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Encounter of the Third Kind — Generalized continua and microstructures

On stress-gradient materials: formulation and homogenization

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Stress-gradient elasticity in a nutshell

The Stress Principle of Cauchy

$$\boldsymbol{\sigma} \cdot \nabla + \mathbf{b} = \mathbf{0} \quad \text{and} \quad [[\boldsymbol{\sigma}]] \cdot \mathbf{n} = \mathbf{0} \quad (\text{SA})$$

Cauchy elasticity

$$W^c[\boldsymbol{\sigma}] = \int w^c(\boldsymbol{\sigma}) \, dV$$

Stress-gradient elasticity

$$W^c[\boldsymbol{\sigma}] = \int w^c(\boldsymbol{\sigma}, \boldsymbol{\sigma} \otimes \nabla) \, dV$$

A mature model

Forest and Sab (2012), Mechanics Research Communications 40 (first derivation)

Sab, Legoll and Forest (2016), Journal of Elasticity 123(2) (mathematical justification)

Forest and Sab (2017), Mathematics and Mechanics of Solids (extension to finite strain)

Alternative model (not discussed here)

Polizzotto (2014, 2016), International Journal of Solids and Structures

In the present talk

A brief overview of the stress-gradient model

- ▶ Decomposition of the stress-gradient
- ▶ Stress boundary conditions

Homogenization of stress-gradient materials

- ▶ Hill–Mandel lemma, boundary conditions
- ▶ Softening size effect

Application to composites with spherical inclusions

- ▶ Eshelby's inhomogeneity problem
- ▶ Mori–Tanaka estimates of effective compliance

[Tran, Brisard, Guilleminot and Sab \(2018\)](#), International Journal of Solids and Structures

Some open questions

Derivation of the stress-gradient model for elasticity

Roadmap

Minimize complementary stress energy under SA constraint

- ▶ Cauchy elasticity: elastic equilibrium of fixed solid is retrieved
- ▶ Stress-gradient elasticity: elastic equilibrium of fixed solid is **defined**
- ▶ At this point, “fixed” not really meaningful, since dofs not (yet) defined
- ▶ “Trace” of the stress-gradient is prescribed

Decomposition of stress-gradient (1/2)

Complementary stress energy of stress-gradient materials

$$W^c[\boldsymbol{\sigma}] = \int w^c(\boldsymbol{\sigma}, \boldsymbol{\sigma} \otimes \nabla) dV$$

Classical equilibrium equation

$$(\boldsymbol{\sigma} \otimes \nabla) : \mathbf{I}_2 = \boldsymbol{\sigma} \cdot \nabla = -\mathbf{b}$$

Orthogonal decomposition of stress gradient

$$\boldsymbol{\sigma} \otimes \nabla = \mathbf{Q} + \mathbf{R} \quad \text{with} \quad \mathbf{R} : \mathbf{I}_2 = \mathbf{0} \quad \text{and} \quad \mathbf{Q} : \mathbf{R} = 0$$

$$\mathbf{R} = \mathbf{I}'_6 \cdot (\boldsymbol{\sigma} \otimes \nabla)$$

(projection onto space of trace-free, third-rank tensors)

Equivalent expression of complementary stress energy

$$W^c[\boldsymbol{\sigma}] = \int w^c(\boldsymbol{\sigma}, \mathbf{Q}, \mathbf{R}) dV$$

Decomposition of stress-gradient (2/2)

Orthogonal decomposition of stress gradient

$$\boldsymbol{\sigma} \otimes \nabla = \mathbf{Q} + \mathbf{R} \quad \text{with} \quad \mathbf{R} : \mathbf{I}_2 = \mathbf{0} \quad \text{and} \quad \mathbf{Q} \cdot \mathbf{R} = 0$$

\mathbf{Q} is in fact fully prescribed

$$\mathbf{Q} = -\frac{1}{2} \mathbf{I}_4 \cdot \mathbf{b}$$

(straightforward linear algebra)

No strain measure attached to \mathbf{Q} (generalized prestress)

Modeling assumption

$$W^c[\boldsymbol{\sigma}] = \int w^c(\boldsymbol{\sigma}, \cancel{\mathbf{Q}}, \mathbf{R}) dV = \int w^c(\boldsymbol{\sigma}, \mathbf{R}) dV$$

$$\text{with} \quad \mathbf{R} = \mathbf{I}'_6 \cdot (\boldsymbol{\sigma} \otimes \nabla)$$

Constrained minimization of energy

Initial problem

$$\text{Minimize: } W^c[\boldsymbol{\sigma}] = \int w^c(\boldsymbol{\sigma}, \mathbf{I}'_6 \text{::} (\boldsymbol{\sigma} \otimes \nabla)) dV$$

$$\text{subject to: } \boldsymbol{\sigma} \cdot \nabla + \mathbf{b} = \mathbf{0}$$

Stress-gradient as independent variable

$$\text{Minimize: } W^c[\boldsymbol{\sigma}, \mathbf{R}] = \int w^c(\boldsymbol{\sigma}, \mathbf{R}) dV$$

$$\text{subject to: } \begin{cases} \boldsymbol{\sigma} \cdot \nabla + \mathbf{b} = \mathbf{0} & \cdot \mathbf{u} \\ \mathbf{R} = \mathbf{I}'_6 \text{::} (\boldsymbol{\sigma} \otimes \nabla) & \text{::} \boldsymbol{\Phi} \end{cases}$$

Lagrange
multipliers



Elastic equilibrium of fixed, SG bodies

Field equations

$$\boldsymbol{\sigma} \cdot \nabla + \mathbf{b} = \mathbf{0}$$

$$\mathbf{R} = \mathbf{I}'_6 \therefore (\boldsymbol{\sigma} \otimes \nabla)$$

Generalized equilibrium equations

$$\mathbf{e} = \partial_{\boldsymbol{\sigma}} W^c$$

$$\boldsymbol{\Phi} = \partial_{\mathbf{R}} W^c$$

Generalized stress-strain relations

$$\mathbf{e} = \boldsymbol{\Phi} \cdot \nabla + \boldsymbol{\varepsilon}[\mathbf{u}]$$

