Herglotz functions and homogenization for waves in random and quasiperiodic composites

Kenneth M. Golden   **University of Utah**

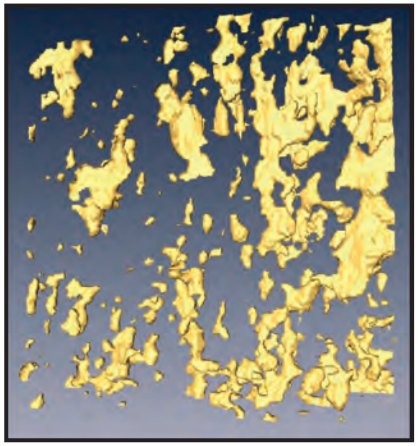
KOZWaves, Melbourne
17 February 2020

Sea Ice is a Multiscale Composite Material

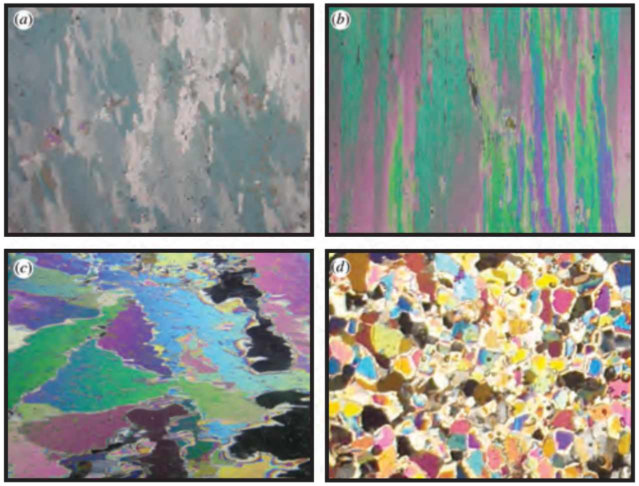
sea ice microstructure

brine inclusions


Weeks & Assur 1969


H. Eicken
Golden *et al. GRL* 2007

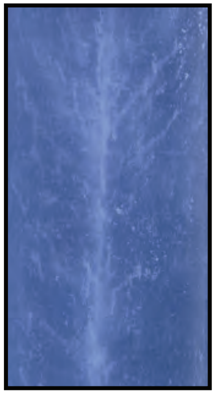
polycrystals



Gully *et al. Proc. Roy. Soc. A* 2015

brine channels


D. Cole


K. Golden

millimeters

centimeters

---

sea ice mesostructure

sea ice macrostructure

Arctic melt ponds


K. Frey

Antarctic pressure ridges


K. Golden

sea ice floes


J. Weller

sea ice pack


NASA

meters

kilometers

What is this talk about?

A tour of Herglotz functions and waves in composite media, motivated by sea ice and its role in the climate system.

Use methods of statistical physics and homogenization to compute effective behavior (and improve climate models).

1. ***EM waves in sea ice, spectral measures, quasiperiodicity***

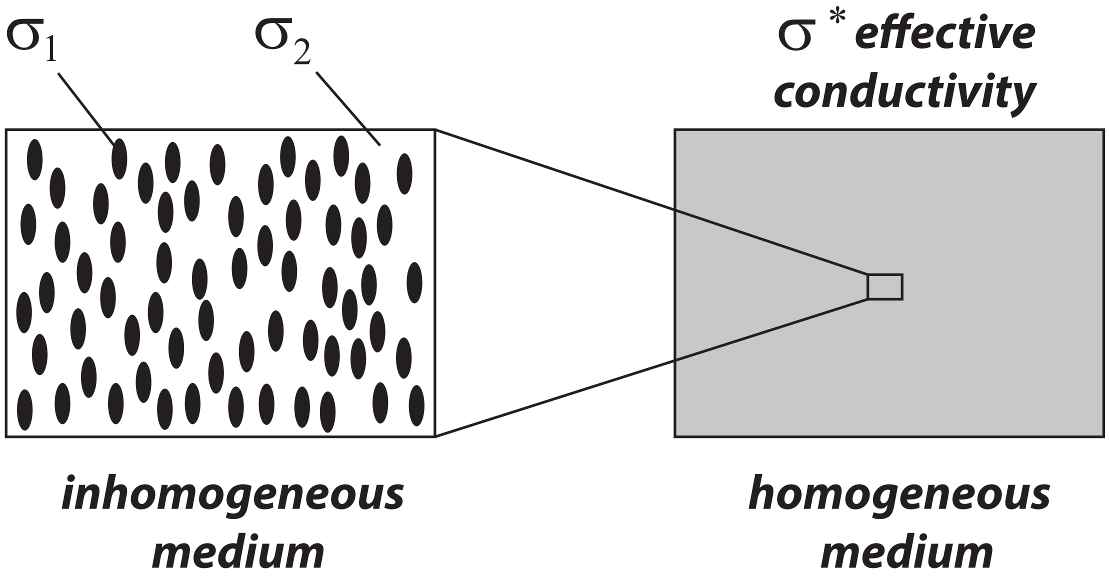
   random matrix theory and Anderson transitions

2. ***Extension to polycrystals, ocean waves in sea ice***

   Stieltjes integral representations, spectral measures

3. ***Light in sea ice, melt ponds***

HOMOGENIZATION - Linking Scales in Composites



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

Maxwell 1873 : effective conductivity of a dilute suspension of spheres
Einstein 1906 : effective viscosity of a dilute suspension of rigid spheres in a fluid

*Wiener 1912 : arithmetic and harmonic mean **bounds** on effective conductivity*
*Hashin and Shtrikman 1962 : variational **bounds** on effective conductivity*

widespread use of composites in late 20th century due in large part to advances in mathematically predicting their effective properties

Remote sensing of sea ice

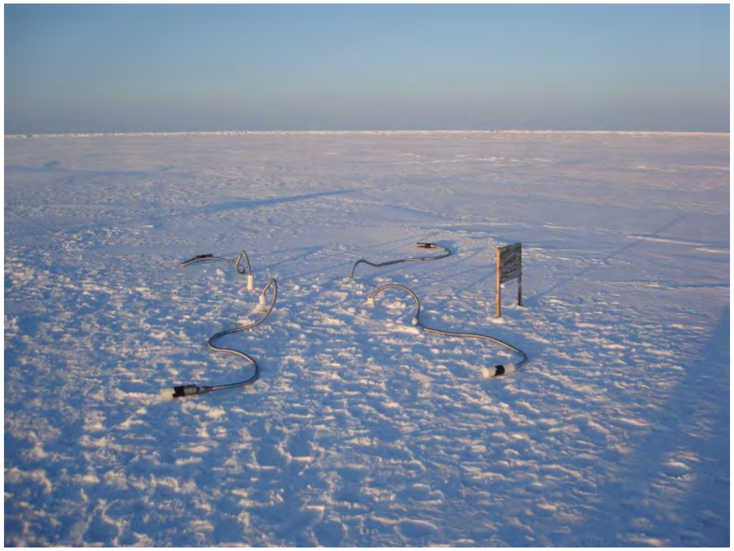
sea ice thickness
ice concentration

INVERSE PROBLEM

Recover sea ice properties from electromagnetic (EM) data

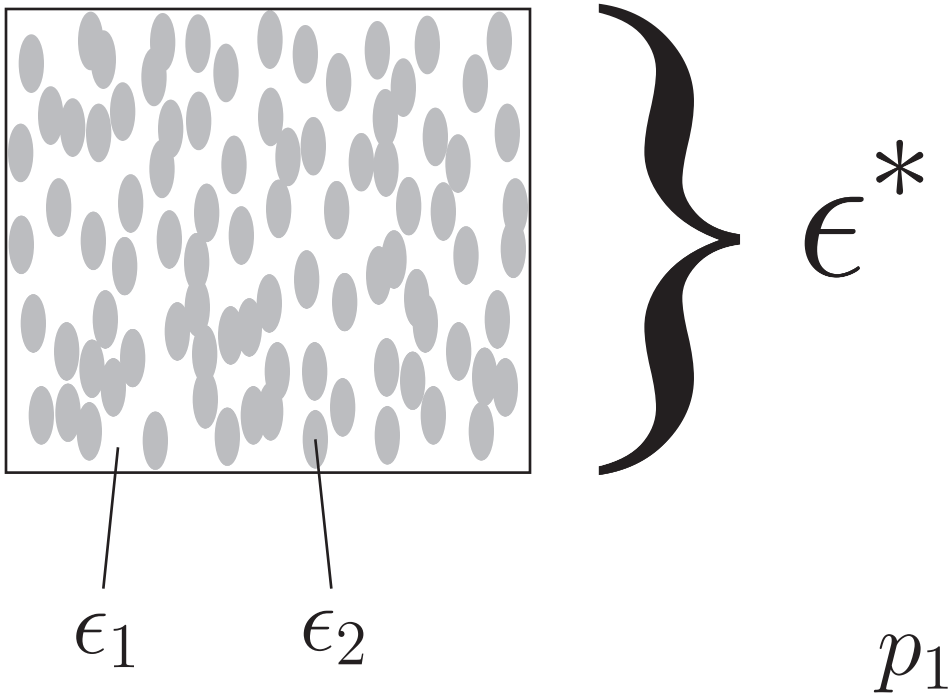
ε^*

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



$$D = \epsilon E$$

$$\nabla \cdot D = 0$$

$$\nabla \times E = 0$$

$$\langle D \rangle = \epsilon^* \langle E \rangle$$

p_1 , p_2 = volume fractions of the components

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

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)

Stieltjes integral representation for homogenized parameter

separates geometry from parameters

geometry

$$F(s) = 1 - \frac{\epsilon^*}{\epsilon_2} = \int_0^1 \frac{d\mu(z)}{s - z} \qquad s = \frac{1}{1 - \epsilon_1 / \epsilon_2}$$

material parameters

μ

- spectral measure of self adjoint operator $\Gamma\chi$
- mass = p_1
- higher moments depend on n-point correlations

$$\Gamma = \nabla(-\Delta)^{-1}\nabla\cdot$$

$\chi =$ characteristic function of the brine phase

$$E = s\,(s + \Gamma\chi)^{-1} e_k$$

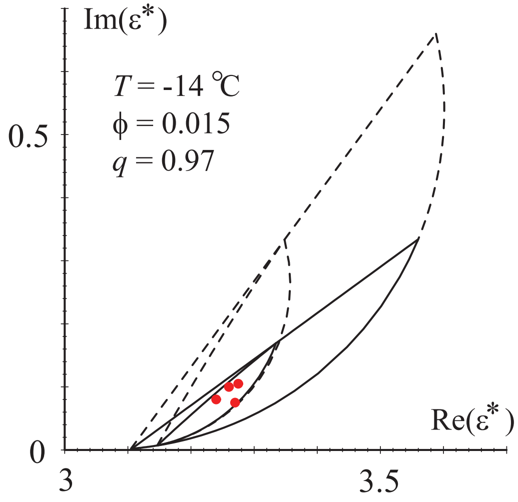
$\Gamma\chi$: **microscale** ⟶ **macroscale**

$\Gamma\chi$ ***links scales***

Golden and Papanicolaou, Comm. Math. Phys. 1983

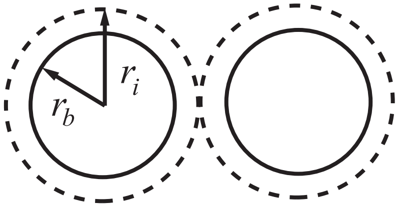
forward and inverse bounds on the complex permittivity of sea ice

forward bounds



4.75 GHz data

matrix particle



$$q = r_b / r_i$$

$$0 < q < 1$$

Golden 1995, 1997

Inverse Homogenization

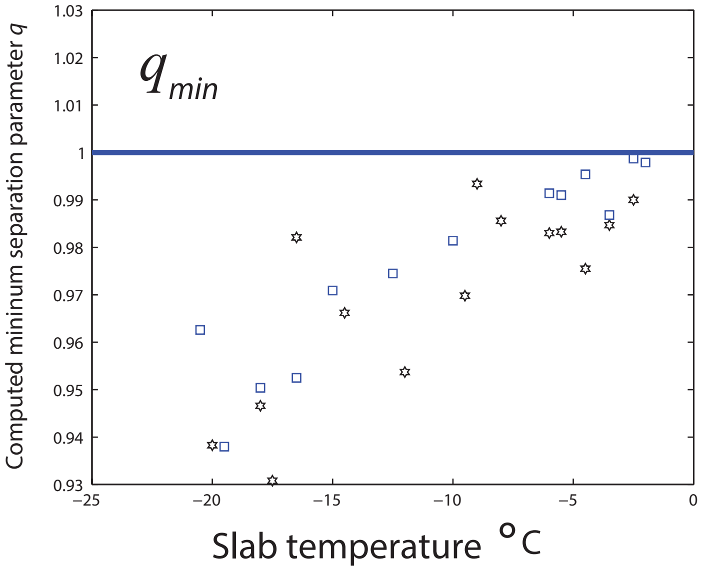
Cherkaev and Golden (1998), Day and Thorpe (1999), Cherkaev (2001), McPhedran, McKenzie, Milton (1982), *Theory of Composites*, Milton (2002)

