

Spectral Properties of Random Cluster Models and Applications to Composite Materials

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**New Interactions between Probability and Geometry
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Composite Materials

- Made from two or more constituent materials with different properties
- Behavior is very random at microscale
- At macroscale the composite behaves like a homogeneous material with **effective parameters**
- **Goal:** Determine effective properties of the composite from statistics of small scale structure
- Further information:
 - Wikipedia: Composite materials
 - Materialism Podcast



Elena Cherkayev



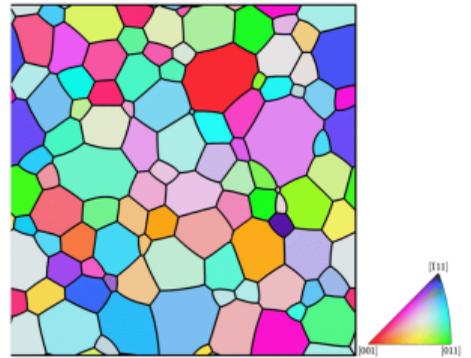
Ken Golden



Benjamin Murphy

Composite Materials: Polycrystals

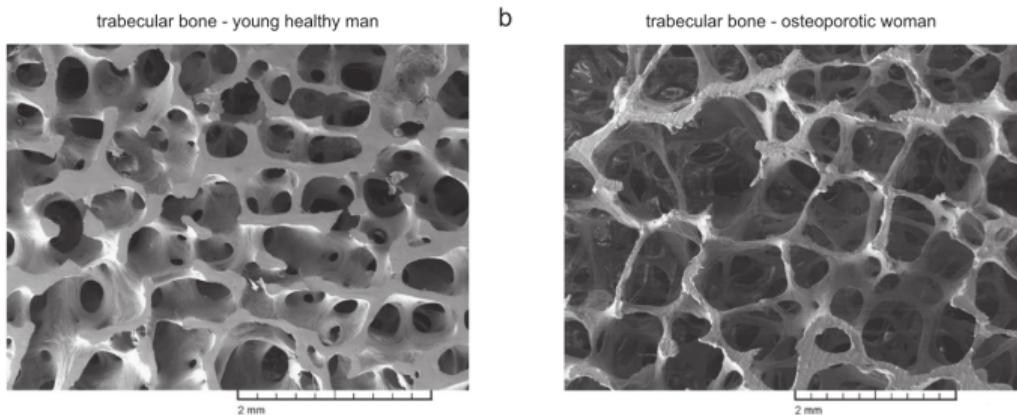
- Made of many small crystals fused together
- Grains vary in size, shape, and spatial orientation
- **Examples:**
 - Metals - Polycrystalline copper - has higher strength than monocrystalline copper
 - Ceramics - Tetragonal Zirconia Polycrystals (TZP) - used in dental implants
 - Sea ice - crystals consisting of frozen water, liquid brine, and air pockets



Kurniawan et al (2020)

Composite Materials: Porous Materials

- Two phase composite of matter and void
- **Examples:**
 - Geological materials - rocks, soils, sandstones
 - Glacial ice - mixture of ice and air pockets
 - Bone - osteoporosis - loss of bone density due to increased porosity



Golden et al (2011) [GBC11]

Composite Materials: Disordered Conductors

- Electrical transport properties determined by connectedness (percolation) of a particular component
- Often exhibit insulator-to-conductor phase transition
- **Examples:**
 - Cermets - ceramic-metal composites used in high temperature applications
 - Polymer composites with conductive fillers - used in flexible electronics
 - Semiconductors with dopants - control electrical properties via random impurities



Mathematical Models

Mathematical Models¹

- Composite materials modeled as random mixtures of two or more phases
- Each phase has different physical properties (e.g. conductivity, elasticity, permittivity)
- **Goal:** Understand effective large scale properties in terms of statistics of small scale structure

¹This slide written by AI

Mathematical Models: Conductors

- Work in \mathbb{R}^2
- $c = c(\mathbf{x}, \omega)$ is **random conductivity tensor** at point \mathbf{x} in random environment ω
- $\mathbf{x} \rightarrow c(\mathbf{x}, \omega)$ is rapidly oscillating
- Given sources and sinks $\rho : \mathbb{R}^d \rightarrow \mathbb{R}$, potential $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ solves

$$\nabla \cdot c \nabla \phi = \rho, \quad +BCs$$

- $E : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ the electric field, $J : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ the current field

$$J(\mathbf{x}) = c(\mathbf{x})E(\mathbf{x}), \quad \nabla \cdot J(\mathbf{x}) = \rho(\mathbf{x}), \quad \nabla \times E(\mathbf{x}) = 0$$