Generalized strain-displacement relations

Boundary conditions

$$\boldsymbol{\Phi} \cdot \mathbf{n} + \text{sym}(\mathbf{u} \otimes \mathbf{n}) = \mathbf{0}$$

6 scalar boundary conditions

Continuity conditions

$$\llbracket \boldsymbol{\Phi} \cdot \mathbf{n} + \text{sym}(\mathbf{u} \otimes \mathbf{n}) \rrbracket = \mathbf{0}$$

Weaker continuity of “displacements”

$$\llbracket \boldsymbol{\sigma} \rrbracket = \mathbf{0}$$

Stronger continuity of “stresses”

Linear elasticity

Complementary stress energy density

$$w^c(\boldsymbol{\sigma}, \mathbf{R}) = \frac{1}{2} \boldsymbol{\sigma} : \mathbf{S} : \boldsymbol{\sigma} + \frac{1}{2} \mathbf{R} :: \mathbf{M} :: \mathbf{R}$$

No $\boldsymbol{\sigma}$ – \mathbf{R} coupling for centrosymmetric materials!

\mathbf{S} and \mathbf{M} have major and minor symmetries

Generalized compliance \mathbf{M} operates on trace-free tensors

$$\mathbf{M} = \mathbf{I}'_6 :: \mathbf{M} :: \mathbf{I}'_6$$

Stress-strain relationships

$$\mathbf{e} = \mathbf{S} :: \boldsymbol{\sigma} \quad \text{and} \quad \boldsymbol{\Phi} = \mathbf{M} :: \mathbf{R}$$

or

$$\mathbf{C} = \mathbf{S}^{-1} \quad \text{and} \quad \mathbf{L} = \mathbf{M}^+$$

$$\boldsymbol{\sigma} = \mathbf{C} :: \mathbf{e} \quad \text{and} \quad \mathbf{R} = \mathbf{L} :: \boldsymbol{\Phi}$$

Isotropic linear elasticity

General isotropic linear stress-gradient elasticity

$$\mathbf{M} = \mathbf{I}'_6 \cdot \mathbf{M} \cdot \mathbf{I}'_6$$

$$2\mu\mathbf{M} = \ell_J^2 \mathbf{J}_6 + \ell_K^2 \mathbf{K}_6 + \ell_H^2 \mathbf{H}_6$$

$$\mathbf{I}'_6 = \mathbf{J}_6 + \mathbf{K}_6$$

\cdot	\mathbf{J}_6	\mathbf{K}_6	\mathbf{H}_6
\mathbf{J}_6	\mathbf{J}_6	$\mathbf{0}$	$\mathbf{0}$
\mathbf{K}_6	$\mathbf{0}$	\mathbf{K}_6	\mathbf{H}_6
\mathbf{H}_6	$\mathbf{0}$	\mathbf{H}_6	\mathbf{H}_6

Simplified model for isotropic linear stress-gradient elasticity

$$2\mu\mathbf{S} = \frac{1-2\nu}{1+\nu} \mathbf{J}_4 + \mathbf{K}_4$$

$$\frac{2\mu}{\ell^2} \mathbf{M} = \frac{1-2\nu}{1+\nu} \mathbf{J}_6 + \mathbf{K}_6$$

[Altan and Aifantis \(1992\)](#), Scripta Metallurgica et Materialia 26(2)

[Altan and Aifantis \(1997\)](#), Journal of the Mechanical behavior of Materials 8(3)

[Gao and Park \(2007\)](#), International Journal of Solids and Structures 44

Homogenization

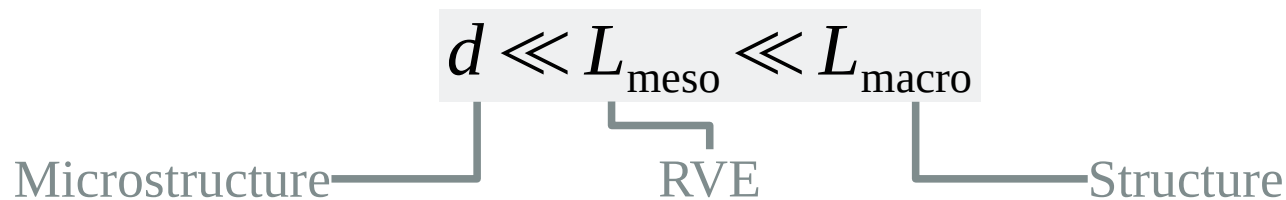
Setting the stage for homogenization

The 3 cases

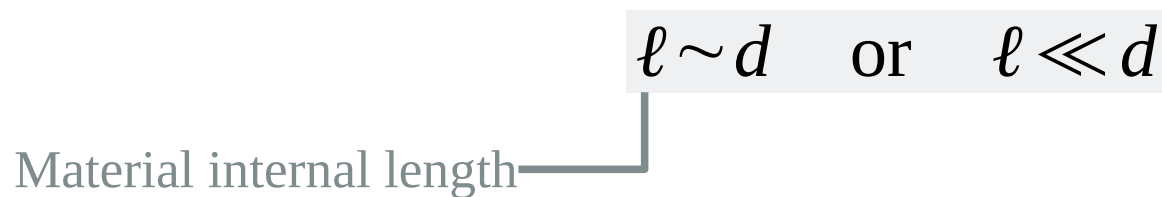
- ▶ Stress-gradient (micro) → stress-gradient (macro)
- ▶ Cauchy (micro) → stress-gradient (macro)
- ▶ **Stress-gradient (micro) → Cauchy (macro)**

Separation of scales

- ▶ Classical condition



- ▶ Additional condition for stress-/strain- gradient materials



Effective and apparent properties

Effective behaviour: stress-gradient \rightarrow Cauchy $(\ell \sim d)$

$$\langle \mathbf{e} \rangle = \mathbf{S}^{\text{eff}} : \langle \boldsymbol{\sigma} \rangle$$

