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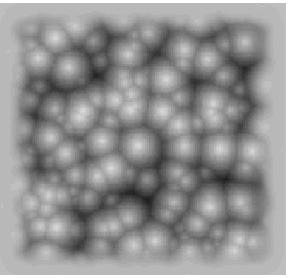

Spatial Randomness in Material Mechanics Models

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in collaboration with

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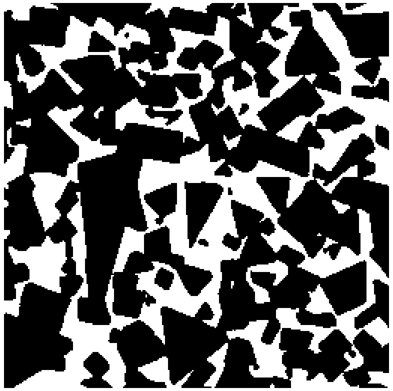
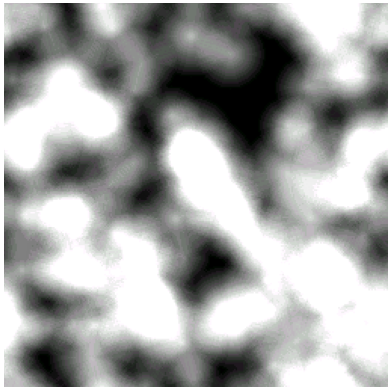
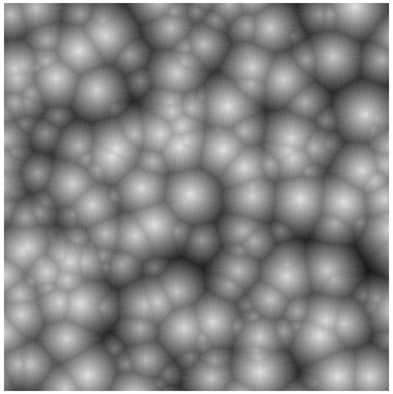
Outline

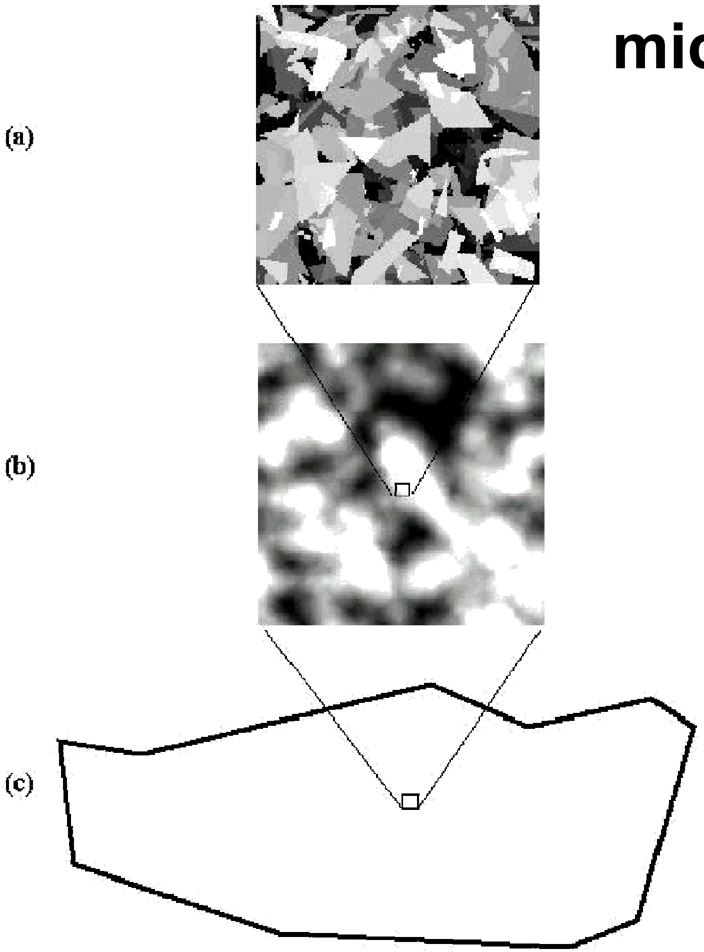


- Separation of scales
- Continuum tensor random fields
- Mesoscale properties
- From scalar to tensor-valued random fields
- Spatial correlations from micromechanics
- Concluding remarks





Separation of Scales?



microscale: d

average size of grain
(microstructure)

mesoscale: L

~~representative volume element (RVE)~~
statistical volume element (SVE)

macroscale: L_{macro}

Separation of scales

$$d << L << L_{macro}$$

does not generally hold!

Continuum Tensor Random Field

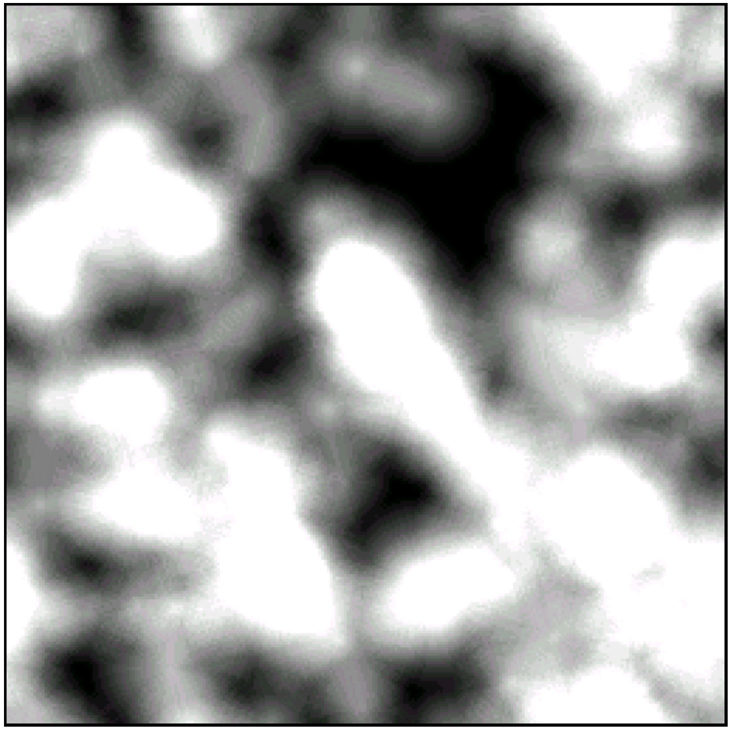
$$\mathbf{C}(\omega, \mathbf{x}) = \overline{\mathbf{C}} + \mathbf{C}'(\omega, \mathbf{x})$$

Can the random field (RF) be assumed isotropic (E, ν) and smooth? **No**

Can we assume a unique tensor RF with anisotropic realizations? **No**

Can we do local averaging of tensor RF for input to stochastic finite elements (SFE)? **No**

Can we assume correlation functions of tensor RF w/o reference to micromechanics? **No**

