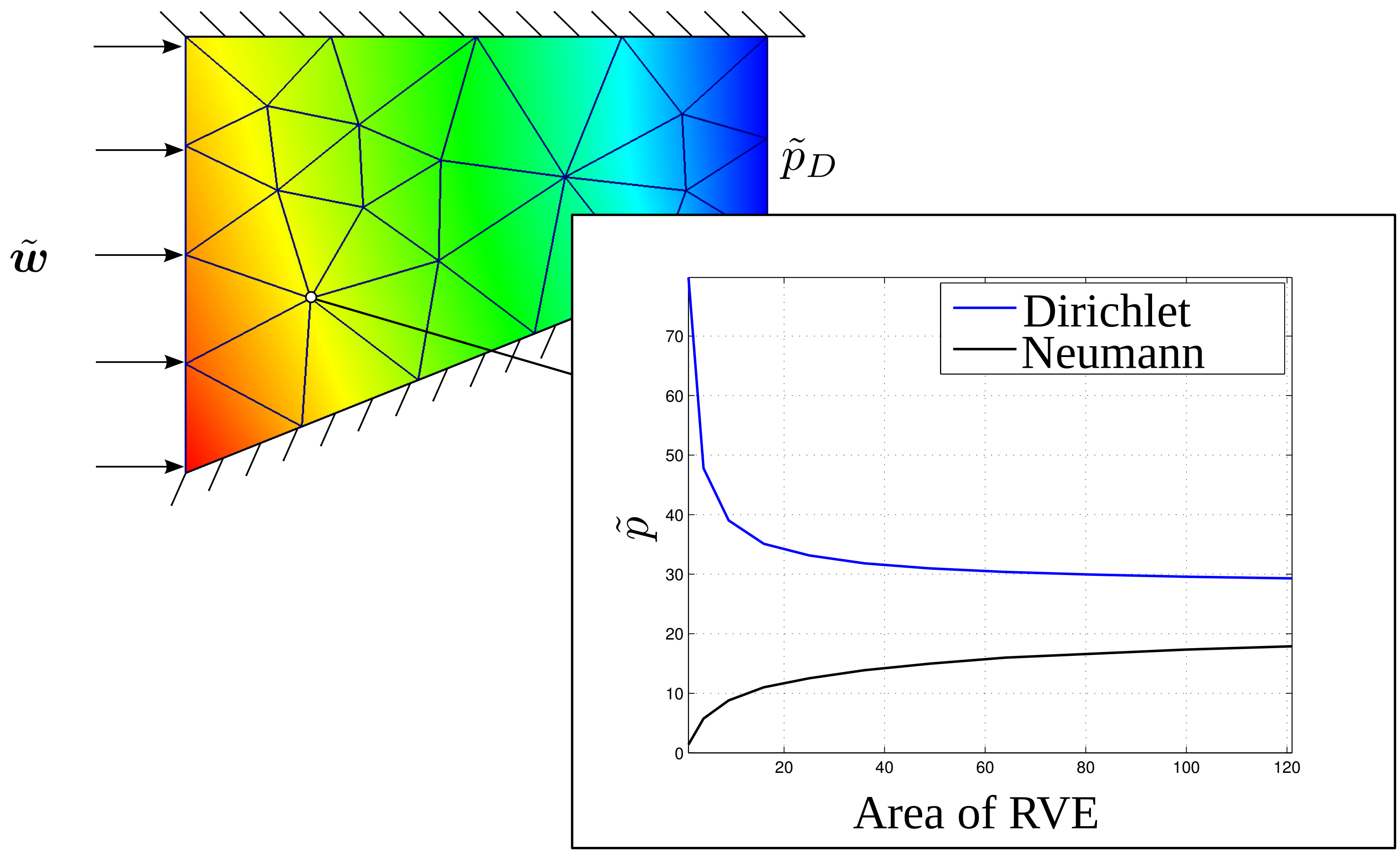
Velocity field



Pressure field

Macroscale permeability tensor

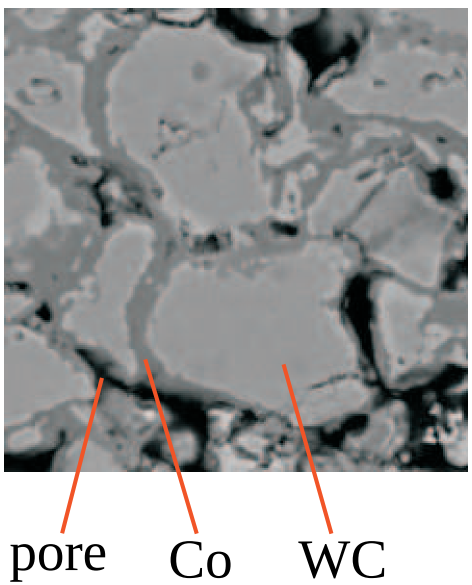
- Nonlinear fluid $\rightsquigarrow$ FE^2

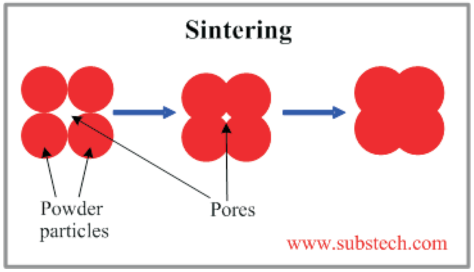


Sintering of hardmetal (WC-Co system)

Öhman, Runesson, Larsson

- WC-particles surrounded by "matrix" of Co, initial pore-space $\sim 20 - 40\%$
  Note: Intrinsically time-dependent deformation + solid diffusion + melt Co





- Sintering driven by surface tension Co-porespace from initial precompacted porosity (inhomogeneous relative density, ρ_0')
- Subscale constitutive modeling:
  - Co-binder: Incompressible, non-Newtonian (visco-plastic) flow $\leadsto$ nonlinear Stokes'
  - WC-particles: "Rigid" $\rightarrow$ incompressible, Newtonian flow with "large" viscosity

$$\boldsymbol{\sigma}_{\text{dev}}(\boldsymbol{d}) = 2\mu\, f(d_{\text{e}})\boldsymbol{d}_{\text{dev}}, \quad d_{\text{e}} \stackrel{\text{def}}{=} \sqrt{\frac{2}{3}}|\boldsymbol{d}_{\text{dev}}|$$

- Macroscale momentum balance.
  Note: Finite macroscale compressibility due to shrinking pore-space

