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Encounter of the Third Kind — Generalized continua and microstructures

# On stress-gradient materials: formulation and homogenization

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LABEX MMCD

4 April 2018

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# Stress-gradient elasticity in a nutshell

## The Stress Principle of Cauchy

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

## 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

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

**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 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

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

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

## Stress-gradient as independent variable

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

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

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

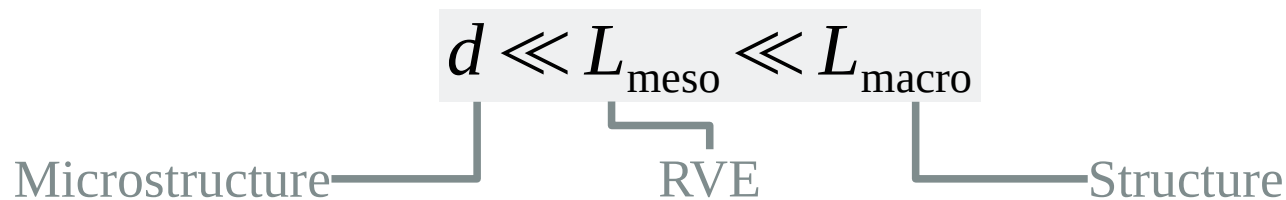
# Setting the stage for homogenization

## 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  $\Omega$

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

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

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

Local problem on SVE  $\Omega$

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

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 $\sigma$ BC)

If  $\mathbf{S}_I \leq \mathbf{S}_{II}$  and  $\mathbf{M}_I \leq \mathbf{M}_{II}$  everywhere in  $\Omega$ , 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

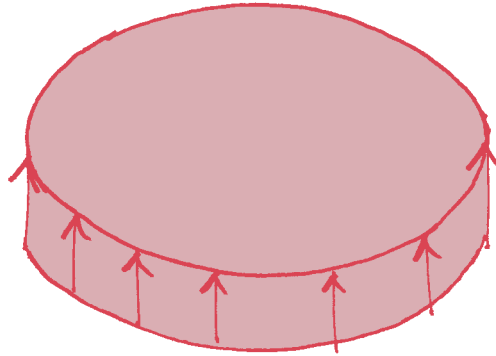
If  $d_I \leq d_{II}$  then  $\mathbf{C}_I^{\text{eff}} \leq \mathbf{C}_{II}^{\text{eff}}$

**Softening size-effect!**

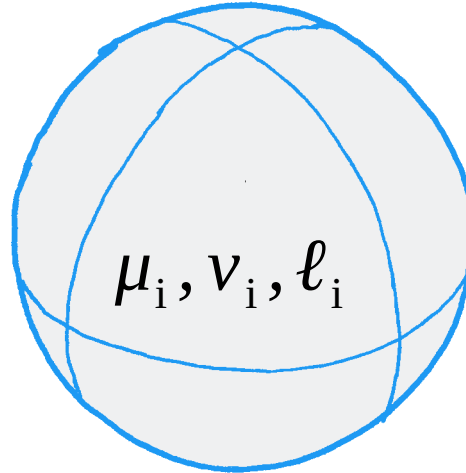
**Eshelby's inhomogeneity  
problem for stress-gradient elasticity**