ε^* → ***composite geometry*** **(spectral measure μ)**

inverse bounds and recovery of brine porosity

Gully, Backstrom, Eicken, Golden
Physica B, 2007

inverse bounds



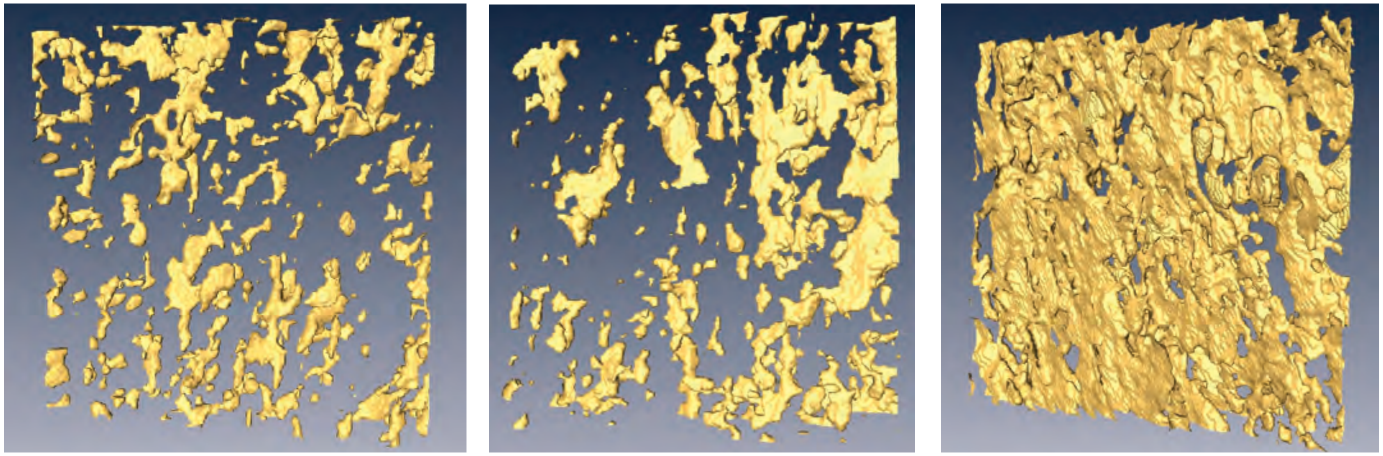
inversion for brine inclusion separations in sea ice from measurements of effective complex permittivity ε^*

rigorous inverse bound
on spectral gap

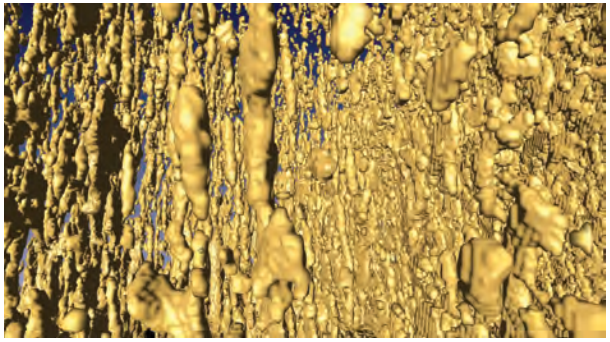
construct algebraic curves which bound admissible region in (p,q)-space

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

brine volume fraction and ***connectivity*** increase with temperature



T = -15 °C, $\phi = 0.033$ | T = -6 °C, $\phi = 0.075$ | T = -3 °C, $\phi = 0.143$



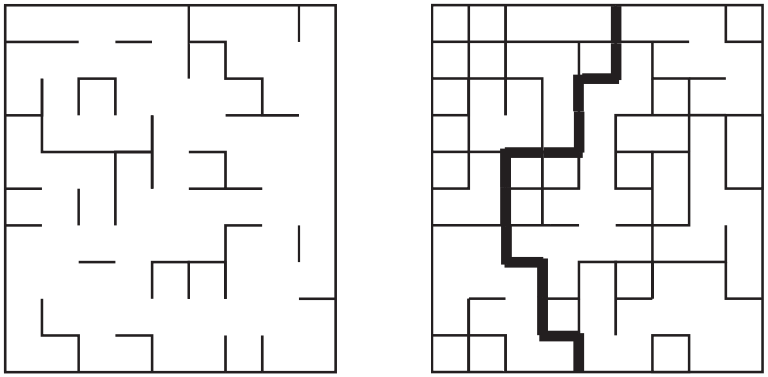
T = -4 °C, $\phi = 0.113$

X-ray tomography for brine phase in sea ice

Golden, Eicken, *et al., Geophysical Research Letters* 2007

PERCOLATION THRESHOLD $\phi_c \approx 5\ \%$

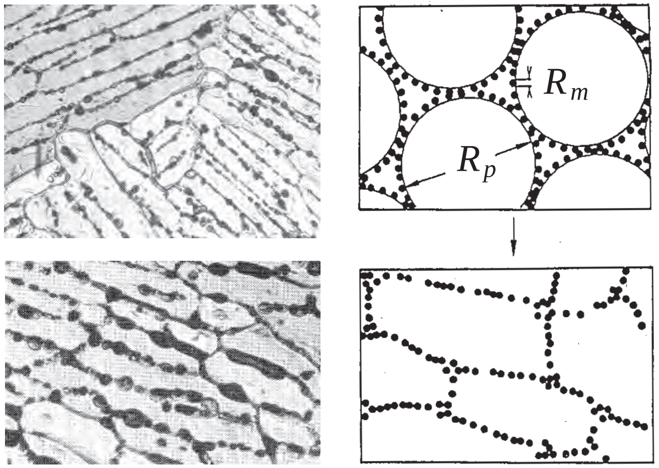
Golden, Ackley, Lytle, *Science* 1998



impermeable | permeable

$p = 1/3$ | $p = 2/3$

lattice percolation



Kusy, Turner
Nature 1971

sea ice | compressed powder

continuum percolation

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

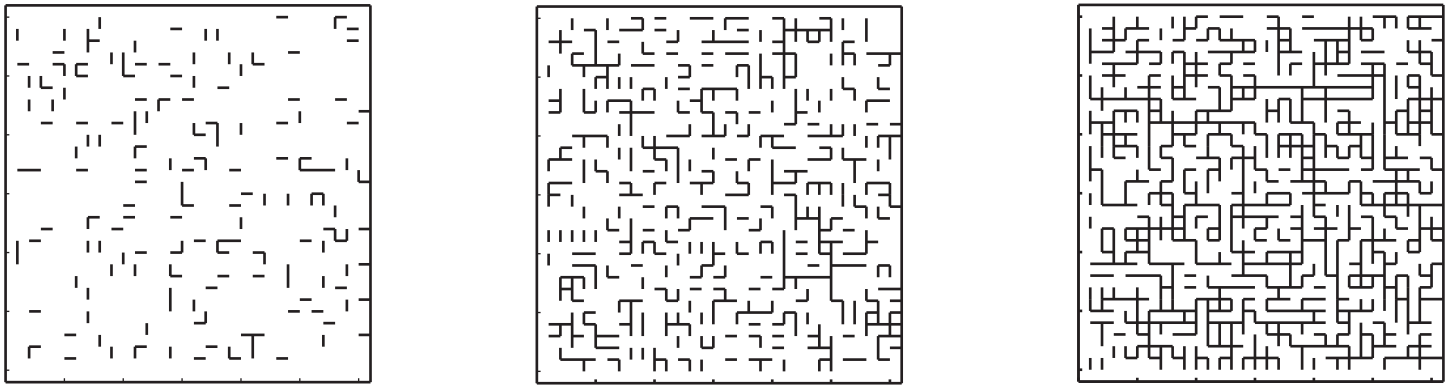
once we have the spectral measure μ it can be used in Stieltjes integrals for other transport coefficients:

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

earlier studies of spectral measures

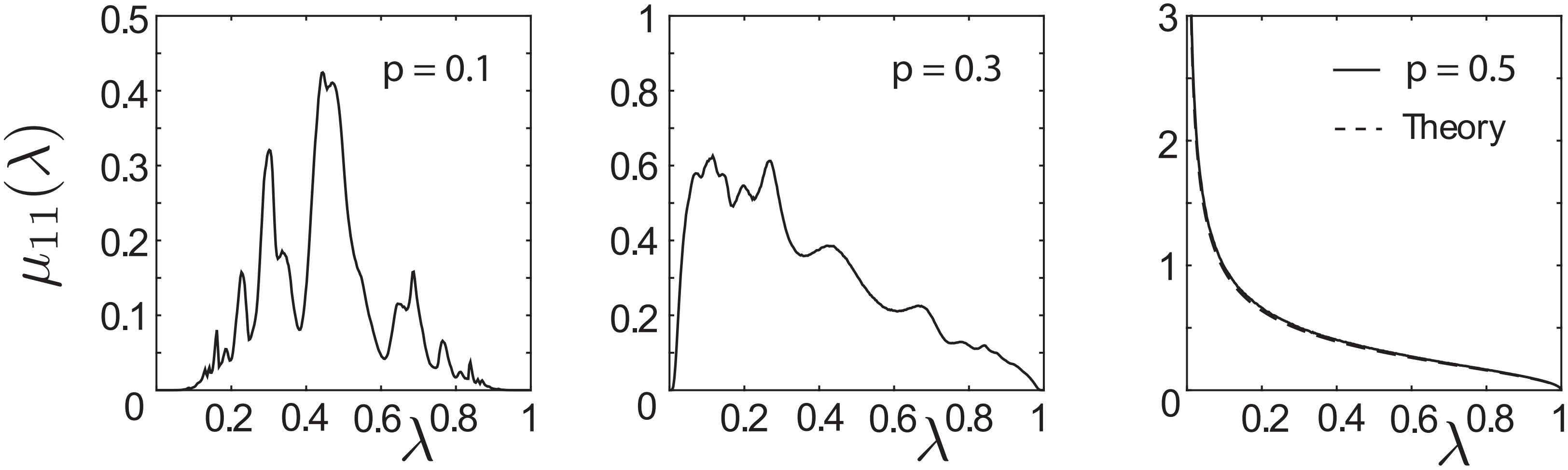
Day and Thorpe 1996
Helsing, McPhedran, Milton 2011

Spectral statistics for 2D random resistor network



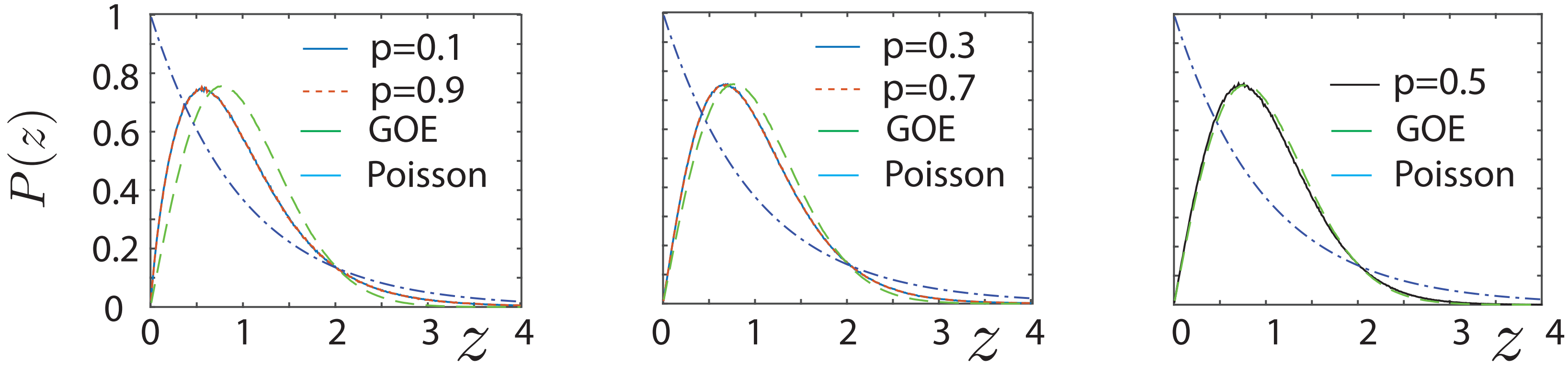
Spectral Measures

Murphy and Golden, *J. Math. Phys.*, 2012
Murphy et al. *Comm. Math. Sci.*, 2015



$p_c = 0.5$

Eigenvalue Spacing Distributions



Murphy, Cherkaev, Golden, *PRL*, 2017

Eigenvalue Statistics of Random Matrix Theory

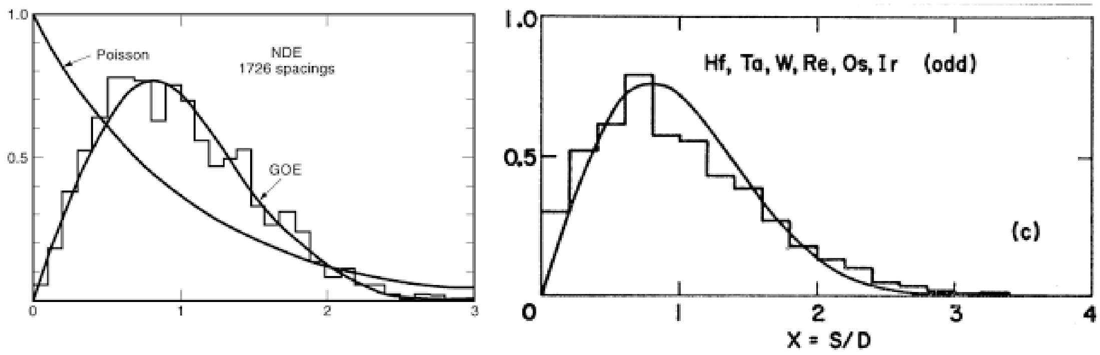
Wigner (1951) and Dyson (1953) first used random matrix theory (RMT) to describe quantized energy levels of heavy atomic nuclei.