Apparent elastic properties of (large) SVE Ω

$$\langle \boldsymbol{\sigma} \rangle = \frac{1}{V} \int_{\Omega} \boldsymbol{\sigma} \, dV$$

$$\langle \mathbf{e} \rangle = \mathbf{S}^{\text{app}}(\Omega) : \langle \boldsymbol{\sigma} \rangle$$

$$\langle \mathbf{e} \rangle = \frac{1}{V} \int_{\Omega} \mathbf{e} \, dV = \frac{1}{V} \int_{\Omega} \boldsymbol{\varepsilon}[\mathbf{u}] \, dV + \frac{1}{V} \int_{\partial\Omega} \boldsymbol{\Phi} \cdot \mathbf{n} \, dS$$

Local problem on SVE Ω

$$\boldsymbol{\sigma} \cdot \nabla = \mathbf{0}$$

No body forces!

$$\mathbf{e} = \mathbf{S} : \boldsymbol{\sigma}$$

$$\boldsymbol{\Phi} = \mathbf{M} : (\boldsymbol{\sigma} \otimes \nabla)$$

+ boundary conditions!

$$\mathbf{e} = \boldsymbol{\Phi} \cdot \nabla + \boldsymbol{\varepsilon}[\mathbf{u}]$$

Boundary conditions

Generalized Hill–Mandel lemma

$$\langle \boldsymbol{\sigma}^* : \mathbf{e} + (\boldsymbol{\sigma}^* \otimes \nabla) :: \boldsymbol{\Phi} \rangle = \langle \boldsymbol{\sigma}^* \rangle : \langle \mathbf{e} \rangle$$

Uniform stress boundary conditions

$$\boldsymbol{\sigma} |_{\partial\Omega} = \bar{\boldsymbol{\sigma}}$$

$$\langle \mathbf{e} \rangle = \mathbf{S}^\sigma(\Omega) : \langle \boldsymbol{\sigma} \rangle = \mathbf{S}^\sigma(\Omega) : \bar{\boldsymbol{\sigma}}$$

Uniform strain boundary conditions

$$\boldsymbol{\Phi} \cdot \mathbf{n} + \mathbf{sym}(u \otimes \mathbf{n}) = \mathbf{sym}[(\bar{\mathbf{e}} \cdot \mathbf{x}) \otimes \mathbf{n}]$$

$$\langle \boldsymbol{\sigma} \rangle = \mathbf{C}^\varepsilon(\Omega) : \langle \mathbf{e} \rangle = \mathbf{C}^\varepsilon(\Omega) : \bar{\mathbf{e}}$$

Uniform traction boundary conditions

$$\boldsymbol{\sigma} |_{\partial\Omega} \cdot \mathbf{n} = \bar{\boldsymbol{\sigma}} \cdot \mathbf{n}$$

$$\langle \mathbf{e} \rangle = \mathbf{S}^T(\Omega) : \langle \boldsymbol{\sigma} \rangle = \mathbf{S}^T(\Omega) : \bar{\boldsymbol{\sigma}}$$

$$\mathbf{a} \cdot [\boldsymbol{\Phi} \cdot \mathbf{n} + \mathbf{sym}(u \otimes \mathbf{n})] \cdot \mathbf{a} = 0$$

$$\mathbf{a} = \mathbf{I}_2 - \mathbf{n} \otimes \mathbf{n}$$

Variational formulation

Minimum of complementary stress energy

$$\bar{\boldsymbol{\sigma}} : \mathbf{S}^\sigma(\Omega) : \bar{\boldsymbol{\sigma}} = \inf \left\{ \langle \boldsymbol{\sigma} : \mathbf{S} : \boldsymbol{\sigma} + (\boldsymbol{\sigma} \otimes \nabla) : \mathbf{M} : (\boldsymbol{\sigma} \otimes \nabla) \rangle \right\}$$

$$\text{subject to: } \boldsymbol{\sigma} \cdot \nabla = \mathbf{0} \quad \text{and} \quad \boldsymbol{\sigma}|_{\partial\Omega} = \bar{\boldsymbol{\sigma}}$$

Minimum of strain energy

$$\bar{\mathbf{e}} : \mathbf{C}^\varepsilon(\Omega) : \bar{\mathbf{e}} = \inf \left\{ \langle \boldsymbol{\varepsilon}[\mathbf{u}] : \mathbf{C} : \boldsymbol{\varepsilon}[\mathbf{u}] + \boldsymbol{\Phi} : \mathbf{L} : \boldsymbol{\Phi} \rangle \right\}$$

$$\text{subject to: } \boldsymbol{\Phi} \cdot \mathbf{n} + \text{sym}(\mathbf{u} \otimes \mathbf{n}) = \text{sym}[(\bar{\mathbf{e}} \cdot \mathbf{x}) \otimes \mathbf{n}]$$

Bounds for finite-size SVEs

$$\mathbf{C}^\sigma(\Omega_I) \leq \mathbf{C}^\sigma(\Omega_{II}) \leq \mathbf{C}^{\text{eff}} \leq \mathbf{C}^\varepsilon(\Omega_{II}) \leq \mathbf{C}^\varepsilon(\Omega_I) \quad \text{for } \Omega_I \subset \Omega_{II}$$

Softening size-effect

Variational definition of apparent compliance (uniform σ BC)

If $\mathbf{S}_I \leq \mathbf{S}_{II}$ and $\mathbf{M}_I \leq \mathbf{M}_{II}$ everywhere in Ω , then $\mathbf{S}_I^{\text{eff}} \leq \mathbf{S}_{II}^{\text{eff}}$

Fixed microstructure, variable material internal length

For $\mathbf{S}_I = \mathbf{S}_{II}$ and $\mathbf{M}_I = \frac{\ell_I^2}{\ell_{II}^2} \mathbf{M}_{II}$: if $\ell_I \leq \ell_{II}$ then $\mathbf{S}_I^{\text{eff}} \leq \mathbf{S}_{II}^{\text{eff}}$

More generally: if $\left(\frac{\ell}{d}\right)_I \leq \left(\frac{\ell}{d}\right)_{II}$ then $\mathbf{S}_I^{\text{eff}} \leq \mathbf{S}_{II}^{\text{eff}}$

Scaled microstructure, constant material internal length

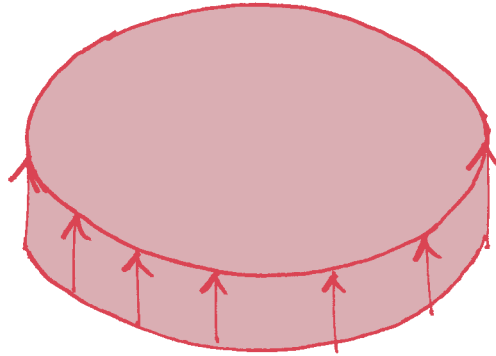
If $d_I \leq d_{II}$ then $\mathbf{C}_I^{\text{eff}} \leq \mathbf{C}_{II}^{\text{eff}}$

Softening size-effect!

