Herglotz Functions and Anderson Transitions in Composites

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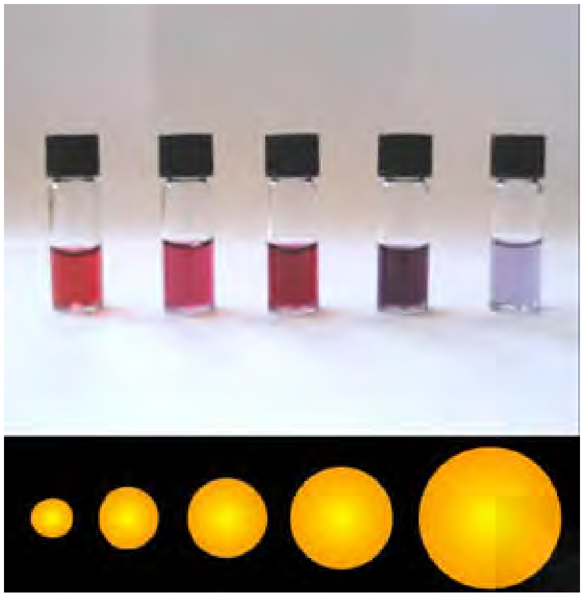
Surface Plasmon Resonances

collective oscillations of electrons on metal / dielectric interface



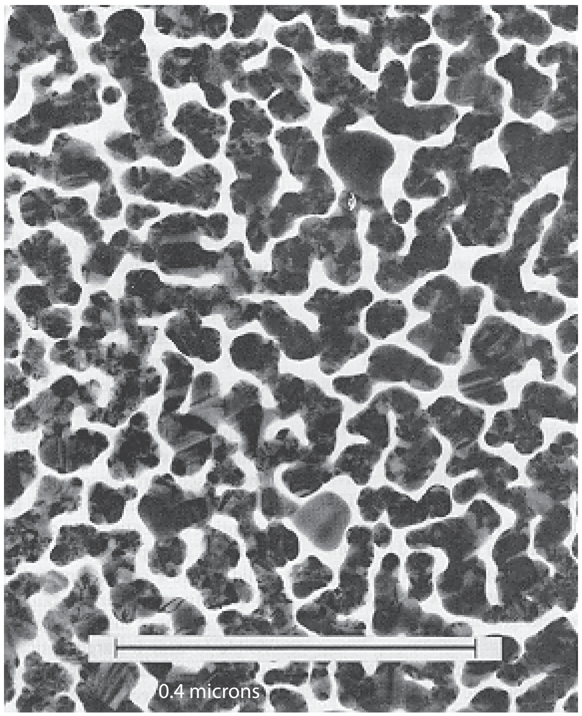
suspension of
gold nanoparticles
absorbs green
and blue light:

WE SEE RED

Michael Faraday's gold colloids - origins of nanoscience 1850s

thin silver film

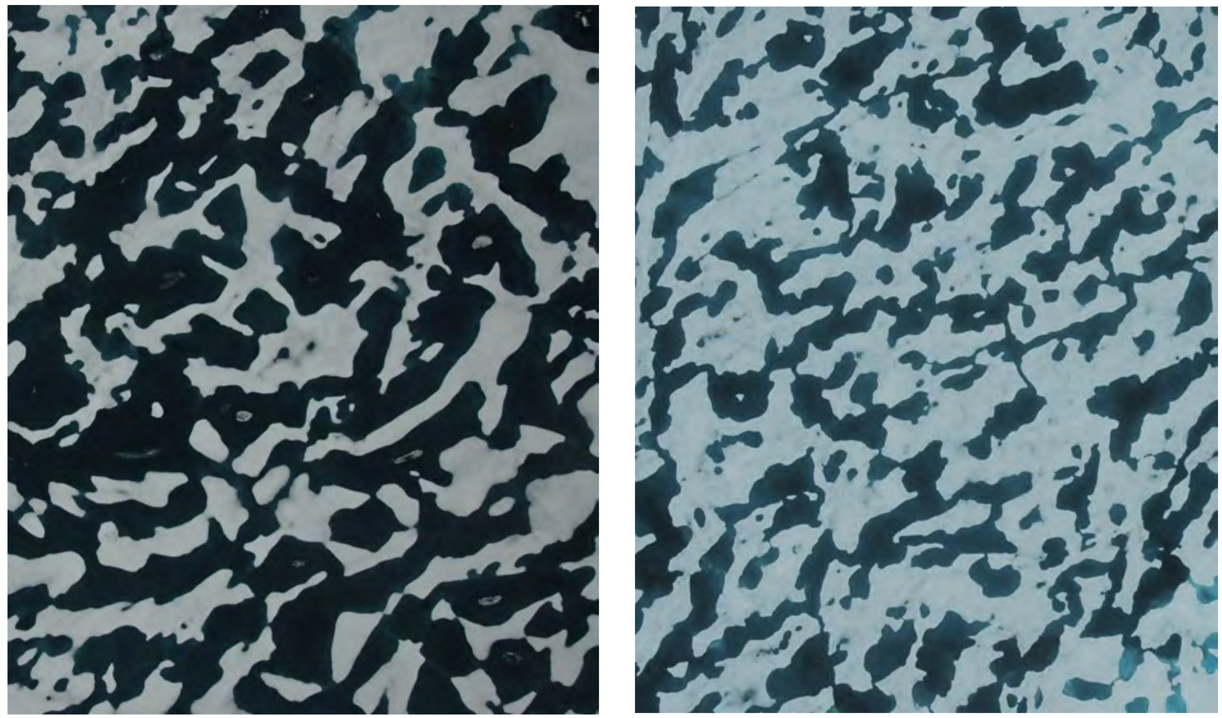
nanometers



(Davis, McKenzie, McPhedran, 1991)