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

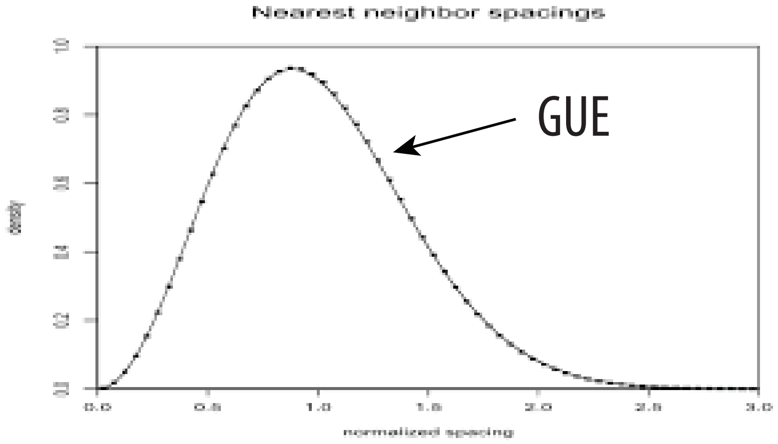
$[\mathbf{N}]_{ij} \sim N(0,1)+iN(0,1)$, $\mathbf{A} = (\mathbf{N}+\mathbf{N}^{\dagger})/2$ ***Gaussian unitary ensemble (GUE)***

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

Spacing distributions of energy levels for heavy atomic nuclei



Spacing distributions of the first billion zeros of the Riemann zeta function



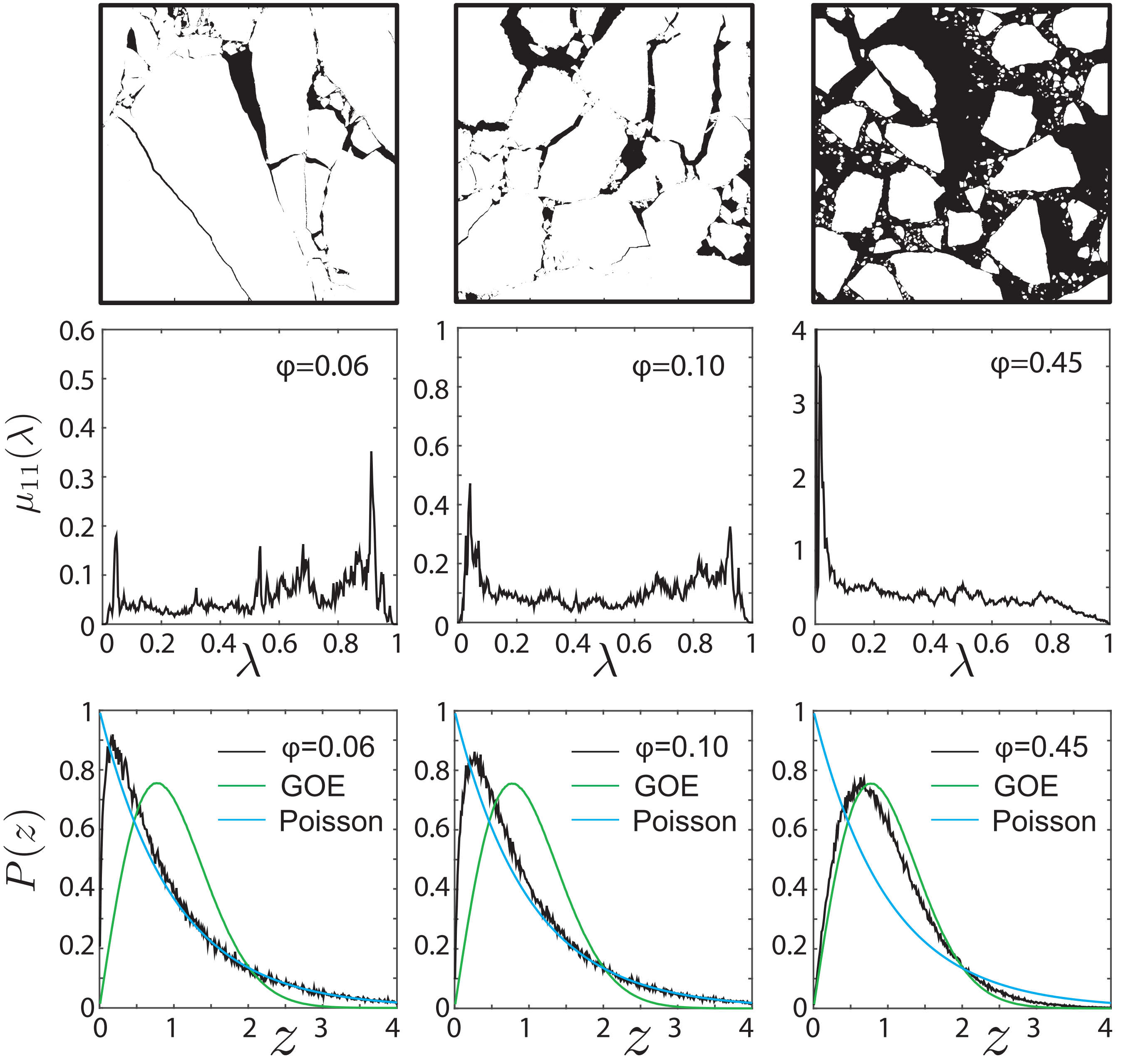
RMT used to characterize disorder-driven transitions in mesoscopic conductors, neural networks, random graph theory, etc.

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

Spectral computations for sea ice floe configurations

spectral measures

eigenvalue spacing distributions

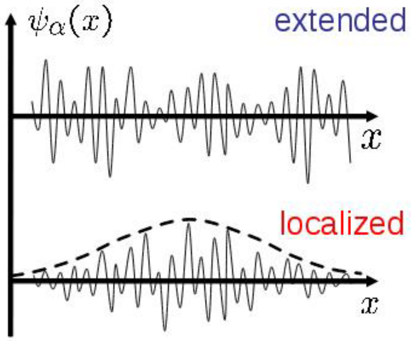


uncorrelated → **level repulsion**

UNIVERSAL Wigner-Dyson distribution

ANDERSON TRANSITION

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



metal / insulator transition

localization

Anderson 1958
Mott 1949
Shklovshii et al 1993
Evangelou 1992

Anderson transition in wave physics:
quantum, optics, acoustics, water waves, ...

we find a surprising analog

Anderson transition for classical transport in composites

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

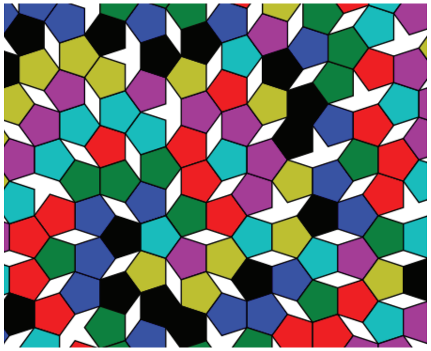
PERCOLATION TRANSITION → **transition to universal eigenvalue statistics (GOE)**
extended states, mobility edges

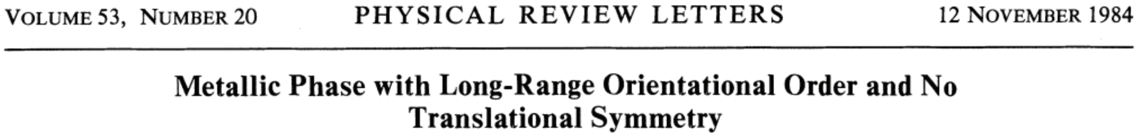
-- but without wave interference or scattering effects ! --

Order to Disorder in Quasiperiodic Materials

Morison, Murphy, Cherkaev, Golden, 2020

Quasiperiodic Microstructure -- Ordered but Not Periodic





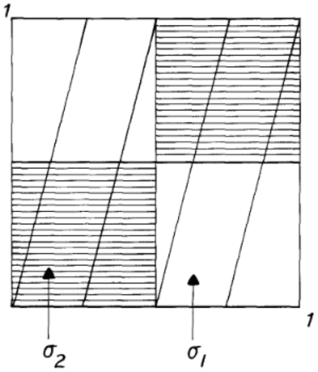
VOLUME 53, NUMBER 20 PHYSICAL REVIEW LETTERS 12 NOVEMBER 1984

Metallic Phase with Long-Range Orientational Order and No Translational Symmetry

In 1984, the discovery of quasicrystals by D. Shechtman opens a new branch of materials science and leads to a Nobel Prize in 2011.

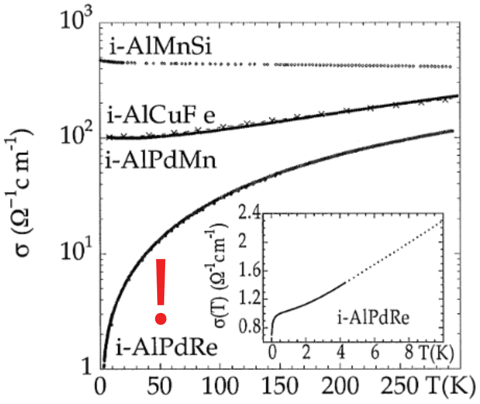
Prior to 1984, quasiperiodicity appears in art, architecture, math, not in phyics of natural systems.

classical transport in quasiperiodic composites



Golden, Goldstein, Lebowitz
Phys. Rev. Lett. 1985

Golden, Goldstein, Lebowitz
J. Stat. Phys. 1990



C. Berger, et al. Physica B: Condensed Matter (2000)

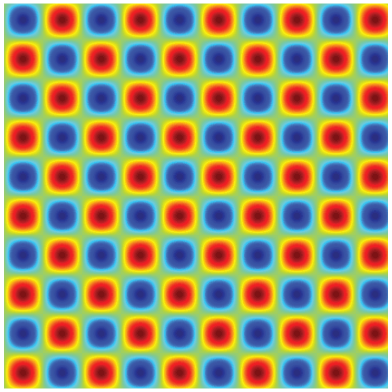
Many quasicrystals exhibit surprising bulk properties, such as aluminum alloys, which are insulating !

Quasiperiodic systems governed by classical physics are of great interest in plasmonics, terahertz and composites research.