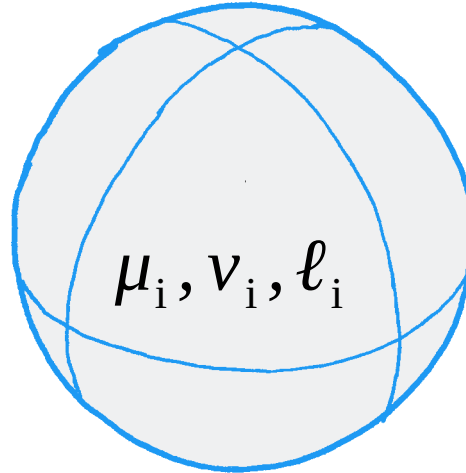
**Eshelby's inhomogeneity
problem for stress-gradient elasticity**

Problem setting

$$\sigma^\infty \mathbf{e}_z$$



Matrix: μ_m, ν_m, ℓ_m

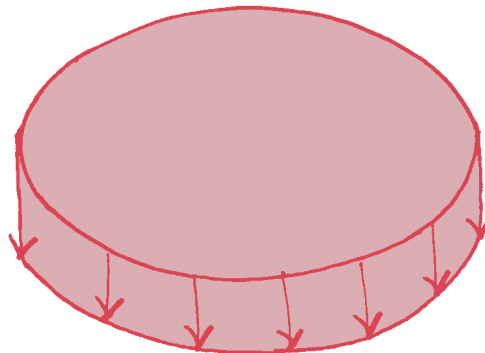


$$\mu_i, \nu_i, \ell_i$$

$$\nu_i = \nu_m = 0.25$$

$$\mu_i = 10 \mu_m$$

$$-\sigma^\infty \mathbf{e}_z$$



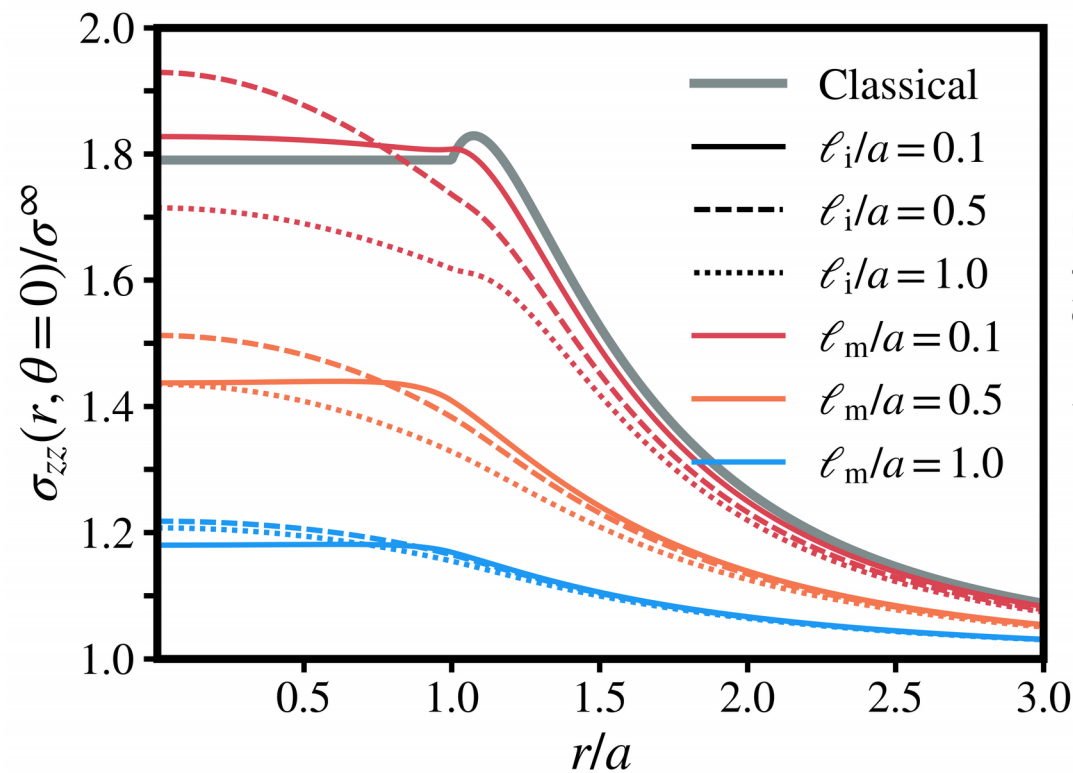


Some tedious calcs later...

