Computational Homogenization and Multiscale Modeling

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Course outline

- Lecture 1
  - Classical homogenization in mechanics - Concepts and assumptions
  - Introduction to computational homogenization - Linear elasticity
- Lecture 2
  - Computational homogenization for nonlinear problems - Nested macro-micro computations (basis for FE^2)
  - The classical prolongation conditions on a Statistical Volume Element (SVE)
  - The concept of weak periodicity on SVE (novel)
- Lecture 3
  - Computational homogenization for nonlinear problems - FE^2 with error estimation and adaptivity
  - Outlook - Selected research at Chalmers University

Homogenization in material mechanics - Which discipline?

- Mathematics
  - Statistics - stochastics
  - Functional analysis - variational methods
  - A posteriori error analysis
- Material physics and science
  - Quantum physics and atomistics
  - Material-specific length scales - Scanning techniques
- Continuum mechanics - general and material modeling
- Experimental techniques
- Computational methods
  - FE
  - Adaptive meshing
  - Parallel computation

Lecture 1: Contents

- Motivation for multiscale modeling – "appetizers"
- Approaches to multiscale modeling
- Classical homogenization – Concepts and assumptions
  - Statistical Volume Element (RVE) versus Representative Volume Element (RVE)
  - Macrohomogeneity (Hill-Mandel) condition
  - Classical prolongation conditions: DBC, TBC, PBC
  - Voigt and Reuss bounds
  - Statistical bounds [without confidence intervals]
- Introduction to computational homogenization – Linear elasticity
  - Effective stiffness tensor for DBC, (TBC, PBC)

Macroscopic versus multiscale modeling

- Macrolevel: Balance equations of mass, momentum, energy, etc., expressed in "flux" quantities, e.g. momentum equation

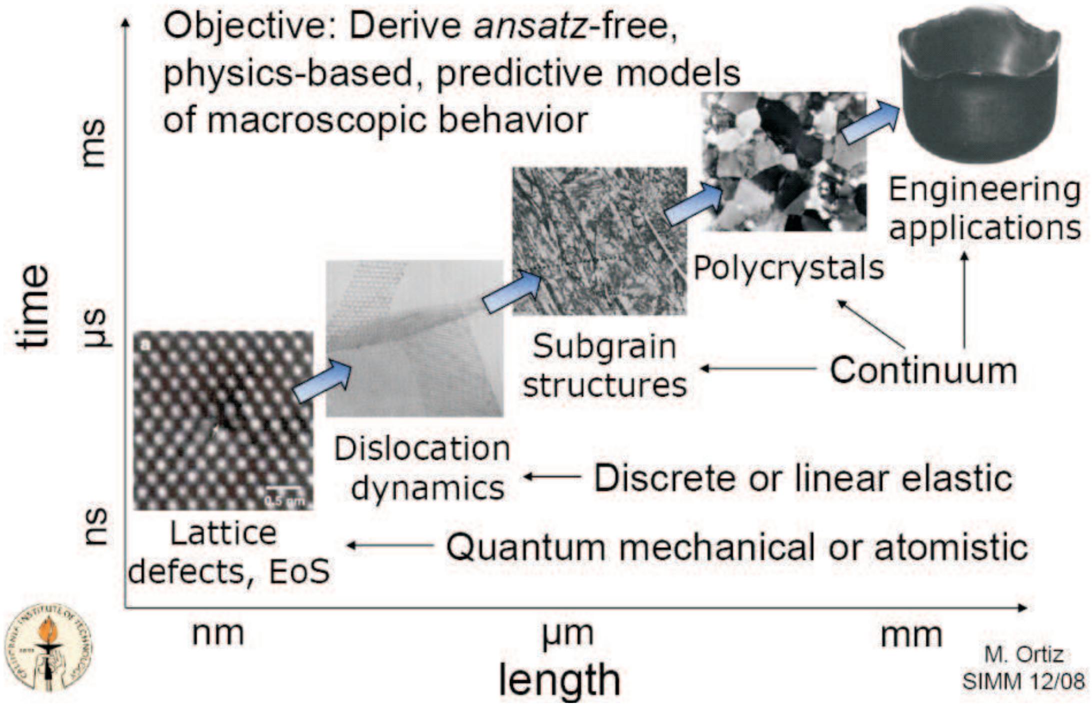
$$-\bar{\boldsymbol{P}} \cdot \bar{\boldsymbol{\nabla}} = \bar{\boldsymbol{f}} \quad \text{Cartesian components:} \quad -\frac{\partial \bar{P}_{ij}}{\partial \bar{X}_j} = \bar{f}_i$$

- **Macroscopic constitutive modeling**:

  $\bar{\boldsymbol{P}} = \bar{\boldsymbol{P}}(\bar{\boldsymbol{H}}, k_\alpha), \quad \bar{\boldsymbol{H}} \overset{\text{def}}{=} \bar{\boldsymbol{u}} \otimes \bar{\boldsymbol{\nabla}} = \bar{\boldsymbol{F}} - \boldsymbol{I}$
  - No explicit account of material (micro)structure, rather implicit via evolution of *internal variables* k_α (e.g. plastic strain, texture tensors, etc.), ODE’s or PDE’s
  - Calibration from macroscale experiments or subscale modeling $\rightarrow$ "upscaling"
- **Multiscale constitutive modeling**: $\bar{\boldsymbol{P}}\{\bar{\boldsymbol{H}}\}$
  - Subscale modeling within RVE $\rightarrow$ homogenization
  - Calibration from macroscale experiments or further lower subscale modeling $\rightarrow$ "upscaling"
  - Always boils down to modeling on (lowest) scale, *ab initio* does not exist!

Length scales

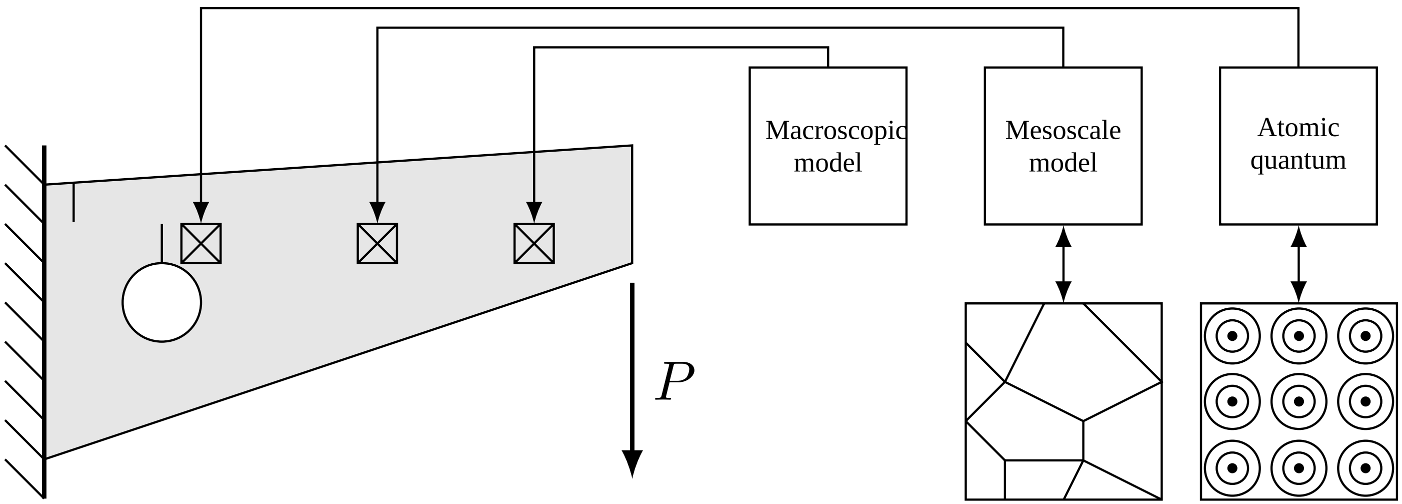
- Example: Multiscale modeling of polycrystalline metals



- "Top-down" strategy
  - Physics at given (lower) scale, "scale of modeling"
  - Engineering output at macroscale
  - Mathematical bridging of scales via accuracy assessment and adaptive choice of "scale of modeling"

Multiscale modeling - Bridging the scales?

- "Vertical" bridging: Computational homogenization
  - Homogenization on RVE, "prolongation conditions" part of model
  - Model adaptivity to account for local defects
- "Horizontal" bridging: Concurrent multiscale modeling
  - Models at different scales coexisting in adjacent parts of the domain (within the component), model coupling along "bridging" domains
  - Model adaptivity to account for local defects



Modeling of selected material classes

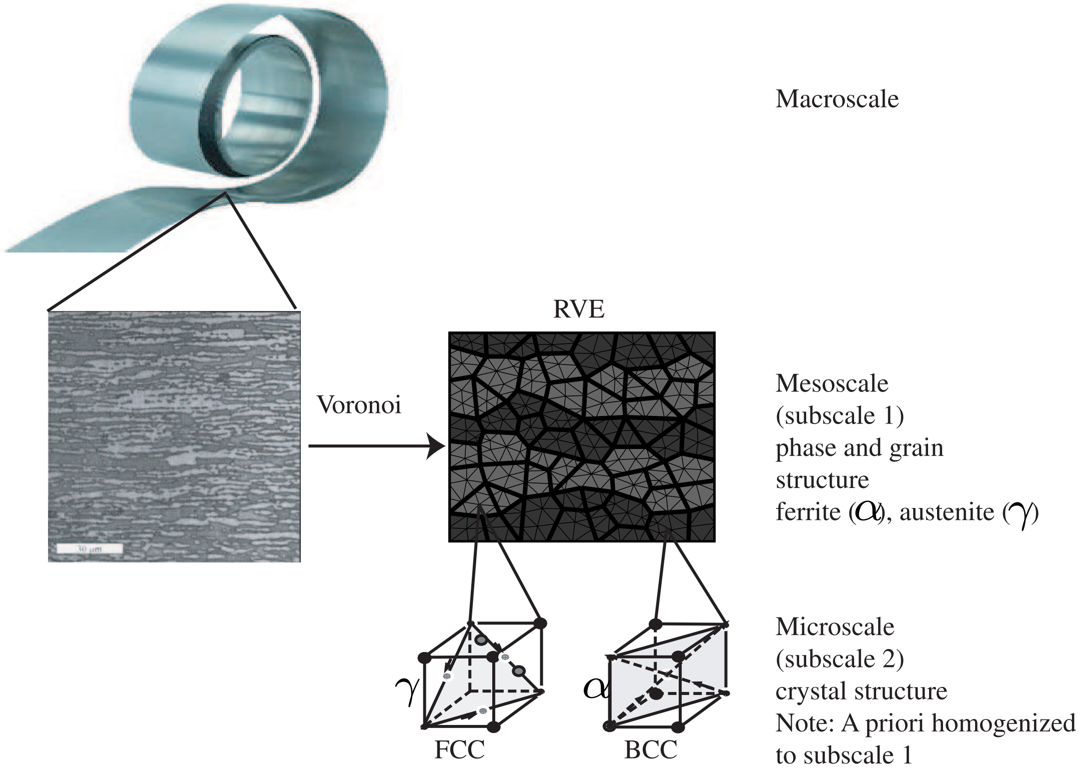
- Nano-materials Prototype material: Graphene (single C-atom layer)
  - *Macroscale*: Hyperelasticity
  - *Mesoscale*: Tershoff-Brenner pair-wise interatomic potential (includes distance and angles), Quasi-Continuum concept for constraining atomic motion
- Polycrystalline metals
  - *Macroscale*: Viscoplasticity with (complicated) mixed isotropic-kinematic-distortional hardening
  - *Mesoscale*: Crystal (visco)plasticity within grains, colonies, etc, grain boundary interaction from crystal orientations $\rightsquigarrow$ "Hall-Petch"-type relation for yield stress. Upscaling to macroscopic yield surface
- PM-products
  - *Macroscale*: Viscoplasticity based on mean-stress dependent yield surface
  - *Mesoscale*: Surface tension along particle/pore interface, moving boundaries of partly (melt) binder metal (liquid-phase sintering)

Modeling of selected material classes

- Porous media saturated with pore fluid
  - *Macroscale*: Porous Media Theory
  - *Mesoscale*: Particles in matrix, homogenization of subscale transient $\leadsto$ "double time-scales", incomplete scale separation cf. "higher order" homogenization scheme in the spatial domain
  - *Microscale*: Modeling of permeability from Stokes' flow, dependence on deformable "particles"

"Appetizer": Duplex Stainless Steel

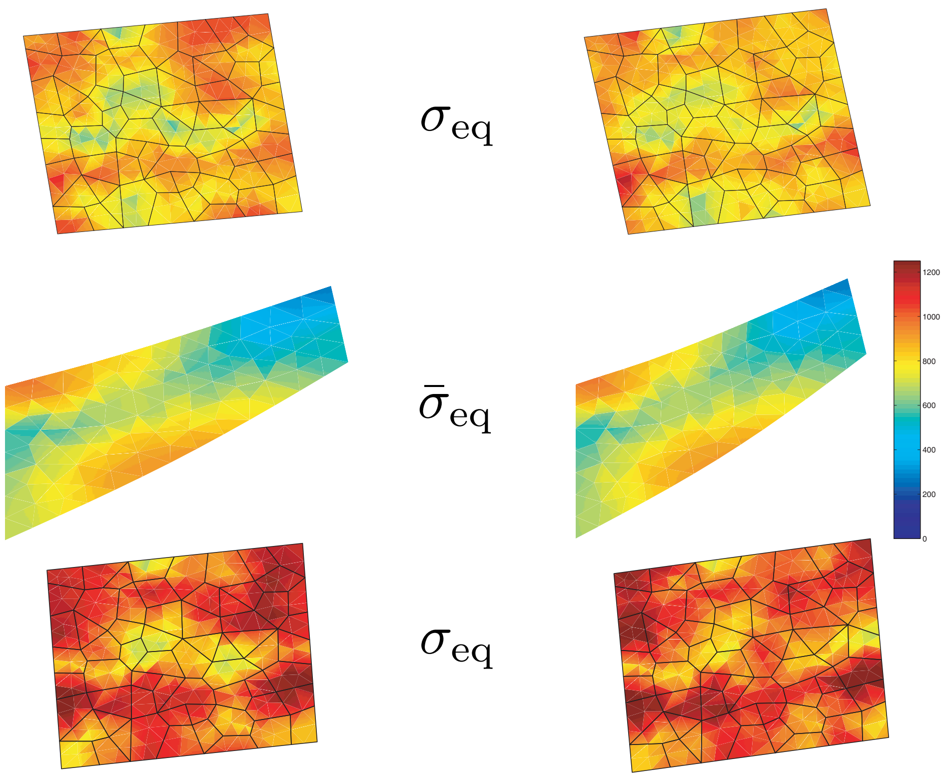
- Multiscale modeling of two-phase (or three-phase) Duplex Stainless Steel (DSS) [Sandvik Materials Technology, Sweden]
- Micro-inhomogeneity: Grain structure, phase structure
- Subscale constitutive modeling: Large strain crystal plasticity, possibly with gradient enhancement to account for grain-size (Hall-Petch) effect