Quasiperiodic geometry determined by (p,q) Moiré pattern

- Moiré Pattern
- Level Set
- Discretization

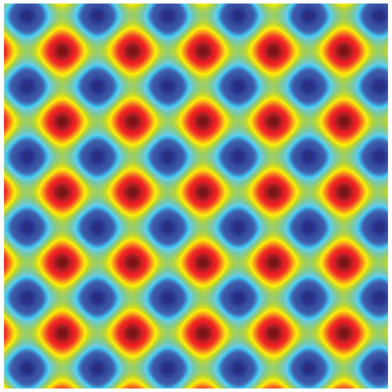
$$\psi_p = \cos\left(\frac{2\pi}{L}px\right)\cos\left(\frac{2\pi}{L}py\right)$$



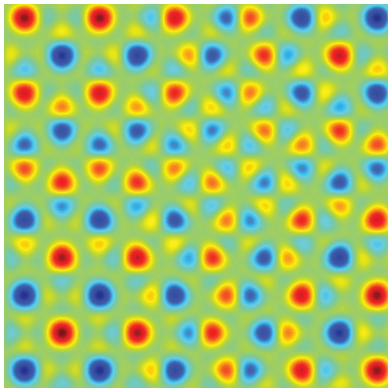
$$u = \frac{1}{2}(x+y)$$

$$v = \frac{1}{2}(x-y)$$

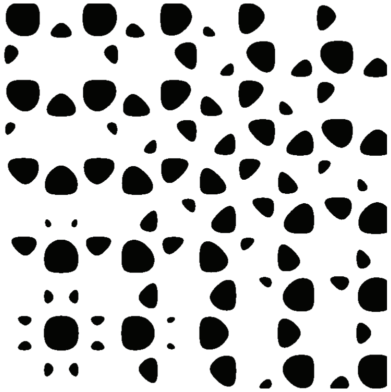
$$\psi_q = \cos\left(\frac{2\pi}{L}qu\right)\cos\left(\frac{2\pi}{L}qv\right)$$



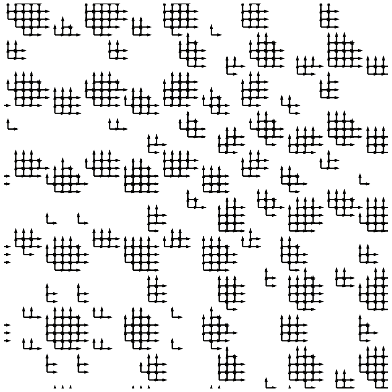
$$\psi = \psi_p \psi_q$$



$$\chi = \begin{cases} 1, \psi \geq \xi \\ 0, \psi < \xi \end{cases}$$

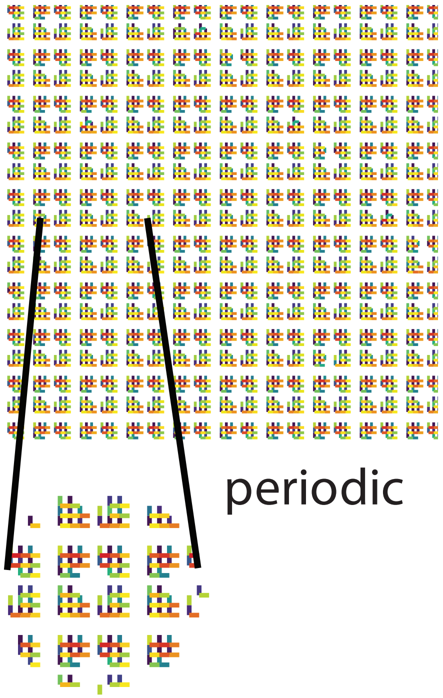


Cartesian Network

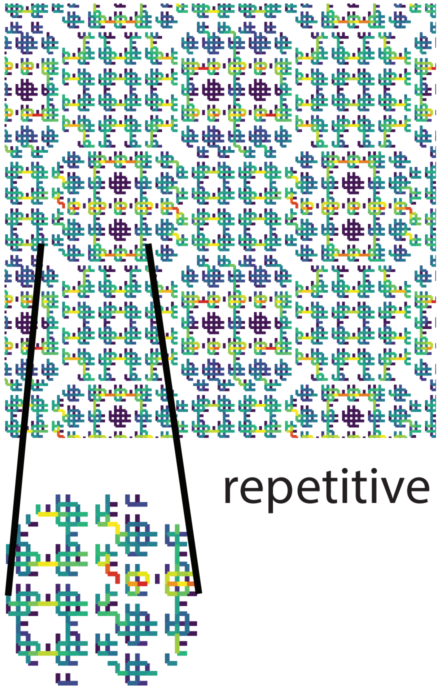


Example Microgeometries

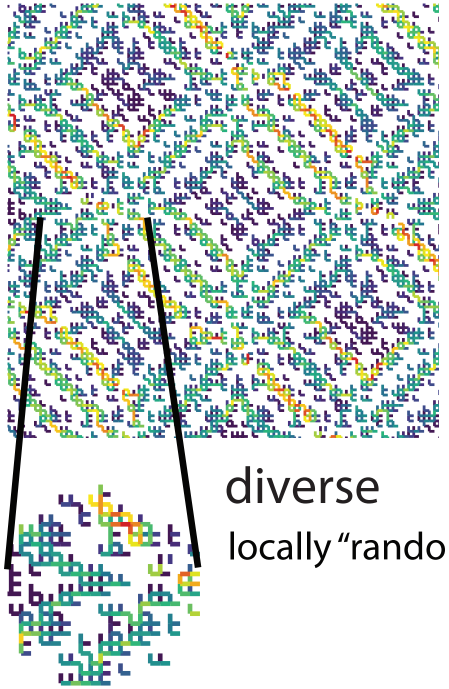
Periodic



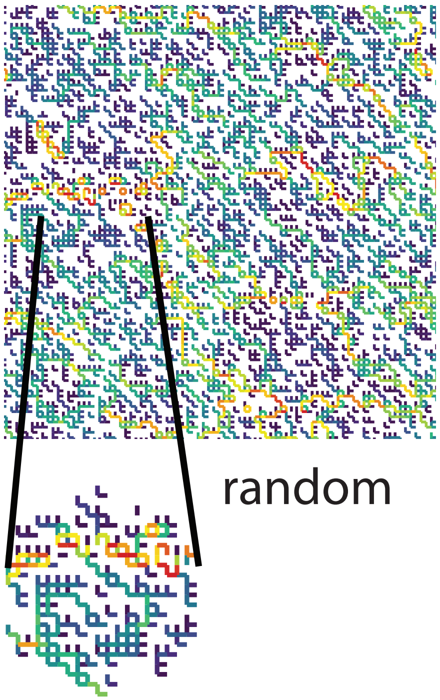
Moiré $p \ll q$



Moiré $p \sim q$



Random



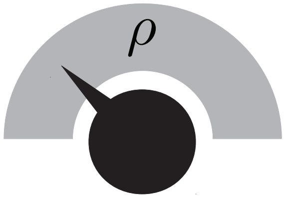
- set a shared system size $L = \mathrm{lcm}\,(p, q)$

quasiperiodicity can interpolate - via spectral measure - between periodic and random

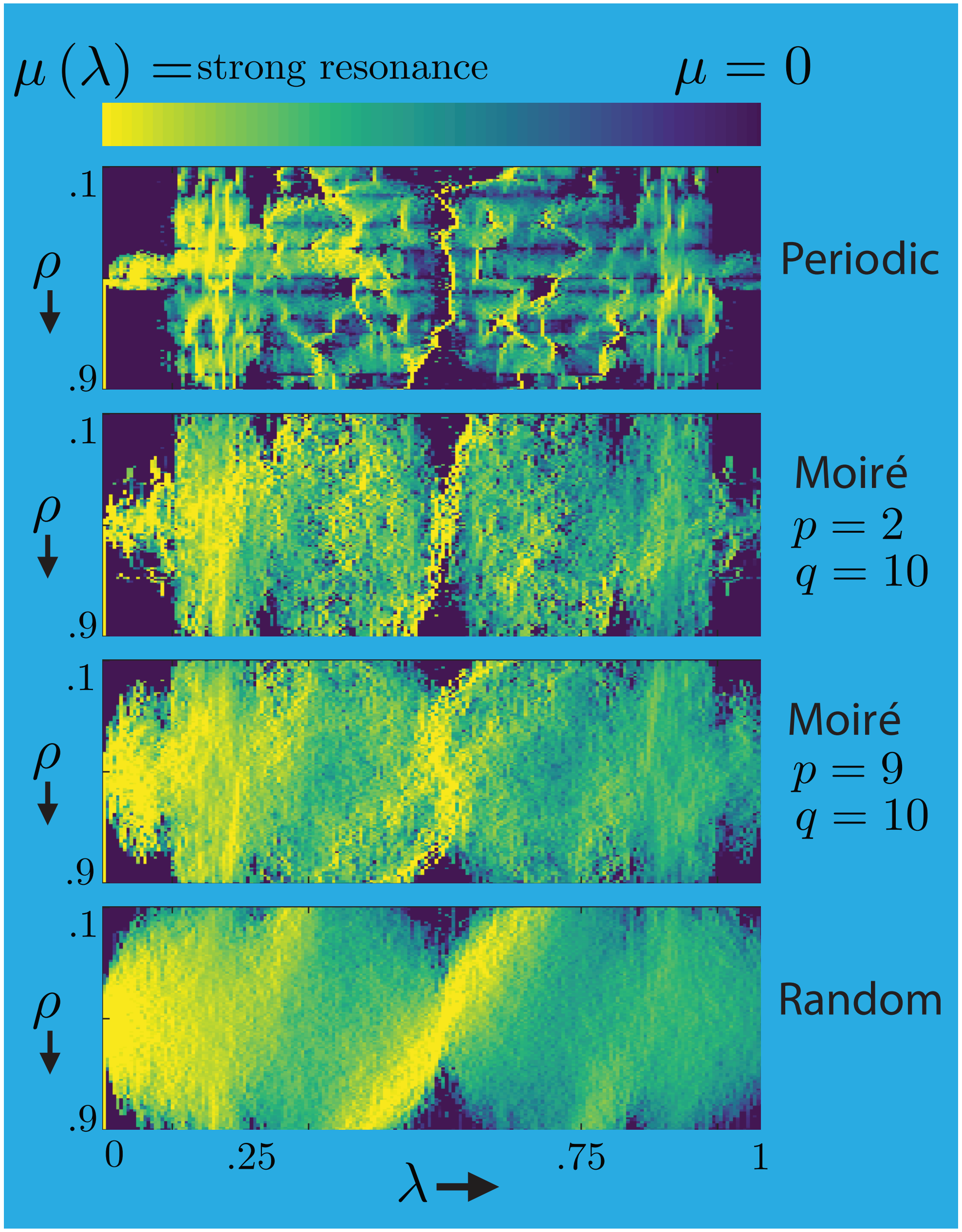
$\mu\left(\lambda\right)$

System Geometry

Bulk Properties



Level Set



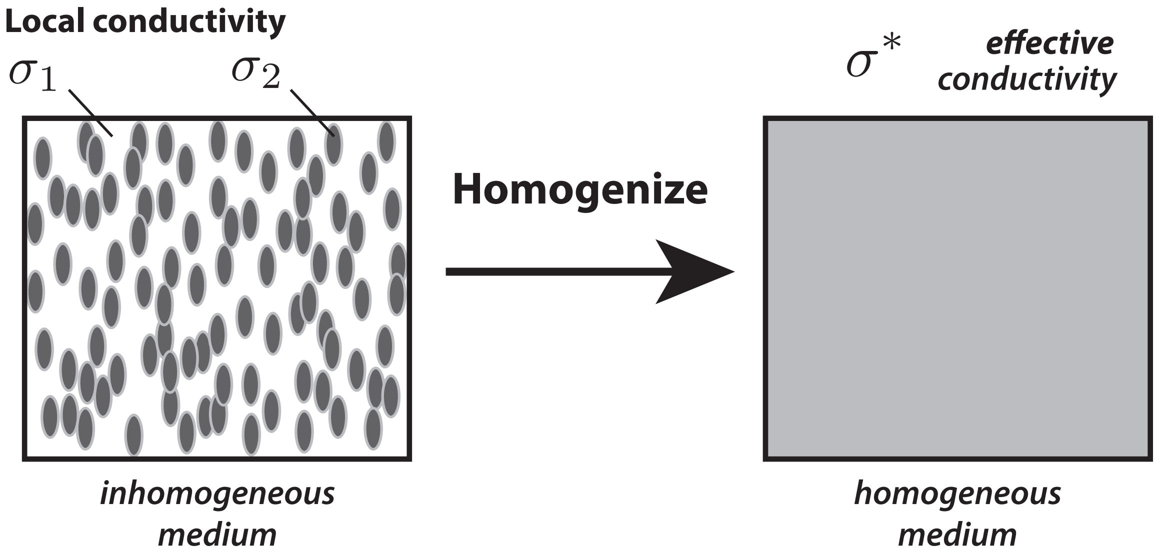
sharp resonances and large eigenvalue gaps

diffuse spectra and correlated eigenvalues

+ results on eigenvalue spacings, localization

Homogenization for polycrystalline materials

Two-component composites



Local conductivity

σ_1 σ_2

inhomogeneous medium

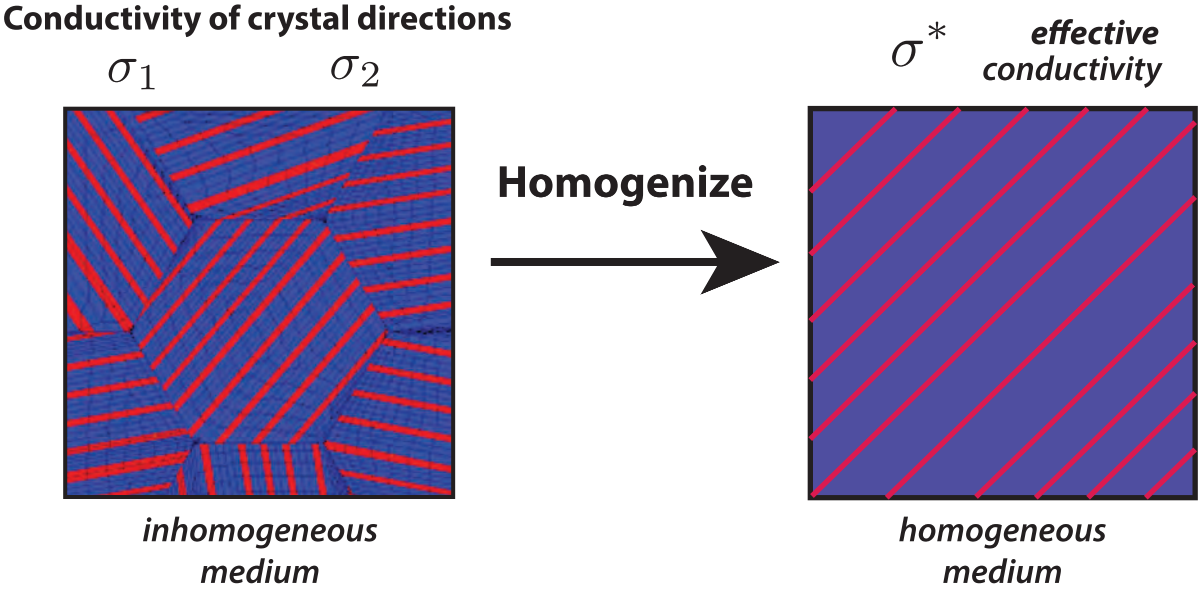
Homogenize

σ^* ***effective conductivity***

homogeneous medium

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

Polycrystalline media



Conductivity of crystal directions

σ_1 σ_2

inhomogeneous medium

Homogenize

σ^* ***effective conductivity***

homogeneous medium

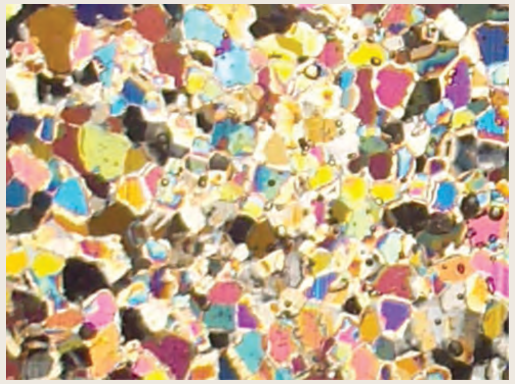
Bounds on the complex permittivity of polycrystalline materials by analytic continuation