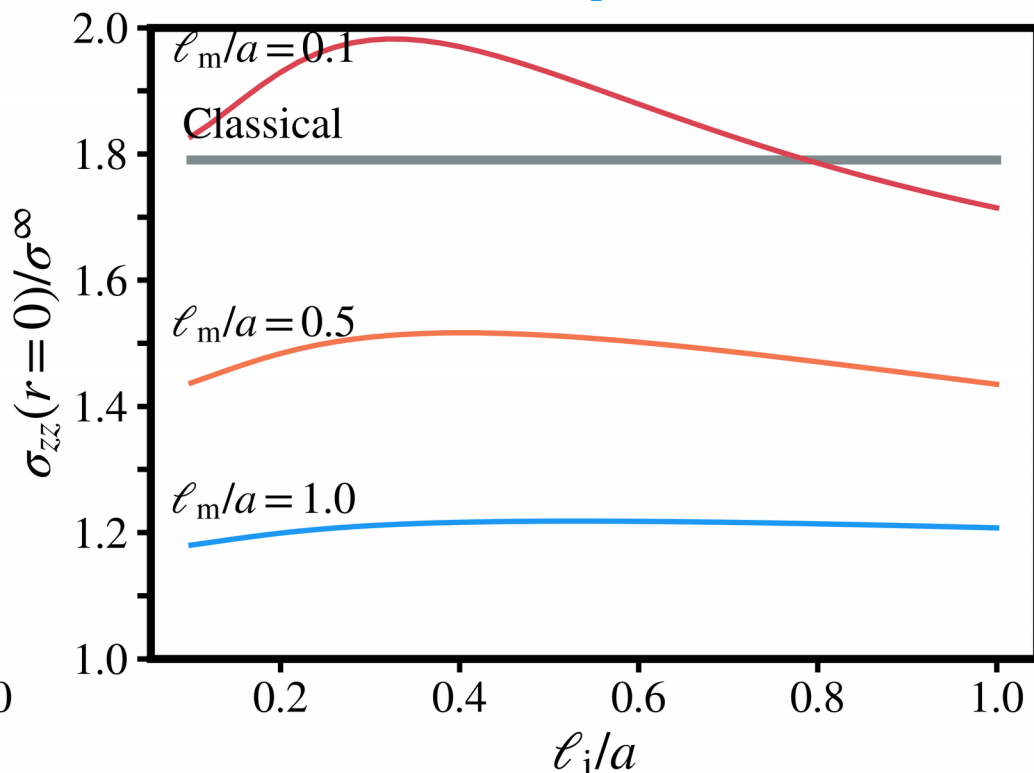


<http://www.sympy.org>

Hat tip to VP Tran!



Axial stress along vertical axis

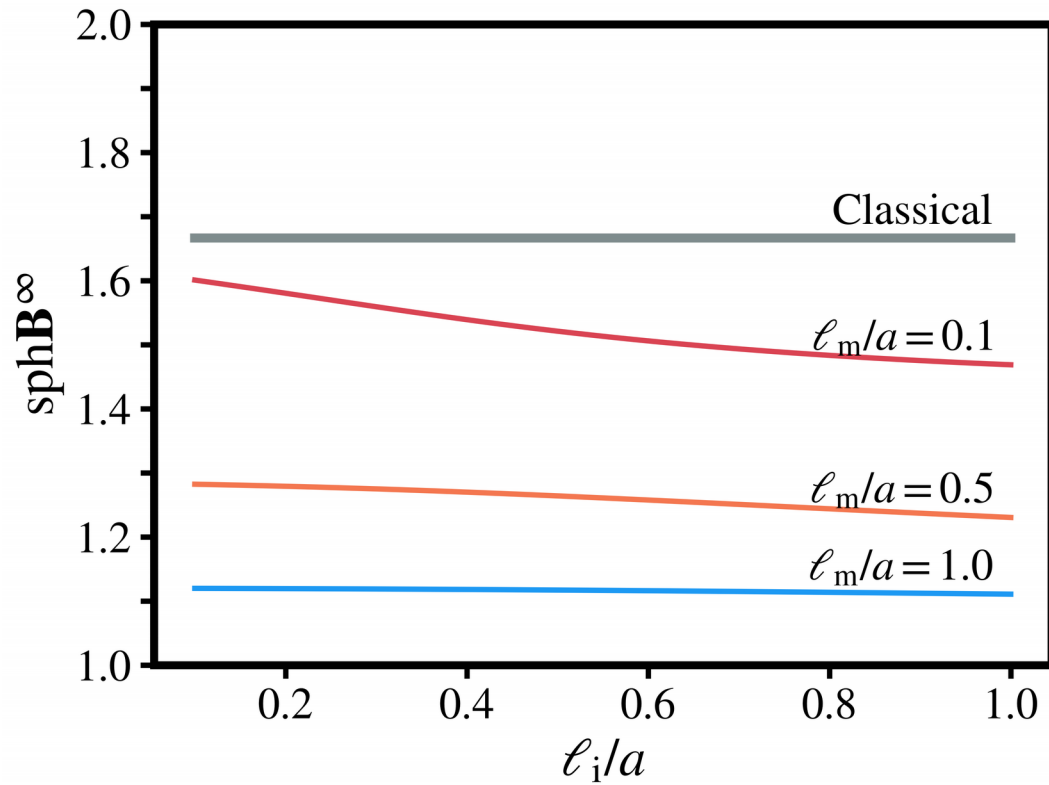


Axial stress at origin

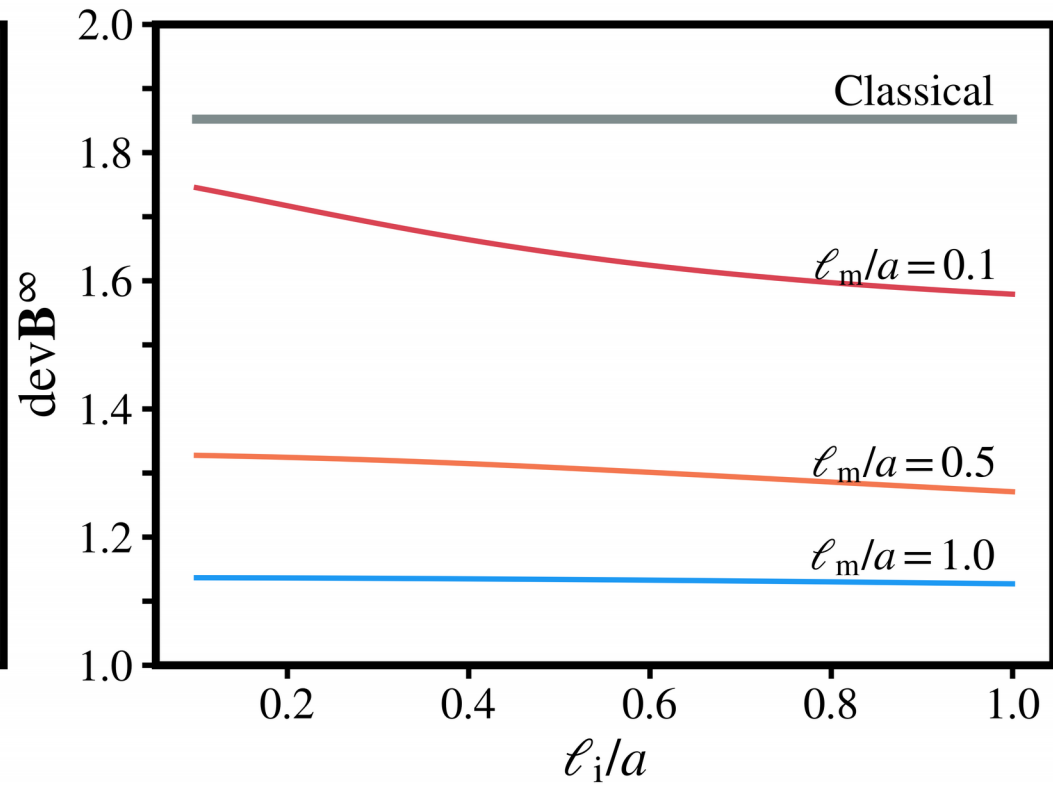
Theorem of Eshelby (1957) does **not** hold!