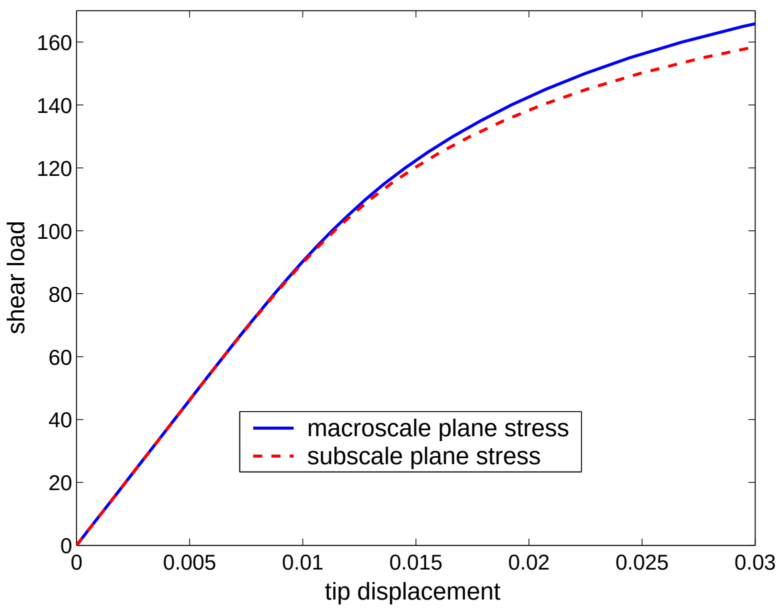
- Homogenization: Dimensional reduction 3D crystal structure $\rightarrow$ plane stress **appropriate definition ?**
- Example of application: Ultrathin foils $\sim$ 0.05 mm

FE^2 applied to thin DSS-membrane

Dimensional reduction on subscale:
macroscale plane stress (left figure)
subscale plane stress (right figure):
σ_{eq} = subscale Mises stress
$\bar{\sigma}_{\mathrm{eq}}$ = macroscale Mises stress



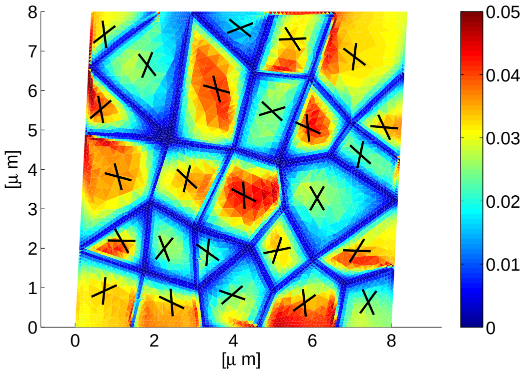
Macroscale response

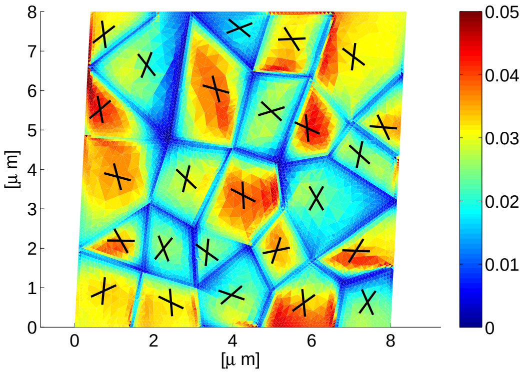


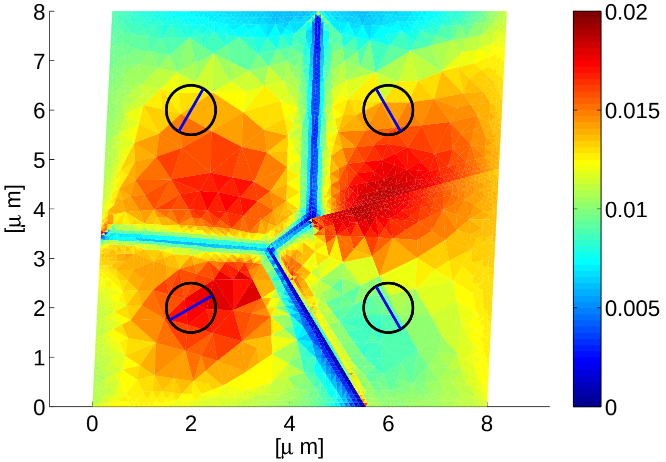
- LILLBACKA ET AL.: *Int. J. Multiscale Comp. Engng.* [2007] Note: No adaptivity

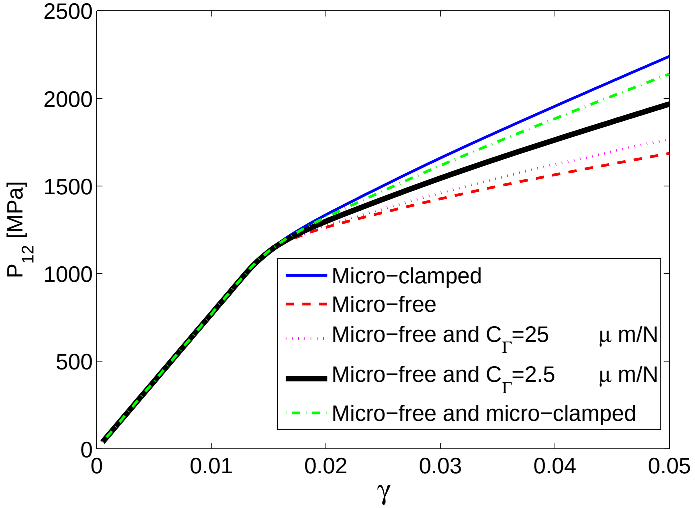
Grain interaction – size effect

- Subscale modeling: Gradient-enhanced theory of crystal (visco)plasticity. Dirichlet b.c. of RVE corresonding to simple shear.
- *Left figure*: Microhard (clamped) grain boundaries. *Right*: Grain boundary interaction dependent on crystal misalignment





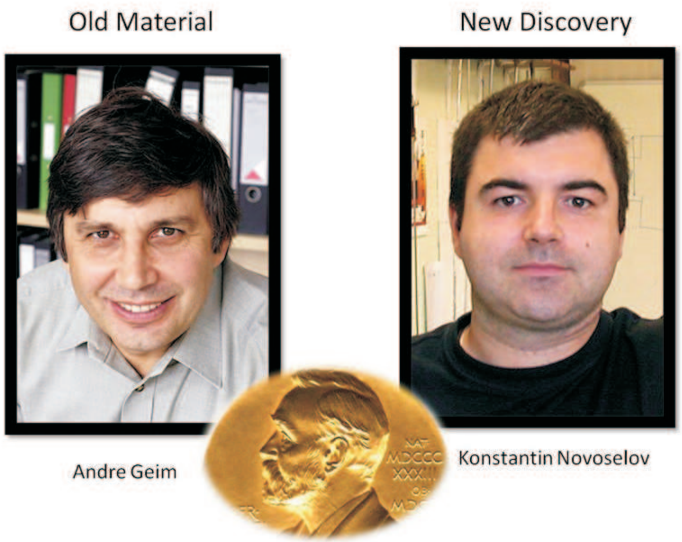


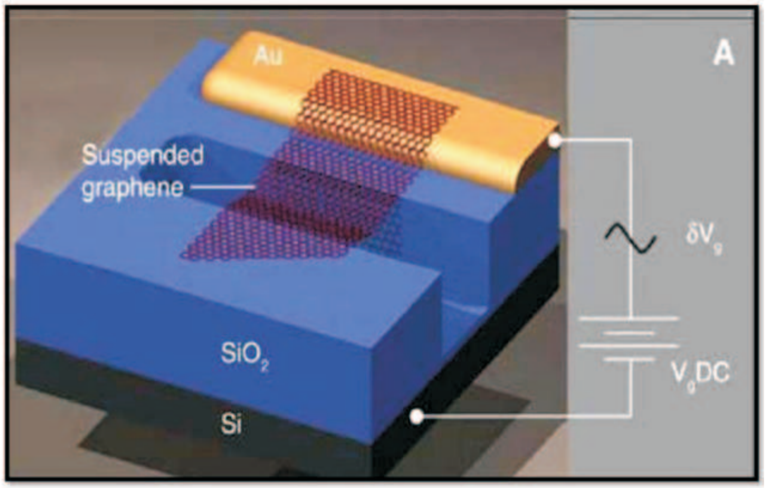


”Appetizer”: Atomistic systems - graphene

Ph.D. project by Kaveh S

- Unique stable 2D lattice, single atom layer
- *Nobel prize 2011*

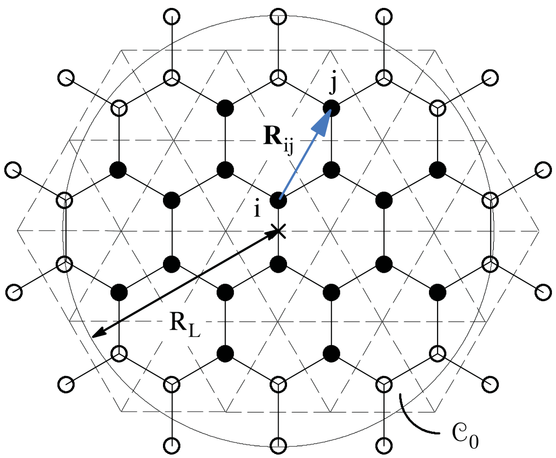


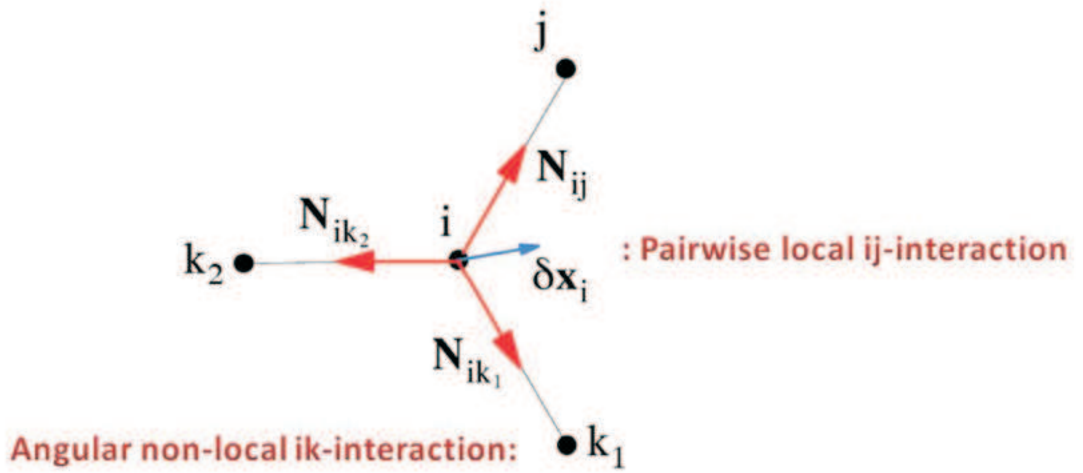


J.S.Bunch *et al.* **Science** 315,490(07)

Atomistic systems - graphene

- Atomic interaction: Tersoff-Brenner pairwise potential, includes angular "non-local" attraction (in addition to conventional "local" pairwise interaction)





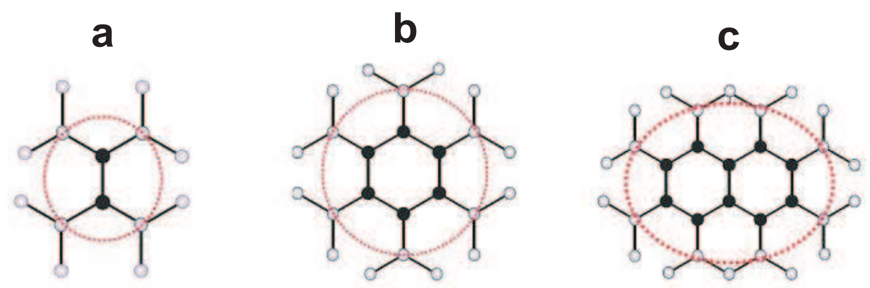
$$\psi_{ij} =_{ij} -\psi_{A_{ij}}\overline{B}_{ij}$$

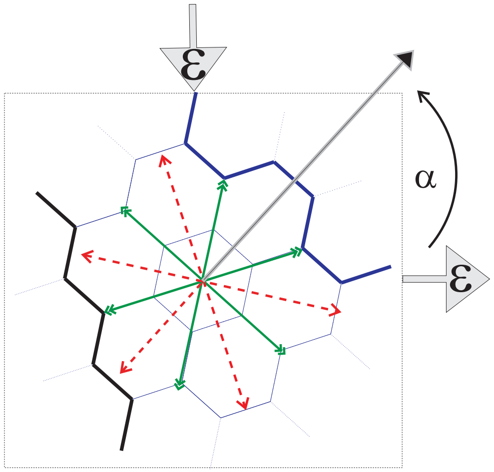
$$\psi_{R_{ij}} \leftrightarrow \text{Repulsion}, \quad \psi_{A_{ij}} \leftrightarrow \text{Attraction}, \quad \overline{B}_{ij} \leftrightarrow \text{Angular term} \qquad (1)$$

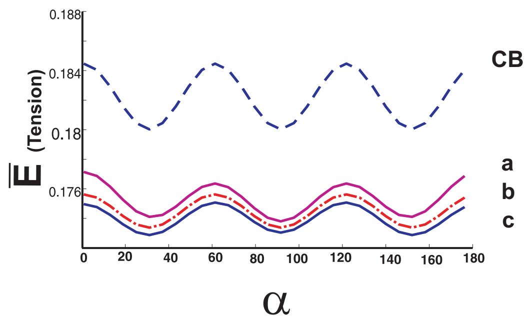
- Homogenized to continuum: Large strain membrane theory – "near-atomic" bending ignored