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

Proc. R. Soc. A | Volume 471 | Issue 2174 | 8 February 2015

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

PROCEEDINGS A

350 YEARS
OF SCIENTIFIC
PUBLISHING

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

THE
ROYAL
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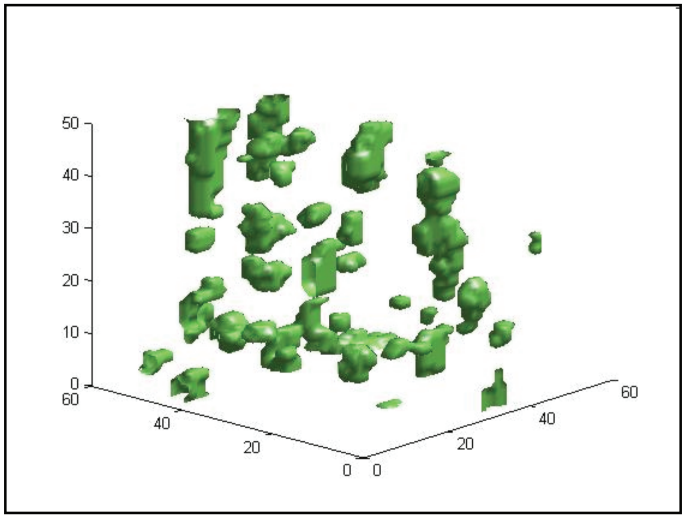
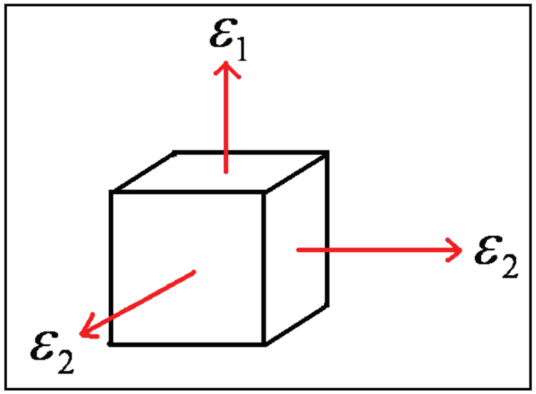
21/01/15 1:47 PM

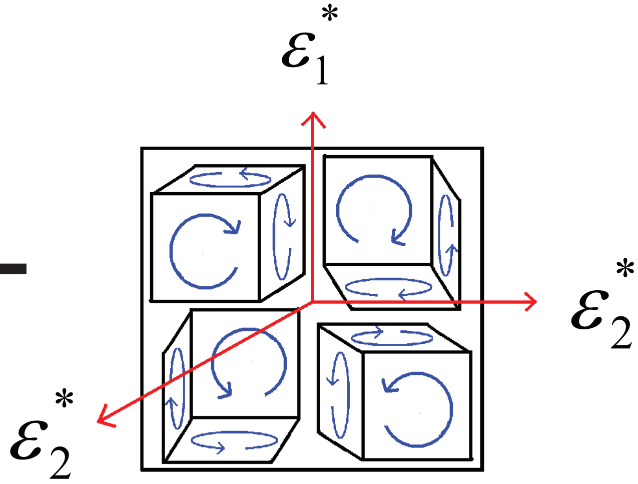
two scale homogenization for polycrystalline sea ice



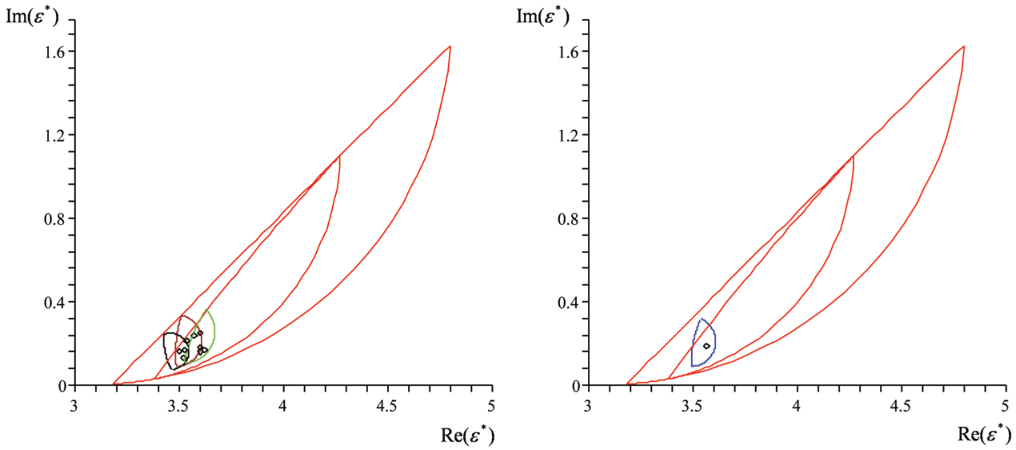
numerical homogenization for single crystal



analytic continuation for polycrystals



bounds



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

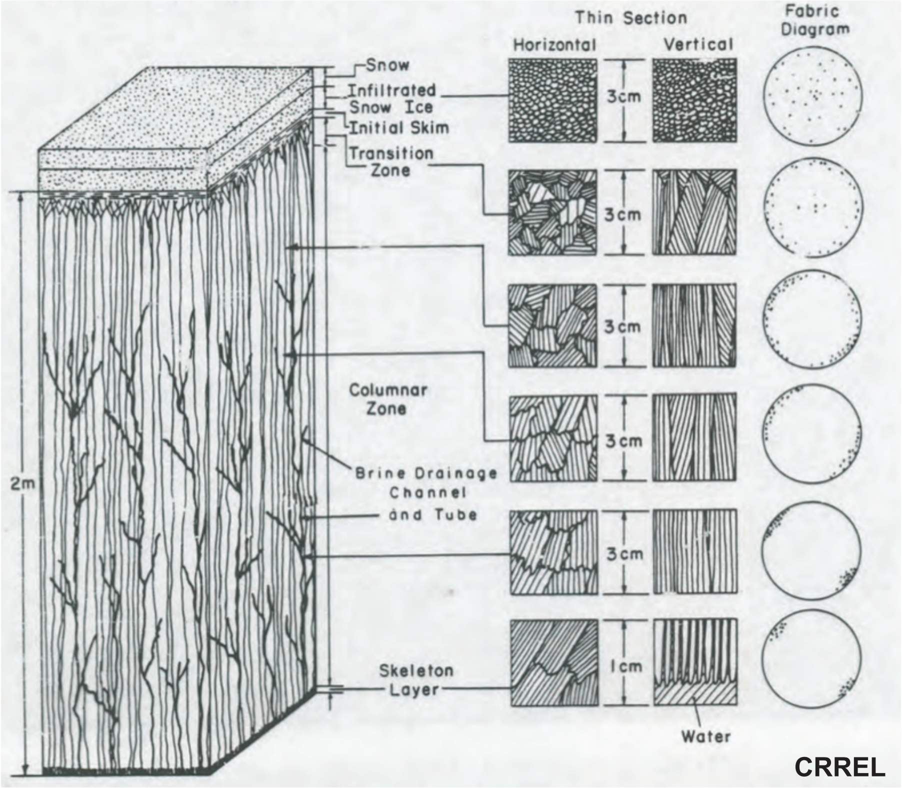
Rigorous bounds on the complex permittivity tensor of sea ice with polycrystalline anisotropy within the horizontal plane

McKenzie McLean, Elena Cherkaev, Ken Golden 2020

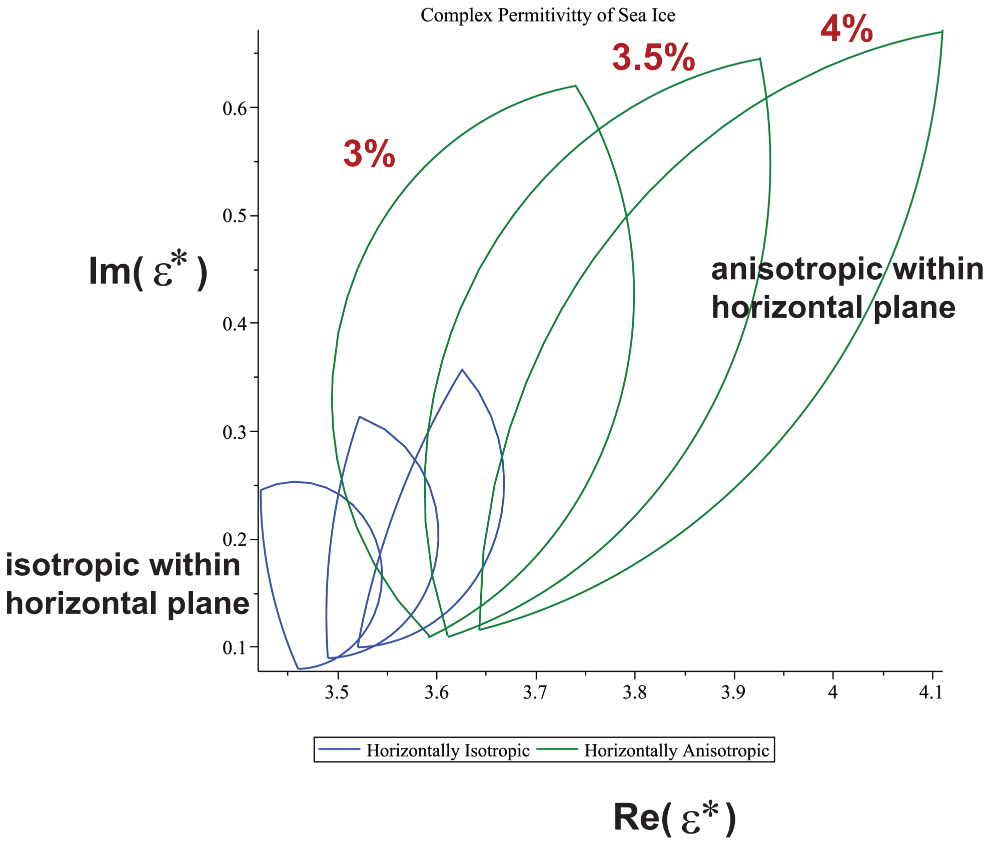
motivated by **Weeks and Gow, *JGR* 1979: c-axis alignment in Arctic fast ice off Barrow**

Golden and Ackley, *JGR* 1981: radar propagation model in aligned sea ice

input: orientation statistics



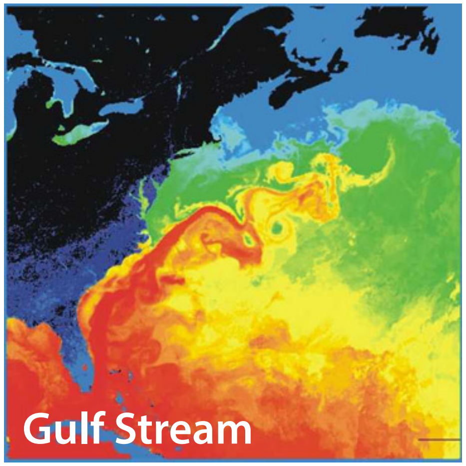
output: bounds

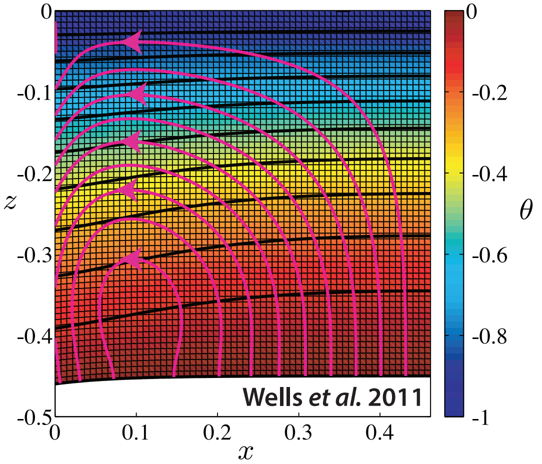


advection enhanced diffusion

effective diffusivity

nutrient and salt transport in sea ice
heat transport in sea ice with convection
sea ice floes in winds and ocean currents
tracers, buoys diffusing in ocean eddies
diffusion of pollutants in atmosphere