Eshelby (1957). Proc. Royal Soc. A 241(1226)

Dilute stress concentration tensor



Axial stress along vertical axis

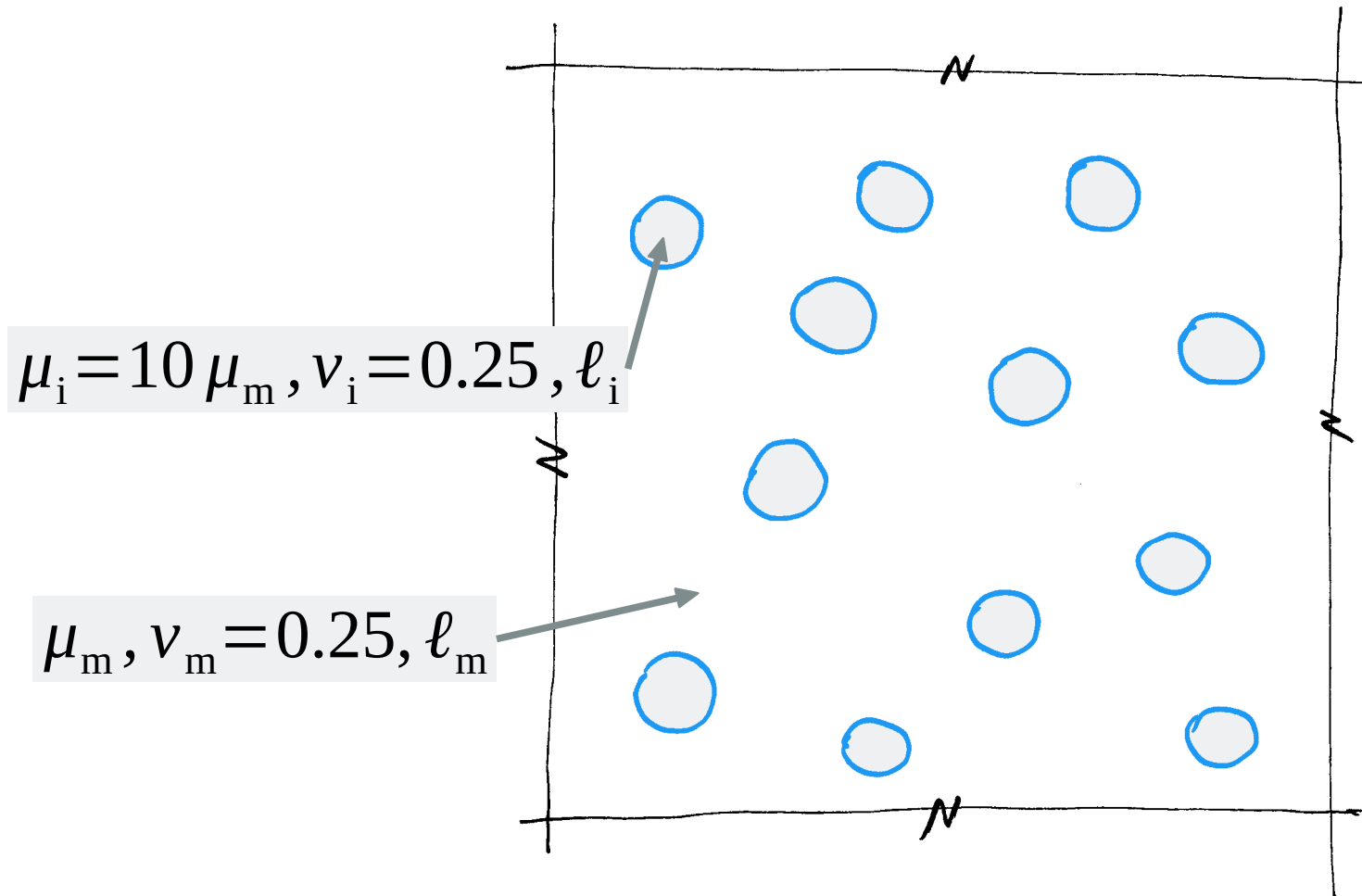


Axial stress at origin

$$\langle \boldsymbol{\sigma} \rangle_i = \frac{1}{V_i} \int_{\Omega_i} \boldsymbol{\sigma} dV = \mathbf{B}^\infty : \boldsymbol{\sigma}^\infty$$