- ϕ, J, E are typically rapidly oscillating at level of microstructure

Mathematical Models: Homogenization

- Transition from micro to macro scale:

$$J_0(\mathbf{x}) = \text{“average of } J \text{ over large box centered at } \mathbf{x}\text{”} \approx \mathbb{E}J(\mathbf{x})$$

- Same for $E_0(\mathbf{x})$
- **Homogenization:** There exists a **non-random** c_* such that

$$J_0(\mathbf{x}) = c_* E_0(\mathbf{x}), \quad \nabla \cdot J_0(\mathbf{x}) = \rho(\mathbf{x}), \quad \nabla \times E_0(\mathbf{x}) = 0$$

- c_* is the **effective conductivity tensor**

$$c_* = \mathcal{F} [\text{Law of } c(\cdot, \omega)]$$

- Existence comes from stationarity and ergodicity of $c(\cdot, \omega)$

Mathematical Models: Homogenization

Forward problem

- Compute c_* from law of $c(\cdot, \omega)$
- Difficult except in special cases
- \mathcal{F} is nonlinear and nonlocal
- Exact expressions given by variational formula over infinite dimensional spaces

Inverse problem

- Infer law of $c(\cdot, \omega)$ from measurements of c_*
- Work with parameterized families of laws
- Infer parameters from effective property measurements

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Takeaway: Understanding \mathcal{F} is crucial for both forward and inverse problems



Analytic Continuation Method

Analytic Continuation Method

- Based on [GP83, Ber80, Mil82]
- Method for effective parameters *without* variational problem
- Based on spectral decomposition of a random operator $\chi\Gamma\chi$
- Perturbative from homogeneous to inhomogeneous
- Useful for estimating effective parameters via simulation



Elena Cherkaev



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Analytic Continuation Method

- Start with a homogeneous material ($c = I$)

$$J_H(\mathbf{x}) = E_H(\mathbf{x}), \quad \nabla \cdot J_H(\mathbf{x}) = \rho(\mathbf{x}), \quad \nabla \times E_H(\mathbf{x}) = 0$$

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- Γ = projection operator onto gradient fields ($\text{Range } \nabla$)
- For a vector field $\theta : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ have

$$\theta = \Gamma\theta + (I - \Gamma)\theta, \quad (I - \Gamma)\theta \in \text{Range}(\nabla)^\perp = \text{Ker}(\nabla \cdot)$$

hence $\nabla \cdot \theta = \nabla \cdot \Gamma\theta$

Takeaway

Find any θ satisfying $\nabla \cdot \theta = \rho$, then $\Gamma\theta = J_H$

Analytic Continuation Method

- Move to an inhomogeneous material (c general)

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Takeaway

$J_I = \Gamma_c \Gamma \theta$ is the current field in the *inhomogeneous* material

Analytic Continuation Method

- J_H = current in homogeneous material ($c = I$)
- J_I = current in inhomogeneous material (c general)
- Using projection ideas from previous slide + further linear algebra:

Theorem

Let $F \subset \mathbb{R}^2$, $\alpha > -1$, and $c(\mathbf{x}) = (1 + \alpha 1_F(\mathbf{x}))I$. Then

$$J_I = J_H + \alpha(I - \Gamma) \int_{(0,1)} \frac{d\mu_{1_F\Gamma 1_F}(\lambda)}{1 + \alpha\lambda} J_H$$

Here $\mu_{1_F\Gamma 1_F}$ is the **spectral resolution** of the operator $1_F\Gamma 1_F$. If F is random, and since J_H is non-random, then

$$\mathbb{E}J_I = J_H + \alpha(I - \Gamma) \int_{(0,1)} \mathbb{E} \left[\frac{d\mu_{1_F\Gamma 1_F}(\lambda)}{1 + \alpha\lambda} \right] J_H$$

Analytic Continuation Method

Spectral resolution:

- For self-adjoint A , μ_A encodes the eigenvalues and eigenvectors of A
 - μ_A is a matrix-valued measure
 - $\mu_A([a, b]) =$ projection onto eigenspaces with eigenvalues in $[a, b]$
- For $A = 1_F \Gamma 1_F$, eigenvalues are in $[0, 1]$ because 1_F and Γ are projections²

²This line written by AI

Analytic Continuation Method

Takeaways:

- For random **two-component** conductivities $c(x) = (1 + \alpha 1_F(x))I$, effective parameters can be expressed in terms of

$$\int_{(0,1)} \mathbb{E} \left[\frac{d\mu_{1_F \Gamma_{1_F}}(\lambda)}{1 + \alpha\lambda} \right]$$

- Above can be approximated by Monte Carlo - no variational problem

Minimally restrictive:

- General conductivities can be expressed as an iterative sequence of two-component conductivities (+ small modifications)
- General approach can be modified for specific physical settings (elasticity, permittivity, etc)

Analytic Continuation Method

Why call it analytic continuation?

$$\alpha \mapsto \int_{(0,1)} \mathbb{E} \left[\frac{d\mu_{1_F \Gamma 1_F}(\lambda)}{1 + \alpha \lambda} \right]$$

is analytic off of the negative real axis



Discrete Setting: Electrical Networks

Discrete Setting

Why move to a discrete setting?

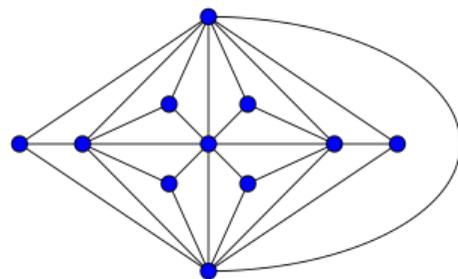
- Linear algebra is cleaner
- Simulations are all graph based
- Connect to statistical mechanics models on graphs
- Deeper understanding of $\mu_{1_F \Gamma 1_F}$ on a realization-by-realization basis

Electrical Networks

- Setup: $G = (V, E, c)$
- $c : E \rightarrow \mathbb{R}_+$ are edge conductivities
- Poisson equation:

$$\nabla' c \nabla \phi = \rho$$

- Solve for $E = \nabla \phi : E \rightarrow \mathbb{R}$ and $J = cE : E \rightarrow \mathbb{R}$

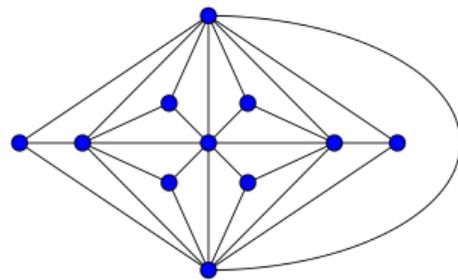


Electrical Networks

- Γ_c = projection onto $\text{Range } c\nabla$ in the inner product

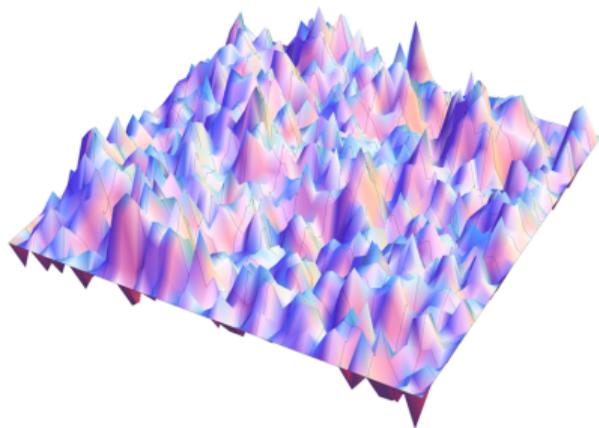
$$\langle \theta, \psi \rangle_r = \sum_{e \in E} r(e) \theta(e) \psi(e), \quad r = c^{-1}$$

- If $\theta : E \rightarrow \mathbb{R}$ satisfies $\nabla' \theta = \rho$, then $J = \Gamma_c \theta$



Probabilistic Interpretation of Γ_c : GFF

- $h : V \rightarrow \mathbb{R}$ a mean zero GFF on G
- Γ is covariance operator for ∇h