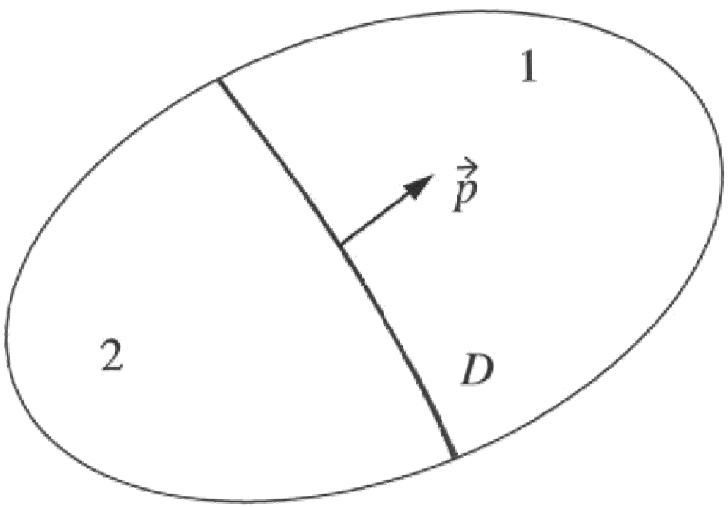


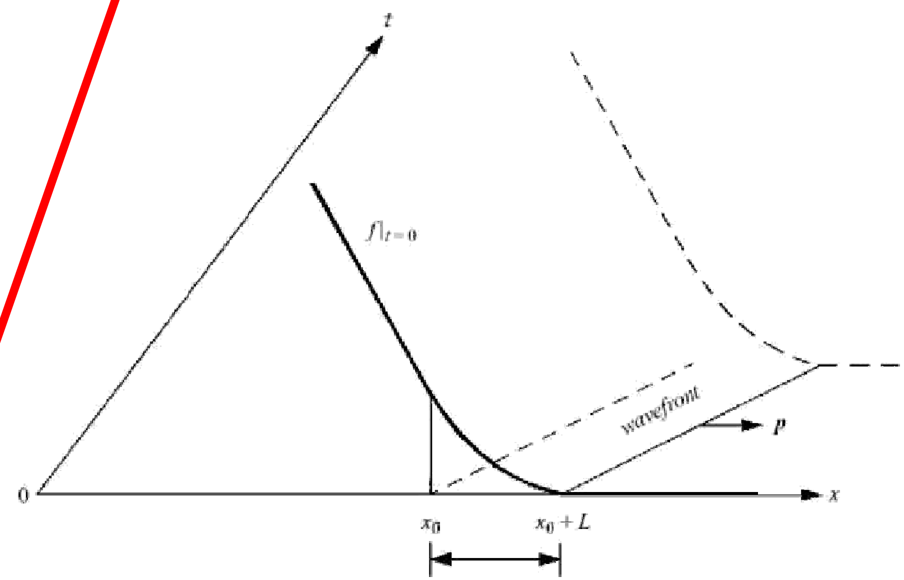
Applications:

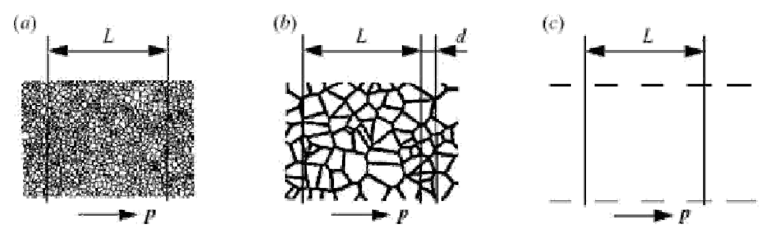
- Random field models
- Uncertainty quantification
- Waves in random media
- FGM …

Continuum Tensor Random Field

For instance, **wavefront** in continuum mechanics is modeled as a **singular surface:**







… an idealized model – homogeneous continuum, **no microstructure**

Continuum Tensor Random Field

* Mesoscale *

$$\mathbf{C}(\omega,\mathbf{x}) = \overline{\mathbf{C}} + \mathbf{C}'(\omega,\mathbf{x}), \quad \omega \in \Omega$$

What is its scale dependence?

Is it isotropic?

Is it uniquely defined?

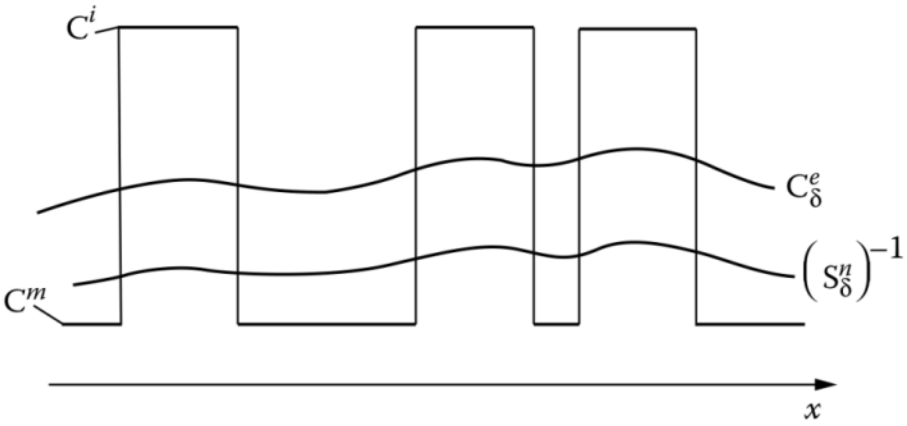
Mesoscale Properties

Local averaging $$Z_L(\omega,\mathbf{x}) = \frac{1}{L^d}\int_{D_L} Z_L(\omega,\mathbf{x}')d\mathbf{x}'$$

is inconsistent with constitutive laws in 2D or 3D

because mechanics involves

boundary value problems…



Mesoscale Properties

Determine mesoscale properties from Hill-Mandel condition; for *Cauchy* materials:

$$\overline{\sigma : \varepsilon} = \overline{\sigma} : \overline{\varepsilon} \qquad \Leftrightarrow \qquad \int_{\partial B_\delta} (t - \overline{\sigma} \cdot n) \cdot (u - \overline{\varepsilon} \cdot x)\, dS = 0$$

Equivalence of mechanical and energetic definitions of properties requires…

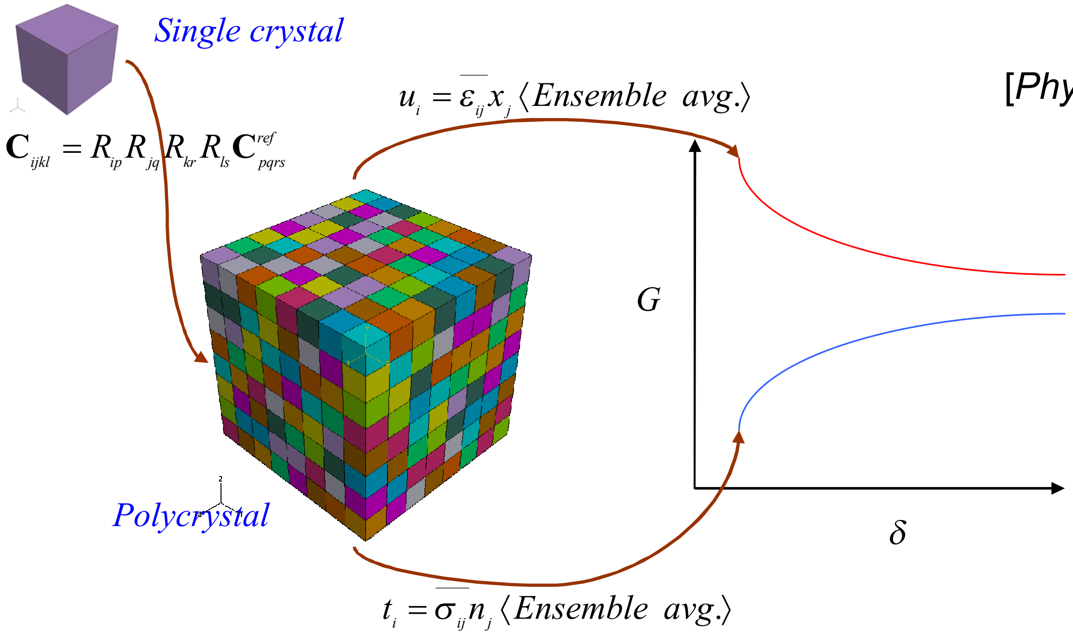
Uniform boundary conditions (BC): $\forall x \in \partial B_\delta$