Arctic melt ponds

kilometers



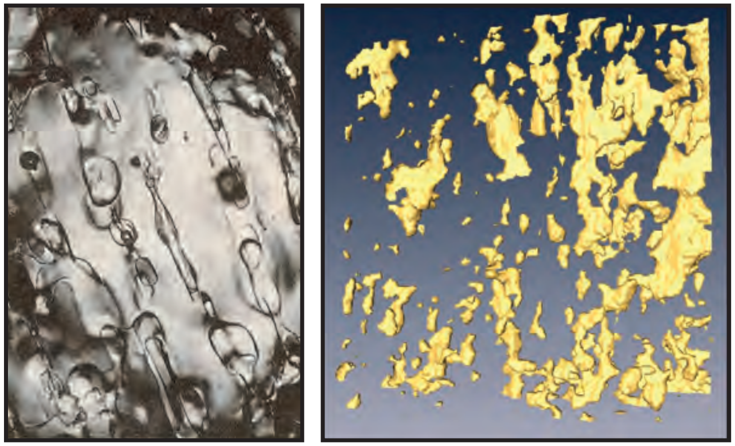
(Perovich, 2005)

optical properties

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

sea ice is a multiscale composite

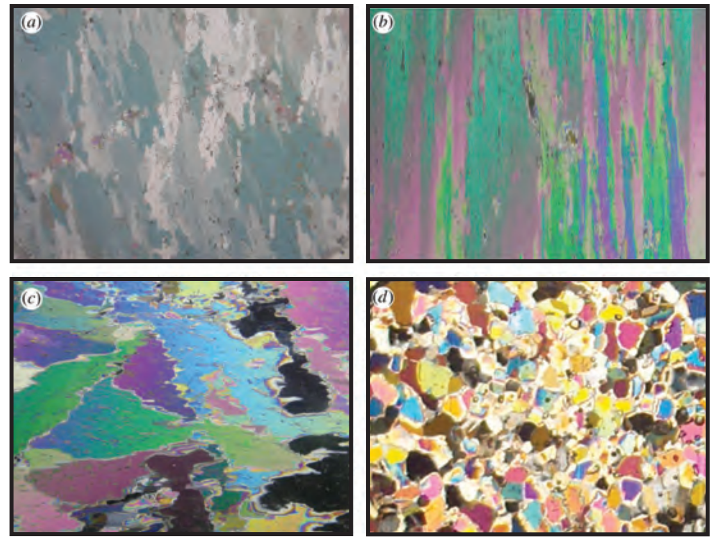
Brine Inclusions



mm

Golden et al GRL 2007

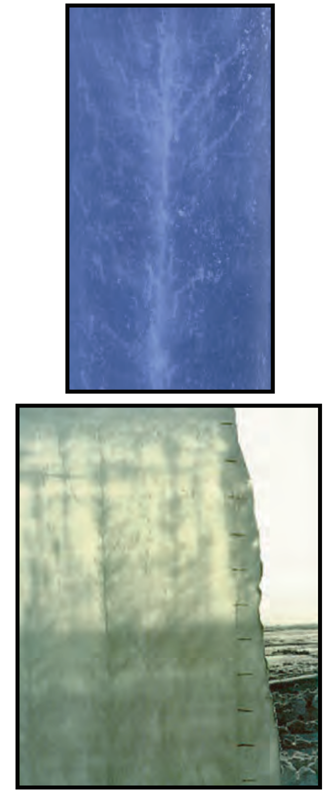
Polycrystals



cm

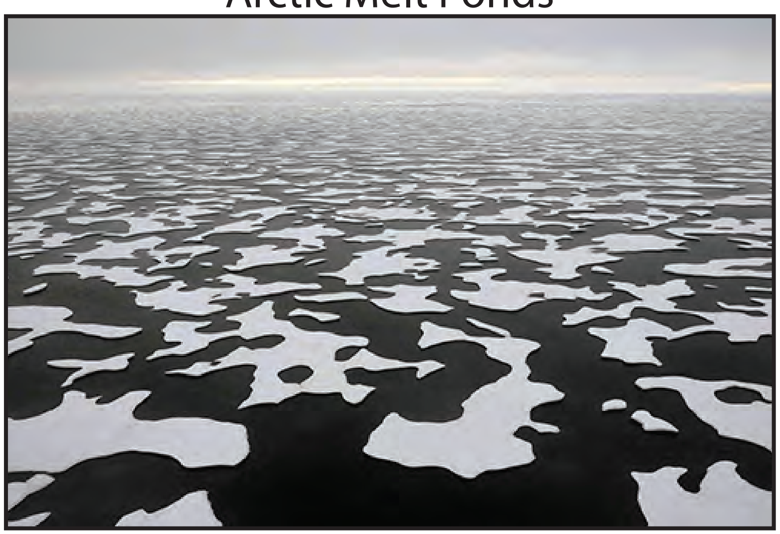
Gully et al. Proc. R. Soc. A 2015

Brine Channels



m

Arctic Melt Ponds



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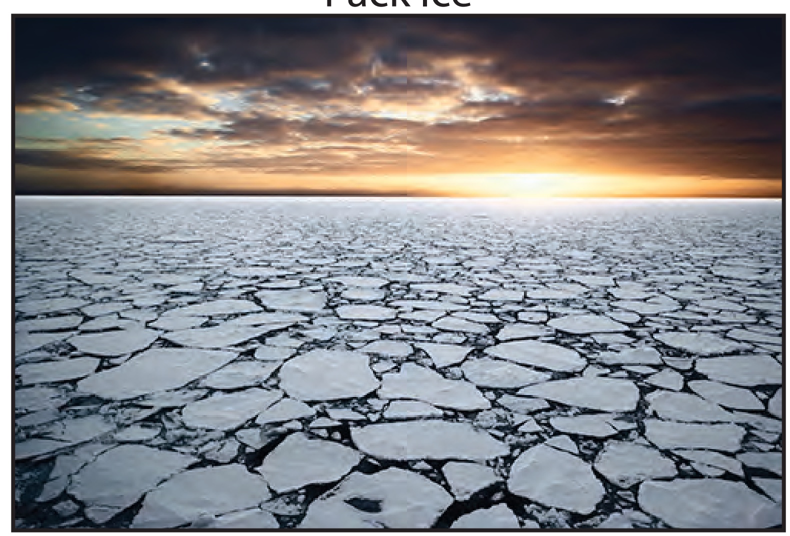
K. Frey

Pack Ice



km

J. Weller

What is this talk about?

A tour of Herglotz functions and how they arise in the study of composites, and sea ice in particular.

Addressing the problem of linking scales in Earth's sea ice system
MULTISCALE HOMOGENIZATION for SEA ICE
drives advances in theory of Herglotz functions for composites.

Find unexpected Anderson transition in composites along the way!

