

Mathematics of Frozen Seas

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Homogenization for Composite Materials



composites & metamaterials











negative index of refraction metamaterials



UC Berkeley

AccSci

acoustic and seismic metamaterials





structural cloak





TheTech Co

Warner Bros.

U. Missouri

porous sea ice



porous rock

Gaspari



Weeks

invisibility cloak



Carbon chemistry and nanomaterials



Central theme:

How do we use "small scale" information to find effective behavior on larger scales relevant to climate and ecological models?

OBJECTIVE: advance how sea ice is represented in climate models improve projections of fate of SEA ICE and its ECOSYSTEMS

HOMOGENIZATION for Composite Materials



Maxwell 1873, Einstein 1906 Wiener 1912, Hashin and Shtrikman 1962



strong, expensive, heavy weak, cheap, light stee reinforced concrete rods concrete breaks apart under tension strong, cheap light WOO. plywood strong in fiber directum strong 0000 in 2 (or all) but fibers can 0 4 00 divections be pulled apart / |° 0 ° 0 00 like a poly cryptal!

O(X) dectrical conductivity $\int \int f(x) = \sigma(x) E(x)$ $\int f(x) = \sigma(x) E(x)$ $\int f(x) = \sigma(x) E(x)$ $\int f(x) = e_x$ $\int f(x) = e_x$ $\int f(x) = e_x$ <E>= IRI E dx curvent electric B.C. on \$ field density \$= electric potential Gauss: $\nabla \cdot J = \int_{\Lambda}$ Sources = 0 5 - 1 $\nabla x E = O$ $\overline{\gamma}, \overline{j} = 0 \Longrightarrow \overline{\gamma}, (\sigma \overline{\gamma} \phi) = 0$ /Laplace in each phase BUT ...

classical transport problems: 'equivalent" permithvity E displacement Delectield E dielectros $D = \varepsilon E = -\varepsilon \nabla \phi$ mag permeability M mag. in an chion B muz field H magnetism - temp-gradient thermal k g=-kPT heat ament g Thermal cond. diffusivity D conc. gradgent DC particle flux dittusion 2=-DVC permeability K fluid vel. V pressure gradient VP Darcy's Law find flow $V = -K \nabla P$

Homo genization $\sigma(x) = \sigma_1 \gamma_1(x) + \sigma_2 \gamma_2(x)$ $|\mathcal{L}| = \sqrt{\frac{5}{62}}$ $\chi_1(\chi) = \begin{cases} 1 & \chi \in med 1 \\ 0 & \chi \in med 2 \end{cases}$ $\chi_2 = 1 - \chi_1$ $\langle \vec{E} \rangle = \frac{1}{V} \int E dx = e_{\kappa}$ $\nabla \cdot J = O$ locally $J(x) = \sigma(x) E(x)$ 7xE=0 homogenized $\langle J \rangle = J^{\star} \langle E \rangle$ effective conductivity $\sigma^* = \frac{1}{\sqrt{\sigma}} = E_k dx$

Variational Formulation of Effective Conductivity
energy dissipated in a conducting medium
$$\mathcal{L}$$

per unit vol.
 $\mathcal{L} = \frac{1}{2V} \int \mathcal{J} \cdot \mathcal{E} \, dx$
 $\langle \mathcal{E} \rangle = \mathcal{E}_{k}$
 $if homogeneous, \quad \sigma(x) = \sigma^{*} \quad \mathcal{L}$
 $\mathcal{L} = \frac{1}{2V} \int \sigma(x) \cdot \mathcal{E}(x) \cdot \mathcal{E}(x) \, dx$

$$\frac{1}{2} \sigma^{*} e_{k} \cdot \bar{e}_{k} = \mathcal{U} = \frac{1}{2} \frac{1}{\sqrt{v}} \int \sigma E \cdot \bar{E} dx$$

$$\sigma^{*} = \frac{1}{\sqrt{v}} \int \sigma E \cdot \bar{E} dx$$

$$\int e^{vergy} \frac{1}{v tegral}$$
Now, do variational calculation of energy integral
$$E = -\nabla \varphi \quad \varphi \rightarrow \varphi + S \varphi \quad , S \varphi \Big|_{\partial D} = 0$$
subject to condition $\nabla x E = 0$,
$$Subject to condition \nabla x E = 0, \quad (Exercise!)$$

$$Dotain minimum that solves \nabla \cdot J = 0$$

$$= \int (I = mM - \int \int \sigma F \cdot F \, dx \qquad \text{Solution} \\ \nabla xF = \sigma \quad \forall \int \sigma F \cdot F \, dx \qquad \text{Solution} \\ \text{Satisfies} \quad \nabla \cdot \sigma F = 0$$