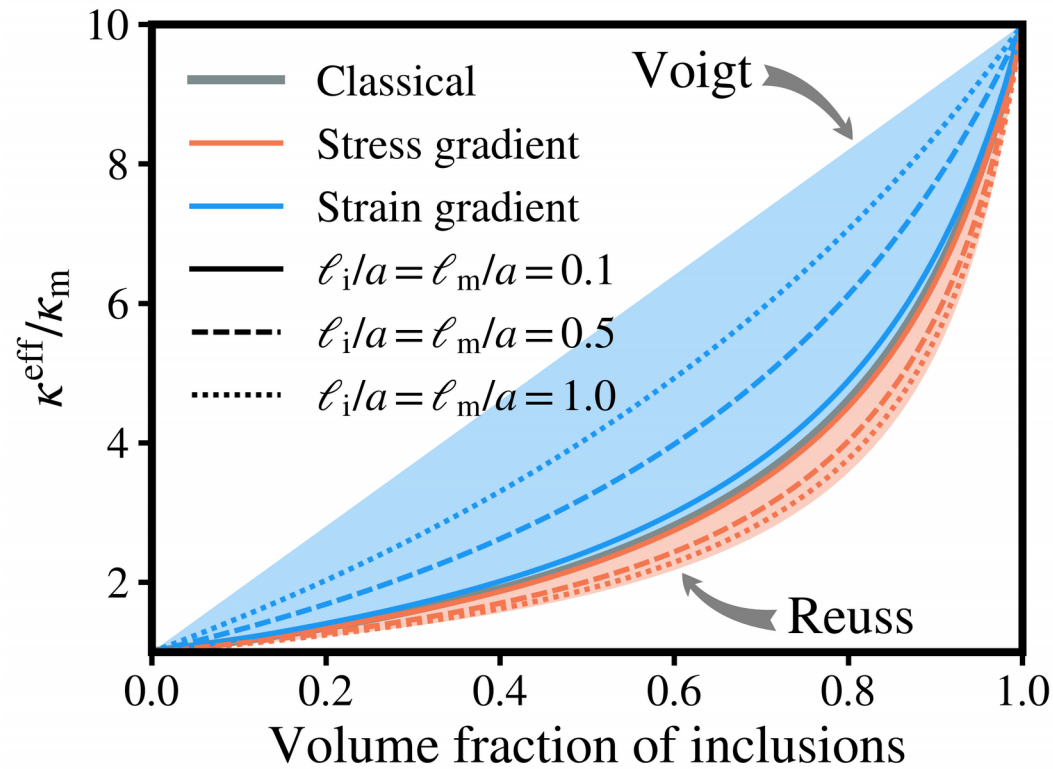
**Mori–Tanaka estimates
for composites
with spherical inclusions**

Problem setting

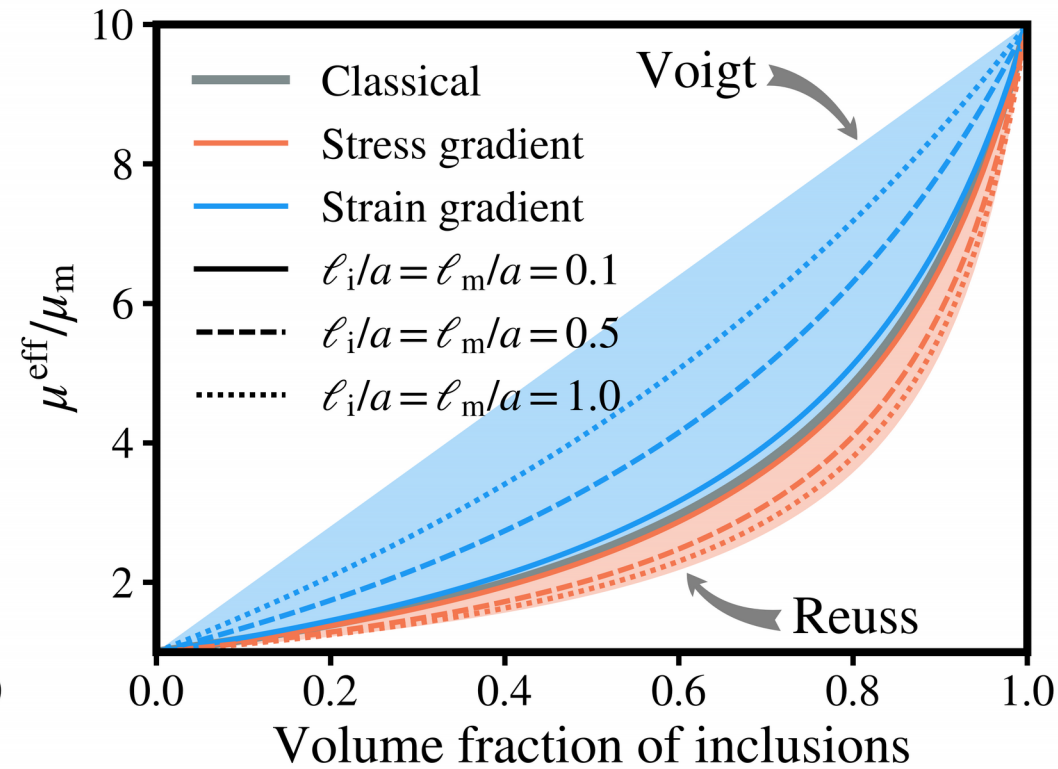


Volume fraction of inclusions: f

Estimates of bulk and shear moduli



Effective bulk modulus



Effective shear modulus

$$\mathbf{S}_{\text{eff}} = \mathbf{S}_m + f (\mathbf{S}_i - \mathbf{S}_m) : \mathbf{B}^\infty : [(1-f) \mathbf{I}_4 + f \mathbf{B}^\infty]^{-1}$$

Strain- and stress- gradient models are not equivalent!

Benveniste (1987), Mechanics of Materials 6(2)

Ma and Gao (2014), Acta Mechanica 225(4-5)

Some questions

The total complementary energy

Assumption 1: Stress Principle of Cauchy

$$\boldsymbol{\sigma} \cdot \nabla = \mathbf{0} \quad \text{and} \quad \boldsymbol{\sigma} \cdot \mathbf{n}|_{\partial\Omega} = \bar{\mathbf{T}}$$