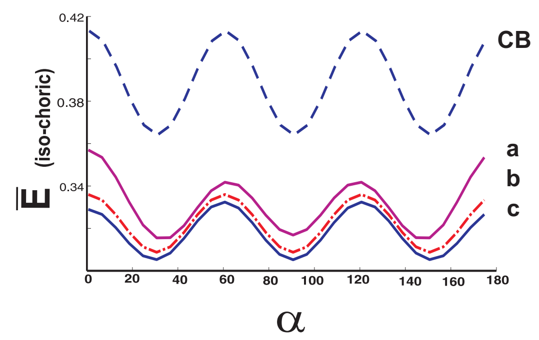
Atomistic systems - graphene

- Homogenized response for increasing size of "Representative Unit Lattice" (RUL): Dirichlet b.c. versus Cauchy-Born (CB) rule, influence of lattice anisotropy



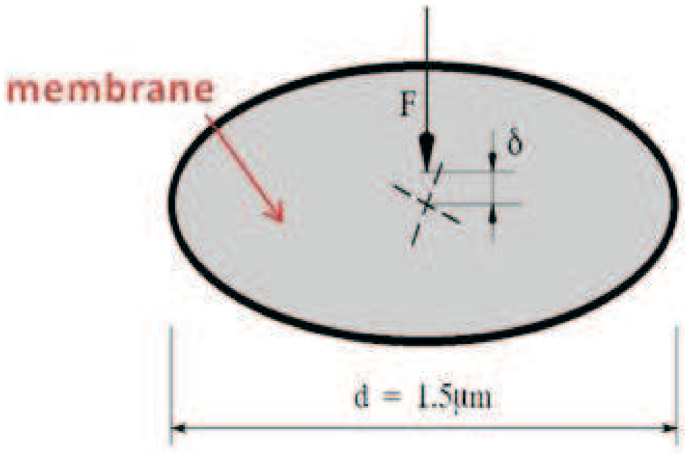


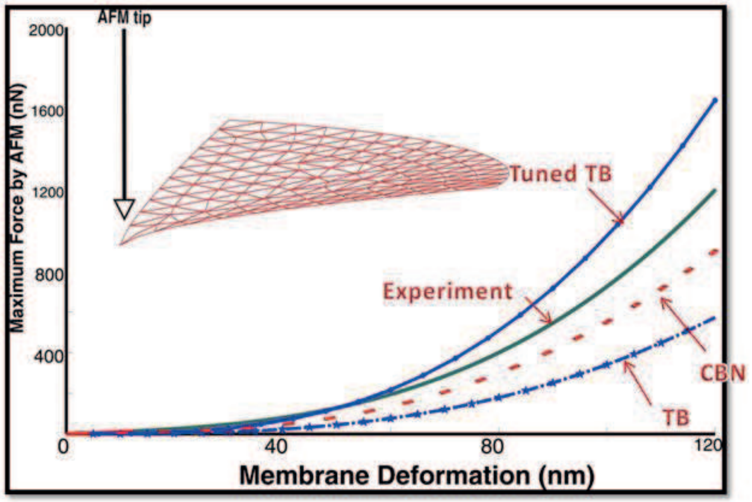




Atomistic systems - graphene

- Eperimental validation using AFM test result, HONE ET AL. 2008





"Appetizer": Moisture/chloride transport in concrete

Ph.D. project by Filip Nilenius

- Composition: Cement paste *permeable*, Ballast stones *impermeable*, Interfacial Transition Zone (ITZ) *highly permeable*
- Transport of chloride and moisture: transient and highly nonlinear coupled phenomena
- High concentration of chloride ions $\rightsquigarrow$ reinforcement corrosion $\rightsquigarrow$ concrete spalling

Figure 1: Corroded re-bars

Figure 2: Concrete specimen

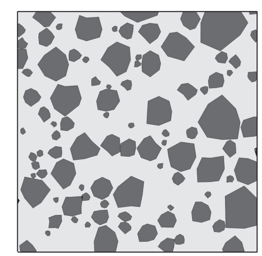
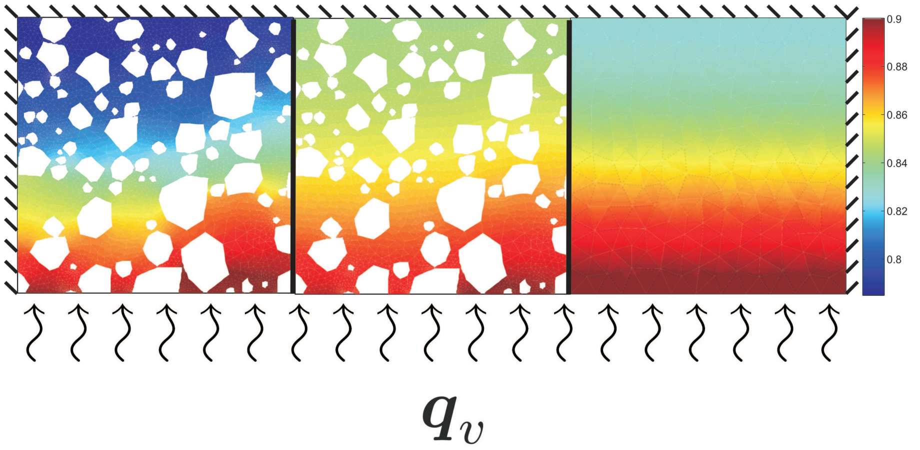


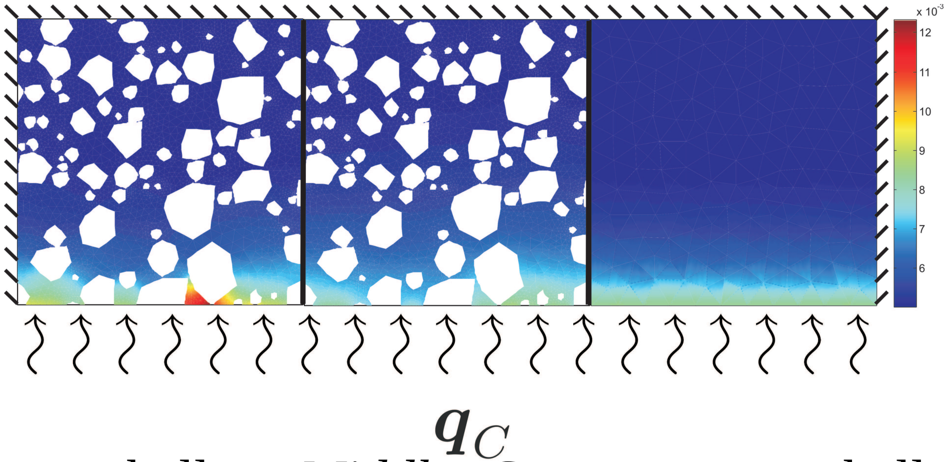
Figure 3: RVE

Computational results for single RVE

- Snapshot of moisture vapor distribution in selected time step



- Snapshot of chloride concentration distribution in selected time step

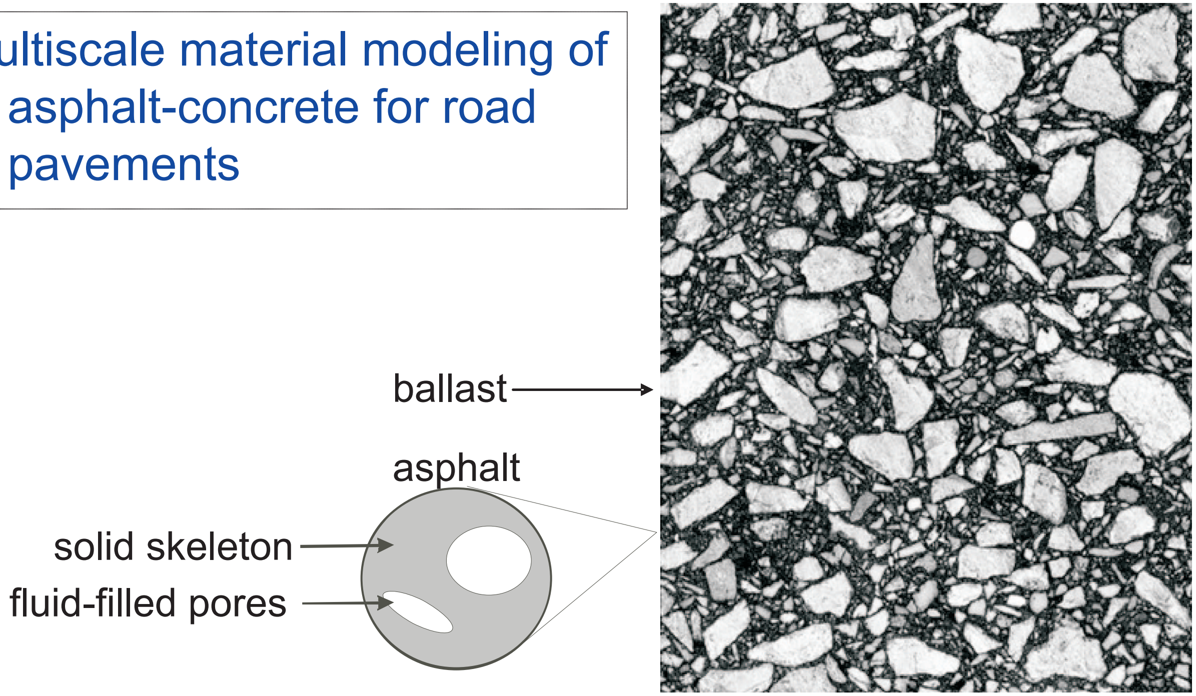


Left: Cement paste + ballast, *Middle*: Cement paste + ballast + ITZ, *Right*: Pure cement paste

”Appetizer”: Consolidation in porous granular media

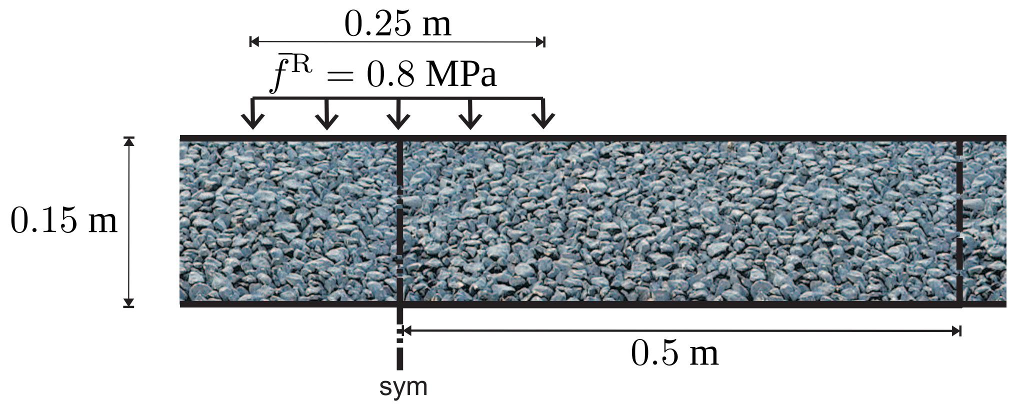
- Multiscale modeling of porous fine-grained granular material with pore-fluid, such as asphalt concrete (sand/bitumen mixture with embedded stones)
- Micro-inhomogeneity: particles in matrix
- **Note**: Intrinsically time-dependent (seepage)

Multiscale material modeling of asphalt-concrete for road pavements

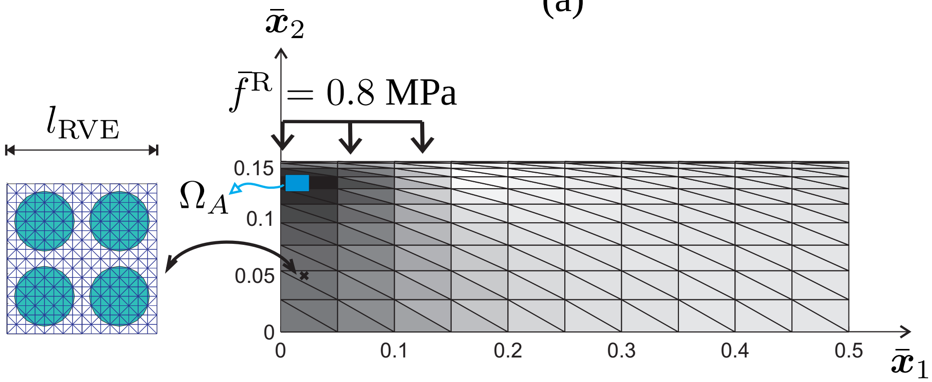


Consolidation of pavement layer

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



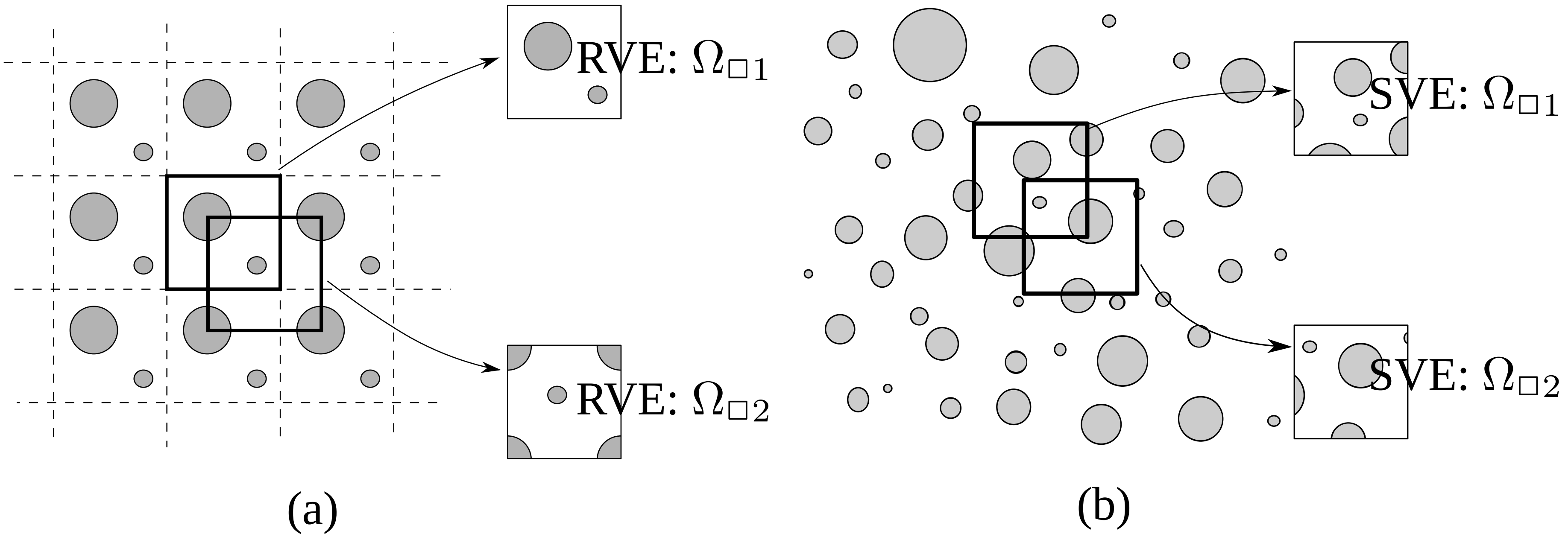
(a)