Jual
Variational vary
$$U = \frac{1}{2V} \int \overline{J} \cdot \overline{J} \, dx$$
 subject to $\overline{P} \cdot \overline{J} = 0$
Principle T minimum satisfies $\overline{Vx}(\overline{J}) = 0$
 $\overline{Vx} = \min_{\overline{V}} \frac{1}{\overline{V}} \int \overline{\sigma(x)} E(x) \cdot \overline{E(x)} \, dx$ (1)
 $\overline{Vx} = -\infty$
 $\frac{1}{\sigma^*} = \min_{\overline{V}} \frac{1}{\sqrt{J}} \int \frac{1}{\sigma(x)} \overline{J(x)} \cdot \overline{J(x)} \, dx$ (2)

Obtain bounds by putting in a "trial field" into the variational principle simplest try: E=ek m (1) $J = \ell_k \quad in \quad (2)$ 07 < <07 Avithmetic Mean Bound (1) =)Harmonic $(2) = \overline{}$ $\frac{1}{\sigma^*} \leq \langle \frac{1}{\sigma} \rangle$ Mean Bound arithmetic harmonic $\frac{1}{\langle \overline{\sigma} \rangle} \leq \sigma^* \leq \langle \sigma \rangle$ mean mean

These bounds are optimal i.e. I actual composité geométries that attain The bounds 2 phase materials $\vec{c} \rightarrow$ $\frac{1}{\frac{P_1}{\sigma_1} + \frac{P_2}{\sigma_2}} \leq O^* \leq P_1 \sigma_1 + P_2 \sigma_2$ Hashin & Shtrikman 1963 Assume iso tropy coated spheres optimal

arithmetic and harmonic mean bounds on transport properties

effective electrical conductivity σ^* for two phase composite of σ_1 and σ_2

optimal bounds on σ^* for known volume fractions p_1 and p_2 :





other approaches · Effective Medylum Theories, CPA replace surroundings with homogeneous medsur TBD $p \ll 1$ · Volume traction expansions (small p) · Expansion around homogeneous medium σ, \sim · Almost touching geometries



Remote sensing of sea ice



sea ice thickness ice concentration

INVERSE PROBLEM

Recover sea ice properties from electromagnetic (EM) data

8*

effective complex permittivity (dielectric constant, conductivity)



brine volume fraction brine inclusion connectivity Effective complex permittivity of a two phase composite in the quasistatic (long wavelength) limit



the components

 $\epsilon^* = \epsilon^* \left(\frac{\epsilon_1}{\epsilon_2} \right)$, composite geometry

What are the effective propagation characteristics of an EM wave (radar, microwaves) in the medium?

Analytic Continuation Method for Homogenization

Bergman (1978), Milton (1979), Golden and Papanicolaou (1983), Theory of Composites, Milton (2002)



Golden and Papanicolaou, Comm. Math. Phys. 1983

complexities of mixture geometry



spectral properties of operator (matrix) ~ quantum states, energy levels for atoms

eigenvectors

eigenvalues

EXTEND to: polycrystals, advection diffusion, waves through ice pack

forward and inverse bounds on the complex permittivity of sea ice



forward bounds



Golden 1995, 1997

_ _

Inverse Homogenization Cherkaev and Golden (1998), Day and Thorpe (1999), Cherkaev (2001), McPhedran, McKenzie, Milton (1982), *Theory of Composites*, Milton (2002)



inverse bounds and recovery of brine porosity Gully, Backstrom, Eicken, Golden Physica B, 2007 inversion for brine inclusion separations in sea ice from measurements of effective complex permittivity ϵ^*

rigorous inverse bound on spectral gap

construct algebraic curves which bound admissible region in (p,q)-space

Orum, Cherkaev, Golden Proc. Roy. Soc. A, 2012

inverse bounds



SEA ICE



young healthy trabecular bone



HUMAN BONE

old osteoporotic trabecular bone





spectral characterization of porous microstructures in human bone

reconstruct spectral measures from complex permittivity data



use regularized inversion scheme

apply spectral measure analysis of brine connectivity and spectral inversion to electromagnetic monitoring of osteoporosis

Golden, Murphy, Cherkaev, J. Biomechanics 2011

the math doesn't care if it's sea ice or bone!