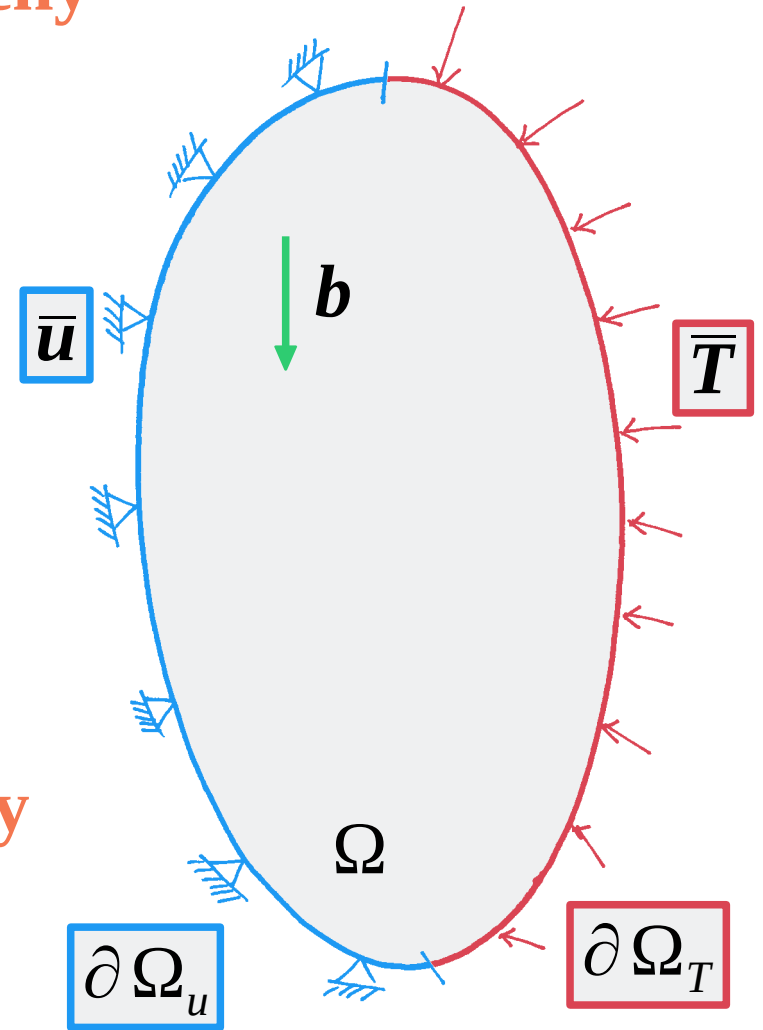
Assumption 2: complementary work of prescribed displacements

$$V^c = \int_{\partial\Omega_u} \bar{\mathbf{u}} \cdot \boldsymbol{\sigma} \cdot \mathbf{n} \, dS$$

Minimization of complementary energy

$$\text{Minimize: } \Pi^c = W^c - V^c$$

$$\text{subject to: } \boldsymbol{\sigma} \cdot \nabla = \mathbf{0} \quad \text{and} \quad \boldsymbol{\sigma} \cdot \mathbf{n}|_{\partial\Omega} = \bar{\mathbf{T}}$$



The general BVP

Field equations

$$\boldsymbol{\sigma} \cdot \nabla + \mathbf{b} = \mathbf{0}$$

$$\mathbf{R} = \mathbf{I}'_6 \therefore (\boldsymbol{\sigma} \otimes \nabla)$$

$$\mathbf{e} = \partial_{\boldsymbol{\sigma}} W^c$$

$$\boldsymbol{\Phi} = \partial_{\mathbf{R}} W^c$$

$$\mathbf{e} = \boldsymbol{\Phi} \cdot \nabla + \boldsymbol{\varepsilon}[\mathbf{u}]$$

Boundary conditions

$$\partial \Omega_T : \begin{cases} \boldsymbol{\sigma} \cdot \mathbf{n}|_{\partial \Omega} = \bar{\mathbf{T}} \\ \mathbf{a} \cdot [\boldsymbol{\Phi} \cdot \mathbf{n} + \mathbf{sym}(\mathbf{u} \otimes \mathbf{n})] \cdot \mathbf{a} = 0 \end{cases}$$

$$\mathbf{a} = \mathbf{I}_2 - \mathbf{n} \otimes \mathbf{n}$$

$$\partial \Omega_u : \boldsymbol{\Phi} \cdot \mathbf{n} + \mathbf{sym}(\mathbf{u} \otimes \mathbf{n}) = \mathbf{sym}(\bar{\mathbf{u}} \otimes \mathbf{n})$$

Continuity conditions

$$[[\boldsymbol{\sigma}]] = \mathbf{0}$$

$$[[\boldsymbol{\Phi} \cdot \mathbf{n} + \mathbf{sym}(\mathbf{u} \otimes \mathbf{n})]] = \mathbf{0}$$

The total potential energy

Potential strain energy

$$W = \int_{\Omega} w(\mathbf{e}, \boldsymbol{\Phi}) dV$$

Work of prescribed body forces and tractions

$$V = \int_{\Omega} \mathbf{b} \cdot \mathbf{u} dV + \int_{\partial\Omega_T} \bar{\mathbf{T}} \cdot [\mathbf{u} + 2\boldsymbol{\Phi} : \mathbf{n} \otimes \mathbf{n} - (\boldsymbol{\Phi} : \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n}) \mathbf{n}] dS$$

Minimization of total potential energy

Minimize: $\Pi = W - V$

$$\mathbf{u} + 2\boldsymbol{\Phi} : \mathbf{n} \otimes \mathbf{n} - (\boldsymbol{\Phi} : \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n}) \mathbf{n} = \bar{\mathbf{u}}$$

subject to:
$$\begin{cases} \partial\Omega_T: \mathbf{a} \cdot [\boldsymbol{\Phi} \cdot \mathbf{n} + \mathbf{sym}(\mathbf{u} \otimes \mathbf{n})] \cdot \mathbf{a} = 0 \\ \partial\Omega_u: \boldsymbol{\Phi} \cdot \mathbf{n} + \mathbf{sym}(\mathbf{u} \otimes \mathbf{n}) = \mathbf{sym}(\bar{\mathbf{u}} \otimes \mathbf{n}) \end{cases}$$

Conclusion & perspectives

Summary

- ▶ Simplified model for isotropic linear elasticity
- ▶ General framework for stress-gradient → Cauchy homogenization
- ▶ Softening size-effect
- ▶ Mori–Tanaka estimates for spherical inclusions

Outlook

- ▶ Hashin–Shtrikman (size-dependent) bounds on effective properties
- ▶ Cauchy → stress-gradient homogenization
- ▶ Understand the meaning of \mathbf{u} (use above)

Thanks for your attention!

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<http://sbrisard.github.io>



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