# Problem setting

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



Matrix:  $\mu_m, \nu_m, \ell_m$

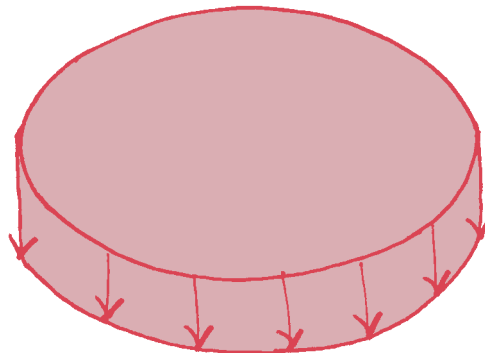


$$\mu_i, \nu_i, \ell_i$$

$$\nu_i = \nu_m = 0.25$$

$$\mu_i = 10 \mu_m$$

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



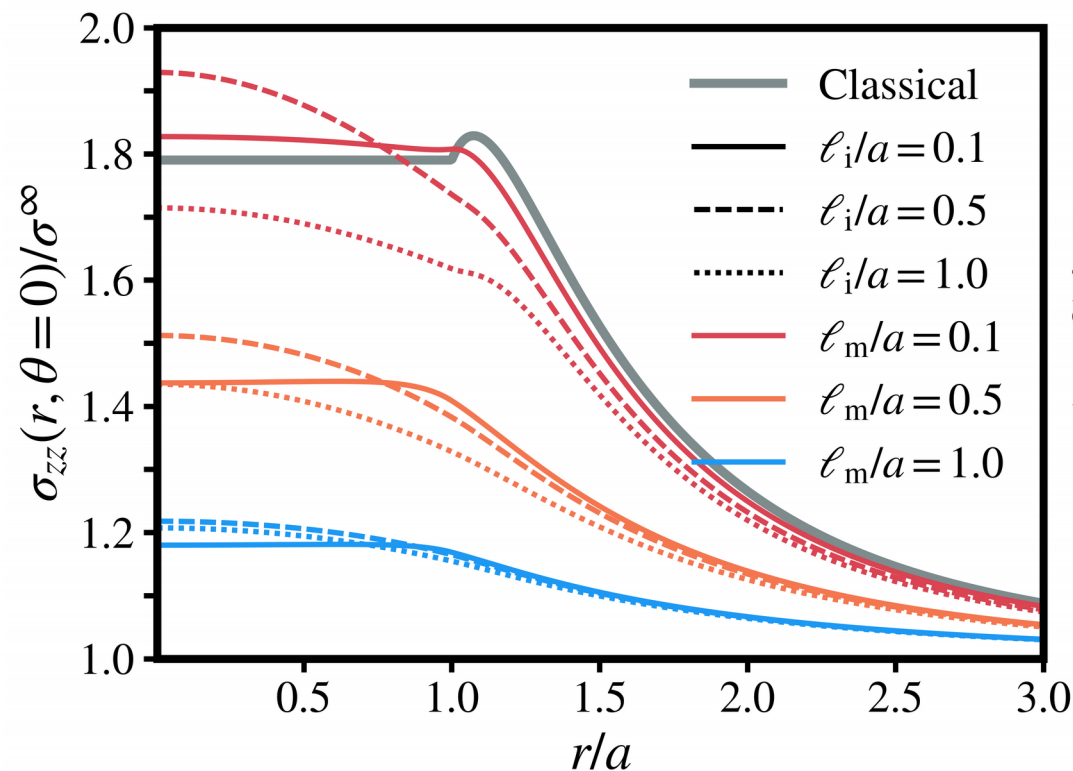


# Some tedious calcs later...

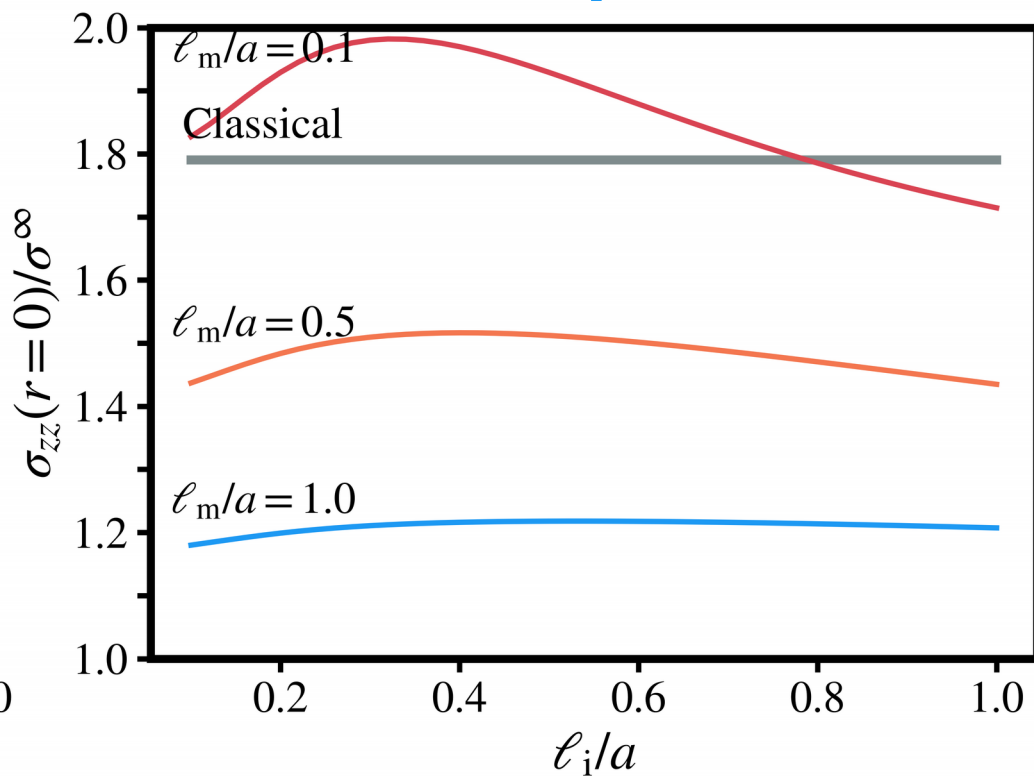


<http://www.sympy.org>

Hat tip to VP Tran!