Homogenization for polycrystalline materials



Find the homogeneous medium which behaves macroscopically the same as the inhomogeneous medium



Mathematical formulation for composite materials



$$\vec{\nabla} \cdot \vec{J} = 0, \quad \vec{\nabla} \times \vec{E} = 0, \quad \vec{J} = \sigma \vec{E}, \quad \vec{E} = \vec{\nabla} \phi + \vec{e}_k, \quad \langle \vec{E} \rangle = \vec{e}_k$$

Polycrystalline material

Local conductivity

$$\sigma = R \operatorname{diag}(\sigma_1, \sigma_2, \sigma_2) R^T$$
$$= \sigma_1 X_1 + \sigma_2 X_2$$

 $X_2 = I - X_1$



Continuum composite



Discrete composite



Random Rotation Matrix

Bounds on the complex permittivity of polycrystalline materials by analytic continuation

> Adam Gully, Joyce Lin, Elena Cherkaev, Ken Golden

 Stieltjes integral representation for effective complex permittivity

Milton (1981, 2002), Barabash and Stroud (1999), ...

- Forward and inverse bounds orientation statistics
- Applied to sea ice using two-scale homogenization
- Inverse bounds give method for distinguishing ice types using remote sensing techniques





Proc. Roy. Soc. A 8 Feb 2015

ISSN 1364-5021 | Volume 471 | Issue 2174 | 8 February 2015

PROCEEDINGS A



An invited review commemorating 350 years of scientific publishing at the Royal Society

A method to distinguish between different types of sea ice using remote sensing techniques A computer model to determine how a human should walk so as to expend the least energy



two scale homogenization for polycrystalline sea ice



Gully, Lin, Cherkaev, Golden, Proc. Roy. Soc. A (and cover) 2015

Rigorous bounds on the complex permittivity tensor of sea ice with polycrystalline anisotropy in the horizontal plane

Kenzie McLean, Elena Cherkaev, Ken Golden 2022

motivated byWeeks and Gow, JGR 1979: c-axis alignment in Arctic fast ice off BarrowGolden and Ackley, JGR 1981: radar propagation model in aligned sea ice

input: orientation statistics

output: bounds



Re(ϵ^*)

direct calculation of spectral measures

Murphy, Hohenegger, Cherkaev, Golden, Comm. Math. Sci. 2015

- depends only on the composite geometry
- discretization of microstructural image gives binary network
- fundamental operator becomes a random matrix
- spectral measure computed from eigenvalues and eigenvectors

once we have the spectral measure μ it can be used in Stieltjes integrals for other transport coefficients:

electrical and thermal conductivity, complex permittivity, magnetic permeability, diffusion, fluid flow properties

earlier studies of spectral measures

Day and Thorpe 1996 Helsing, McPhedran, Milton 2011

Spectral computations for sea ice floe configurations



Murphy, Cherkaev, Golden, Phys. Rev. Lett. 2017

Eigenvalue Statistics of Random Matrix Theory

Wigner (1951) and Dyson (1953) first used random matrix theory (RMT) to describe quantized energy levels of heavy atomic nuclei.

 $[N]_{ij} \sim N(0,1),$ $A = (N+N^T)/2$ Gaussian orthogonal ensemble (GOE) $[N]_{ij} \sim N(0,1) + iN(0,1),$ $A = (N+N^T)/2$ Gaussian unitary ensemble (GUE)

Short range and long range correlations of eigenvalues are measured by various eigenvalue statistics.



Universal eigenvalue statistics arise in a broad range of "unrelated" problems!



Anderson localization

disorder-driven

metal / insulator transition

Anderson 1958 Mott 1949 Evangelou 1992 Shklovshii et al 1993

Wave equations

propagation vs. localization in wave physics: quantum, optics, acoustics, water waves

Laplace + Diffusion equations

we find percolation-driven

Anderson transition for classical transport in composites

mobility edges, localization, universal spectral statistics

Murphy, Cherkaev, Golden Phys. Rev. Lett. 2017

but no wave interference or scattering effects at play!

Where to look to see this behavior exploited in tunable media that display rich transport properties?

Go back to the dawn of ordered, aperiodic materials quasicrystals.