1. Fluid flow through sea ice, percolation

2. Analytic continuation for two phase composites
   remote sensing, inversion, spectral measures

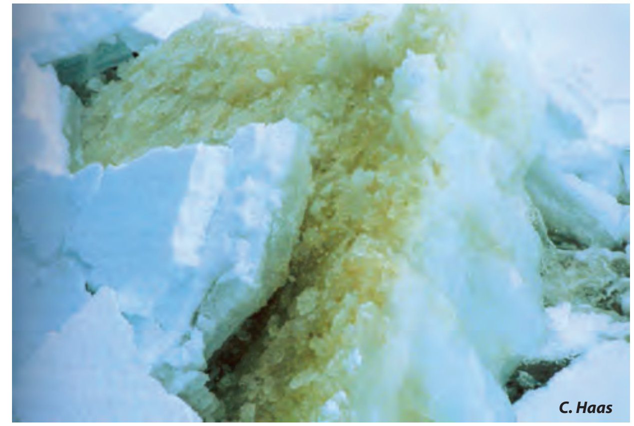
   random matrix theory and Anderson transitions

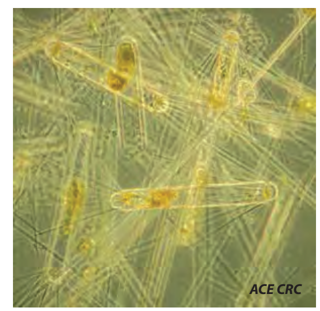
3. Stieltjes representations for advection diffusion,
   polycrystals, ocean waves in the sea ice pack

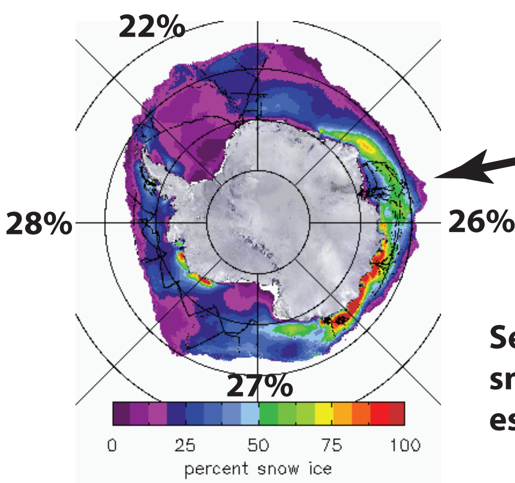
fluid flow through the porous microstructure of sea ice governs key processes in polar climate and ecosystems

evolution of Arctic melt ponds and sea ice albedo

nutrient flux for algal communities







T. Maksym and T. Markus, 2008

September snow-ice estimates

Antarctic surface flooding and snow-ice formation

- *evolution of salinity profiles*
- *ocean-ice-air exchanges of heat, CO_2*

fluid permeability of a porous medium

how much water gets through the sample per unit time?