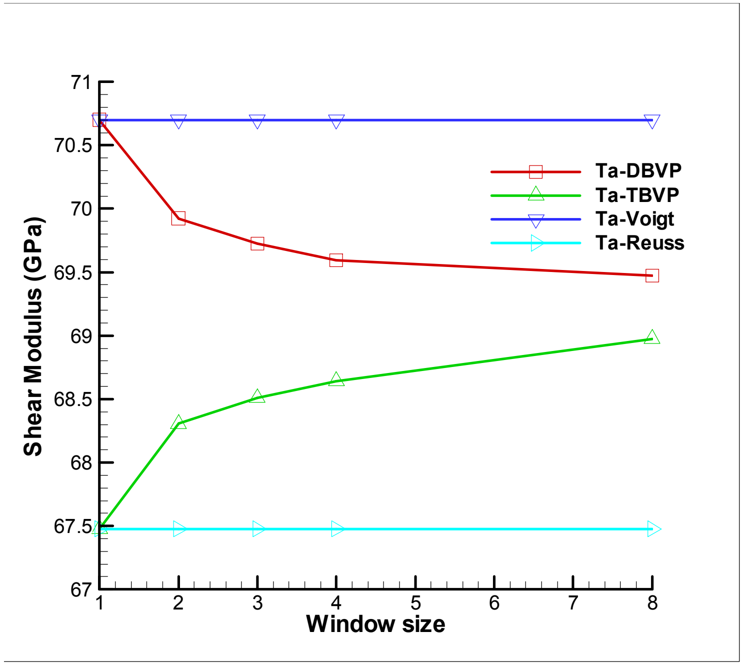
1. Displacement (or *Dirichlet*) BC: $u = \overline{\varepsilon} \cdot x$
2. Traction (or *Neumann*) BC: $t = \overline{\sigma} \cdot n$
3. Displacement-traction (or mixed-orthogonal) BC: $(t - \overline{\sigma} \cdot n) \cdot (u - \overline{\varepsilon} \cdot x) = 0$

Mesoscale Properties

Scale-dependent homogenization

[*Phys. Rev. B*, 2008: *JMPS*, 2008; *IJES*, 2010]





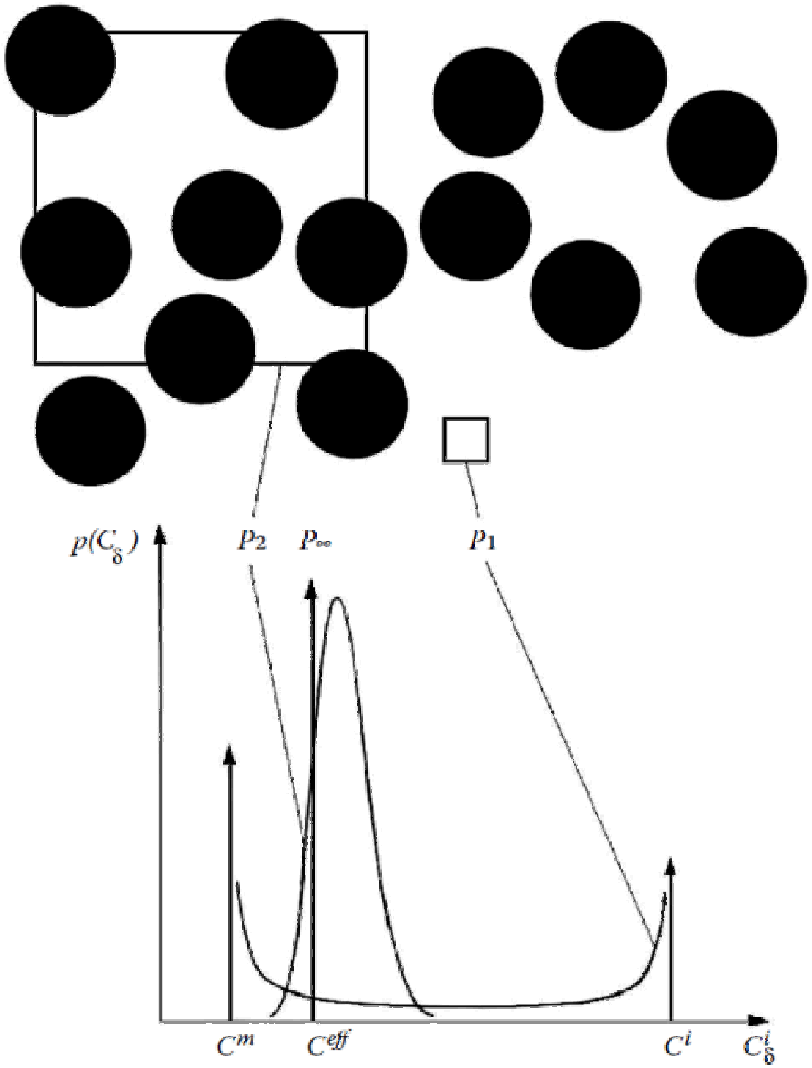
$$t = \bar{\sigma} \cdot n \rightarrow \mathbf{S}^t, \quad u = \bar{\varepsilon} \cdot x \rightarrow \mathbf{C}^d$$

Hierarchy of bounds:

$$\left\langle \mathbf{S}^t_1 \right\rangle^{-1} \le \ldots \le \left\langle \mathbf{S}^t_{\delta'} \right\rangle^{-1} \le \left\langle \mathbf{S}^t_{\delta} \right\rangle^{-1} \le \ldots \le \mathbf{C}^{eff}_{\infty} \ldots \le \left\langle \mathbf{C}^d_{\delta} \right\rangle \le \left\langle \mathbf{C}^d_{\delta'} \right\rangle \ldots \le \left\langle \mathbf{C}^d_1 \right\rangle$$

Mesoscale Properties

Two-phase composite material



In two-phase media, the

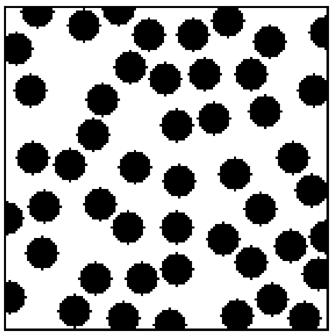
beta probability distribution function

approximates the scale change
for entire range of mesoscales:
from SVE to RVE

[*IJSS*, 1998]