Shechtman et al. 1984 Levine & Steinhardt 1984

Order to Disorder in Quasiperiodic Composites

D. Morison (Physics), N. B. Murphy, E. Cherkaev, K. M. Golden, Communications Physics 2022



quasiperiodic checkerboard Stampfli, 2013



energy surface Al-Pd-Mn quasicrystal Unal et al., 2007

quasiperiodic crystal

quasicrystal



dense packing of dodecahedra 3D Penrose tiling Tripkovic, 2019

ordered but aperiodic

lacks translational symmetry

Shechtman et al., *Phys. Rev. Lett.*, 1984 Levine & Steinhardt, *Phys. Rev. Lett.*, 1984

classical transport in quasiperiodic media

Golden, Goldstein & Lebowitz, *Phys. Rev. Lett.*, 1985 Golden, Goldstein & Lebowitz, *J. Stat. Phys.*, 1990



Holmium-magnesium-zinc quasicrystal



aperiodic tiling of the plane - R. Penrose 1970s

:

1D, 2D inhomogeneous materials - quasiperiodic

$$\sigma(x) = 3 + \cos x + \cos kx$$

effective conductivity

$$\sigma^*(k) = \begin{cases} \text{constant} & k \text{ irrational } \text{quasiperiodic} \\ f(k) & k \text{ rational } \text{periodic} \end{cases}$$

Golden, Goldstein, Lebowitz Classical transport in modulated structures, Phys. Rev. Lett. 1985

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G. Bouchitté, S. Guenneau, F. Zolla, SIAM Multiscale Modeling & Simulation, 2010

E. Cherkaev, S. Guenneau, N. Wellander, IEEE Metamaterials, 2017

N. Wellander, S. Guenneau, E. Cherkaev, Math. Methods in the Applied Sci., 2017


line of slope k through an infinite checkerboard

Classical transport in quasiperiodic media

Golden, Goldstein, and Lebowitz Phys. Rev. Lett. 1985 J. Stat. Phys. 1990

1D two component composite material

effective conductivity $\sigma^*(k)$ effective resistivity $1/\sigma^*(k) = 1 - G(k)$

$$G(k) = \begin{cases} 0, & k \text{ irrational} \\ 1/pq, & k = p/q \text{ rational} \end{cases}$$

continuous at *k* irrational discontinuous at *k* rational



Moiré patterns generate two component composites on any scale

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quantum dots artificial atoms

Tran et al. Nature 2019



Small Difference in Moiré Parameters

Big Difference in Material Properties

Wide Variety of Microgeometries





Wide Variety of Microgeometries





Order to disorder in quasiperiodic composites

Morison, Murphy, Cherkaev, Golden, Comm. Phys. 2022



twisted bilayer composites

sea ice - inspired high tech spin off

tunable Moiré composites with exotic properties

(optical, electrical, thermal, ...), Anderson localization; our Moiré patterned geometries are similar to twisted bilayer graphene

but can be engineered on any scale!



we bring the solid state physics framework for electronic transport and band gaps in semiconductors to classical transport in periodic and quasiperiodic composites

Anderson transition as twist angle is tuned

photonic crystals and quasicrystals

communications physics

Explore content Y About the journal Y Publish with us Y

<u>nature</u> > communications physics

Order to disorder in quasiperiodic composites

constellation of periodic systems in a sea of randomness



David Morison, N. Benjamin Murphy ... Kenneth M. Golden Article 14 June 2022

Moiré parameter space

Featured

Article Open Access 10 Jan 2023	Versatile tuning of Kerr soliton microcombs in crystalline microresonators High-repetition rate microresonator-based frequency combs offer powerful and compact optical frequency comb sources that are of great importance to various applications. Here, the authors extend the tunability of the Kerr soliton frequency combs by exploiting thermal effects and frequency stabilization techniques. Shun Fujii, Koshiro Wada Takasumi Tanabe	
Article	Compliant mechanical response of the ultrafast folding protein EnHD	b c 250-1 (01.07) (01
Open Access	under force	200- 201 2 150-
12 Jan 2023	Exhibiting low-energy (un)folding barriers and fast kinetics, ultrafast folding proteins are enticing models to study protein dynamics. The authors use single molecule force spectroscopy AFM to capture the compliant behaviour hallmarking the dynamics of ultrafast folding proteins under force.	