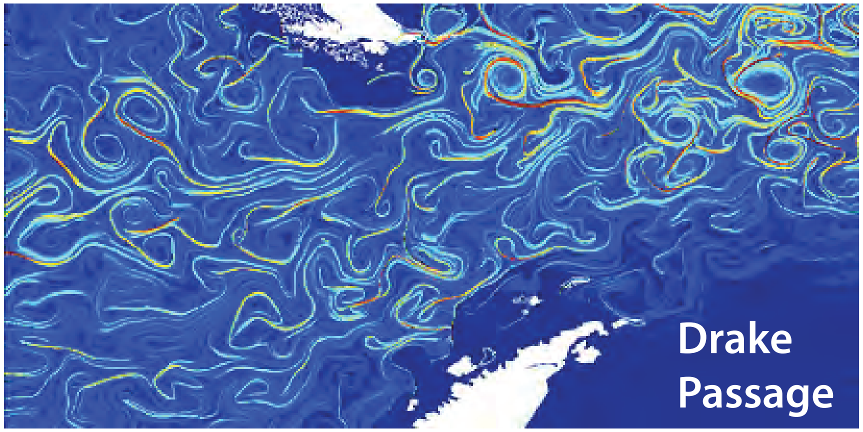
advection diffusion equation with a velocity field $\vec{u}$

$$\frac{\partial T}{\partial t} + \vec{u} \cdot \vec{\nabla} T = \kappa_0 \Delta T$$

$$\vec{\nabla} \cdot \vec{u} = 0$$

$$\Big\downarrow \quad \textit{homogenize}$$

$$\frac{\partial \overline{T}}{\partial t} = \kappa^* \Delta \overline{T}$$



κ^* ***effective diffusivity***

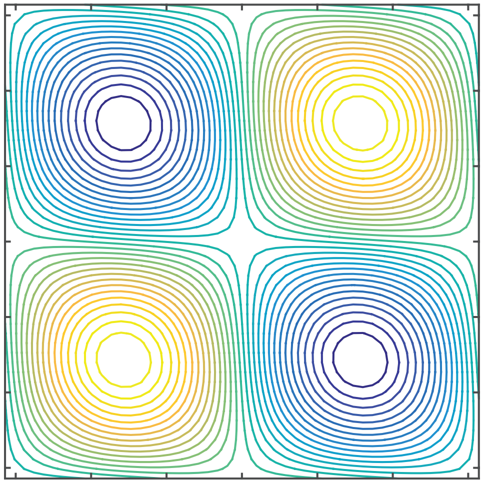
Stieltjes integral for κ^* with spectral measure

Avellaneda and Majda, PRL 89, CMP 91

Murphy, Cherkaev, Xin, Zhu, Golden, *Ann. Math. Sci. Appl.* 2017
Murphy, Cherkaev, Zhu, Xin, Golden, *J. Math. Phys.* 2020

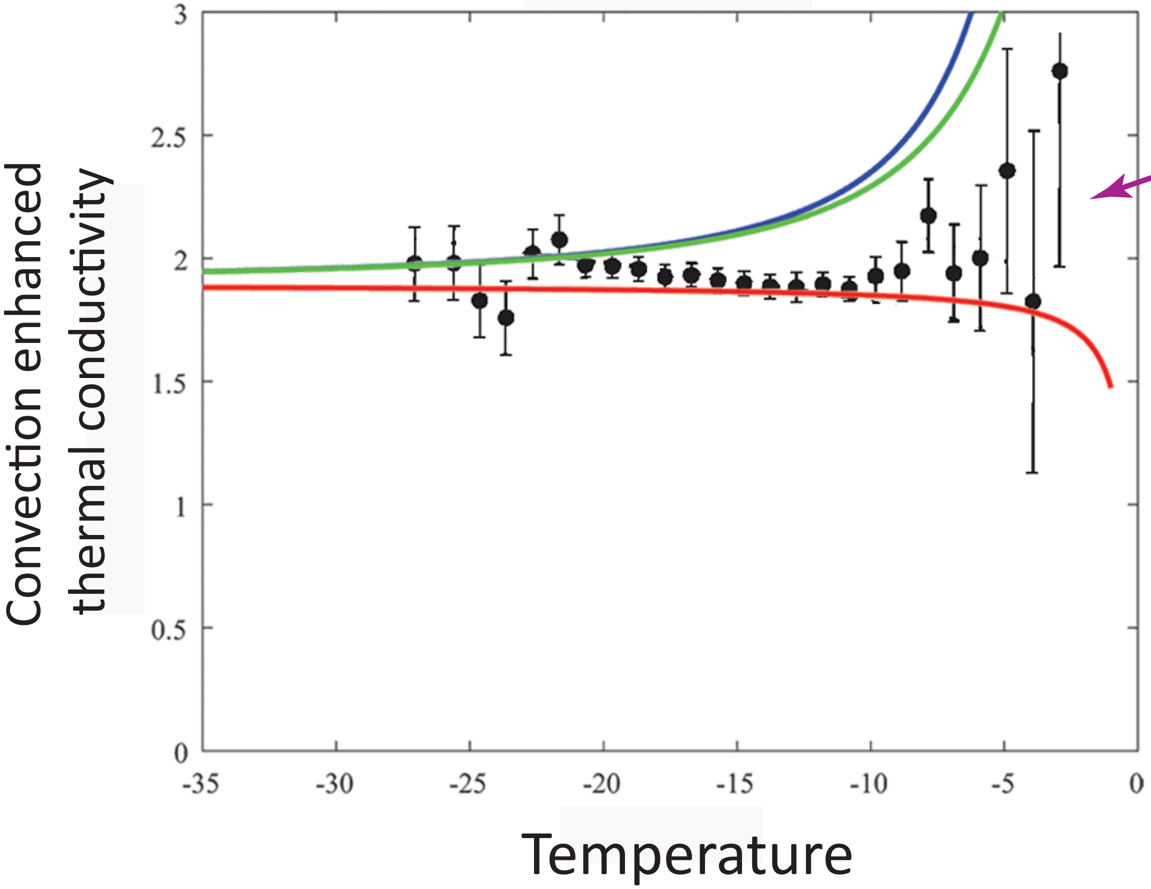
Rigorous bounds on convection enhanced thermal conductivity of sea ice

Kraitzman, Hardenbrook, Dinh, Murphy, Zhu, Cherkaev, Golden 2020



cat’s eye flow model for brine convection cells

similar bounds
for shear flows



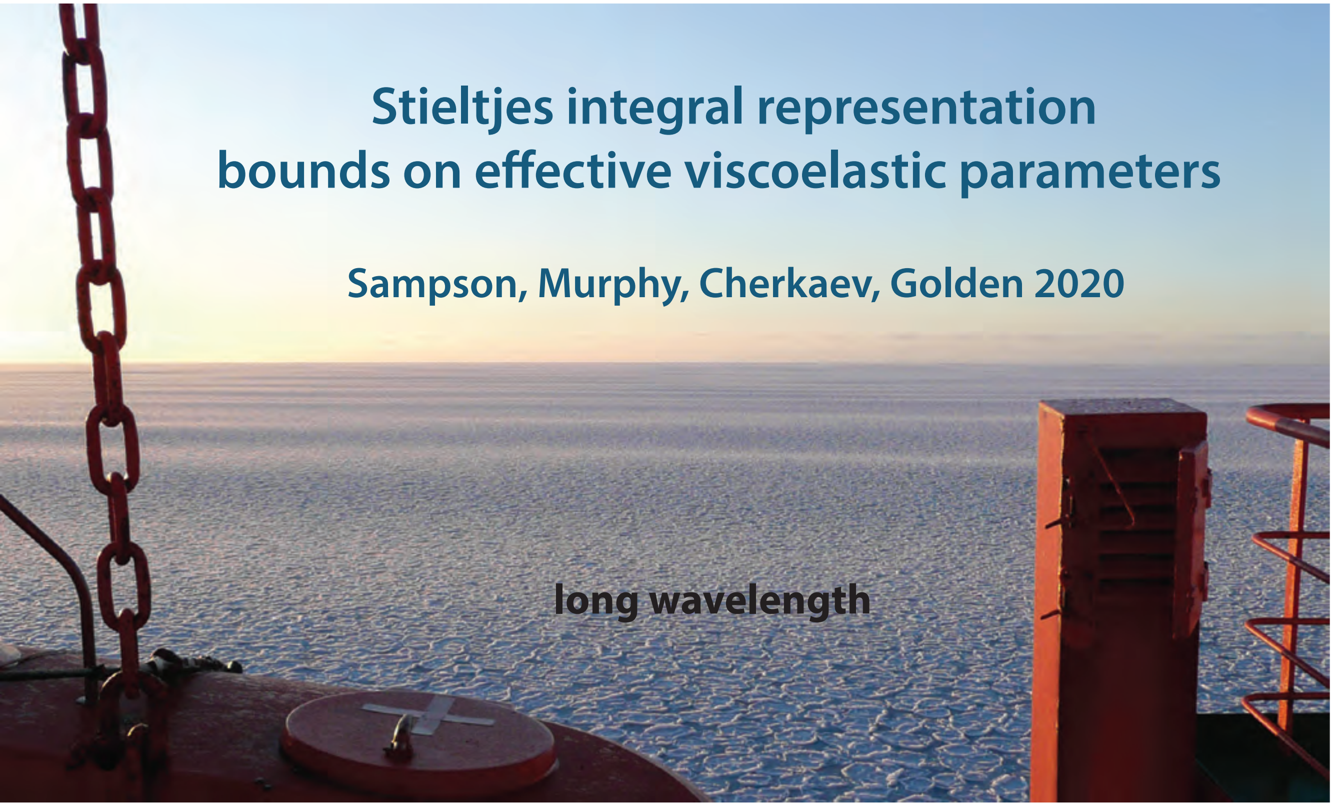
data Trodahl et al. 2001

rigorous Padé bounds from Stieltjes integral + analytical calculations of moments of measure

rigorous bounds assuming information on flow field INSIDE inclusions

Kraitzman, Cherkaev, Golden
in revision, 2020

wave propagation in the marginal ice zone



Stieltjes integral representation
bounds on effective viscoelastic parameters

Sampson, Murphy, Cherkaev, Golden 2020

long wavelength

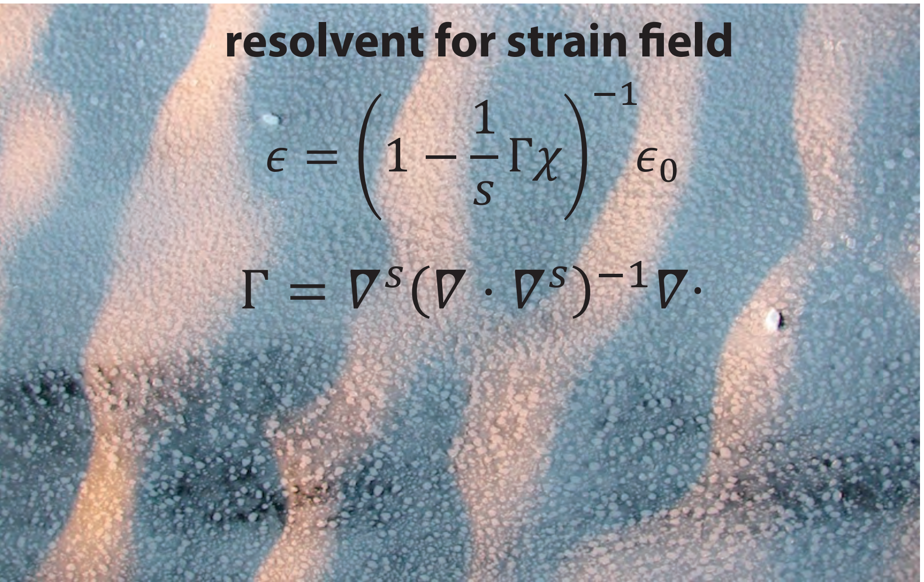
$$\langle \sigma_{ij} \rangle = C^*_{ijkl} \langle \epsilon_{kl} \rangle$$