Mesoscale Properties

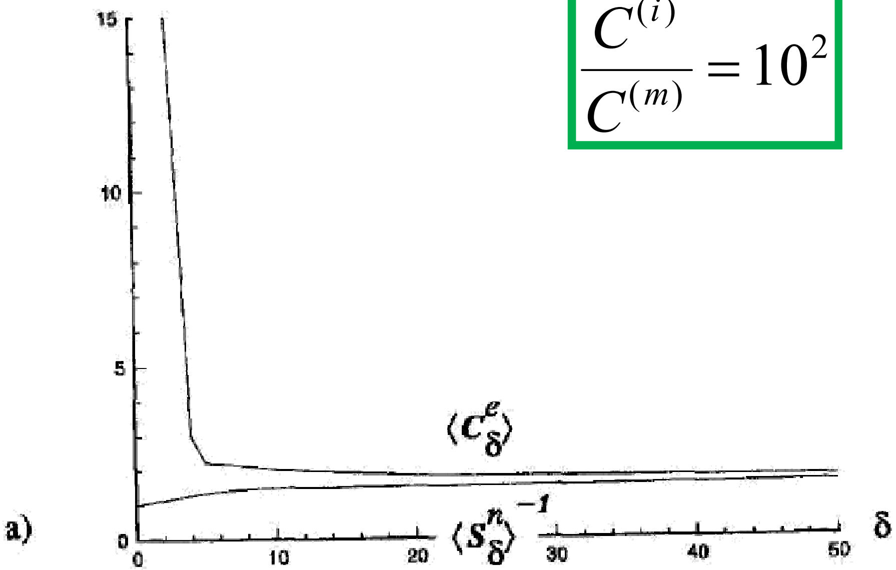
Two-phase composite material



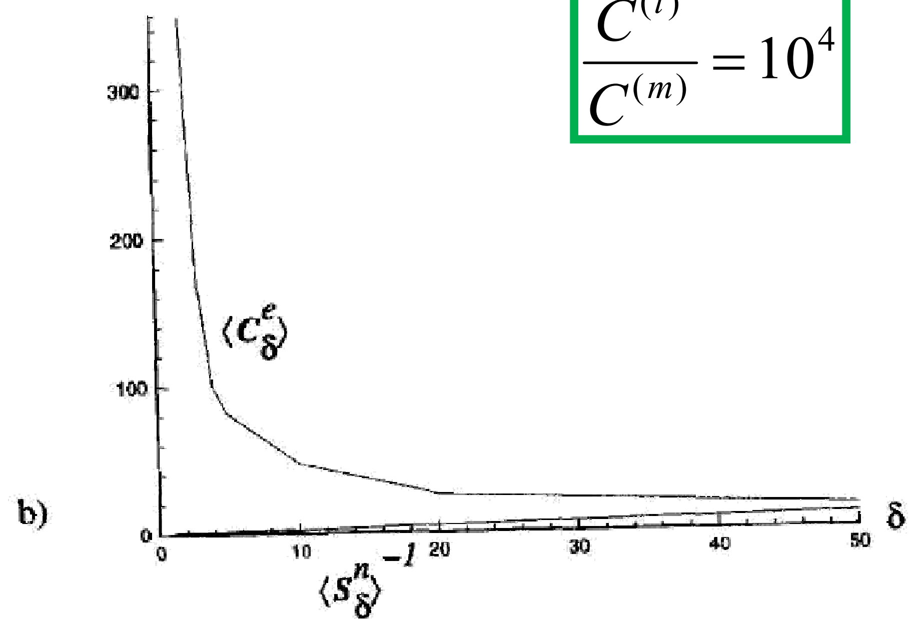
Effect of contrast in C :

stiff inclusions in soft matrix

$$\frac{C^{(i)}}{C^{(m)}} = 10^2$$

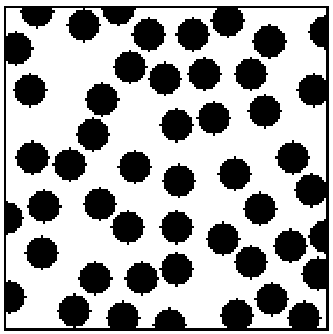


$$\frac{C^{(i)}}{C^{(m)}} = 10^4$$



Mesoscale Properties

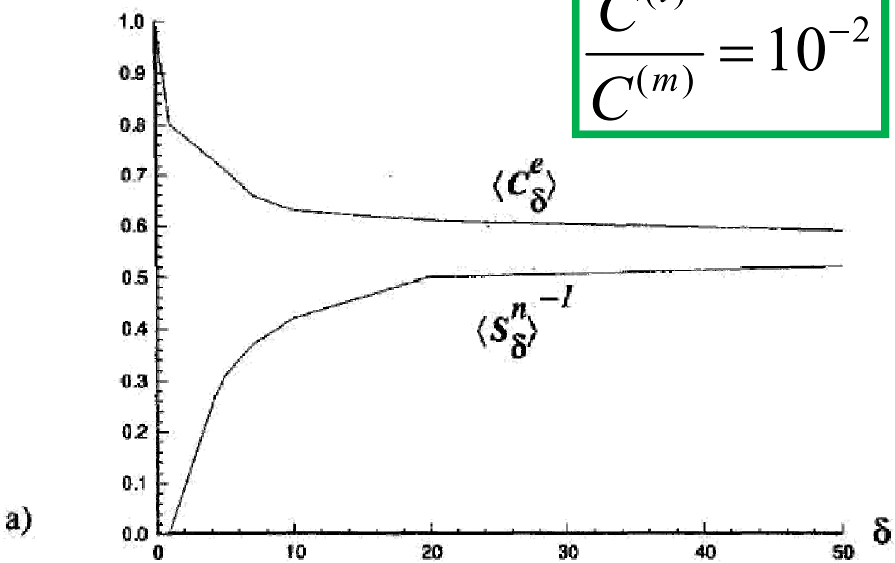
Two-phase composite material



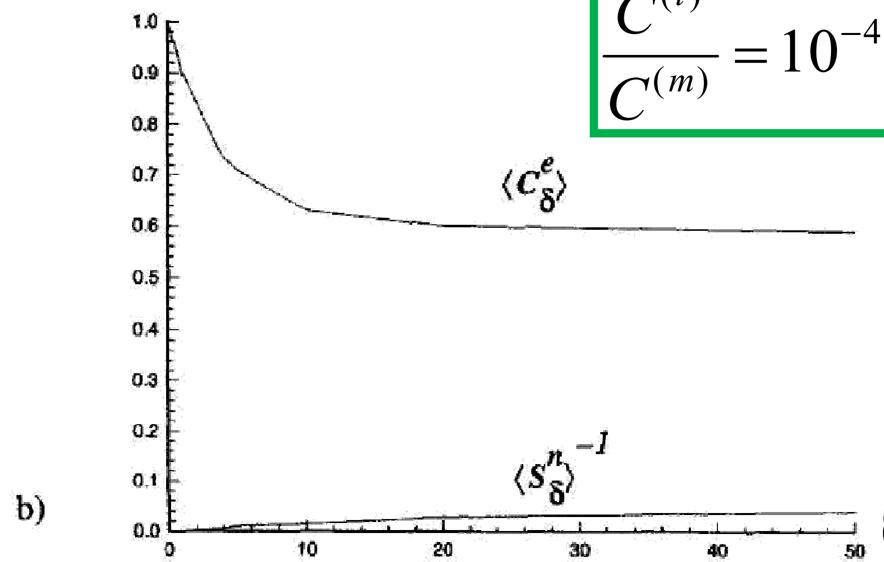
Effect of contrast in C :

soft inclusions in stiff matrix

$$\frac{C^{(i)}}{C^{(m)}} = 10^{-2}$$



$$\frac{C^{(i)}}{C^{(m)}} = 10^{-4}$$



Mesoscale Random Fields

Scalar RFs

$$Z : \Omega \times X \to \mathrm{R}^1, \quad Z(\omega, \mathbf{x}) = z, \ \mathbf{x} \in X$$

$$F_n(\mathbf{z}_1, \ldots, \mathbf{z}_n; \mathbf{x}_1, \ldots, \mathbf{x}_n) = P\{\mathbf{Z}(\mathbf{x}_1) \le \mathbf{z}_1, \ldots, \mathbf{Z}(\mathbf{x}_n) \le \mathbf{z}_n\}$$

$$\langle Z(\mathbf{x}) \rangle = \mu, \quad \langle Z(\mathbf{x}_1) Z(\mathbf{x}_1 + \mathbf{x}) \rangle = R_Z(\mathbf{x}) < \infty$$

$$R(\mathbf{x}_1, \mathbf{x}_2) = \langle [Z(\mathbf{x}_1) - \langle Z(\mathbf{x}_1) \rangle][Z(\mathbf{x}_2) - \langle Z(\mathbf{x}_2) \rangle] \rangle$$

$$\rho(\mathbf{x}_1, \mathbf{x}_2) = \frac{R(\mathbf{x}_1, \mathbf{x}_2)}{\sigma(\mathbf{x}_1)\sigma(\mathbf{x}_2)}$$

$$\rho(\mathbf{x}) = \rho(x), \quad x \equiv \|\mathbf{x}\| = \sqrt{x_i x_i}$$

$$\rho(x) \ge -1/D$$

Mesoscale Random Fields

Constructing correlation functions

Using simpler models, one may construct new, more complex correlation functions:

1. A convex combination of probability distributions is a probability distribution (and the same holds for density functions)

2. A convex combination of correlation functions is a correlation function

3. A finite product of correlation functions is a correlation function

Mesoscale Random Fields

Basic models of correlation functions

$$\rho(x) = \exp[-Ax^{\alpha}], \quad A > 0, \quad 0 < \alpha \le 2$$

$$\rho(x) = [1 + Ax^{\alpha}]^{-1}, \quad A > 0, \quad 0 < \alpha \le 2$$

$$\rho(x) = \frac{\exp[-Ax^{\alpha}]}{1 + Bx^{\alpha}}, \quad A, B > 0, \quad 0 < \alpha, \beta \le 2$$

$$\rho(x) = \exp[-\sum_{s=1}^{r} Ax^{\alpha_s}], \quad A_s > 0, \quad 0 < \alpha_s \le 2, \quad s = 1, \ldots, r$$

$$\rho(x) = [-\prod_{s=1}^{r} (1 + B_s x^{\beta_s}) l_s], \quad B_s > 0, \quad 0 < \beta_s \le 2, \quad l_s = 1, 2, \ldots$$

$$\rho(x) = \exp[-Ax^{\alpha}](\cosh Bx^{\alpha})^{s}, \quad A + B(2l - s) > 0, \quad 0 < \alpha \le 2, \quad s = 1, \ldots, r$$

$$\rho(x) = \frac{(\cosh Bx^{\alpha})^{s}}{1 + Ax^{\alpha}}, \quad A + B(2l - s) > 0, \quad 0 < \alpha \le 2, \quad s = 1, \ldots, r$$

NOTE: These do not separate **local** from **long-range** effects

Mesoscale Random Fields

Vector RFs

$$\mathbf{Z} : \Omega \times \mathbf{X} \to \mathrm{R}^2, \quad \mathbf{Z}(\omega, \mathbf{x}) = \mathbf{z}, \ \mathbf{x} \in \mathbf{X}$$

Wide Sense Stationary (WSS)

$$\langle Z_i(\mathbf{x}) \rangle = \mu_i, \quad \langle Z_i(\mathbf{x}_1) Z_j(\mathbf{x}_1 + \mathbf{x}) \rangle = R_{ij}(\mathbf{x}) < \infty$$

$$R_{ij}(\mathbf{x}_1, \mathbf{x}_2) = \langle [Z_i(\mathbf{x}_1) - \langle Z_i(\mathbf{x}_1) \rangle][Z_j(\mathbf{x}_2) - \langle Z_j(\mathbf{x}_2) \rangle] \rangle$$

$$\rho_{ij}(\mathbf{x}_1, \mathbf{x}_2) = \frac{R_{ij}(\mathbf{x}_1, \mathbf{x}_2)}{\sigma_i(\mathbf{x}_1) \sigma_j(\mathbf{x}_2)}$$

$$\rho_{ij}(\mathbf{x}_1, \mathbf{x}_2) = \rho_{ij}(|\mathbf{x}_1 - \mathbf{x}_2|)$$

Mesoscale Random Fields

Tensor RFs

2nd rank tensor RF correlation:

$$\rho_{ij}^{kl}(\mathbf{x}_1,\mathbf{x}_2)=\frac{\langle[C_{ij}(\mathbf{x}_1)-\langle C_{ij}(\mathbf{x}_1)\rangle][C_{kl}(\mathbf{x}_2)-\langle C_{kl}(\mathbf{x}_2)\rangle]\rangle}{\sigma_{ij}(\mathbf{x}_1)\sigma_{kl}(\mathbf{x}_2)}$$

- Stationary RF: $\langle C_{ij}(\mathbf{x})\rangle = \mathrm{const} \quad \forall \mathbf{x}$

$$\rho_{ij}^{kl}(\mathbf{x}_1,\mathbf{x}_2)=\rho_{ij}^{kl}(\mathbf{x}) \qquad \mathbf{x}=|\mathbf{x}_1-\mathbf{x}_2|$$

- Isotropic RF: $\langle C_{ij}(\mathbf{x})\rangle = C\delta_{ij} \quad \forall \mathbf{x} \qquad x=\|\mathbf{x}\|$

$$\begin{aligned}\rho_{ij}^{kl}(x)=&K_4(x)\delta_{ij}\delta_{kl}+K_6(x)\left[\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\right]\\&+\left[K_5(x)-K_6(x)\right]\left[n_jn_k\delta_{il}+n_in_l\delta_{jk}+n_in_k\delta_{jl}+n_jn_l\delta_{ik}\right]\\&+\left[K_3(x)-K_4(x)\right]\left[n_in_j\delta_{kl}+n_kn_l\delta_{ij}\right]\\&+\left[K_1(x)+K_2(x)-2K_3(x)-4K_5(x)\right]n_in_jn_kn_l,\end{aligned}$$

Five functions K_i: $\qquad K_4+2K_6-K_2=0$

Mesoscale Random Fields

Tensor RFs

2nd rank tensor RF correlation:

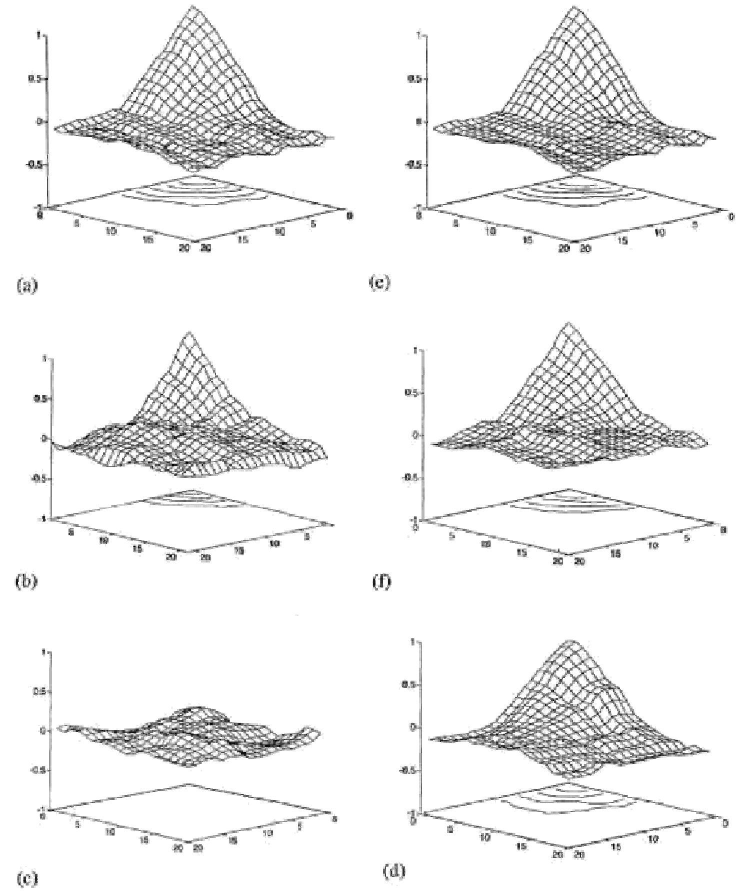
$$\rho_{ij}^{kl}(\mathbf{x}_1,\mathbf{x}_2)=\frac{\langle[C_{ij}(\mathbf{x}_1)-\langle C_{ij}(\mathbf{x}_1)\rangle][C_{kl}(\mathbf{x}_2)-\langle C_{kl}(\mathbf{x}_2)\rangle]\rangle}{\sigma_{ij}(\mathbf{x}_1)\sigma_{kl}(\mathbf{x}_2)}$$