Axial stress along vertical axis

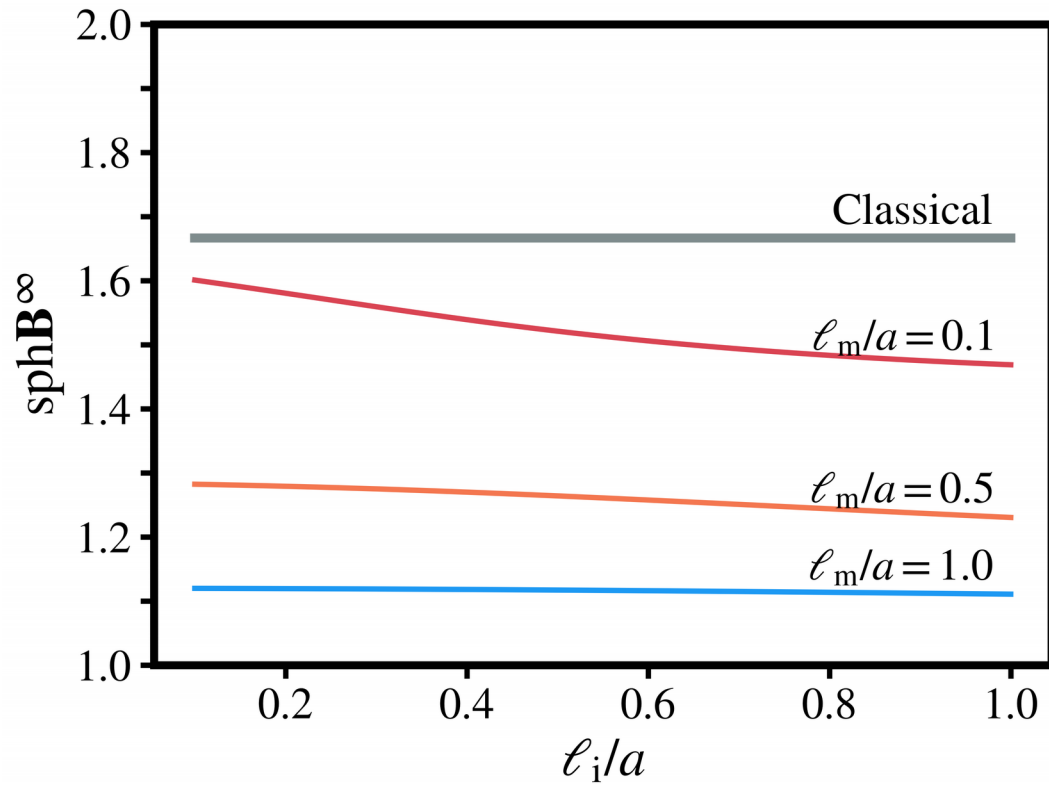


Axial stress at origin

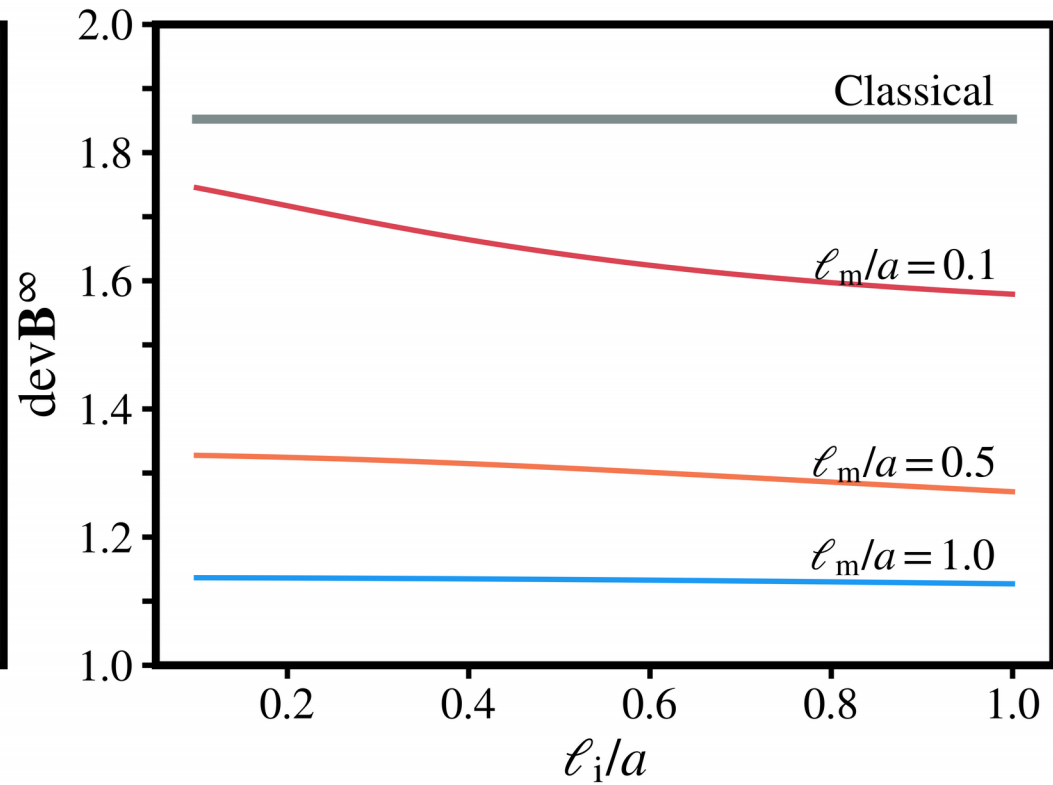
## Theorem of Eshelby (1957) does **not** hold!