ϵ_0 **avg strain**

$$C^*_{ijkl} = \nu^* \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl} \right) = \nu^* \lambda_s$$

$$F(s) = 1 - \frac{\nu^*}{\nu_2} \qquad s = \frac{1}{1 - \frac{\nu_1}{\nu_2}}$$

$$F(s) = ||\epsilon_0||^{-2} \int_\Sigma \frac{d\mu(\lambda)}{s - \lambda}$$



resolvent for strain field

$$\epsilon = \left(1 - \frac{1}{s}\Gamma\chi\right)^{-1} \epsilon_0$$

$$\Gamma = \nabla^s (\nabla \cdot \nabla^s)^{-1} \nabla \cdot$$

local

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}$$

quasistatic

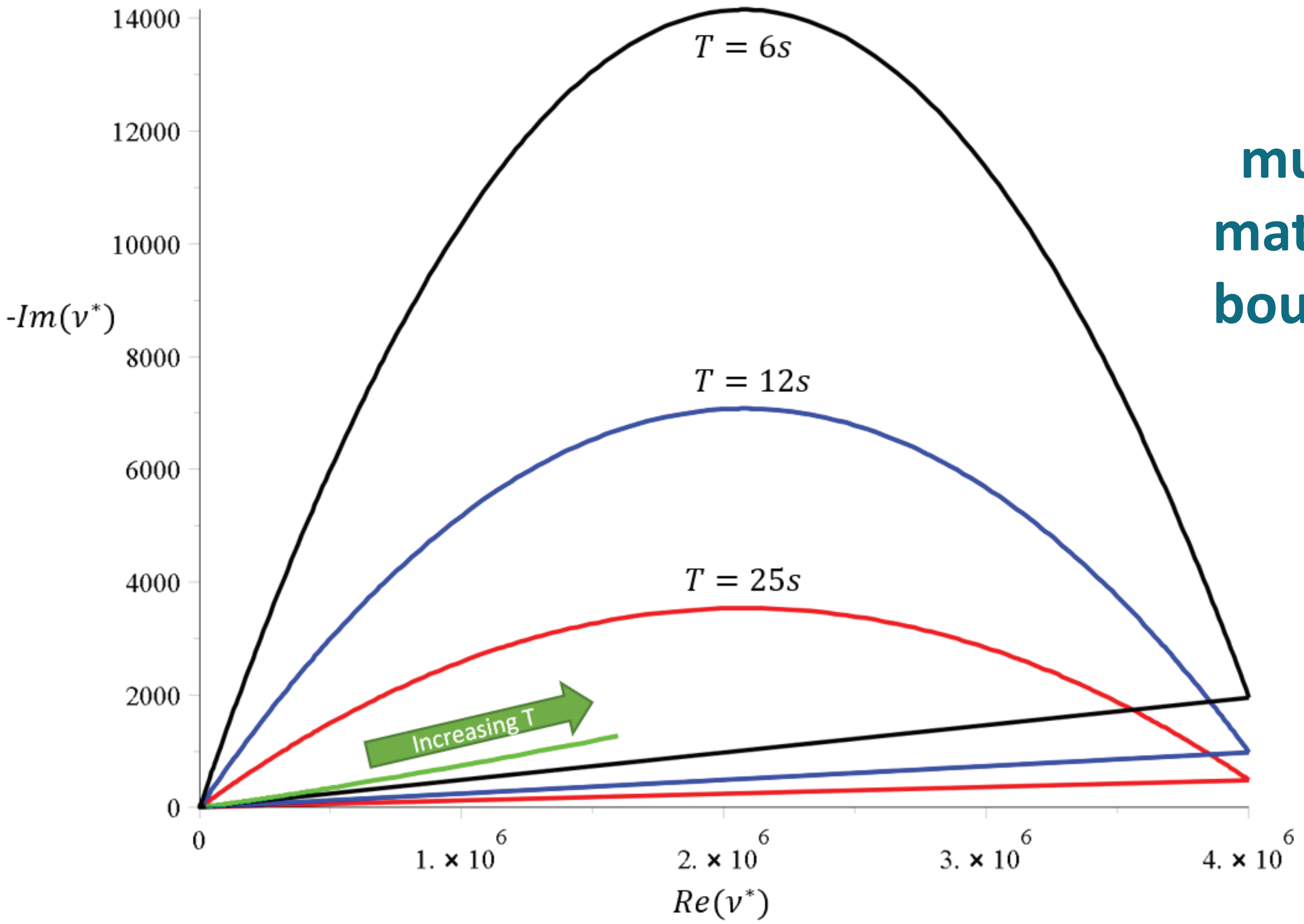
$$\nabla \cdot \sigma = 0$$

bounds on the effective complex viscoelasticity

complex elementary bounds (fixed area fraction of floes)

$\nu_1 = 10^7 + i\,4875$ **pancake ice**

$\nu_2 = 5 + i\,0.0975$ **slush / frazil**



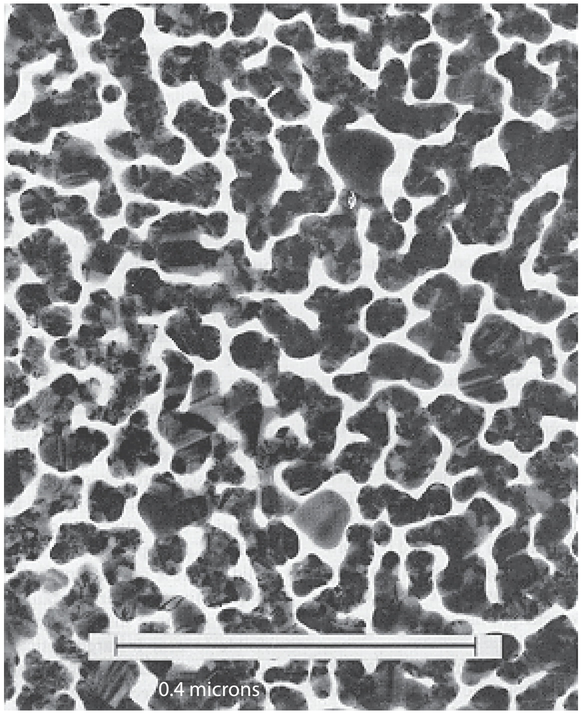
+ much tighter matrix particle bounds + data

Sampson, Murphy, Cherkaev, Golden 2019

Interaction of light with sea ice

thin silver film

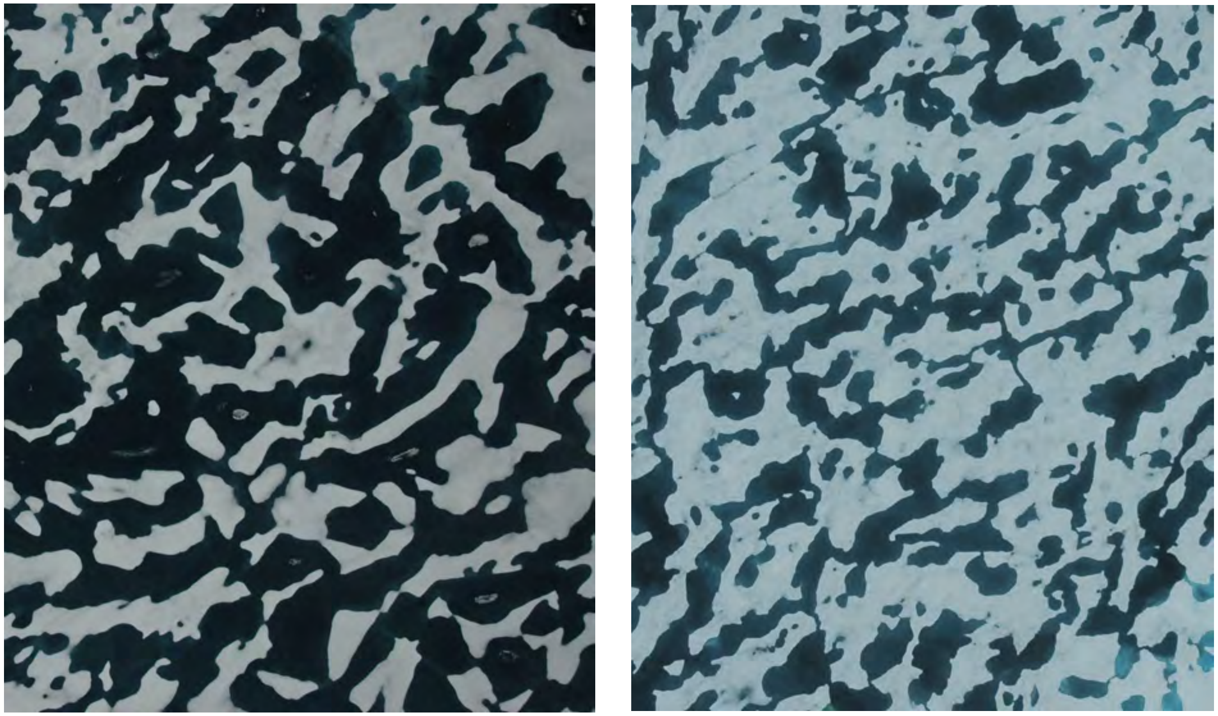
microns



(Davis, McKenzie, McPhedran, 1991)

Arctic melt ponds

kilometers



(Perovich, 2005)

optical properties

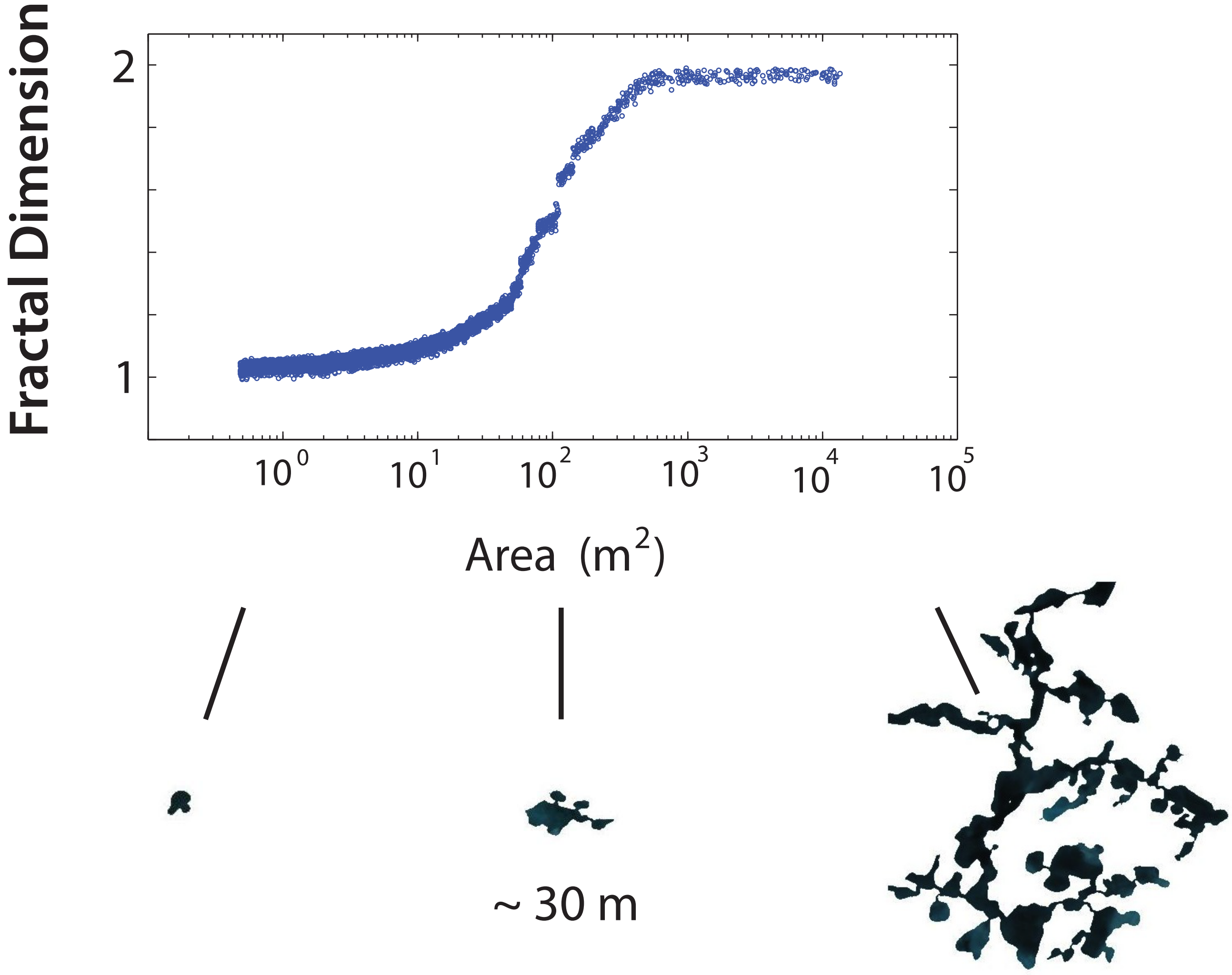
composite geometry -- area fraction of phases, connectedness, necks