Tensor RFs of constitutive responses (from micromechanics)

in **anti-plane elasticity** of a matrix-inclusion composite $\longrightarrow C_{ij}$

$$R_{ij}^{kl}(\mathbf{x})=R_1(x_1)R_2(x_2)$$

$$R_{ij}^{kl}(\mathbf{x})=\prod_{d=1}^{D}R_d(x_d) \qquad D=1,2,3$$



Mesoscale Random Fields

Tensor RFs

4th rank tensor RF correlation:

$$\rho_{ijkl}^{prst}(\mathbf{x}_1,\mathbf{x}_2)=\frac{\langle[C_{ijkl}(\mathbf{x}_1)-\langle C_{ijkl}(\mathbf{x}_1)\rangle][C_{prst}(\mathbf{x}_2)-\langle C_{prst}(\mathbf{x}_2)\rangle]\rangle}{\sigma_{ijkl}(\mathbf{x}_1)\sigma_{prst}(\mathbf{x}_2)}$$

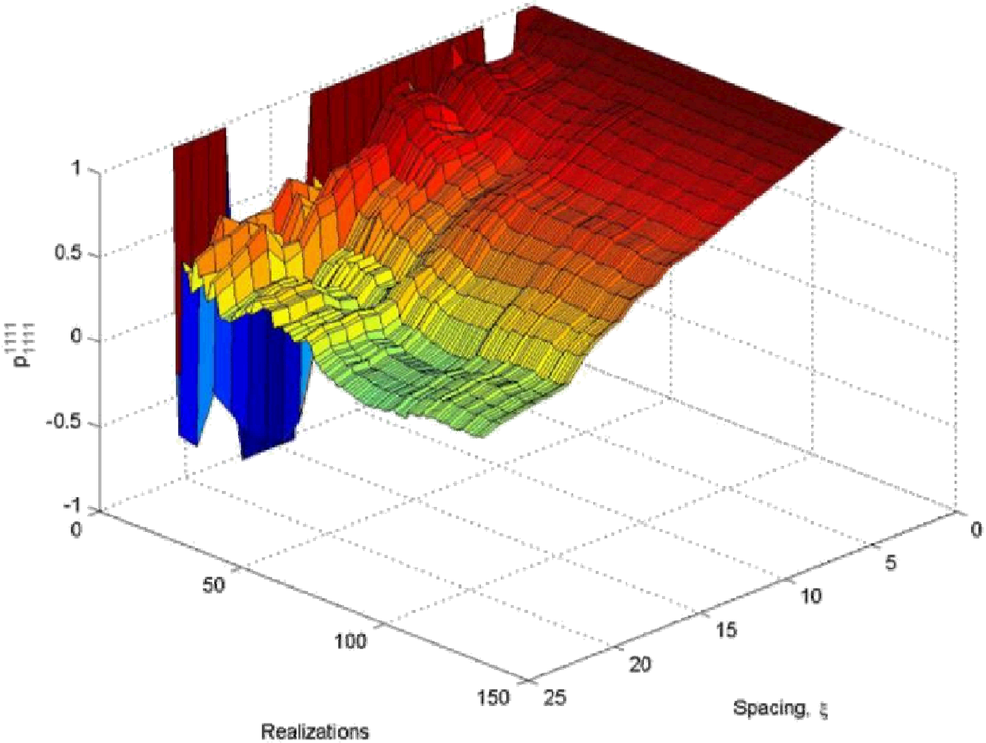
Tensor RFs of constitutive responses (from micromechanics)

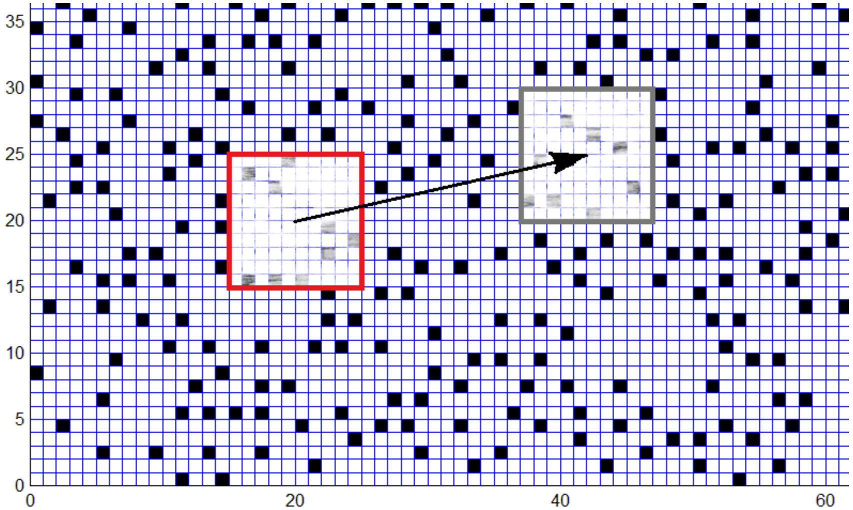
in **2D elasticity** of a matrix-inclusion composite $\longrightarrow C_{ijkl}$