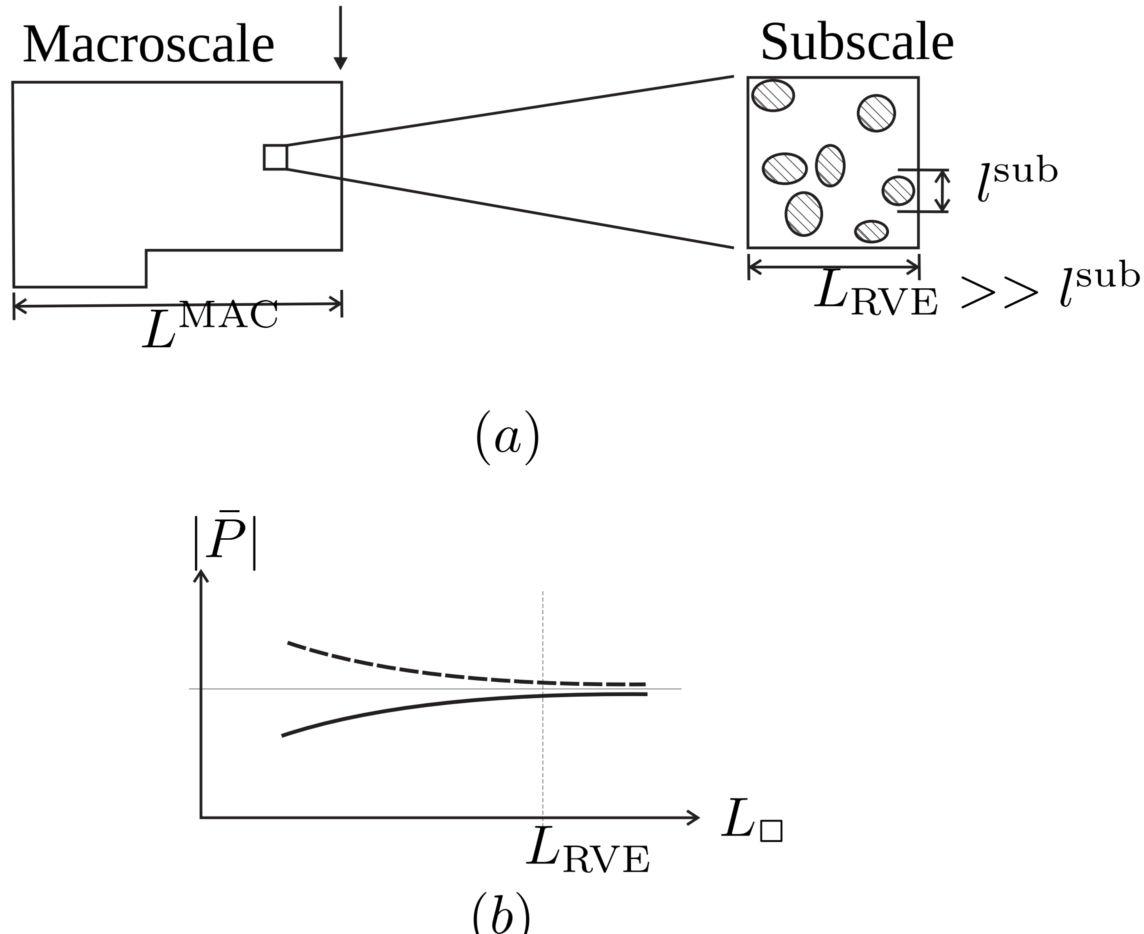
(b)

Periodic versus random substructures

- Periodic micro-structure with two selected equivalent RVE's obtained by "translation" of the centroid (Figure a)
- Aperiodic (random) micro-structure with SVE's (Statistical Volume Element, coined by OSTOJA-S.), taken from a single realization of random structure (Figure b). The microstructure is characterized by the same average volume fractions of matrix and particles as the periodic structure.



Representative Volume Element



- Conditions on size of RVE
  - Sufficiently small compared to the typical macroscale dimension of the structural component, $L_{\mathrm{RVE}} << L^{\mathrm{MAC}}$.
  - Sufficiently large compared to the typical subscale dimension of micro-constituents, e.g. grains, $l^{\mathrm{sub}} << L_{\mathrm{RVE}}$.

Average strain and stress representations

- Volume average on $\Omega_\square$, boundary $\Gamma_\square$

$$\langle \bullet \rangle_\square \stackrel{\text{def}}{=} \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \bullet \, \mathrm{d}\Omega$$

- Strain ($\boldsymbol{H} = \boldsymbol{u} \otimes \boldsymbol{\nabla}$), $\boldsymbol{N}$ = normal

$$\langle \boldsymbol{H} \rangle_\square = \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{H} \, \mathrm{d}\Omega = \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{u} \otimes \boldsymbol{N} \, \mathrm{d}\Gamma$$

- Stress ($-\boldsymbol{P} \cdot \boldsymbol{\nabla} = \boldsymbol{f}$), $\boldsymbol{t} = \boldsymbol{P} \cdot \boldsymbol{N}$ = traction

$$\langle \boldsymbol{P} \rangle_\square = \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{P} \, \mathrm{d}\Omega = \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \otimes \boldsymbol{X} \, \mathrm{d}\Gamma + \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{f} \otimes \boldsymbol{X} \, \mathrm{d}\Omega$$

Special case: $\boldsymbol{f} = \boldsymbol{0}$ (usual assumption)

$$\langle \boldsymbol{P} \rangle_\square = \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t} \otimes \boldsymbol{X} \, \mathrm{d}\Gamma$$

Effective properties – Linear elasticity

- Subscale linear elasticity (Lagrangian setting). Small deformations: E is standard elasticity stiffness tensor with major and minor symmetries

$$\boldsymbol{P} = \mathsf{E} : \boldsymbol{H}, \quad \boldsymbol{H} = \mathsf{C} : \boldsymbol{P}, \quad \mathsf{E} = \mathsf{C}^{-1}$$

  - $\boldsymbol{P}$ becomes symmetrical due to first *minor* symmetry of E
  - Only the symmetric part of $\boldsymbol{H}$, which may be non-symmetric, contributes to $\boldsymbol{P}$

- Effective constitutive relation, assume $L_\square \to \infty$ (RVE)

$$\bar{\boldsymbol{P}} = \bar{\mathsf{E}} : \bar{\boldsymbol{H}}, \quad \bar{\boldsymbol{H}} = \bar{\mathsf{C}} : \bar{\boldsymbol{P}}$$

- Strain concentration tensor

$$\boldsymbol{H}(\boldsymbol{X}) = \mathsf{A}(\boldsymbol{X}) : \bar{\boldsymbol{H}}, \quad \boldsymbol{X} \in \Omega_\square \quad \Rightarrow \quad \bar{\mathsf{E}} = \langle \mathsf{A} : \boldsymbol{H} \rangle_\square$$

Effective properties – Linear elasticity, cont'd

- Macrohomogeneity

$$\langle \boldsymbol{P} : \boldsymbol{H} \rangle_{\square} = \langle \boldsymbol{P} \rangle_{\square} : \langle \boldsymbol{H} \rangle_{\square} (= \bar{\boldsymbol{P}} : \bar{\boldsymbol{H}})$$

$$\Rightarrow \quad \bar{\mathsf{E}} = \langle \mathsf{A}^{\mathrm{T}} : \mathsf{E} : \mathsf{A} \rangle_{\square}$$

  Major symmetry!

- Challenge: $\bar{\mathsf{E}}$ not computable for $L_{\square} \to \infty$ (RVE) in principle. Common strategies (in the classical literature on homogenization) aim for
  - sharp bounds on (the eigenvalues) of $\bar{\mathsf{E}}$
  - or a good approximation of $\bar{\mathsf{E}}$ via a suitable choice of the strain concentration field A, or "clever" approximations of the displacement gradient and stress fields within the RVE

Homogenization – Effective properties

- Closed-form homogenization approaches – linear elasticity
  - Mean field methods for matrix-inclusions composites: Eshelby solution for dilute inclusions ESHELBY 1959, Mori-Tanaka-type approaches for non-dilute composite MORI, TANAKA 1973, HASHIN-SHTRIKMAN 1962,
  - Classical bounds based on "rule of mixtures": Upper bound VOIGT 1887, TAYLOR 1938 (polycrystalline structure), CAUCHY-BORN 1890 (atomistic structure). Lower bound REUSS, HILL 1970, SACHS 1928 (polycrystalline structure)
- Computational homogenization
  - Direct FE-computation on "unit cell" SUQUET 1985
  - Bounds based on "virtual statistical testing", HAZANOV AND HUET 1994, ZOHDI 2004
  - Hybrid techniques: Windowing (embedding of "unit cell" in larger domain), ...
- Selected texts (classical theory): NEMAT-NASSER & HORI (1993), SUQUET (1997), TORQUATO (2002), OSTOJA-STARZEWSKI (2007)

Classical prolongation conditions on SVE

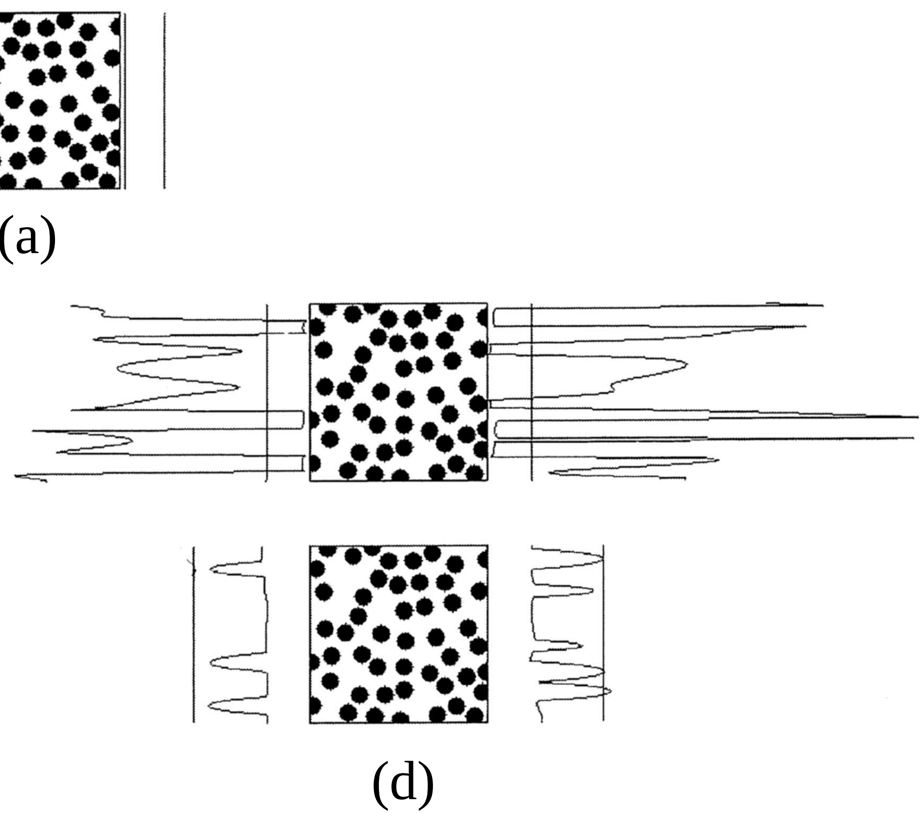
- Major issue: Boundary conditions on SVE that ensure best possible approximation of $\bar{\mathsf{E}}$
- Classical conditions:
  - Boundary displacements generated by a macroscale strain $\bar{\boldsymbol{H}}$ (denoted the DBC-problem) – Dirichlet b.c.
  - Boundary tractions generated by a macroscale stress $\bar{\boldsymbol{P}}$ (denoted the TBC-problem) – Neumann b.c.
  - Periodic boundary displacements and antiperiodic tractions (denoted the PBC-problem), realizable in practice only for a cubic in 3D (square in 2D) SVE
- Type of "load control" independent on prolongation conditions:
  - Macroscale "strain control": $\langle \boldsymbol{H} \rangle_\square$ is prescribed to value $\bar{\boldsymbol{H}}$
  - Macroscale "stress control": $\langle \boldsymbol{P} \rangle_\square$ is prescribed to value $\bar{\boldsymbol{P}}$
- **Note**: Strain control useful for (i) standard displacement-based FE on macroscale, (ii) core-algorithm in constitutive driver for plane stress, etc

Classical prolongation conditions on SVE, cont'd

- Assessment of prolongation conditions
  - Periodic microstructure: PBC exact for $L_\square = L_{\rm per}$
  - Random microstructure: PBC "good"
- **Remarks**:
  - All prolongation conditions: Convergence to $\bar{\mathbf{E}}$ for $L_\square \to \infty$
  - No prolongation condition gives guaranteed "best" approximation to $\bar{\mathbf{E}}$ (in some measure) $\Rightarrow$ Not possible to establish "model hierarchy"
  - No prolongation condition gives guaranteed upper or lower bound to $\bar{\mathbf{E}}$ for a single realization of a random microstructure
  - Possible to obtain guaranteed bounds (within given confidence interval) using "statistical sampling" of random microstructure

Classical prolongation conditions on SVE, cont'd

- Assessment of prolongation conditions: Effect depends on degree of microheterogeneity [Figure from OSTOJA-STARZEWSKI (2007)]



Fluctuations of boundary fields for different mismatch of the shear modulus G. (a) Homogenous: $G^{(\mathrm{p})}/G^{(\mathrm{m})} = 1$. (b) $G^{(\mathrm{p})}/G^{(\mathrm{m})} = 0.2$. (c)$G^{(\mathrm{p})}/G^{(\mathrm{m})} = 0.05$. (d) $G^{(\mathrm{p})}/G^{(\mathrm{m})} = 0.02$.