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

# Dilute stress concentration tensor



Axial stress along vertical axis

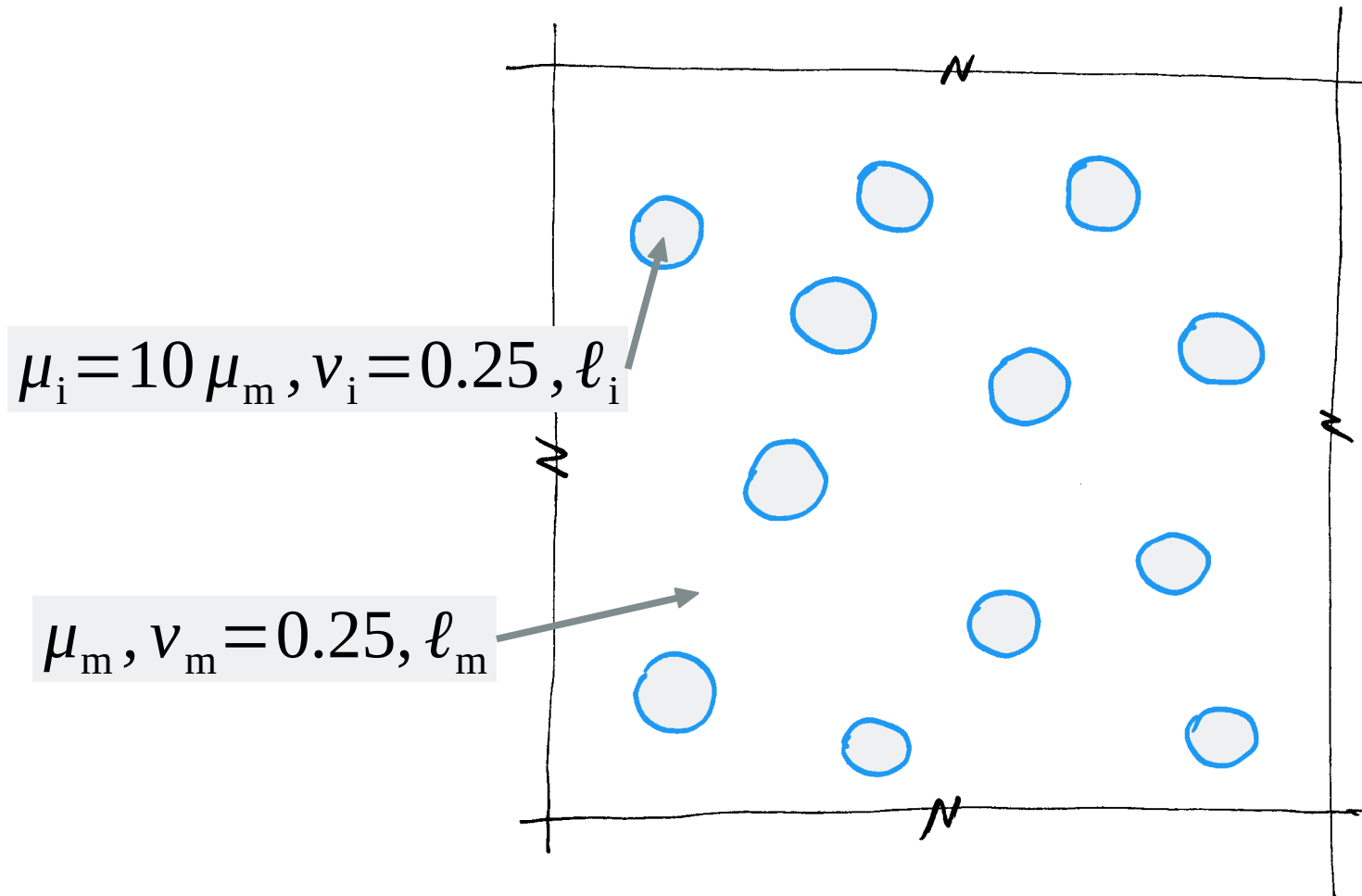


Axial stress at origin

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