$$R_{ijkl}(\mathbf{x})=\prod_{d=1}^{D}R_d(x_d) \qquad D=1,2,3$$

Spatial Correlations of Random Fields

Sample realization
of random binary checkerboard
at 50/50%

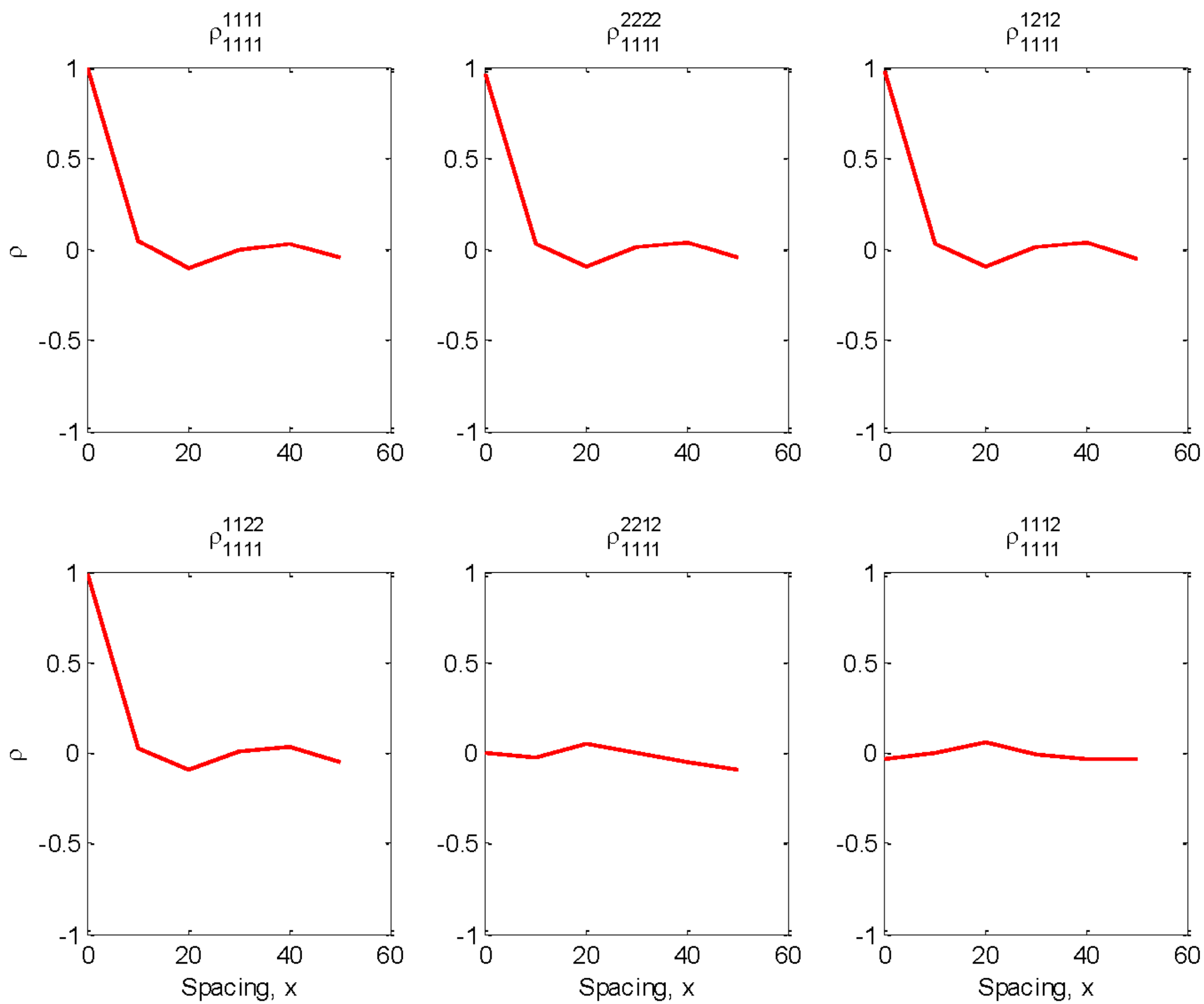




Spatial Correlations of Random Fields

ΔX

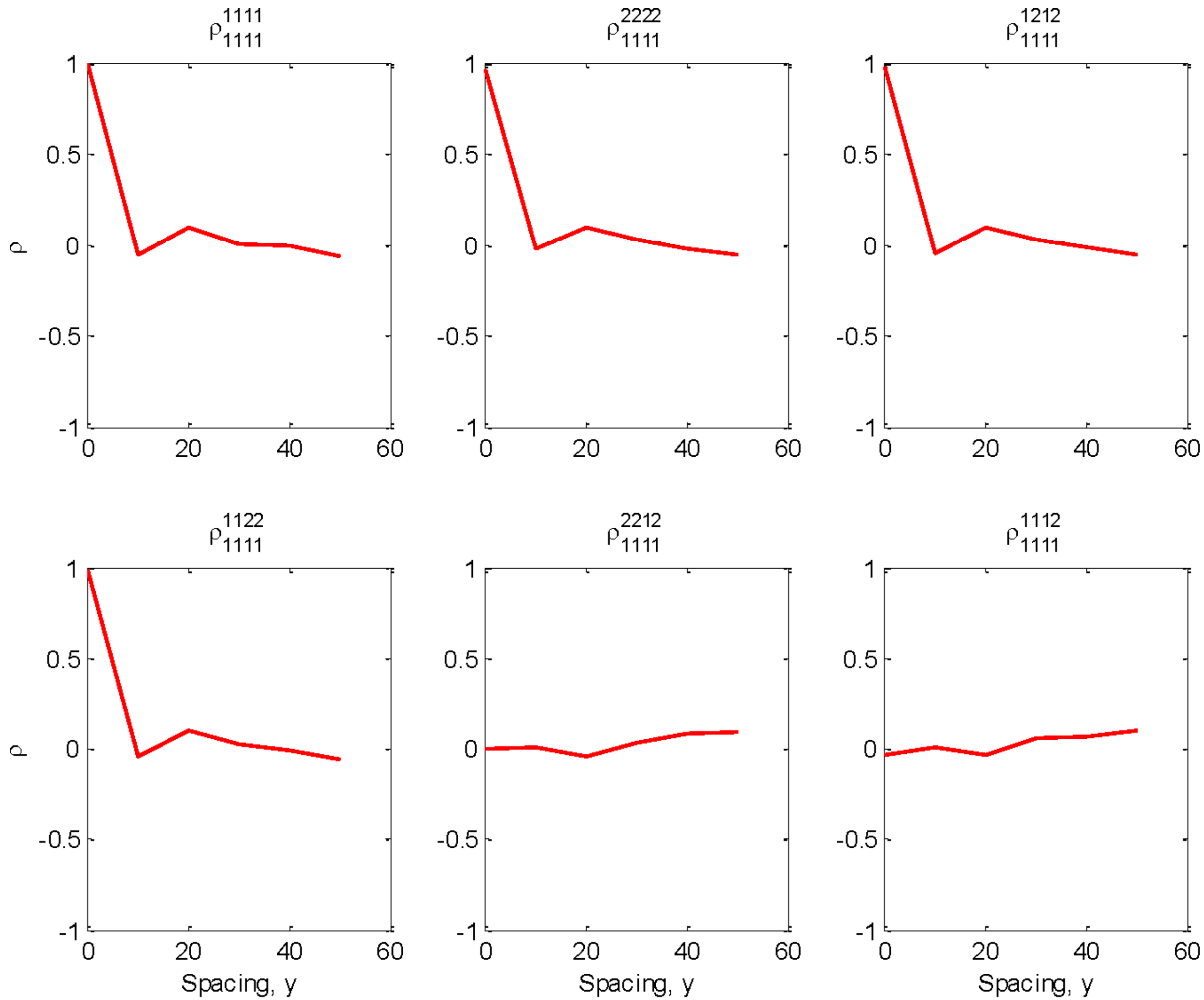
$$L = 10$$
$$v_f = 0.59$$
$$\alpha = 2$$
$$N = 400$$



Spatial Correlations of Random Fields

$$\boxed{\Delta Y}$$

$$L = 10$$
$$v_f = 0.59$$
$$\alpha = 2$$
$$N = 400$$



Concluding Remarks

- **For tensor-type properties of materials, need RFs consistent with mechanics**
- Consistent with mechanics iff mechanical definition of properties = energetic definition of properties (Hill Mandel condition)
- Random fields of properties are functions of microstructure + mesoscale
- Micromechanics analyses lead to counterintuitive results
- Can construct correlation functions from products of basic 1D models
- Can go to: coupled field phenomena, inelastic properties, fractal versus long-range effects…

Thank you kindly for your attention

We acknowledge the support for this work
from the Defense Threat Reduction Agency (DTRA)
under grant HDTRA1-08-10-BRCWMD