Hill-Mandel macrohomogeneity condition

- "Virtual work" identity for macro- and subscales: For *statically admissible* $\boldsymbol{P}'$ and *kinematically admissible* $\boldsymbol{H}''$

$$\langle \boldsymbol{P}' : \boldsymbol{H}'' \rangle_\square = \langle \boldsymbol{P}' \rangle_\square : \langle \boldsymbol{H}'' \rangle_\square$$

- Useful identity

$$\langle \boldsymbol{P}' : \boldsymbol{H}'' \rangle_\square \quad = \quad \frac{1}{|\Omega_\square|} \int_{\Omega_\square} \boldsymbol{P}' : \boldsymbol{H}'' \,\mathrm{d}\Omega = \frac{1}{\Omega_\square} \left[\int_{\Omega_\square} \boldsymbol{f} \cdot \boldsymbol{u}'' \,\mathrm{d}\Omega + \int_{\Gamma_\square} \boldsymbol{t}' \cdot \boldsymbol{u}'' \,\mathrm{d}\Gamma \right.$$

$$\overset{\boldsymbol{f}=\boldsymbol{0}}{=} \quad \frac{1}{|\Omega_\square|} \int_{\Gamma_\square} \boldsymbol{t}' \cdot \boldsymbol{u}'' \,\mathrm{d}\Gamma$$

- Decomposition into "macro" and "fluctuation" parts

$$\boldsymbol{u}'' = \bar{\boldsymbol{u}}'' + \bar{\boldsymbol{H}}'' \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}] + (\boldsymbol{u}^{\mathrm{s}})'' \quad \Rightarrow \quad (\boldsymbol{H}^{\mathrm{s}})'' \overset{\mathrm{def}}{=} \boldsymbol{H}'' - \bar{\boldsymbol{H}}'', \quad \langle (\boldsymbol{H}^{\mathrm{s}})'' \rangle_\square = \boldsymbol{0}$$

$$\boldsymbol{P}' = \bar{\boldsymbol{P}}' + (\boldsymbol{P}^{\mathrm{s}})', \quad \langle (\boldsymbol{P}^{\mathrm{s}})' \rangle_\square = \boldsymbol{0}$$

$$\rightsquigarrow \qquad \langle (\boldsymbol{P}^{\mathrm{s}})' : (\boldsymbol{H}^{\mathrm{s}})'' \rangle_\square = 0$$

Hill-Mandel macrohomogeneity condition, cont'd

- Alternative classical formulation of HM-condition

$$\int_{\Gamma_\square} \left[\boldsymbol{t}' - \bar{\boldsymbol{P}}' \cdot \boldsymbol{N}\right] \cdot \left[\boldsymbol{u}'' - \bar{\boldsymbol{u}}'' - \bar{\boldsymbol{H}}'' \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}]\right] \, \mathrm{d}\Gamma = 0$$

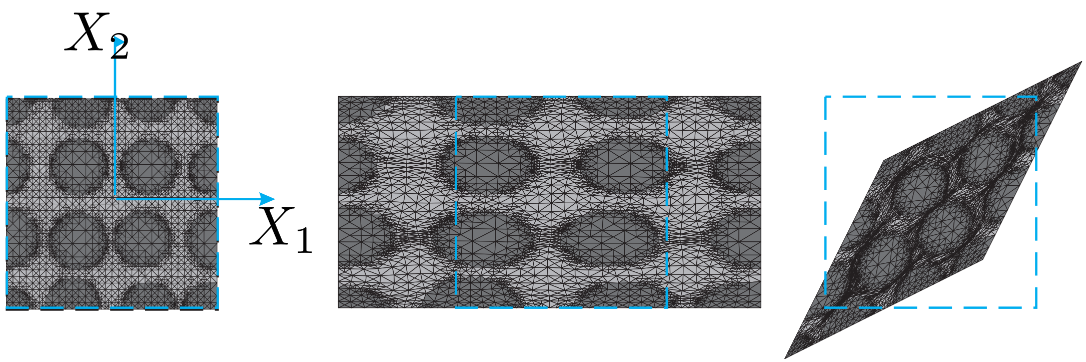
Displacement boundary condition (DBC)

- Model assumption

$$\boldsymbol{u}(\boldsymbol{X}) = \bar{\boldsymbol{u}} + \bar{\boldsymbol{H}} \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}], \quad \text{or} \quad \boldsymbol{u}^{\mathrm{s}}(\boldsymbol{X}) = \boldsymbol{0}, \quad \boldsymbol{X} \in \Gamma_{\square}$$

$$\Rightarrow \quad \langle \boldsymbol{H} \rangle_{\square} = \bar{\boldsymbol{H}}$$

- **Note**: HM-condition satisfied a priori



Examples of deformed shapes of square RVE with particles in matrix subjected to DBC. (Left) Undeformed RVE. (Middle) Normal displacement gradient: Only $\bar{H}_{11}$ is non-zero. (Right) Shear strain: Only $\bar{H}_{12} = \bar{H}_{21}$ is non-zero.

Traction boundary condition (TBC)

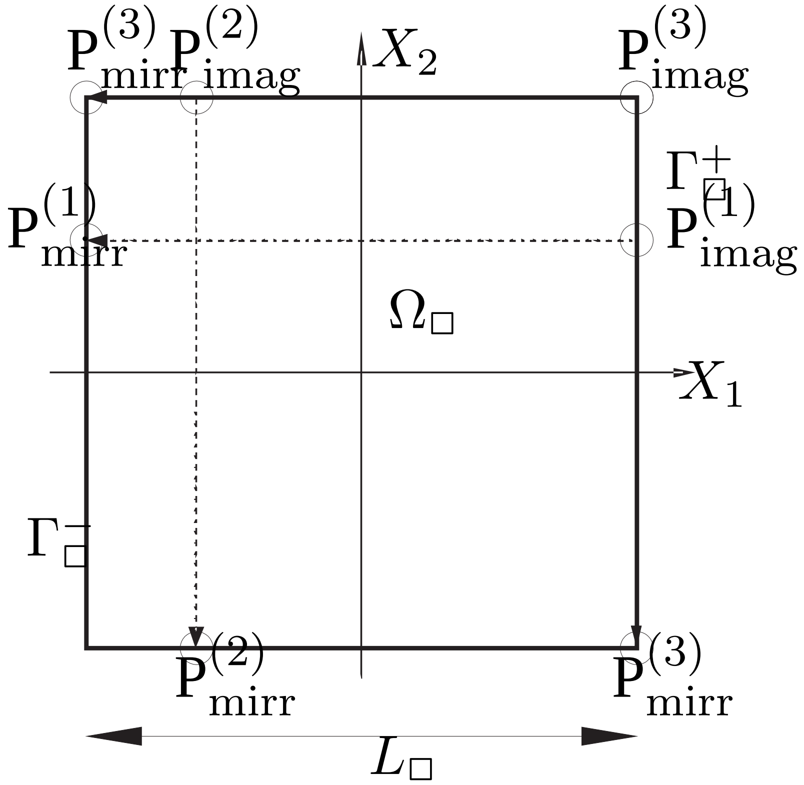
- Model assumption

$$\boldsymbol{t}(\boldsymbol{X}) = \bar{\boldsymbol{P}} \cdot \boldsymbol{N}(\boldsymbol{X}) \quad \text{or} \quad \boldsymbol{t}^{\text{s}}(\boldsymbol{X}) = \boldsymbol{0}, \quad \boldsymbol{X} \in \Gamma_{\Box}$$

$\Rightarrow \quad \langle \boldsymbol{P} \rangle_{\Box} = \bar{\boldsymbol{P}}$

- **Note**: HM-condition satisfied a priori

Periodic boundary condition (PBC)



- Cubic (square) SVE with assumed microperiodicity in coordinate directions: $\Gamma_{\square} = \Gamma^{-}_{\square} \cup \Gamma^{+}_{\square}$
  - Image boundary $\Gamma^{+}_{\square}$ computational domain
  - Mirror boundary $\Gamma^{-}_{\square}$

Periodic boundary condition (PBC), cont'd

- Model assumption: Assumed periodicity of displacement fluctuation

$$\boldsymbol{u}^{\mathrm{s}}(\boldsymbol{X}^{+}) = \boldsymbol{u}^{\mathrm{s}}(\boldsymbol{X}^{-}) \quad \text{or} \quad [\![\boldsymbol{u}^{\mathrm{s}}]\!] = \boldsymbol{0}$$

- Model assumption: Assumed anti-periodicity of traction

$$\boldsymbol{t}(\boldsymbol{X}^{+}) = -\boldsymbol{t}(\boldsymbol{X}^{-}) \quad \text{or} \quad \boldsymbol{t}(\boldsymbol{X}^{+}) + \boldsymbol{t}(\boldsymbol{X}^{-}) = \boldsymbol{0}$$

  - Necessary assumption [literature somewhat vague on this point]
  - Anti-periodic $\boldsymbol{t}$ can be interpreted as periodic $\boldsymbol{P}$
- **Note**: HM-condition satisfied a priori

Classical energy bounds

- Bounds
  - "Apparant" stiffness (compliance) for single SVE (single realization),
  - Effective properties based on "numerical statistical testing"
- Tool: Fundamental extremal properties
  - DBC with strain control
  - TBC with stress control

DBC – Extremal properties

- Admissible spaces
  - Kinematically admissible displacements

$$\mathbb{U}_{\square}^{\mathrm{D}} = \{\boldsymbol{u} \text{ "sufficiently regular"},\ \boldsymbol{u} = \bar{\boldsymbol{H}} \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}] \text{ on } \Gamma_{\square}\}$$

$$\mathbb{U}_{\square}^{\mathrm{D},0} = \{\boldsymbol{u} \text{ "sufficiently regular"},\ \boldsymbol{u} = \boldsymbol{0} \text{ on } \Gamma_{\square}\}$$

  - Statically admissible stresses

$$\mathbb{S}_{\square}^{\mathrm{D}} = \{\boldsymbol{P} \text{ "sufficiently regular"},\ -\boldsymbol{P} \cdot \boldsymbol{\nabla} = \boldsymbol{0} \text{ in } \Omega_{\square}\}$$

- Fundamental DBC-problem with strain control: Find $\boldsymbol{u} \in \mathbb{U}_{\square}$ which, for given $\bar{\boldsymbol{H}}$, solves

$$\langle \boldsymbol{H} : \mathsf{E} : \delta\boldsymbol{H} \rangle_{\square} = 0 \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0}$$

Post-processing: $\bar{\boldsymbol{P}}^{\mathrm{D}} \stackrel{\mathrm{def}}{=} \langle \boldsymbol{P} \rangle_{\square}$

DBC – Extremal properties, cont'd

- Min of potential energy

$$\Pi_\square^{\mathrm{D}}(\boldsymbol{u}) \leq \Pi_\square^{\mathrm{D}}(\hat{\boldsymbol{u}}) \quad \forall \hat{\boldsymbol{u}} \in \mathbb{U}_\square^{\mathrm{D}}, \quad \Pi_\square^{\mathrm{D}}(\hat{\boldsymbol{u}}) \stackrel{\mathrm{def}}{=} \frac{1}{2}\langle \hat{\boldsymbol{H}} : \mathsf{E} : \hat{\boldsymbol{H}}\rangle_\square$$

- Strain energy obtained obtained from min of $\Pi_\square^{\mathrm{D}}(\boldsymbol{u})$ using HM-condition

$$\bar{\psi}_\square^{\mathrm{D}}(\bar{\boldsymbol{H}}) \stackrel{\mathrm{def}}{=} \frac{1}{2}\bar{\boldsymbol{H}} : \bar{\mathsf{E}}_\square^{\mathrm{D}} : \bar{\boldsymbol{H}}$$

- Min of complementary potential energy

$$\Pi_\square^{*\mathrm{D}}(\boldsymbol{P}) \leq \Pi_\square^{*\mathrm{D}}(\hat{\boldsymbol{P}}) \quad \forall \hat{\boldsymbol{P}} \in \mathbb{S}_\square^{\mathrm{D}} \quad \Pi_\square^{*\mathrm{D}}(\hat{\boldsymbol{P}}) \stackrel{\mathrm{def}}{=} \frac{1}{2}\langle \hat{\boldsymbol{P}} : \mathsf{C} : \hat{\boldsymbol{P}}\rangle_\square - \langle \hat{\boldsymbol{P}}\rangle_\square : \bar{\boldsymbol{H}}$$

- Combining min-properties gives fundamental result to be used in constructing bounds:

$$\langle \hat{\boldsymbol{P}}\rangle_\square : \bar{\boldsymbol{H}} - \frac{1}{2}\langle \hat{\boldsymbol{P}} : \mathsf{C} : \hat{\boldsymbol{P}}\rangle_\square \leq \bar{\psi}_\square^{\mathrm{D}}(\bar{\boldsymbol{H}}) \leq \frac{1}{2}\langle \hat{\boldsymbol{H}} : \mathsf{E} : \hat{\boldsymbol{H}}\rangle_\square \quad \forall \hat{\boldsymbol{u}} \in \mathbb{U}_\square^{\mathrm{D}},\ \forall \hat{\boldsymbol{P}} \in \mathbb{S}_\square^{\mathrm{D}}$$

TBC – Extremal properties

- Admissible spaces
  - Kinematically admissible displacements

$$\mathbb{U}_{\square}^{\mathrm{N}} = \{\boldsymbol{u} \text{ "sufficiently regular"}, \ \boldsymbol{u}(\bar{\boldsymbol{X}}) = \boldsymbol{0}\}$$