Darcy's Law

for slow viscous flow in a porous medium

averaged fluid velocity

pressure gradient

$$\mathbf{v} = -\frac{\mathbf{k}}{\eta}\,\nabla p$$

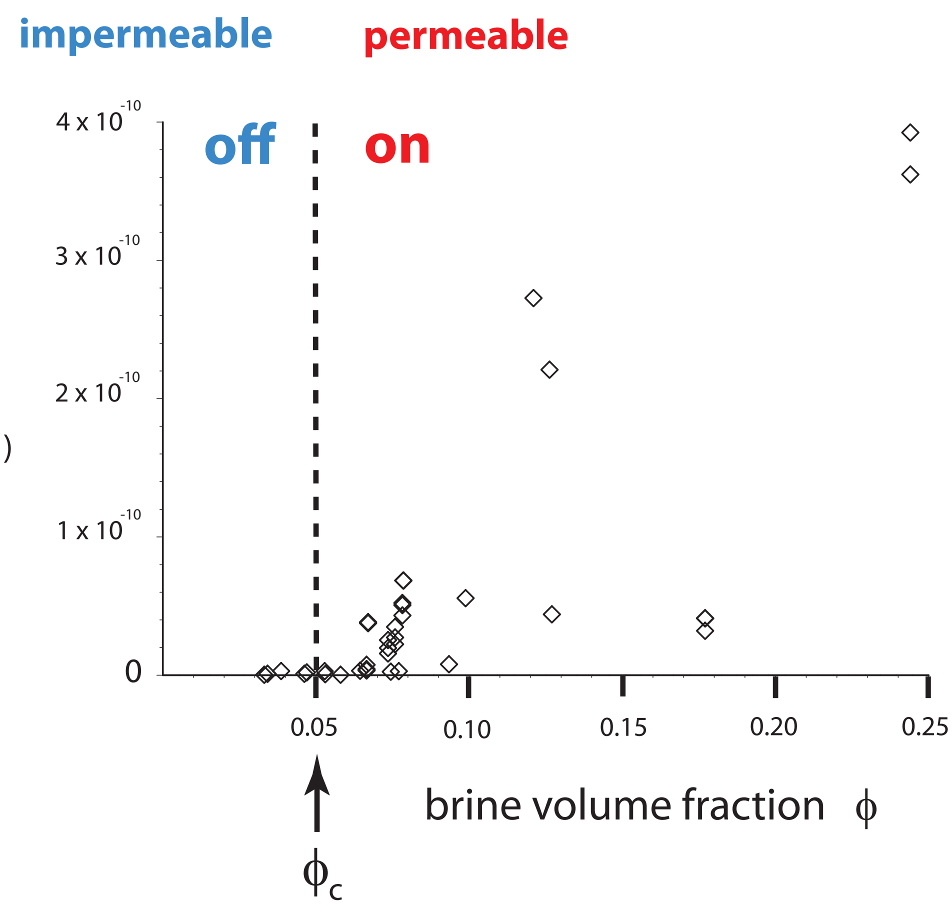
viscosity

$\mathbf{k}$ = fluid permeability tensor

HOMOGENIZATION

mathematics for analyzing effective behavior of heterogeneous systems

Critical behavior of fluid transport in sea ice



Arctic field data

vertical fluid permeability k (m ^{2})

on - off switch for fluid flow

critical brine volume fraction $\phi_c \approx 5\% \longleftrightarrow T_c \approx -5^\circ C, \; S \approx 5$ ppt

RULE OF FIVES

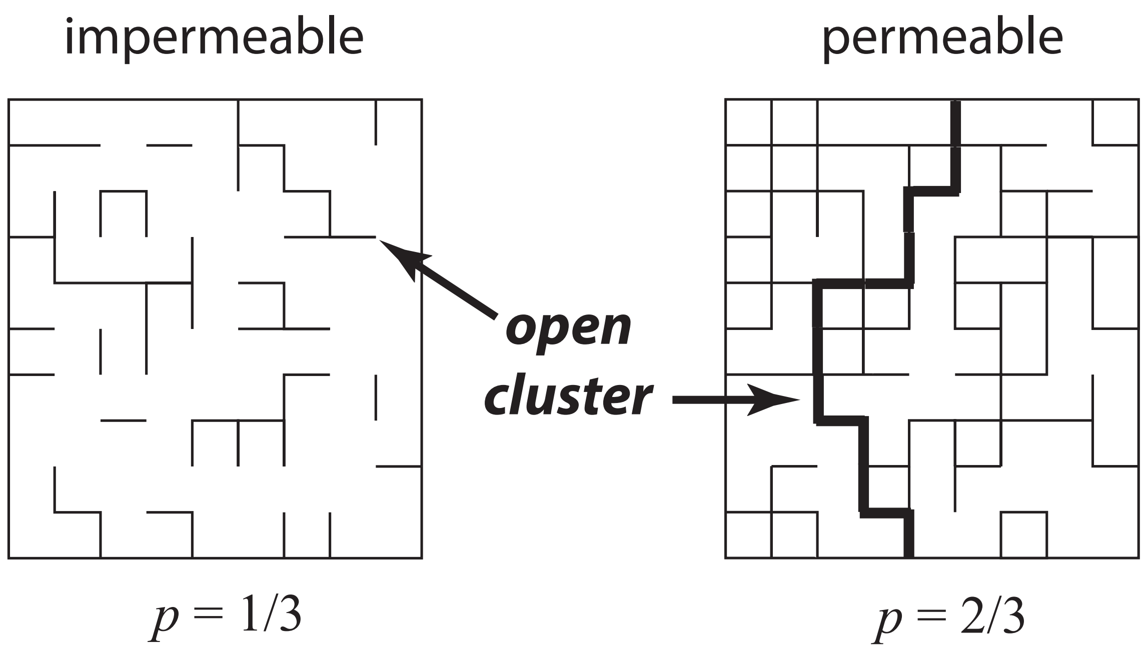
Golden, Ackley, Lytle *Science* 1998

Golden, Eicken, Heaton, Miner, Pringle, Zhu, *Geophys. Res. Lett.* 2007

Pringle, Miner, Eicken, Golden *J. Geophys. Res.* 2009

percolation theory

probabilistic theory of connectedness



bond → **open** *with probability* p
closed *with probability* $1\text{-}p$

percolation threshold

$$p_c = 1/2 \quad \text{for} \quad d = 2$$

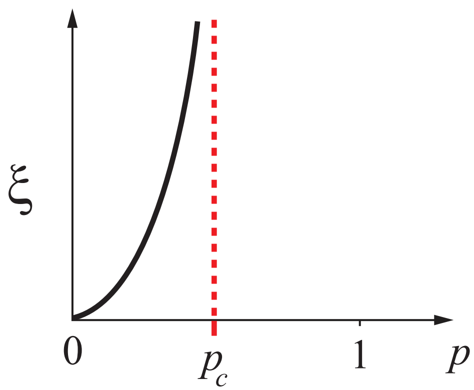
smallest p for which there is an infinite open cluster