ADDITIONAL SLIDES FOLLOW

Dynamics

Determine mesoscale properties from Hill-Mandel condition for dynamics of Cauchy materials:

$$\overline{\sigma_{ji}\ \dot{\varepsilon}_{ji}} = \overline{\sigma_{ji}}\ \overline{\dot{\varepsilon}_{ji}} \quad \Leftrightarrow \quad \frac{1}{V}\int_S \left(t_i - \overline{\sigma_{ki}}\ n_k\right)\left(\dot{u}_i - \overline{\dot{\varepsilon}_{ij}}\ x_j\right)\, dS - \overline{\dot{k}_c} + (\overline{k_c})^{\cdot} = 0$$

Determine mesoscale properties from Hill-Mandel condition for dynamics of Cosserat materials:

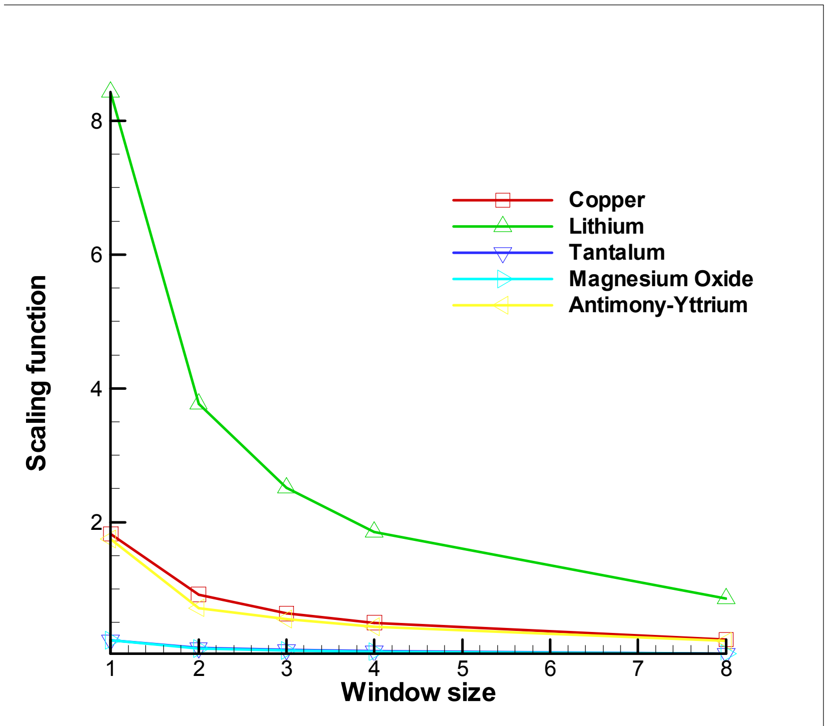
$$\overline{\tau_{ji}\ \dot{\gamma}_{ji}} - \overline{\tau_{ji}}\ \overline{\dot{\gamma}_{ji}} + \overline{\mu_{ji}\ \dot{\kappa}_{ji}} - \overline{\mu_{ji}}\ \overline{\dot{\kappa}_{ji}} =$$

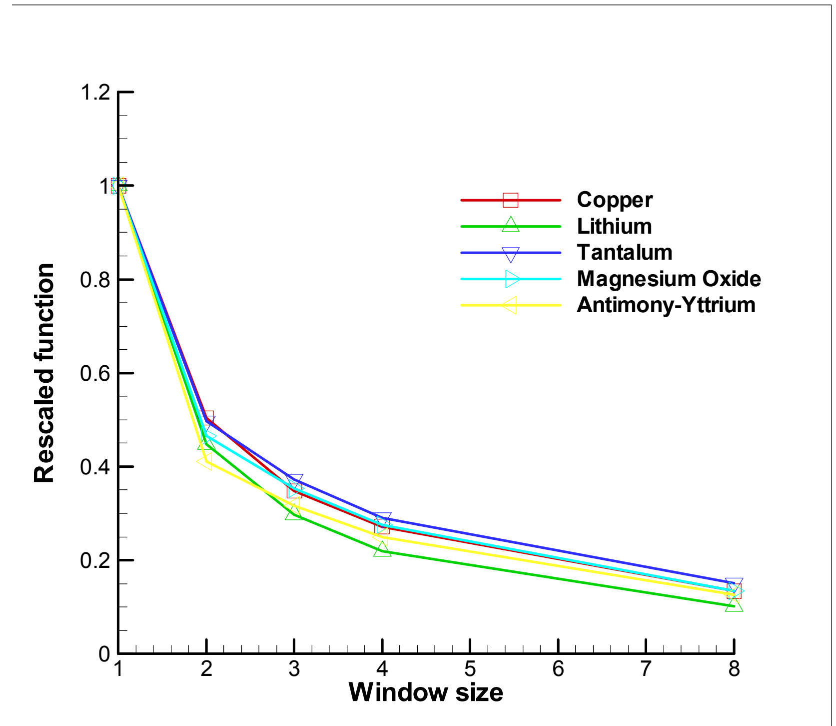
$$\tfrac{1}{V}\int_S \left(t_i - \overline{\tau_{ki}}\ n_k\right)\left(\dot{u}_i - \overline{\dot{u}_{i,j}}\ x_j\right)\, dS + \tfrac{1}{V}\int_S \left(m_i - \overline{\mu_{ki}}\ n_k\right)\left(\dot{\phi}_i - \overline{\dot{\phi}_{i,j}}\ x_j\right)\, dS +$$

$$- \overline{\dot{k}_c} + (\overline{k_c})^{\cdot} - \overline{\dot{k}_m} + (\overline{k_m})^{\cdot}$$

Scale-Dependent Response

3D random polycrystal





Scaling function: $$f(A,\delta) = \frac{6}{5}\left(\sqrt{A} - \frac{1}{\sqrt{A}}\right)^2 \exp\left[-0.767(\delta - 1)^{0.504}\right], \quad \delta = N_G^{\frac{1}{3}}$$

Zener anisotropy index

[*JMPS*, 2008; *IJES*, 2009]

Fractals and Hurst Effect

Two new Gaussian RFs are able to grasp

fractals
(i.e. roughness)

and **Hurst effect**
(i.e. heavy-tail behavior of covariance function)

1. Cauchy correlation function:

$$\rho(x) = \left(1 + x^{\theta}\right)^{-\eta/\theta}, \quad \theta \in (0,2], \quad \eta > 0$$

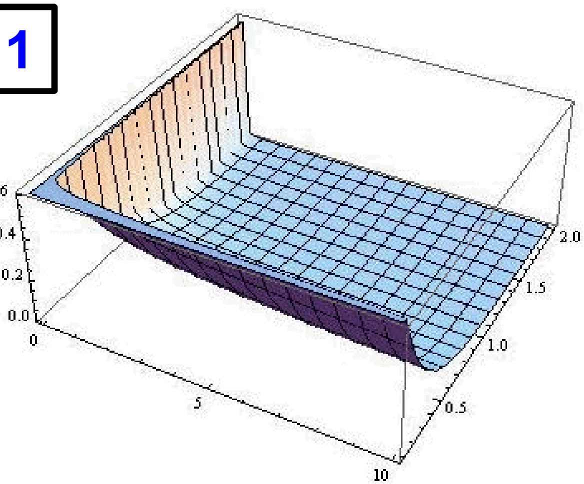
[Gneiting & Schlather, *SIAM Review*, 2004]

2. Dagum correlation function:

$$\rho(x) = 1 - \left(1 + \lambda x^{-\theta}\right)^{-\varepsilon}, \quad \theta < \left(7 - \varepsilon\right)\left(1 + 5\varepsilon\right), \quad \varepsilon < 7$$

[Porcu *et al.*, PEM 2007, 2011, *Stat. Probab. Lett*, 2007, *Bernoulli*, 2008]

1



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