  - Statically admissible stresses

$$\mathbb{S}_{\square}^{\mathrm{N}} = \{\boldsymbol{P} \text{ "sufficiently regular"}, \ -\boldsymbol{P} \cdot \boldsymbol{\nabla} = \boldsymbol{0} \text{ in } \Omega_{\square}, \ \boldsymbol{t} = \bar{\boldsymbol{P}} \cdot \boldsymbol{N} \text{ on } \Gamma_{\square}\}$$

- Fundamental TBC-problem with stress control: Find $\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{N}}$ which, for given $\bar{\boldsymbol{P}}$, solves

$$\langle \boldsymbol{H} : \mathsf{E} : \delta \boldsymbol{H} \rangle_{\square} = \bar{\boldsymbol{P}} : \langle \delta \boldsymbol{H} \rangle_{\square} \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{N}}$$

Post-processing: $\bar{\boldsymbol{H}}^{\mathrm{N}} \overset{\mathrm{def}}{=} \langle \boldsymbol{H} \rangle_{\square}$

TBC – Extremal properties, cont'd

- Min of complementary potential energy

$$\Pi^{*\mathrm{N}}_{\Box}(\boldsymbol{P}) \leq \Pi^{*\mathrm{N}}_{\Box}(\hat{\boldsymbol{P}}) \quad \forall \hat{\boldsymbol{P}} \in \mathbb{S}^{\mathrm{N}}_{\Box} \quad \Pi^{*\mathrm{D}}_{\Box}(\hat{\boldsymbol{P}}) \stackrel{\mathrm{def}}{=} \frac{1}{2}\langle \hat{\boldsymbol{P}} : \mathsf{C} : \hat{\boldsymbol{P}} \rangle_{\Box}$$

- Complementary strain (stress) energy obtained from min of $\Pi^{*\mathrm{N}}_{\Box}(\boldsymbol{P})$ using HM-condition

$$\bar{\psi}^{*\mathrm{N}}_{\Box}(\bar{\boldsymbol{P}}) \stackrel{\mathrm{def}}{=} \frac{1}{2}\bar{\boldsymbol{P}} : \bar{\mathsf{C}}^{\mathrm{N}}_{\Box} : \bar{\boldsymbol{P}}$$

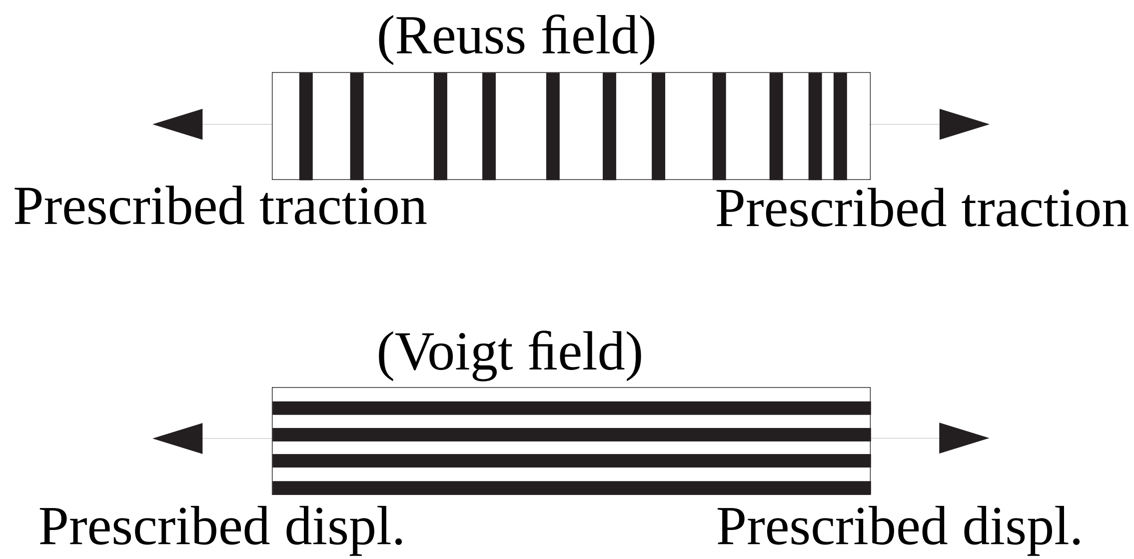
- Min of potential energy

$$\Pi^{\mathrm{N}}_{\Box}(\boldsymbol{u}) \leq \Pi^{\mathrm{N}}_{\Box}(\hat{\boldsymbol{u}}) \quad \forall \hat{\boldsymbol{u}} \in \mathbb{U}^{\mathrm{N}}_{\Box}, \quad \Pi^{\mathrm{N}}_{\Box}(\hat{\boldsymbol{u}}) \stackrel{\mathrm{def}}{=} \frac{1}{2}\langle \hat{\boldsymbol{H}} : \mathsf{E} : \hat{\boldsymbol{H}} \rangle_{\Box} - \bar{\boldsymbol{P}} : \langle \hat{\boldsymbol{H}} \rangle_{\Box}$$

- Combining min-properties gives fundamental result to be used in constructing bounds:

$$\bar{\boldsymbol{P}} : \langle \hat{\boldsymbol{H}} \rangle_{\Box} - \frac{1}{2}\langle \hat{\boldsymbol{H}} : \mathsf{E} : \hat{\boldsymbol{H}} \rangle_{\Box} \leq \bar{\psi}^{*\mathrm{N}}_{\Box}(\bar{\boldsymbol{P}}) \leq \frac{1}{2}\langle \hat{\boldsymbol{P}} : \mathsf{C} : \hat{\boldsymbol{P}} \rangle_{\Box} \quad \forall \hat{\boldsymbol{u}} \in \mathbb{U}^{\mathrm{N}}_{\Box},\ \forall \hat{\boldsymbol{P}} \in \mathbb{S}^{\mathrm{N}}_{\Box}$$

Voigt (upper) and Reuss (lower) bounds



- Voigt (Taylor) assumption $\hat{\boldsymbol{H}}(\boldsymbol{X}) = \bar{\boldsymbol{H}}, \ \forall \boldsymbol{X}$

$$\bar{\psi}_{\square}^{\mathrm{D}}(\bar{\boldsymbol{H}}) \leq \frac{1}{2}\bar{\boldsymbol{H}} : \langle \mathbf{E} \rangle_{\square} : \bar{\boldsymbol{H}} = \frac{1}{2}\bar{\boldsymbol{H}} : \bar{\mathbf{E}}_{\square}^{\mathrm{V}} : \bar{\boldsymbol{H}} \overset{\mathrm{def}}{=} \bar{\psi}_{\square}^{\mathrm{V}}(\bar{\boldsymbol{H}}), \quad \bar{\mathbf{E}}_{\square}^{\mathrm{V}} \overset{\mathrm{def}}{=} \langle \mathbf{E} \rangle_{\square}$$

- Reuss (Sachs) assumption $\hat{\boldsymbol{P}}(\boldsymbol{X}) = \bar{\boldsymbol{P}}, \ \forall \boldsymbol{X}$

$$\bar{\psi}_{\square}^{*\mathrm{N}}(\bar{\boldsymbol{P}}) \leq \frac{1}{2}\bar{\boldsymbol{P}} : \langle \mathbf{C} \rangle_{\square} : \bar{\boldsymbol{P}} = \frac{1}{2}\bar{\boldsymbol{P}} : \bar{\mathbf{C}}_{\square}^{\mathrm{R}} : \bar{\boldsymbol{P}} \overset{\mathrm{def}}{=} \bar{\psi}_{\square}^{*\mathrm{R}}(\bar{\boldsymbol{P}}), \quad \bar{\mathbf{C}}_{\square}^{\mathrm{R}} \overset{\mathrm{def}}{=} \langle \mathbf{C} \rangle_{\square}$$

Voigt and Reuss bounds, cont'd

- Only info used is volume fraction of microconstituents $\Rightarrow$ Valid also for effective properties (when $L_{\square} \to \infty$) $\Rightarrow$ Hill-Reuss-Voigt bounds

$$\bar{\mathsf{E}}^{\mathrm{R}} \leq \bar{\mathsf{E}} \leq \bar{\mathsf{E}}^{\mathrm{V}}$$

Bounds for single SVE-realization

- Fundamental inequality for DBC-problem can be used to obtain bounds for strain energy

$$\bar{\psi}_{\Box}^{\mathrm{R}}(\bar{\boldsymbol{H}}) \leq \bar{\psi}_{\Box}^{\mathrm{N}}(\bar{\boldsymbol{H}}) \leq \bar{\psi}_{\Box}^{\mathrm{D}}(\bar{\boldsymbol{H}}) \leq \bar{\psi}_{\Box}^{\mathrm{V}}(\bar{\boldsymbol{H}}) \quad \forall \bar{\boldsymbol{H}} \in \mathbb{R}^{3\times 3}$$

- Fundamental inequality for TBC-problem can be used to obtain bounds for stress energy

$$\bar{\psi}_{\Box}^{*\mathrm{V}}(\bar{\boldsymbol{P}}) \leq \bar{\psi}_{\Box}^{*\mathrm{D}}(\bar{\boldsymbol{P}}) \leq \bar{\psi}_{\Box}^{*\mathrm{N}}(\bar{\boldsymbol{P}}) \leq \bar{\psi}_{\Box}^{*\mathrm{R}}(\bar{\boldsymbol{P}}) \quad \forall \bar{\boldsymbol{P}} \in \mathbb{R}^{3\times 3}$$

- **Note**: All stiffness-compliance tensors can be expressed in the fundamental tensors:
  - $\bar{\mathsf{E}}_{\Box}^{\mathrm{D}}$ from the DBC-problem
  - $\bar{\mathsf{C}}_{\Box}^{\mathrm{N}}$ from the TBC-problem
  - $\bar{\mathsf{E}}_{\Box}^{\mathrm{V}} = \langle \mathsf{E} \rangle_{\Box}$
  - $\bar{\mathsf{C}}_{\Box}^{\mathrm{R}} = \langle \mathsf{C} \rangle_{\Box}$

  and their inverses

Bounds on effective stiffness

- Aim for guaranteed upper and lower bounds on $\bar{\psi}(\bar{\boldsymbol{H}}) \leftrightarrow \bar{\mathsf{E}}$
- Identities for effective properties:

$$\bar{\psi}(\bar{\boldsymbol{H}}) = \lim_{L_{\square}\to\infty} \bar{\psi}_{\square}^{\mathrm{N}}(\bar{\boldsymbol{H}}) = \lim_{L_{\square}\to\infty} \bar{\psi}_{\square}(\bar{\boldsymbol{H}}) = \lim_{L_{\square}\to\infty} \bar{\psi}_{\square}^{\mathrm{D}}(\bar{\boldsymbol{H}})$$

$$\bar{\psi}^{*}(\bar{\boldsymbol{P}}) = \lim_{L_{\square}\to\infty} \bar{\psi}_{\square}^{*\mathrm{D}}(\bar{\boldsymbol{P}}) = \lim_{L_{\square}\to\infty} \bar{\psi}_{\square}^{*}(\bar{\boldsymbol{P}}) = \lim_{L_{\square}\to\infty} \bar{\psi}_{\square}^{*\mathrm{N}}(\bar{\boldsymbol{P}})$$

- Strategy to obtain upper bound: Introduce "large" SVE with size $L_{(\square)} > L_{\square}$

$$\bar{\psi}(\bar{\boldsymbol{H}}) = \lim_{L_{(\square)}\to\infty} \bar{\psi}_{(\square)}^{\mathrm{D}}\{\bar{\boldsymbol{H}}, \omega_1\}$$

- Strategy of "numerical testing" using ergodicity arguments, HAZANOV AND HUET (1994)

$$\bar{\psi}(\bar{\boldsymbol{H}}) \leq \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \bar{\psi}_{\square}^{\mathrm{D}}\{\bar{\boldsymbol{H}}, \omega_i\} = E\left[\bar{\psi}_{\square}^{\mathrm{D}}\{\bar{\boldsymbol{H}}, \tilde{\omega}\}\right]$$

Bounds on effective stiffness, cont'd

- Approximation for $N < \infty$

$$\bar{\psi}(\bar{\boldsymbol{H}}) \leq \bar{\psi}^{\mathrm{UB}}(\bar{\boldsymbol{H}}) \quad \text{with} \quad \bar{\psi}^{\mathrm{UB}}(\bar{\boldsymbol{H}}) \approx \bar{\psi}^{\mathrm{D-V}}(\bar{\boldsymbol{H}})$$

and

$$\bar{\psi}^{\mathrm{D-V}}(\bar{\boldsymbol{H}}) \stackrel{\mathrm{def}}{=} \frac{1}{2}\bar{\boldsymbol{H}} : \bar{\mathsf{E}}_{\square}^{\mathrm{D-V}} : \bar{\boldsymbol{H}} \quad \text{with} \quad \bar{\mathsf{E}}_{\square}^{\mathrm{D-V}} \stackrel{\mathrm{def}}{=} \frac{1}{N}\sum_{i=1}^{N} \bar{\mathsf{E}}_{\square}^{\mathrm{D}}(\omega_i)$$

- Similar arguments for lower bound, involving Legendre transformations

$$\bar{\psi}(\bar{\boldsymbol{H}}) \geq \bar{\psi}^{\mathrm{LB}}(\bar{\boldsymbol{H}}) \quad \text{with} \quad \bar{\psi}^{\mathrm{LB}}(\bar{\boldsymbol{H}}) \approx \bar{\psi}^{\mathrm{N-R}}(\bar{\boldsymbol{H}})$$

and

$$\bar{\psi}^{\mathrm{N-R}}(\bar{\boldsymbol{H}}) \stackrel{\mathrm{def}}{=} \frac{1}{2}\bar{\boldsymbol{H}} : \bar{\mathsf{E}}_{\square}^{\mathrm{N-R}} : \bar{\boldsymbol{H}} \quad \text{with} \quad \bar{\mathsf{E}}_{\square}^{\mathrm{N-R}} \stackrel{\mathrm{def}}{=} \left[\frac{1}{N}\sum_{i=1}^{N} \left[\bar{\mathsf{E}}_{\square}^{\mathrm{N}}(\omega_i)\right]^{-1}\right]^{-1}$$