Transition in the fractal geometry of Arctic melt ponds

Christel Hohenegger, Bacim Alali, Kyle Steffen, Don Perovich, Ken Golden

The Cryosphere, 2012

complexity grows with length scale

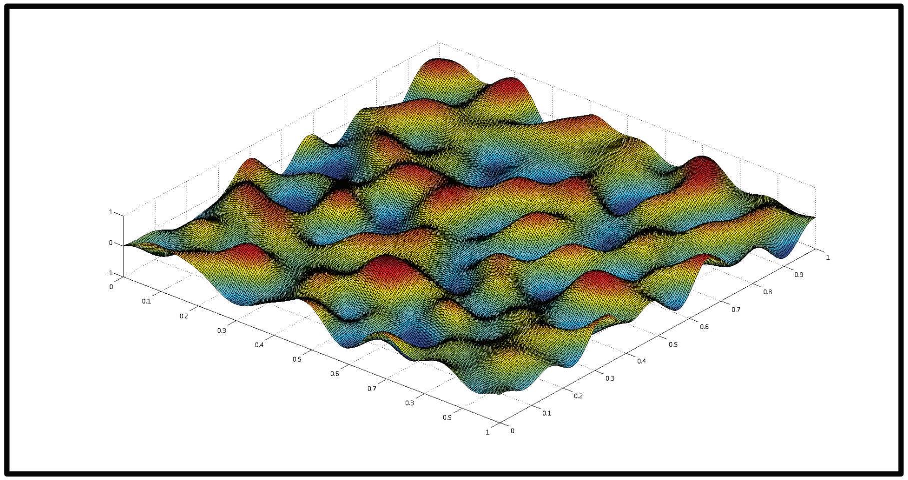


simple pond ***transitional pond*** ***complex pond***

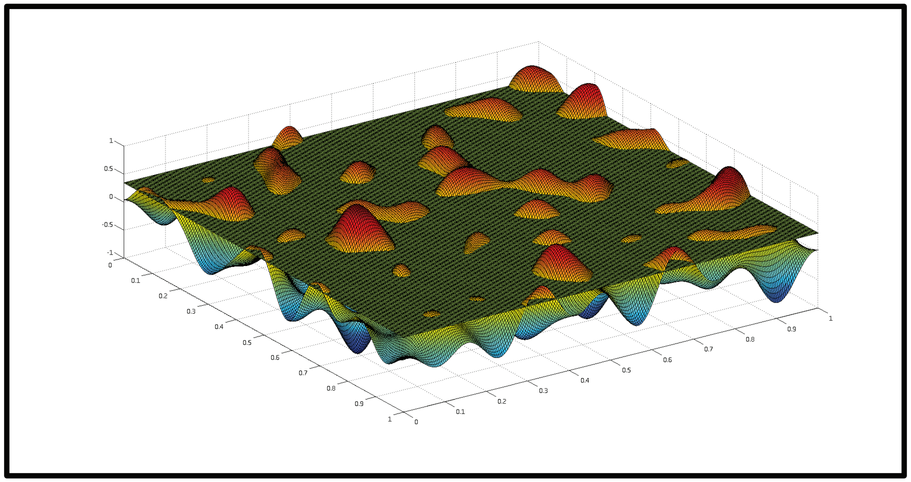
Continuum percolation model for melt pond evolution

level sets of random surfaces

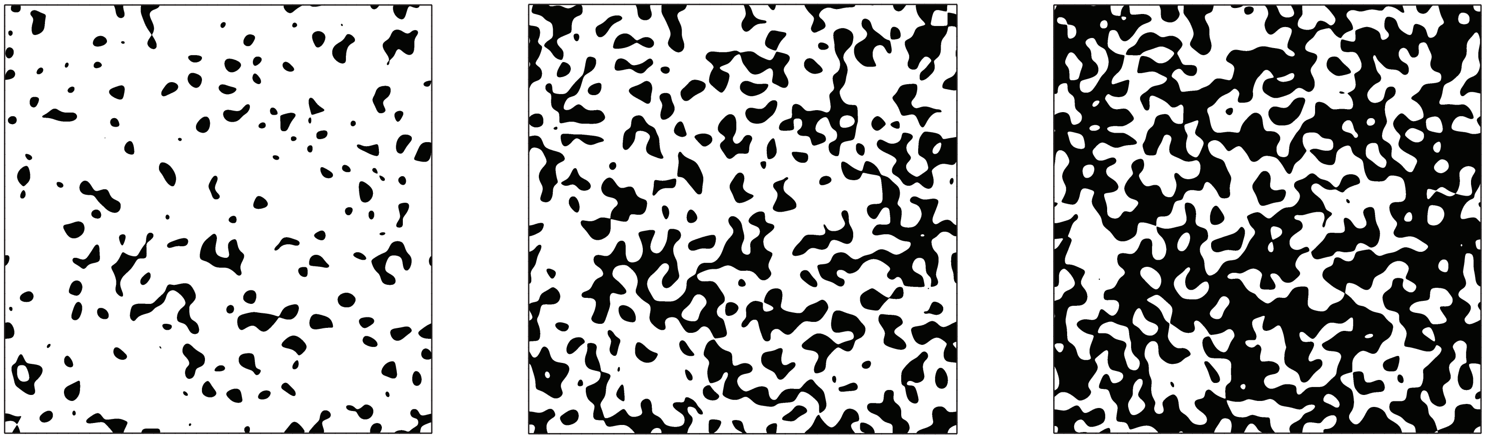
Brady Bowen, Court Strong, Ken Golden, J. Fractal Geometry 2018



random Fourier series representation of surface topography



intersections of a plane with the surface define melt ponds



electronic transport in disordered media *diffusion in turbulent plasmas* *Isichenko, Rev. Mod. Phys., 1992*

Ising model for ferromagnets ⟶ Ising model for melt ponds

Ma, Sudakov, Strong, Golden, *New J. Phys.*, 2019

$$\mathcal{H} = -\sum_{i}^{N} H_i\, s_i - J \sum_{<i,j>}^{N} s_i s_j \qquad s_i = \begin{cases} \uparrow & +1 \quad \text{water} \quad \text{(spin up)} \\ \downarrow & -1 \quad \text{ice} \quad \text{(spin down)} \end{cases}$$

random magnetic field represents snow topography

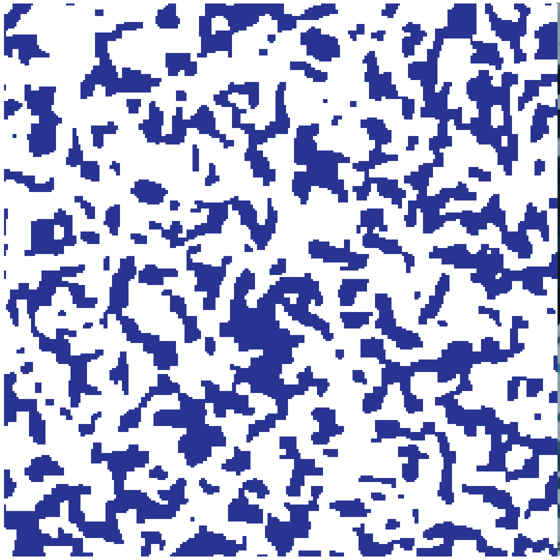
magnetization M **pond coverage** $\dfrac{(M+1)}{2}$

~ albedo

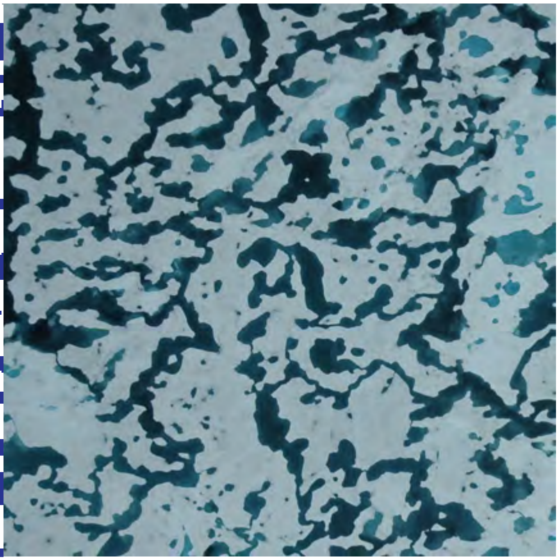
only nearest neighbor patches interact

Starting with random initial configurations, as Hamiltonian energy is minimized by Glauber spin flip dynamics, system "flows" toward metastable equilibria.

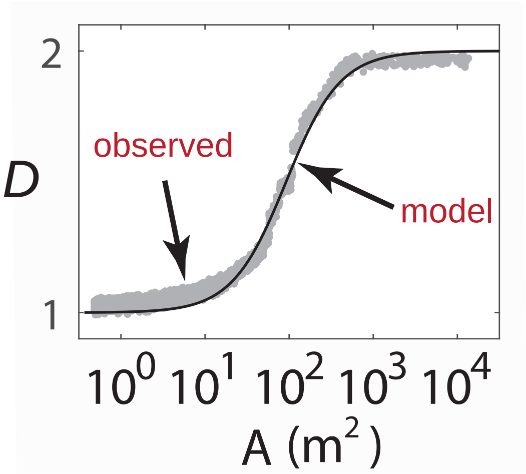
Order from Disorder



Ising model



melt pond photo **(Perovich)**



pond size distribution exponent

observed	-1.5
	(Perovich, *et al.* 2002)
model	-1.58

ONLY MEASURED INPUT = LENGTH SCALE (GRID SIZE) from snow topography data

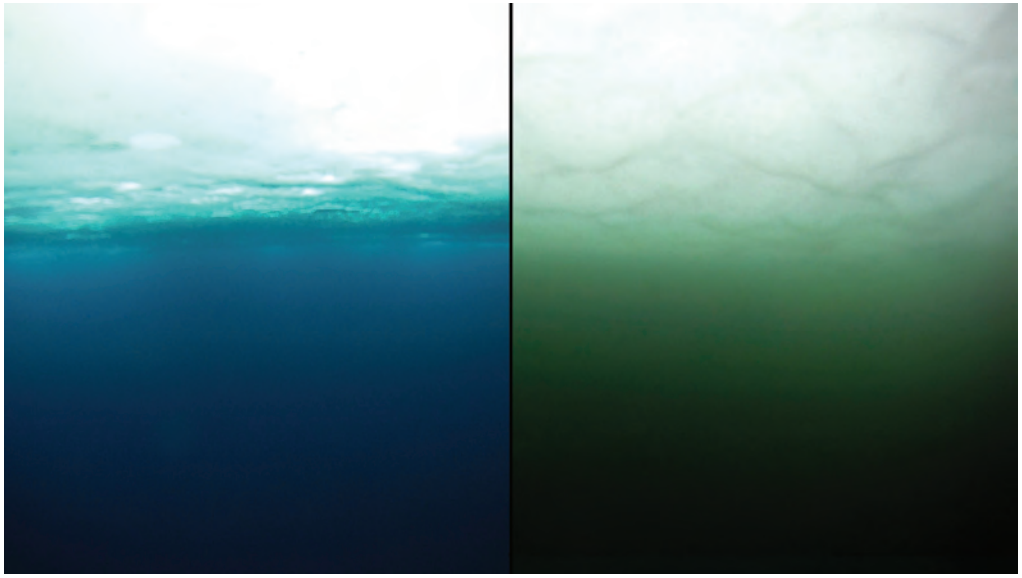
2011 massive under-ice algal bloom

Arrigo et al., *Science* 2012

melt ponds act as

WINDOWS

allowing light through sea ice



no bloom **bloom**

Have we crossed into a new ecological regime?

The frequency and extent of sub-ice phytoplankton blooms in the Arctic Ocean

Horvat, Rees Jones, Iams, Schroeder, Flocco, Feltham, *Science Advances*, 2017

(2015 AMS MRC, Snowbird)

The effect of melt pond geometry on the distribution of solar energy under ponded first-year sea ice

Horvat, Flocco, Rees Jones, Roach, Golden, *Geophys. Res. Lett.*, 2020

- Model for 3D light field under ponded sea ice.
- Distribution of solar energy at depth influenced by ***shape and connectivity*** of melt ponds, as well as area fraction.
- Aggregate properties of the sub-ice light field, such as a significant enhancement of available solar energy under the ice, are controlled by parameter closely related to pond fractal geometry.
- Model and analysis explain how melt pond geometry ***homogenizes*** under-ice light field, affecting habitability.

Pond geometry affects the ecology of the Arctic Ocean.

Conclusions

1. Wave phenomena arise naturally in the sea ice system.

2. Homogenization and statistical physics help *link scales* and provide rigorous methods for finding effective behavior, and advance how sea ice is represented in climate models.

3. Herglotz functions and Stieltjes integrals provide powerful methods of homogenization for wave phenomena in composite media.

4. Quasiperiodic media display fascinating effective properties.

5. Our research will help to improve projections of climate change and the fate of the Earth sea ice packs.

THANK YOU

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THE UNIVERSITY OF UTAH

Buchanan Bay, Antarctica   Mertz Glacier Polynya Experiment   July 1999