order parameters in percolation theory

geometry

correlation length

characteristic scale
of connectedness

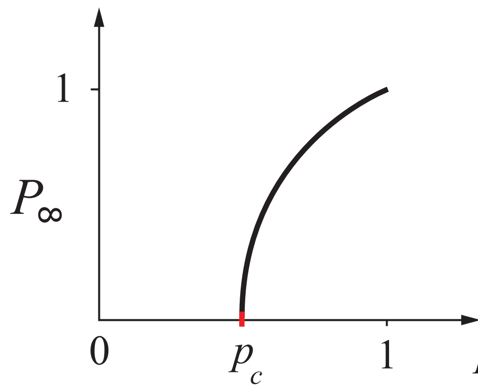


$$\xi(p) \sim |p - p_c|^{-\nu}$$

$$p \rightarrow p_c$$

infinite cluster density

probability the origin
belongs to infinte cluster

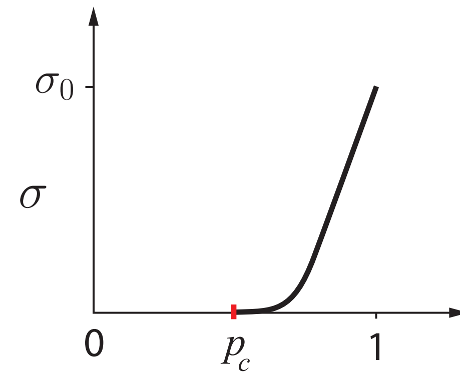


$$P_\infty(p) \sim (p - p_c)^{\beta}$$

$$p \rightarrow p_c^+$$

transport

effective conductivity or fluid permeability



$$\sigma(p) \sim \sigma_0 \, (p - p_c)^t$$

$$p \rightarrow p_c^+$$

UNIVERSAL critical exponents for lattices -- depend only on dimension

1 $\leq$ *t* $\leq$ 2 (for idealized model), Golden, *Phys. Rev. Lett.* 1990 ; *Comm. Math. Phys.* 1992

non-universal behavior in continuum

Thermal evolution of permeability and microstructure in sea ice

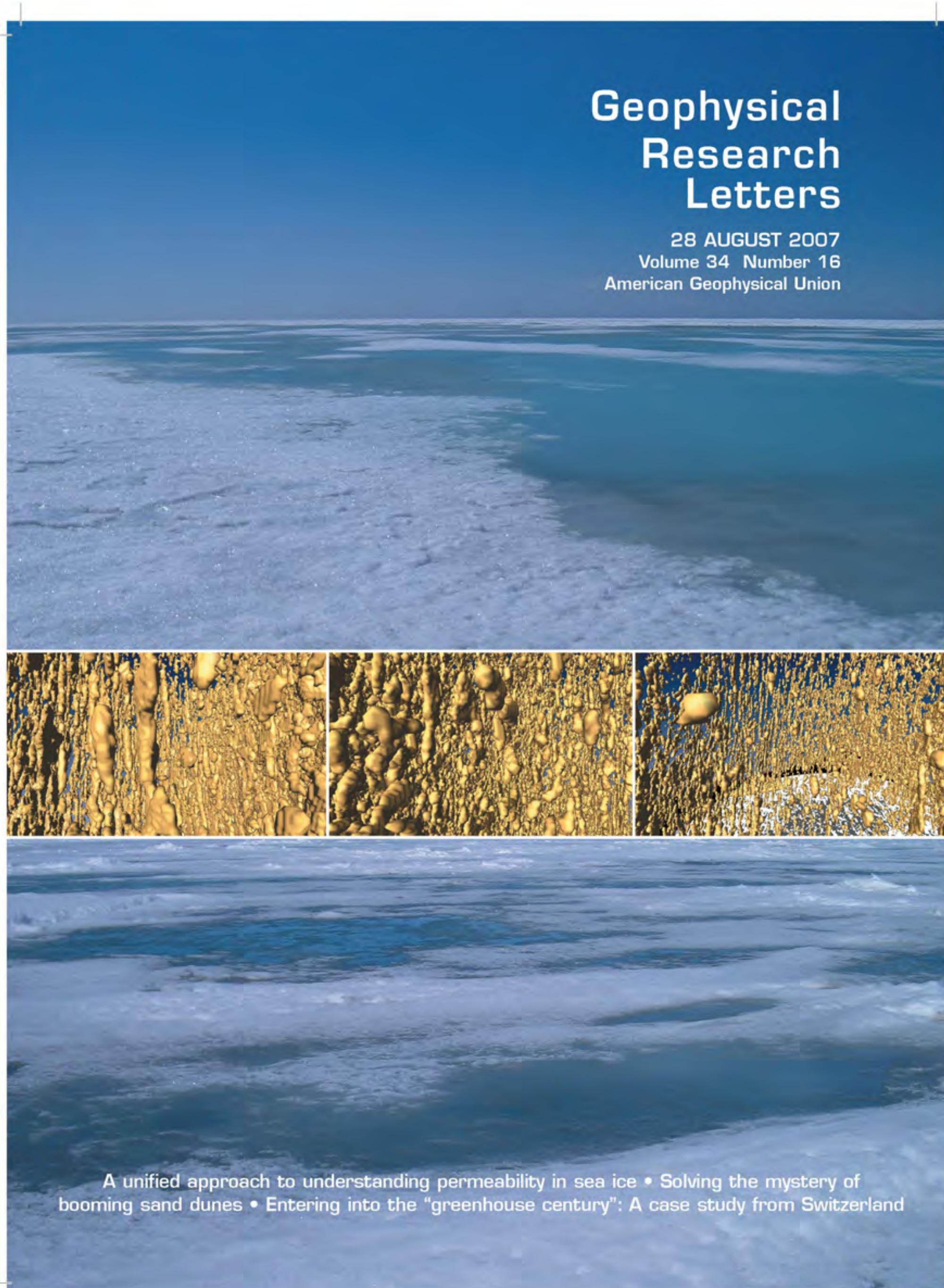
Golden, Eicken, Heaton, Miner, Pringle, Zhu, Geophysical Research Letters 2007