Bounds on effective stiffness, cont'd

- Summary

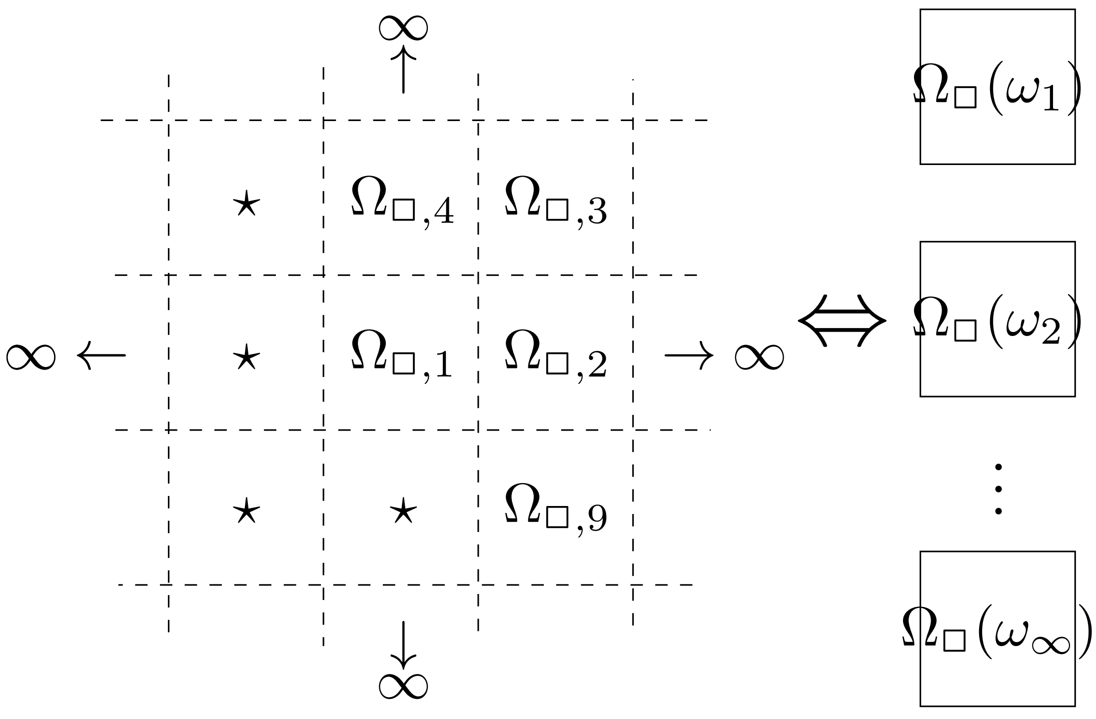
$$\bar{\psi}_{\square}^{\mathrm{N-R}}(\bar{\boldsymbol{H}}) \leq \bar{\psi}(\bar{\boldsymbol{H}}) \leq \bar{\psi}_{\square}^{\mathrm{D-V}}(\bar{\boldsymbol{H}})$$

  "V" and "R" denote "Voigt-type sampling" and "Reuss-type sampling", respectively

- **Remarks**:
  - Bounds become more reliable when number of "samples" increase
  - Guaranteed bounds within confidence intervals can be constructed assuming Gaussian distribution (manuscript in preparation) New result, even for elasticity!

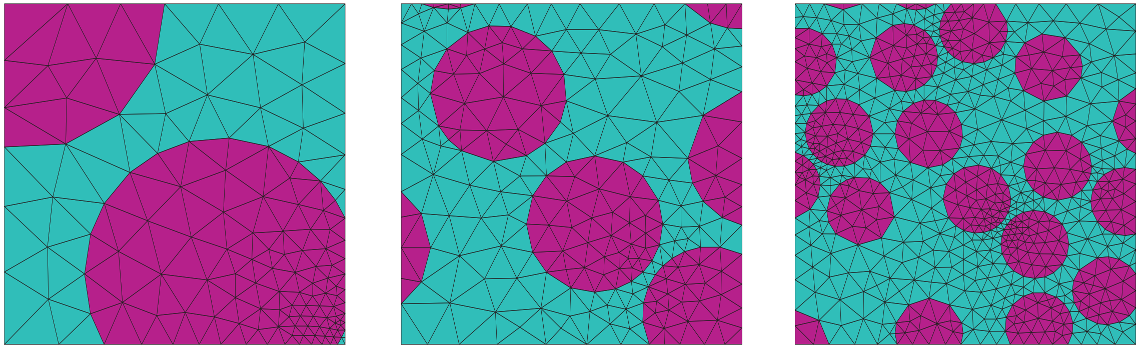
Strategy of ”numerical statistical testing”

- Single realization ω_0 for large domain $\Omega_{(\square)}$: N subdomains of the same size obtained by subdivision into subdomains of size $L_\square$, $\{\Omega_{\square,i}(\omega_0)\}_1^N$
- Single domain $\Omega_\square$ of size $L_\square$: N different realizations in $\Omega_\square$, $\{\Omega_\square(\omega_i)\}_1^N$
- Ergodicity and statistical uniformity: $\{\Omega_{\square,i}(\omega_0)\}_1^\infty \quad \equiv \quad \{\Omega_\square(\omega_i)\}_1^\infty$



Computational results of bounds

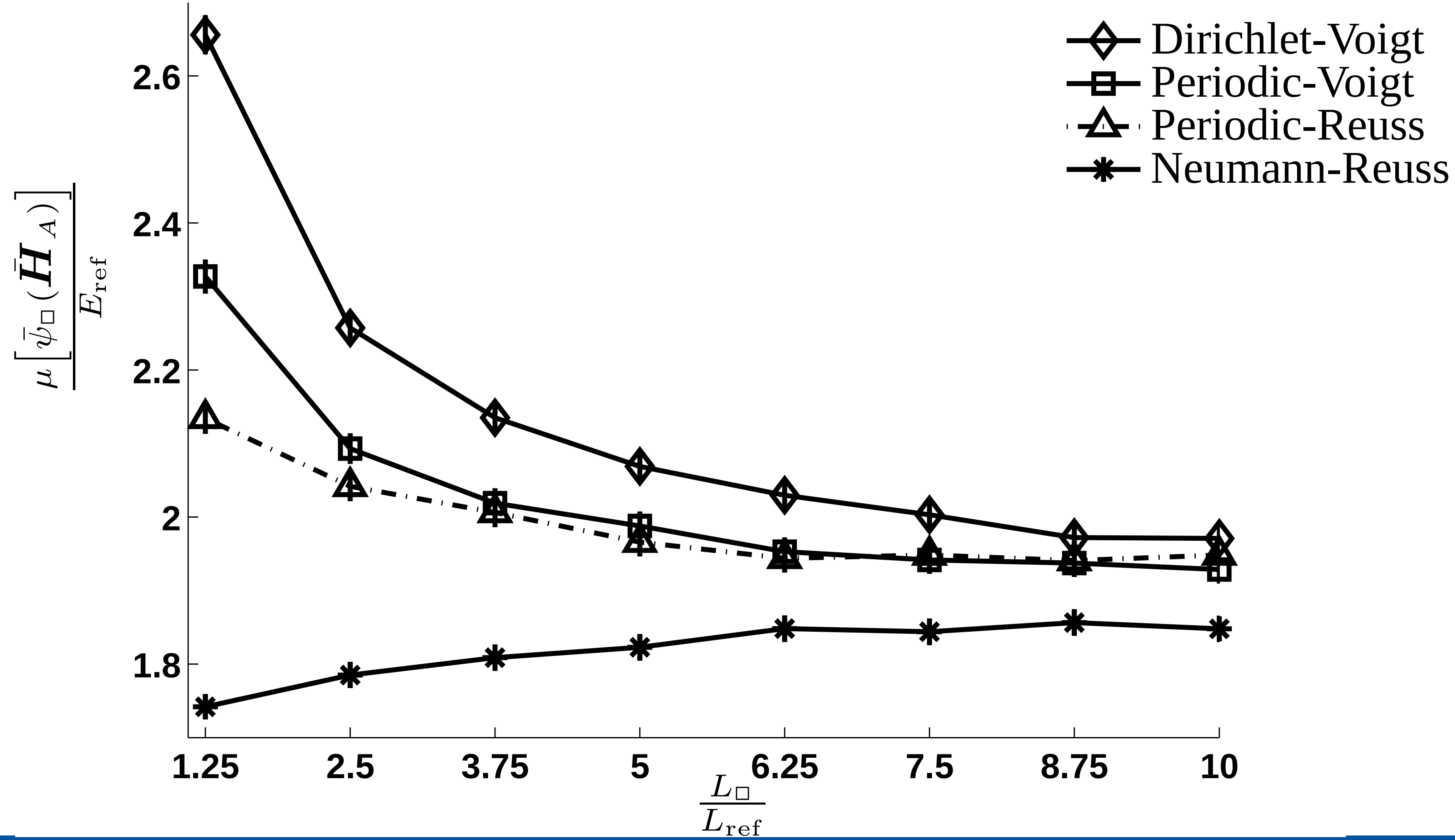
- Single realization of random microstructure for different RVE-sizes: Stiff (hard) particles (p) in a compliant (soft) matrix material: $E_\mathrm{p} = 15E_\mathrm{ref}$, $\nu_\mathrm{p} = 0.3$ and $E_\mathrm{m} = E_\mathrm{ref}$, $\nu_\mathrm{m} = 0.49$. Volume fraction $n_\mathrm{p} = 0.40$.



$\frac{L_\square}{L_\mathrm{ref}} = 1.25$ $\quad$ $\frac{L_\square}{L_\mathrm{ref}} = 2.50$ $\quad$ $\frac{L_\square}{L_\mathrm{ref}} = 5.00$

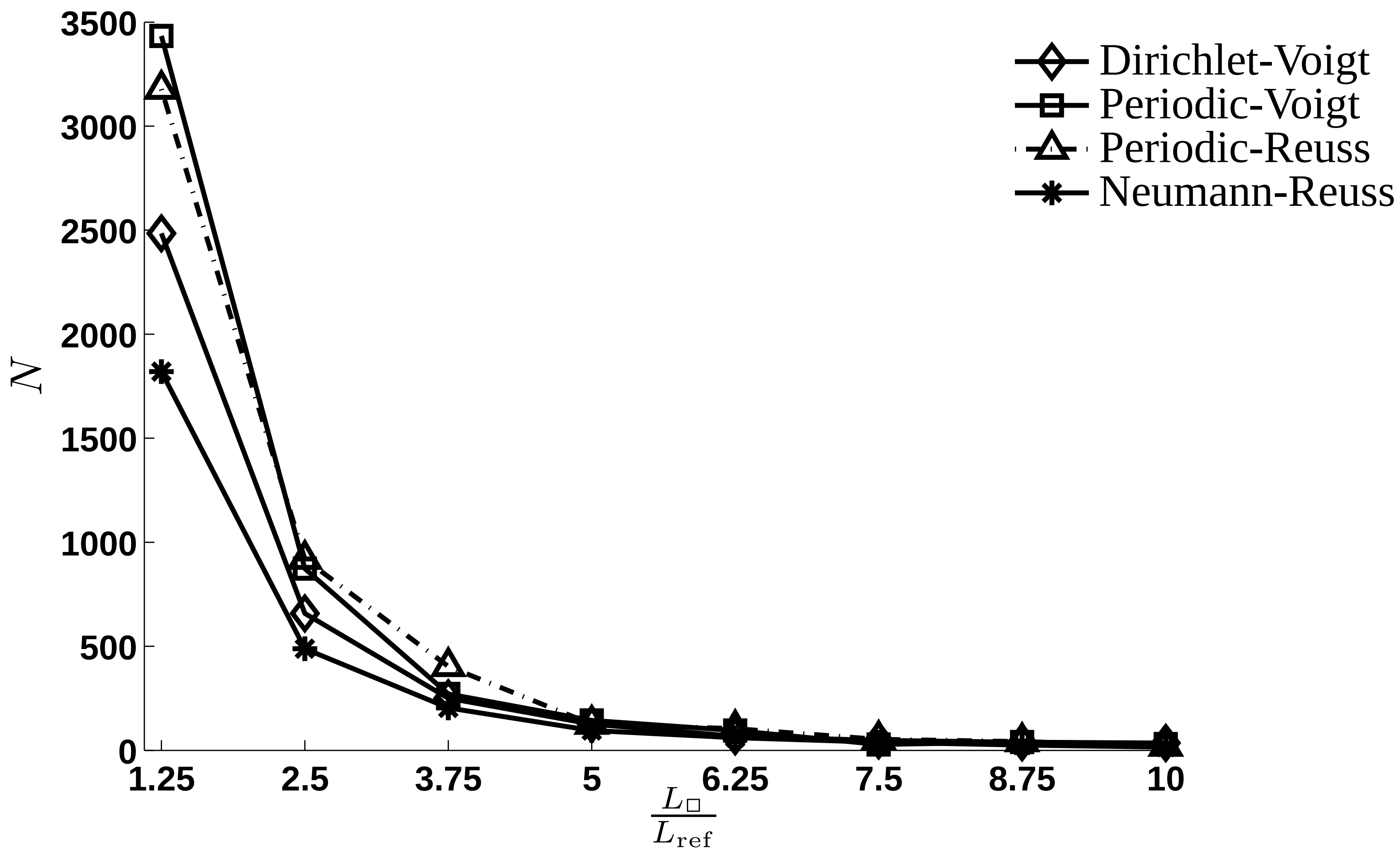
Computational results of bounds, cont'd

- Convergence of mean value of strain energy $\bar{\psi}_{\square}(\bar{\boldsymbol{H}}_A)$ with SVE-size. Uniaxial strain: $\bar{\boldsymbol{H}}_A = \boldsymbol{e}_1 \otimes \boldsymbol{e}_1$