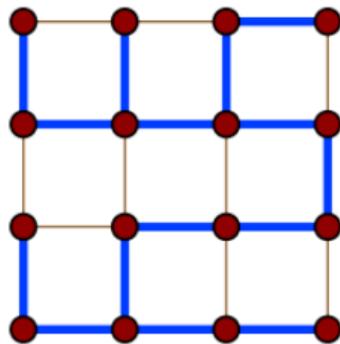
Probabilistic Interpretation of Γ_c : UST

- \mathcal{T} a uniform spanning tree on G , with weights

$$\mathbb{P}_G(\mathcal{T}) \propto \prod_{e \in \mathcal{T}} c(e)$$

- $\mathcal{F} \subset E$ is determinantal with kernel Γ_c

$$\mathbb{P}_G(\mathcal{F} \subset \mathcal{T}) = \det(\Gamma_c|_{\mathcal{F} \times \mathcal{F}})$$

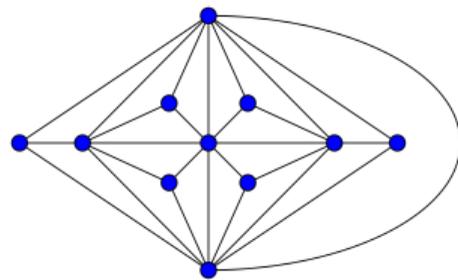


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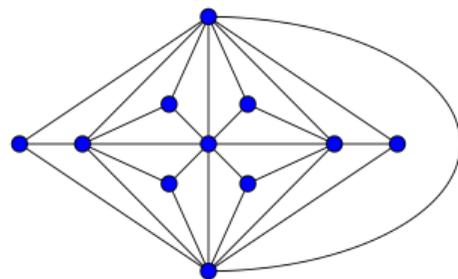


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Theorem

Let $F \subset E$ and $\alpha > -1$. Then

$$\Gamma_{(1+\alpha 1_F)c} = \Gamma_c + \alpha(I - \Gamma_c) [1_F + (I + \alpha 1_F \Gamma_c 1_F)^{-1}] \Gamma_c,$$

equivalently

$$\Gamma_{(1+\alpha 1_F)c} = \Gamma_c + \alpha(I - \Gamma_c) \int_{(0,1)} \frac{d\mu_{1_F \Gamma_c 1_F}(\lambda)}{1 + \alpha \lambda} \Gamma_c$$

Electrical Networks

Theorem

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Proof:

- Application of Sherman-Morrison-Woodbury formula
- Only matters that the perturbation is two-component

Takeaways:

- Spectral decomposition of $1_F \Gamma_c 1_F$ is only relevant object
- $\sigma(1_F \Gamma_c 1_F) \subset [0, 1]$ for same reason as continuum
- Only the spectrum in $(0, 1)$ is needed



Spectral Properties of

$$1_F \Gamma 1_F$$

Spectral Properties of $1_F \Gamma 1_F$

Theorem

Table 1: Spectrum of $\chi \Gamma \chi$, for χ the indicator matrix of edges $F \subset E$

Eigenvalues	Dimension of Eigenspace	Eigenvectors
$\{0\}$	$ E - V + K(G \setminus F)$	deleted edges + cycles in percolated graph
$(0, 1)$	$ V - K(G \setminus F) - K(G \setminus F^c) + 1$	vectors that are cycles on the contracted graph and gradients on the percolated graph
$\{1\}$	$K(G \setminus F^c) - 1$	gradients on contracted graph

For the spectrum in $(0, 1)$, eigenvectors are of the form $\chi_F \nabla f$ where f satisfies

$$\nabla' \chi_F \nabla f = \lambda \nabla' \nabla f$$

Spectral Properties of $1_F \Gamma 1_F$



Li-Fu Chen

Theorem

$$\lambda \in \sigma(1_F \Gamma 1_F) \iff \mathbb{E} \left[\lambda^{|F \cap \mathcal{T}|} (1 - \lambda)^{|F^c \cap \mathcal{T}|} \right] = 0$$

Spectral Properties of $1_F \Gamma 1_F$: Dirichlet case



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- Also have modifications for the Dirichlet setting:

$$\nabla' c \nabla \phi = f \text{ on } V \setminus \partial V, \quad \phi = 0 \text{ on } \partial V$$

- $\Gamma_c^{\partial V}$ = projection onto gradient fields that satisfy BCs
- Spectral decomposition of $1_F \Gamma_c^{\partial V} 1_F$ is relevant for two-component perturbations
- As before: sizes of clusters determine eigenvalue counts in $(0, 1)$
- Partial info about eigenspaces