micro-scale

controls

macro-scale

processes



percolation theory

$$k(\phi) = k_0 (\phi - 0.05)^2$$

critical exponent t

$$k_0 = 3 \times 10^{-8}\ \mathrm{m}^2$$

hierarchical model
network model
rigorous bounds

agree closely
with field data

X-ray tomography for brine inclusions

unprecedented look at thermal evolution of brine phase and its connectivity

confirms rule of fives

Pringle, Miner, Eicken, Golden
J. Geophys. Res. 2009

Remote sensing of sea ice

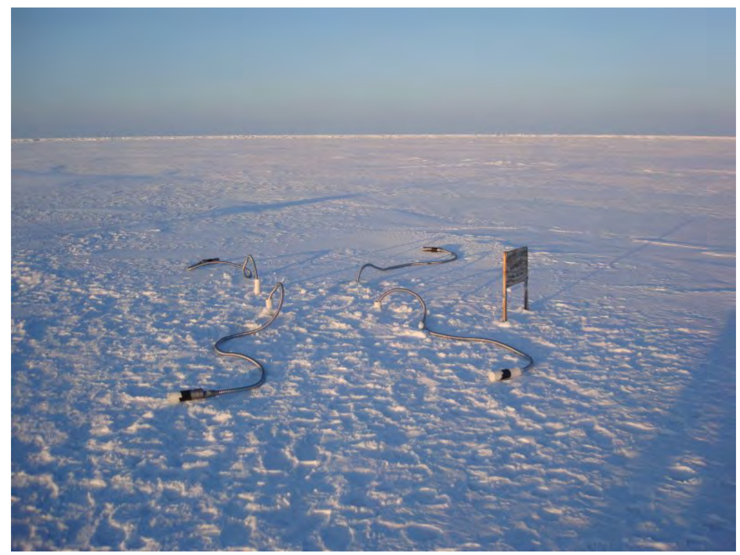
sea ice thickness
ice concentration

INVERSE PROBLEM

Recover sea ice properties from electromagnetic (EM) data

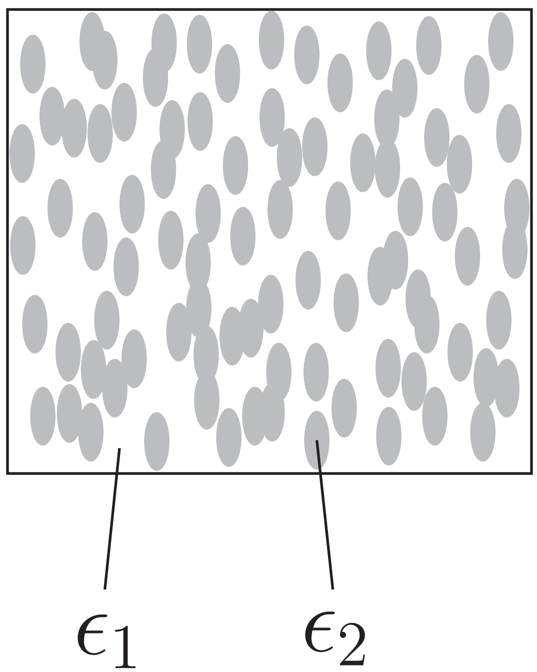
ε^*

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



ϵ^*

$$D = \epsilon E$$

$$\nabla \cdot D = 0$$

$$\nabla \times E = 0$$

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

p_1 , p_2 = volume fractions of the components

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

Herglotz function

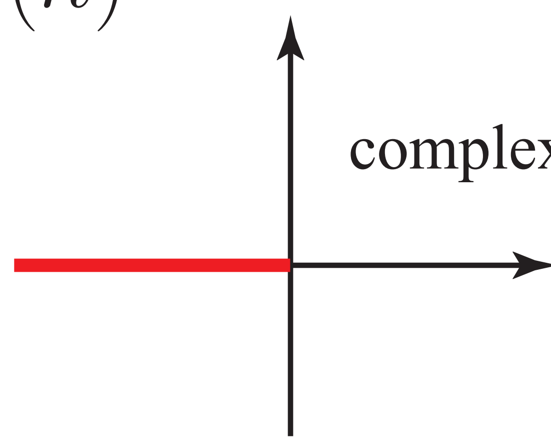
Analytic continuation method for bounding complex ϵ^*

Bergman (1978), Milton (1979), Golden and Papanicolaou (1983)

$$m(h) = \frac{\epsilon^*}{\epsilon_2}\left(\frac{\epsilon_1}{\epsilon_2}\right) \qquad h = \frac{\epsilon_1}{\epsilon_2}$$

Exploit analytic properties of $m(h)$

- $m(h)$ analytic off negative real axis



- $m(h)$: UHP $\longrightarrow$ UHP

Theory of Effective Electromagnetic Behavior of Composites

analytic continuation method

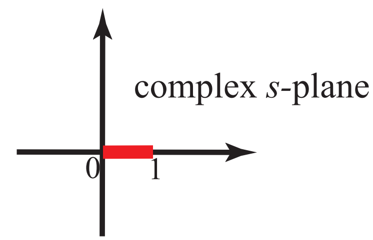
Forward Homogenization Bergman (1978), Milton (1979), Golden and Papanicolaou (1983)
Theory of Composites, Milton (2002)

composite geometry
(spectral measure μ) ⟶ ε^*

integral representations, rigorous bounds, approximations, etc.