Model-based homogenization of viscous sintering

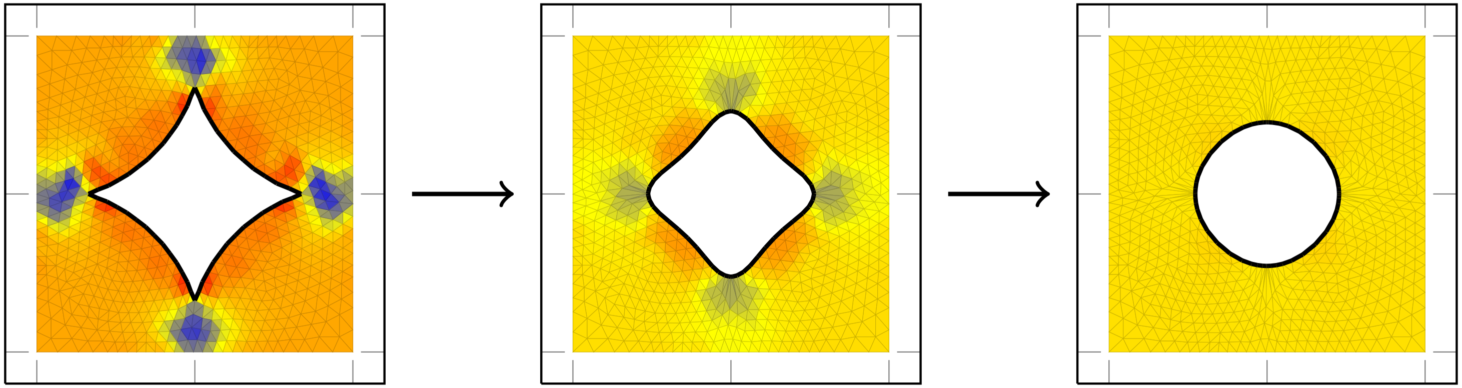


Figure 1: Evolution of free surface within a typical RVE

- RVE-problem with Dirichlet b.c. (example), "driven" by macroscale rate-of-deformation $\bar{\boldsymbol{d}} \rightarrow$ subscale velocity: $\boldsymbol{v} = \boldsymbol{v}^{\mathrm{M}}(\bar{\boldsymbol{d}}) + \boldsymbol{v}^{\mathrm{s}}$

  For given $\bar{\boldsymbol{d}}$, solve for $\boldsymbol{v}^{\mathrm{s}} \in \mathbb{V}_{\square}^{(\mathrm{D})}$, $p \in \mathbb{P}_{\square}$:

$$
\begin{aligned}
a_{\square}(\boldsymbol{v}^{\mathrm{M}}(\bar{\boldsymbol{d}}) + \boldsymbol{v}^{\mathrm{s}}; \delta\boldsymbol{v}^{\mathrm{s}}) + b_{\square}(p, \delta\boldsymbol{v}^{\mathrm{s}}) &= l_{\square}(\delta\boldsymbol{v}^{\mathrm{s}}) && \forall \delta\boldsymbol{v}^{\mathrm{s}} \in \mathbb{V}_{\square}^{(\mathrm{D})}, \\
b_{\square}(\delta p, \boldsymbol{v}^{\mathrm{M}}(\bar{\boldsymbol{d}}) + \boldsymbol{v}^{\mathrm{s}}) &= 0 && \forall \delta p \in \mathbb{P}_{\square}.
\end{aligned}
$$

  $l_{\square}(\delta\boldsymbol{v}^{\mathrm{s}})$: loading by "sintering stresses" = surface tension tractions on $\Gamma_{\square}^{\mathrm{pore}}$
- Surface-tension driven microflow of single "unit cell" RVE
  - macroscopically rigid (RVE-boundaries are rigid)
  - macroscopically isochoric

Simulation of sintering

- Macroscale problem for "free" (special case) sintering obtained from variationally consistent macro-homogeneity condition

$$\bar{a}\{\bar{\boldsymbol{v}};\delta\bar{\boldsymbol{v}}\} \stackrel{\text{def}}{=} \int_{\Omega} \bar{\boldsymbol{\sigma}}\{\bar{\boldsymbol{d}}\} : \delta\bar{\boldsymbol{d}}\,\mathrm{d}\bar{v} = 0$$

  Energy-conjugated macroscale stress: $\bar{\boldsymbol{\sigma}} = \frac{1}{|\hat{\Omega}_{\square}|}\int_{\hat{\Gamma}_{\square}} (\boldsymbol{t}\otimes[\boldsymbol{x}-\bar{\boldsymbol{x}}])^{\mathrm{sym}}\,\mathrm{d}a$

  $\bar{\boldsymbol{x}}$ = center of RVE

- FE^2 of free sintering for non-Newtonian microflow
  - homogeneous initial relative density (but lower boundary is artificially fixed)
  - non-homogeneous initial relative density, truly unrestrained macroscopic boundaries, single-phase
  - non-homogeneous initial relative density, truly unrestrained macroscopic boundaries, two-phase (with near-rigid particles)
- Modeling and computational strategies of surface tension: ZHOU & DERBY, PERIC ET AL., JAVILI & STEINMANN among others

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