

# **Mathematics of Frozen Seas**

Ken Golden, University of Utah

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

classical transport problems: 'equivalent" permithvity E displacement Delectield E dielectros  $D = \varepsilon E = -\varepsilon \nabla \phi$ mag permeability M maz. induction B muz field H magnetism - temp-gradient thermal k g=-kPT heat ament g Thermal cond. diffusibily 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  $\nabla x E = 0$ ,
$$\int e^{vercise!}$$

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

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  $\sigma^*$  for two phase composite of  $\sigma_1$  and  $\sigma_2$ 

*optimal bounds* on  $\sigma^*$  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  $\sigma, \sim$ · 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  $\epsilon^*$ 

### 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



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

### **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(**  $\epsilon^*$  )

# 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  $\mu$  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

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<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	<b>Versatile tuning of Kerr soliton microcombs in crystalline microresonators</b> 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- 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**



 $\nu$ 

Viscous fluid layer (Keller 1998) Effective Viscosity  $\nu$ 

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

 $\nabla \cdot \sigma_s = 0$ 

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

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



### of the American Mathematical Society

November 2020

Volume 67, Number 10







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

**Overall goal:** Build an advanced, competitive U.S. STEM workforce.

- Strengthen our graduate and postdoctoral programs in applied math to attract top students in the nation, and place them in top jobs.
  - Provide transformative experiences that draw students into math.

### Arctic Mathpeditions - May 2024 & 2026

# **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