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

$$s = \frac{1}{1 - \epsilon_1 / \epsilon_2}$$



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)

recover brine volume fraction, connectivity, etc.

Stieltjes integral representation

separates geometry from parameters

geometry

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

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

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

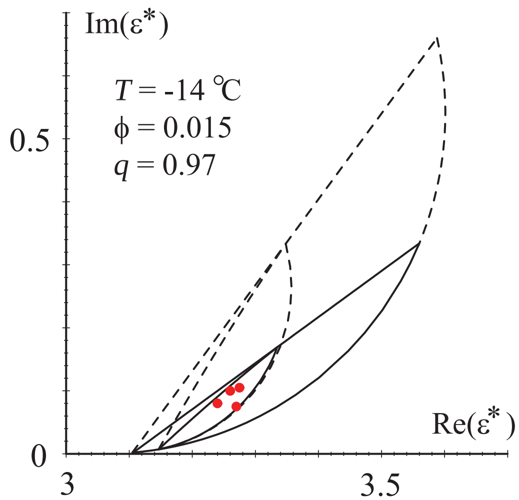
$\Gamma\chi$: microscale $\longrightarrow$ macroscale

$\Gamma\chi$ links scales

Golden and Papanicolaou, Comm. Math. Phys. 1983

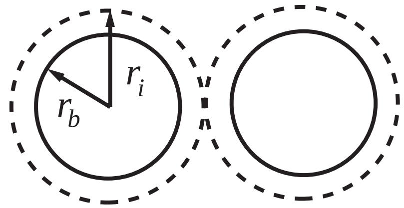
forward and inverse bounds on the complex permittivity of sea ice

forward bounds



4.75 GHz data

matrix particle



$$q = r_b / r_i$$

$$0 < q < 1$$

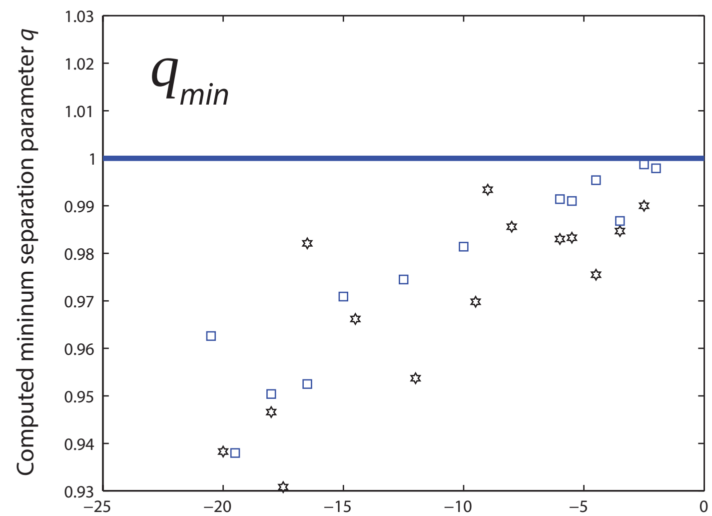
Golden 1995, 1997

Bruno 1991

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

direct calculation of spectral measure

1. Discretization of composite microstructure gives lattice of 1's and 0's (random resistor network).

2. The fundamental operator $\chi\Gamma\chi$ becomes a random matrix depending only on the composite geometry.

3. Compute the eigenvalues λ_i and eigenvectors of $\chi\Gamma\chi$ with inner product weights α_i

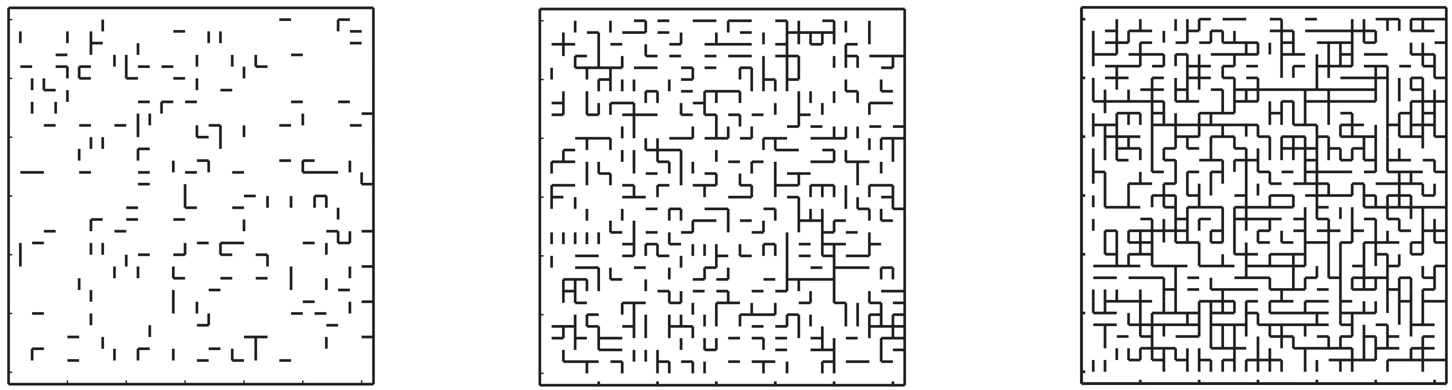
$$\mu(\lambda) = \sum_i \alpha_i \, \delta(\lambda - \lambda_i)$$