Cycle Overlap Matrix

Cycle Overlap Matrix

- For spanning tree microstructure eigenvalues can be computed by counting tree overlaps

Theorem

Let \mathcal{T} be a spanning tree of G . The $(0, 1)$ eigenvalues of $\chi_{\mathcal{T}} \Gamma_G \chi_{\mathcal{T}}$ are

$$\frac{1}{1 + \lambda}$$

where λ are the eigenvalues of the *cycle overlap matrix*. The latter is the $E \setminus \mathcal{T} \times E \setminus \mathcal{T}$ Gram matrix with entries

$$\langle \mathcal{P}_e, r \mathcal{P}_{e'} \rangle,$$

where

$\mathcal{P}_e =$ unique path in \mathcal{T} connecting the endpoints of e .

Cycle Overlap Matrix

Proof:



Han Le

- Every spanning tree gives a natural basis of $\text{Range}(\nabla)$
- Compute Γ via this basis, cycle overlap matrix appears



Random Iterated Function Systems

Random Iterated Function Systems

- Choose μ_0 a probability measure on \mathbb{R}_+
- Define random iterated function system via

$$\mu_{j+1} = \text{Law} \left(\frac{X_1^{(j)} X_2^{(j)}}{X_1^{(j)} + X_2^{(j)}} + \frac{X_3^{(j)} X_4^{(j)}}{X_3^{(j)} + X_4^{(j)}} \right)$$

where $X_k^{(j)}$, $k = 1, 2, 3, 4$, are iid with law μ_j

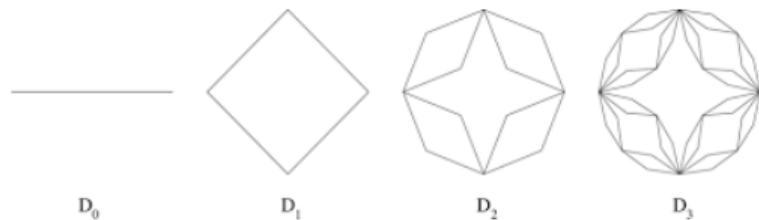
- **Question:** Does

$$\lim_{j \rightarrow \infty} \mu_j$$

exist, and how does it depend on μ_0 ?

Random Iterated Function Systems

- IFS arises as effective resistance on diamond hierarchical lattice



- Extensive literature on existence of limit
[H000, WW99, LR99, Jor02, SWW00, Weh97, Shn87]
- Limit is always a delta mass at a constant

$$\lim_{j \rightarrow \infty} \mu_j = \delta_c, \quad c = F(\mu_0)$$

- Dependence of c on μ_0 is poorly understood

Random Iterated Function Systems



Loren Santana

Theorem

For $h > 0$ and $\mu_0 = p\delta_h + (1-p)\delta_1$,

$$\lim_{n \rightarrow \infty} \mathcal{ER}(D_n) = 1 + \sum_{k=1}^3 M_k(p)(h-1)^k + O((h-1)^4),$$

where $M_k(p)$ are explicit polynomials in p :

$$M_1(p) = -p, \quad M_2(p) = \frac{p}{3}(2+p), \quad M_3(p) = -\frac{p}{9}(4+6p-p^2)$$

Random Iterated Function Systems



Sudheesh
Surendranath

Theorem

For $h > 0$ and $\mu_0 = p\delta_h + (1 - p)\delta_1$,

$$\lim_{n \rightarrow \infty} \mathbb{E}[\text{Tr}(1_{\mathbb{F}} \Gamma_n 1_{\mathbb{F}})^k] = Q_k(p),$$

where $M_k(p)$ are explicit polynomials in p , computed for $k \leq 4$.

Work in progress:

- Limit for every k to get limiting empirical spectral measure
- Computation via enumeration of maps
- Relation to Bell polynomials
- Rank one perturbations and changes to Stieltjes transform



Future Directions

Future Directions

- Probabilistic characterizations of spectral properties
- Changes in spectral properties under exploration/growth of F
- Random graphs $G = (V, E, c)$ with random edge set $F \subset E$:
 - Spectral statistics through hamburger-cheeseburger bijection
 - Effective parameters via ergodicity plus local graph properties
- Infinite volume versions
- Exploit conformal symmetries in continuum setting
- Connections to random matrix distributions

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