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

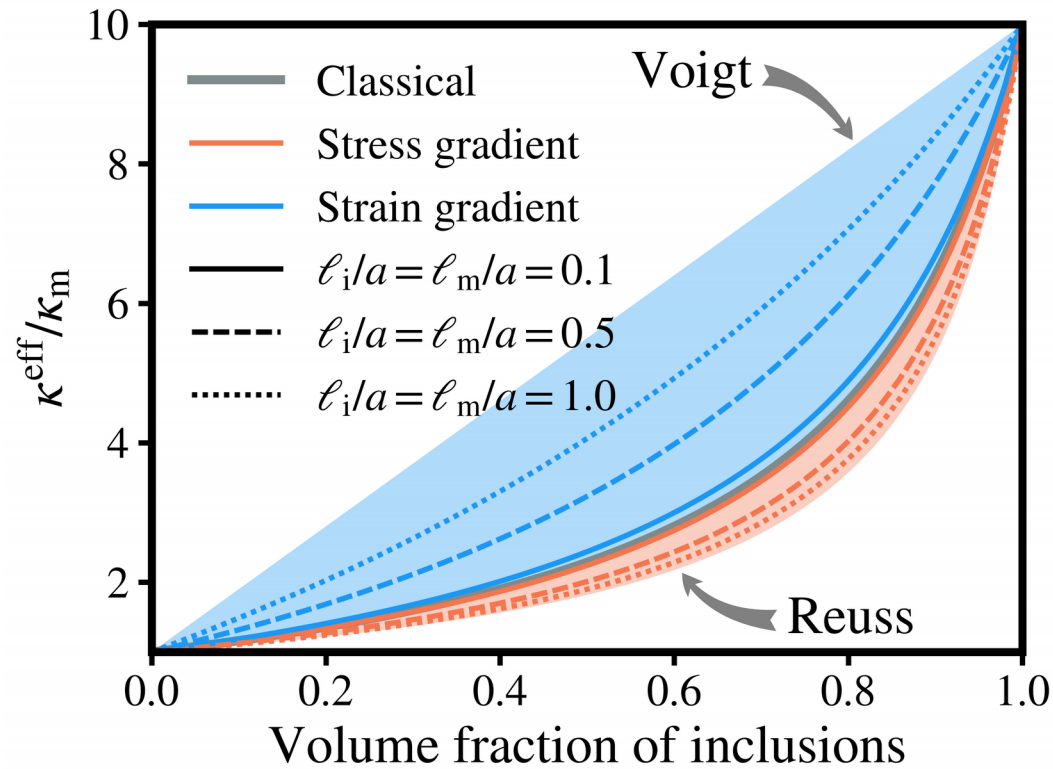
# Problem setting



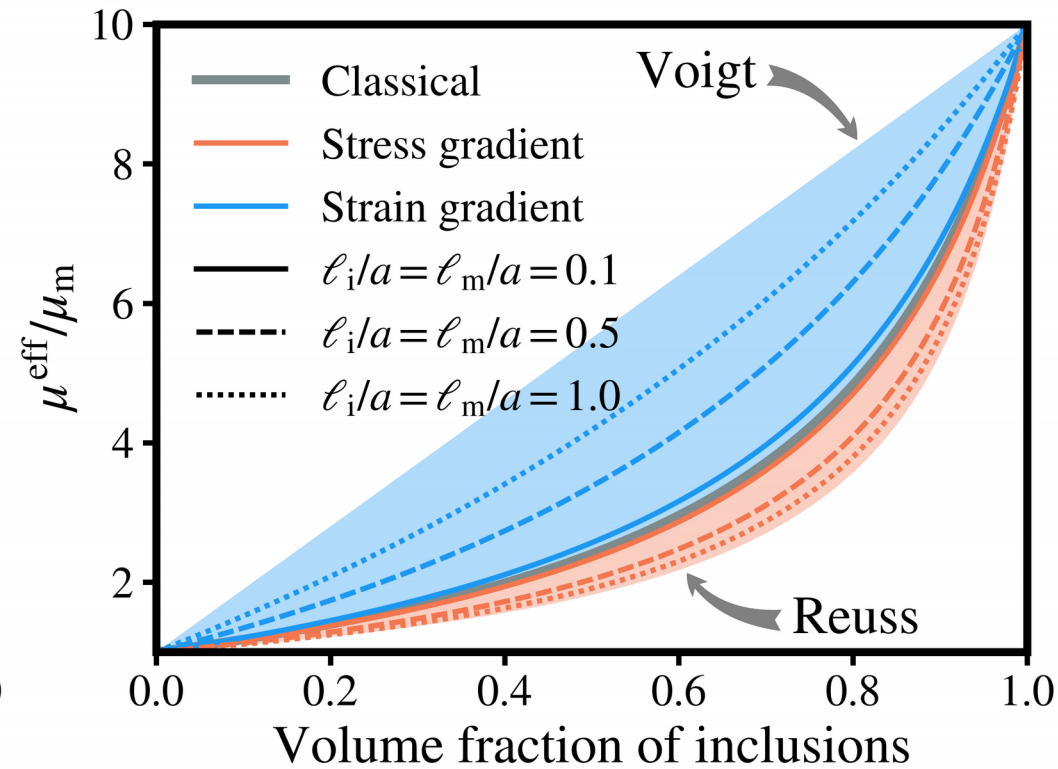
Volume fraction of inclusions:  $f$



# 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

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