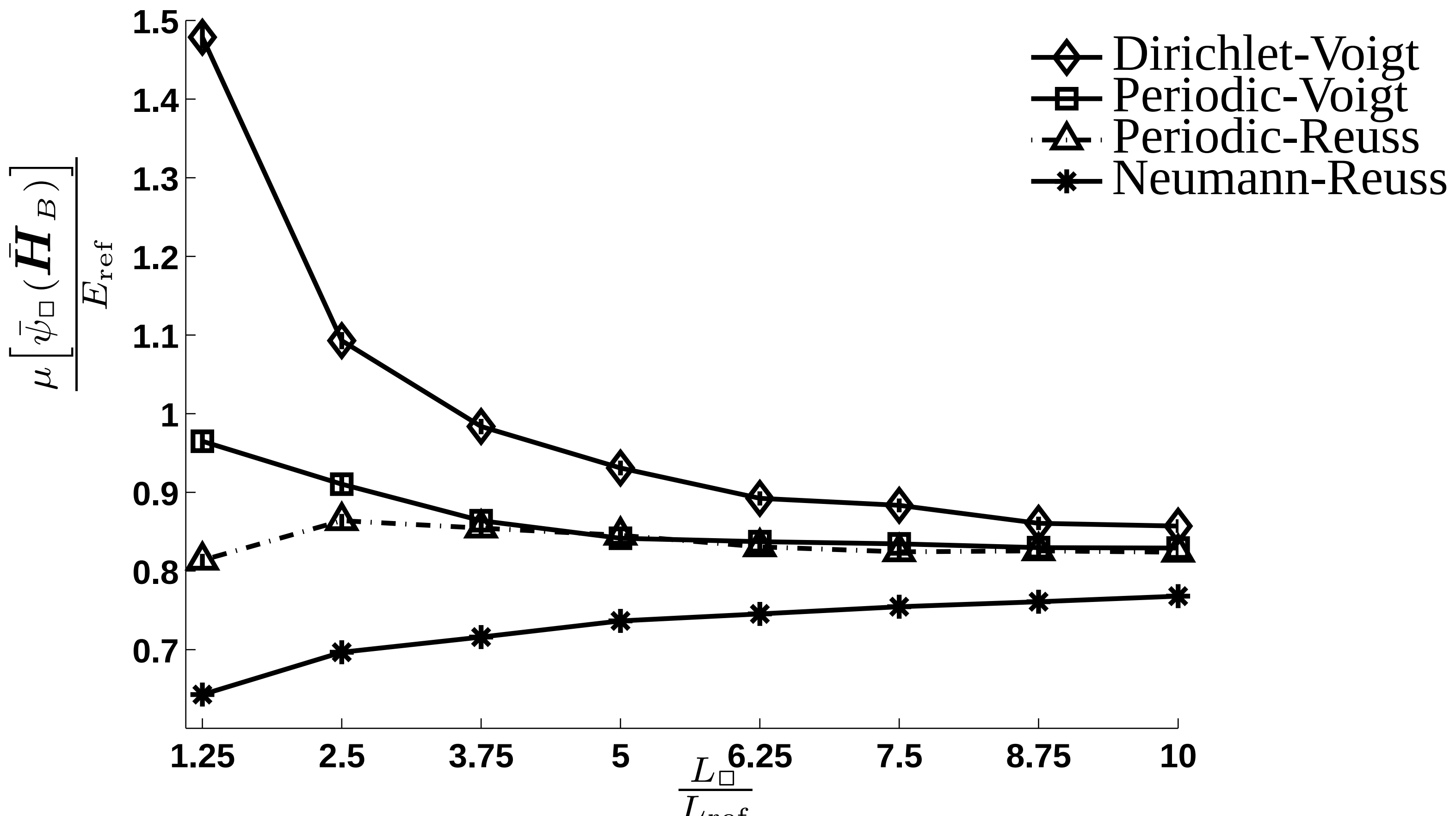
Computational results of bounds, cont'd

- Development of the number of realizations N, required to estimate $\bar{\psi}_{\square}(\bar{\boldsymbol{H}}_A)$ within a given confidence interval, with SVE-size



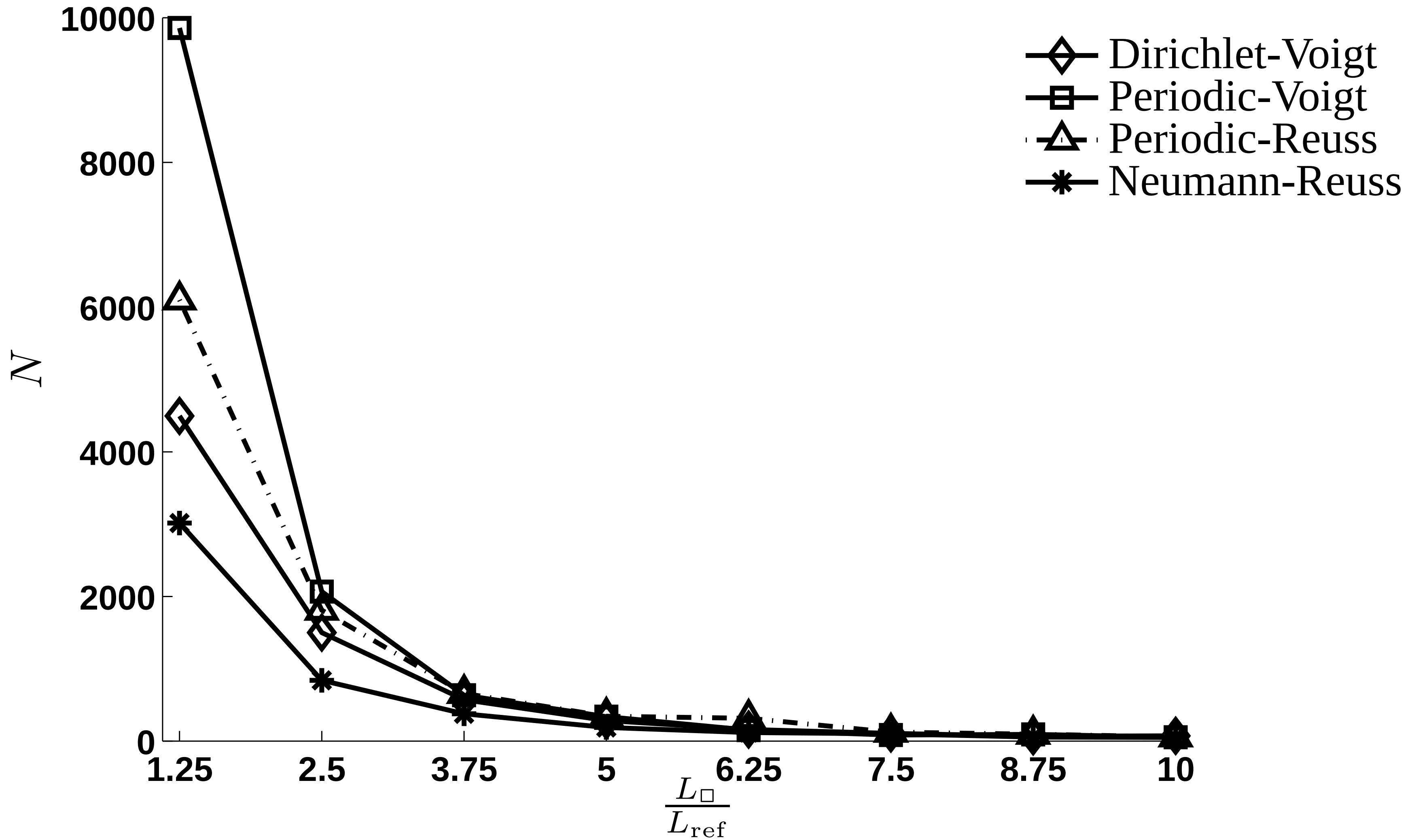
Computational results of bounds, cont'd

- Convergence of mean value of strain energy $\bar{\psi}_{\square}(\bar{\boldsymbol{H}}_B)$ with SVE-size. Pure shear: $\bar{\boldsymbol{H}}_B = \frac{1}{2}[\boldsymbol{e}_1 \otimes \boldsymbol{e}_2 + \boldsymbol{e}_2 \otimes \boldsymbol{e}_1]$. Since the results are scaled by the modulus of elasticity for the matrix material, E_{ref}, the ratio $\mu\left[\bar{\psi}_{\square}(\bar{\boldsymbol{H}}_B)\right]/E_{\text{ref}}$ may become smaller than unity



Computational results of bounds, cont'd

- Development of the number of realizations N, required to estimate $\bar{\psi}_{\square}(\bar{\boldsymbol{H}}_B)$ within a given confidence interval, with SVE-size



Computational homogenization – Introduction

- Aim: establish most general expression for $\bar{\mathsf{E}}_\square$ for given prolongation conditions
- Upscaling for linear problems: Need to establish
  - the strain concentration tensor $\mathsf{A}(\boldsymbol{X})$, $\boldsymbol{X} \in \Omega_\square$, in $\boldsymbol{H}(\boldsymbol{X}) = \mathsf{A}(\boldsymbol{X}) : \bar{\boldsymbol{H}}$ in terms of the macroscale and fluctuation fields,
  - the RVE-problem from which A can be computed,
  - $\bar{\mathsf{E}}_\square$ using the fields $\mathsf{E}(\boldsymbol{X})$ and $\mathsf{A}(\boldsymbol{X})$.
  - **Note**: For linear problems $\mathsf{A}(\boldsymbol{X})$ is independent of the actual $\bar{\boldsymbol{H}}$ $\Rightarrow$ $\bar{\mathsf{E}}_\square$ can be established once and for all (for a given realization SVE).

Effective stiffness for DBC

- SVE-problem (general): Find $\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D}}$ which, for given value of $\bar{\boldsymbol{H}}$, solves

$$\langle \boldsymbol{H} : \mathsf{E} : \delta \boldsymbol{H} \rangle_{\square} = 0 \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0}$$

- Additive split

$$\boldsymbol{u}(\boldsymbol{X}) = \boldsymbol{u}^{\mathrm{M}}(\boldsymbol{X}) + \boldsymbol{u}^{\mathrm{s}}(\boldsymbol{X}), \quad \boldsymbol{u}^{\mathrm{M}}(\boldsymbol{X}) = \bar{\boldsymbol{H}} \cdot [\boldsymbol{X} - \bar{\boldsymbol{X}}], \quad \boldsymbol{X} \in \Omega_{\square}$$

$$\rightsquigarrow \quad \langle \boldsymbol{H}^{\mathrm{s}} : \mathsf{E} : \delta \boldsymbol{H} \rangle_{\square} = -\langle \boldsymbol{H}^{\mathrm{M}} : \mathsf{E} : \delta \boldsymbol{H} \rangle_{\square} \quad \forall \delta \boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0}$$

Effective stiffness for DBC, cont'd

- Unit displacement fields

$$\boldsymbol{u}^{\mathrm{M}}(\boldsymbol{X}) = \bar{\boldsymbol{H}}\cdot[\boldsymbol{X}-\bar{\boldsymbol{X}}] = \sum_{i,j} \hat{\boldsymbol{u}}^{\mathrm{M}(ij)}(\boldsymbol{X})\bar{H}_{ij} \quad \Rightarrow \quad \hat{\boldsymbol{u}}^{\mathrm{M}(ij)} = \boldsymbol{e}_i \otimes \boldsymbol{e}_j \cdot[\boldsymbol{X}-\bar{\boldsymbol{X}}]$$

$$\rightsquigarrow \quad \boldsymbol{H}^{\mathrm{M}} = \boldsymbol{u}^{\mathrm{M}} \otimes \boldsymbol{\nabla} = \bar{\boldsymbol{H}} = \sum_{i,j} \hat{\boldsymbol{H}}^{\mathrm{M}(ij)} \bar{H}_{ij} \quad \Rightarrow \quad \hat{\boldsymbol{H}}^{\mathrm{M}(ij)} = \boldsymbol{e}_i \otimes \boldsymbol{e}_j$$

- *Ansatz* for fluctuation $\boldsymbol{u}^{\mathrm{s}}(\boldsymbol{X}) = \sum_{i,j} \hat{\boldsymbol{u}}^{\mathrm{s}(ij)}(\boldsymbol{X})\bar{H}_{ij}$

$$\rightsquigarrow \quad \boldsymbol{H}(\boldsymbol{X}) = \bar{\boldsymbol{H}} + \boldsymbol{H}^{\mathrm{s}}(\boldsymbol{X}) = [\mathbf{I} + \sum_{i,j} \hat{\boldsymbol{H}}^{\mathrm{s}(ij)}(\boldsymbol{X}) \otimes \hat{\boldsymbol{H}}^{\mathrm{M}(ij)}] : \bar{\boldsymbol{H}} = \mathbf{A}(\boldsymbol{X}) : \bar{\boldsymbol{H}}$$

SVE-problem must hold for any choice of $\bar{\boldsymbol{H}}$ $\rightsquigarrow$ Problem for unit fields: Find $\hat{\boldsymbol{u}}^{\mathrm{s}(ij)} \in \mathbb{U}_{\square}^{\mathrm{D},0}$ for $i, j = 1, 2, NDIM$ s. t.

$$\langle \hat{\boldsymbol{H}}^{\mathrm{s}(ij)} : \mathbf{E} : \delta\boldsymbol{H} \rangle_{\square} = -\langle \hat{\boldsymbol{H}}^{\mathrm{M}(ij)} : \mathbf{E} : \delta\boldsymbol{H} \rangle_{\square} = -\langle \boldsymbol{e}_i \otimes \boldsymbol{e}_j : \mathbf{E} : \delta\boldsymbol{H} \rangle_{\square} \quad \forall \delta\boldsymbol{u} \in \mathbb{U}_{\square}^{\mathrm{D},0}$$

Effective stiffness for DBC, cont'd

- Effective stiffness tensor

$$\bar{\boldsymbol{P}} = \langle \boldsymbol{P} \rangle_\square = \langle \mathsf{E} : \boldsymbol{H} \rangle_\square = \underbrace{\langle \mathsf{E} : \mathsf{A} \rangle_\square}_{=\bar{\mathsf{E}}_\square} : \bar{\boldsymbol{H}}$$

$$\begin{aligned} \bar{\mathsf{E}}_\square &= \langle \mathsf{E} : \mathsf{A} \rangle_\square \\ &= \bar{\mathsf{E}}_\square^{\mathrm{V}} + \sum_{i,j} \langle \mathsf{E} : \hat{\boldsymbol{H}}^{\mathrm{s}(ij)} \rangle_\square \otimes \boldsymbol{e}_i \otimes \boldsymbol{e}_j = \sum_{i,j} \langle \mathsf{E} : \hat{\boldsymbol{H}}^{(ij)} \rangle_\square \otimes \boldsymbol{e}_i \otimes \boldsymbol{e}_j \end{aligned}$$

- **Remarks**:
  - Major symmetry of $\bar{\mathsf{E}}_\square$ ensured by HM-condition
  - Taylor assumption: $\hat{\boldsymbol{H}}^{\mathrm{s}(ij)} = \boldsymbol{0}$ (fluctuation omitted) $\rightarrow$ No SVE-problem to be solved
  - Isotropic microconstituents does not ascertain isotropic macroscopic response for single (or even averaged) realizations