Antonio Reifs, Irene Ruiz Ortiz ... Raul Perez-Jimenez

Fractal arrangement of periodic systems



Sequential insets zooming into smaller regions of parameter space.

size of the dots ~ length of period

(large dot ~ small period; small dot ~ large period; white space ~ "infinite" period)

ocean wave propagation through the sea ice pack





- wave-ice interactions critical to growth and melting processes
- break-up; pancake promotion floe size distribution

effective layer parameter previously fit to wave data

Keller 1998 Mosig, Montiel, Squire 2015 Wang, Shen 2012

Analytic Continuation Method Bergman 1978, Milton 1979 Golden and Papanicolaou 1983 Milton, *Theory of Composites* 2002



homogenized parameter depends on sea ice concentration and ice floe geometry

like EM waves



Storm-induced sea-ice breakup and the implications for ice extent

Kohout et al., Nature 2014

- during three large-wave events, significant wave heights did not decay exponentially, enabling large waves to persist deep into the pack ice.
- Iarge waves break sea ice much farther from the ice edge than would be predicted by the commonly assumed exponential decay





ice extent compared with significant wave height

Waves have strong influence on both the floe size distribution and ice extent.

Two Layer Models and Effective Parameters



 ν

Viscous fluid layer (Keller 1998) Effective Viscosity ν

Equations of $\frac{\partial U}{\partial t} = -\frac{1}{\rho}\nabla P + \nu\nabla^2 U + g$

Viscoelastic fluid layer (Wang-Shen 2010) Effective Complex Viscosity $\nu_e = \nu + iG/\rho\omega$

Equations of $\frac{\partial U}{\partial t} = -\frac{1}{\rho}\nabla P + \nu_e \nabla^2 U + g$

Viscoelastic thin beam (Mosig et al. 2015) Effective Complex Shear Modulus $G_v = G - i\omega\rho\nu$

Stieltjes integral representation for effective complex viscoelastic parameter; bounds

Sampson, Murphy, Cherkaev, Golden 2017



Single effective rheological parameter (Mosig et al. 2015)

$$u^* = G - i\omega\rho v$$

Effective complex viscoelasticity

 $\frac{i\omega\rho v}{i\omega\rho v} \quad \frac{\nu}{\nu_2} = ||\epsilon_s^0||^2(1-F(s))$ $\frac{\rho}{\nu_2} = |\epsilon_s^0||^2(1-F(s))$ $F(s) = \int_0^1 \frac{d\mu(\lambda)}{s-\lambda}$ microscale

z=h

z=0

7=-H

 u^*

divergence-free deviatoric stress

 $\nabla \cdot \sigma_s = 0$

$$egin{aligned} rac{ extsf{microscale}}{\sigma_s = 2
u \epsilon_s} & rac{ extsf{\sigma}_s}{\langle \sigma_s
angle = 2
u^* \epsilon_s^0} &
u(ec{x}) = \chi_1
u_1 + \chi_2
u_2 & \langle \epsilon_s
angle = \epsilon_s^0 &
extsf{vector} \end{aligned}$$

Kelvin-Voigt model

Ice

Ocean

Integral representation

Bottom

Forward bounds for the effective viscoelasticity are fitted to well known wave-ice datasets, including *Wadhams et al. 1988, Newyear & Martin 1997, Wang & Shen 2010, Meylan et al. 2014,* and several others!



Waves in sea ice and solid state physics



PR



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The cover is based on "Modeling Sea Ice," page 1535.

NSF Research Training Grant (RTG) with 15 Applied Math faculty:

optimization and inverse problems

July 2022 - June 2027

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 - Provide transformative experiences that draw students into math.

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OPEN POSITIONS: Postdoctoral, Ph.D., Undergraduate

Arctic Mathpedition 2024

NSF RTG Arctic Mathpedition, May 2024

on the frozen Arctic Ocean north of Utqiagvik, AK

We took 7 math students working on sea ice models to the Arctic to do *experiments* on the physics and biology of sea ice.

Jody Reimer, Ken Golden [Seth & Tarn] Anthony Lee David Gluckman Kathy Lin Nash Ward Daniel Hallman Anthony Jajeh Delaney Mosier Marco Lozzi High School Undergraduate Undergraduate Undergraduate Graduate Student Graduate Student Graduate Student Student Photojournalist

see what you're modeling; close the gap between theory and experiment; connect physics & bio; experience climate change first-hand; math outreach to locals

Math Dept Colloquium, Nov 21

NSF RTG Arctic Mathpedition 2, May 2026

















bottom of a sea ice core