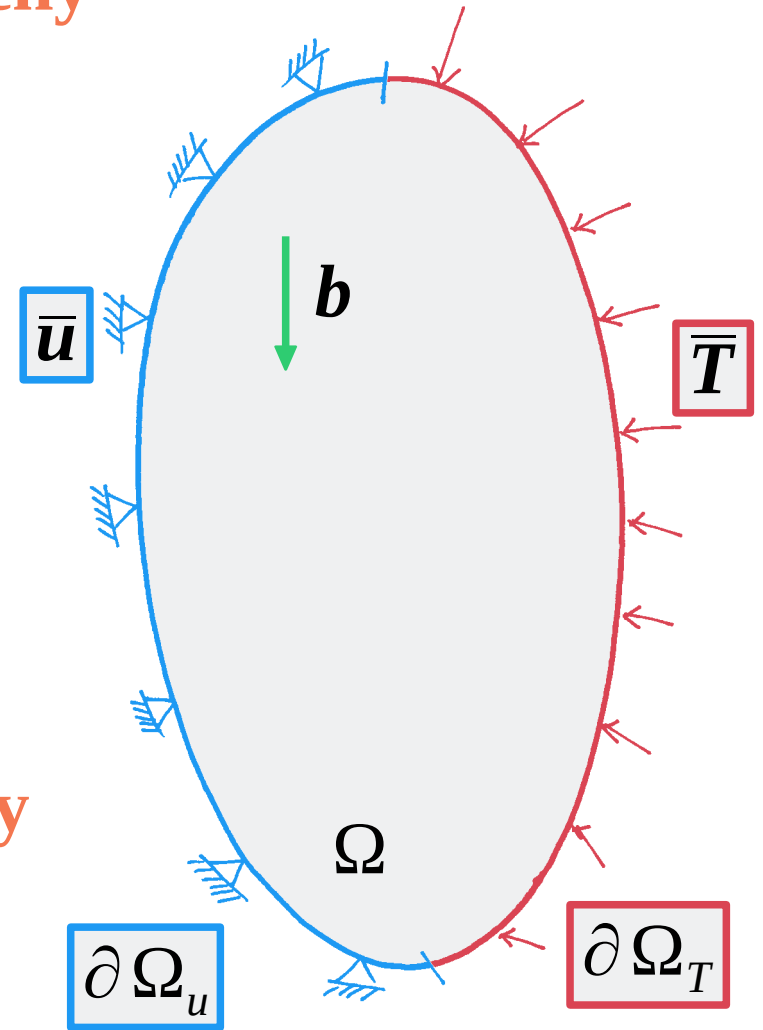
## Assumption 2: complementary work of prescribed displacements

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

## 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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