Dirac point measure (Dirac delta)

earlier studies of spectral measures

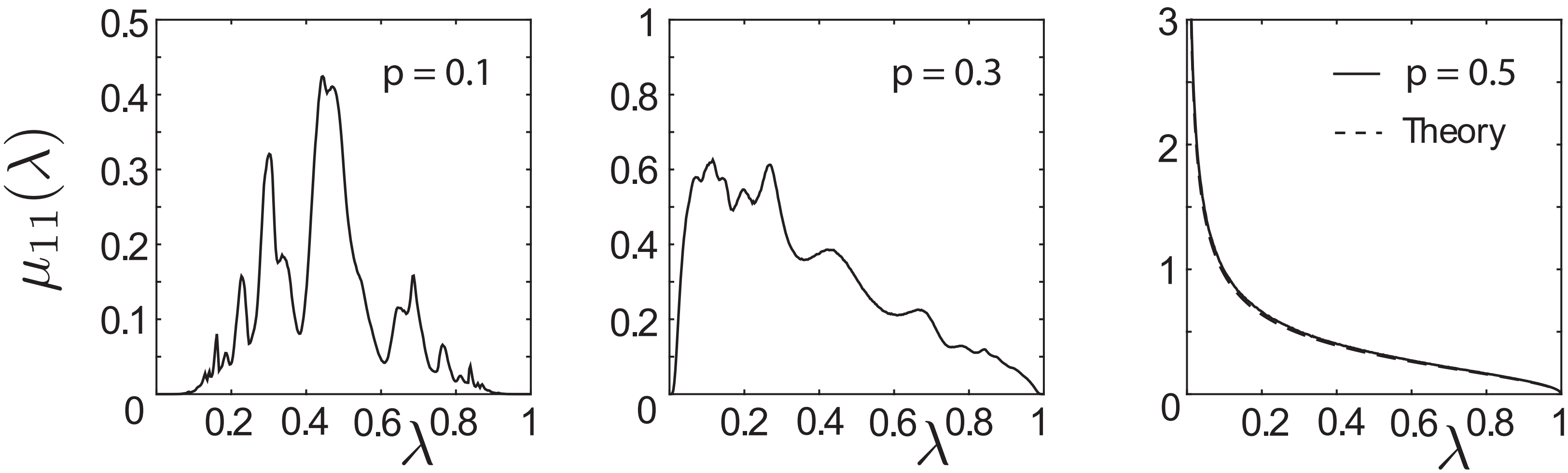
Day and Thorpe 1996
Helsing, McPhedran, Milton 2011

Spectral statistics for 2D random resistor network



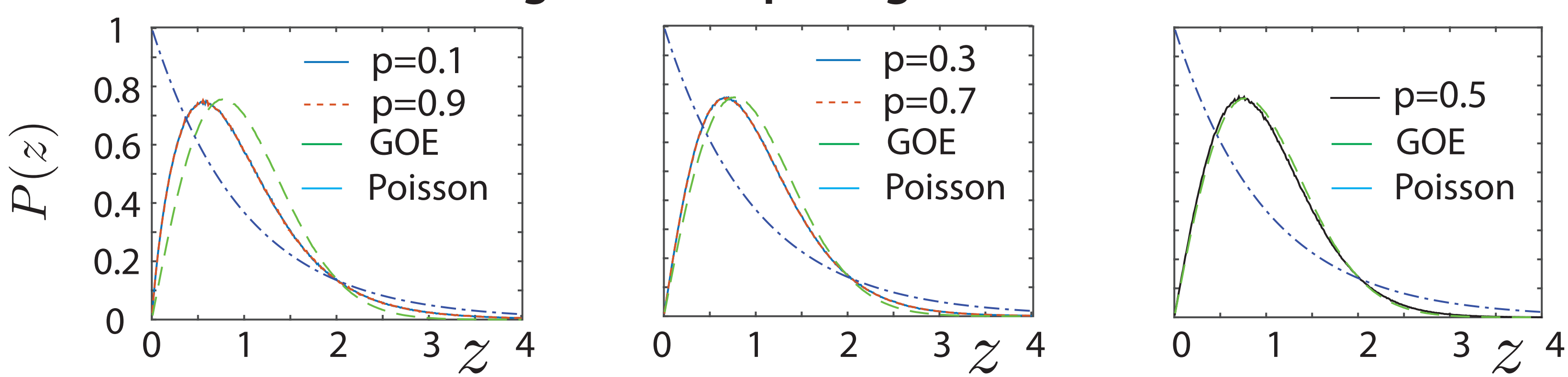
Spectral Measures

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

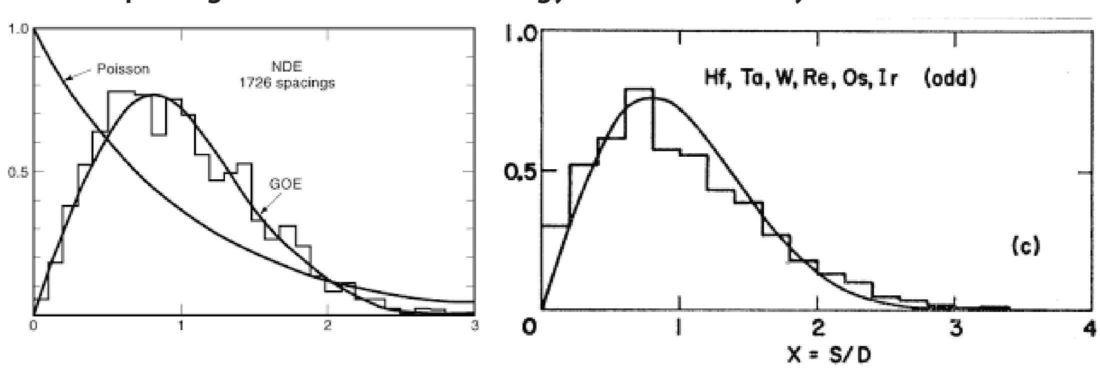
Wigner (1951) and Dyson (1953) first used random matrix theory (RMT) to describe quantized energy levels of heavy atomic nuclei.

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

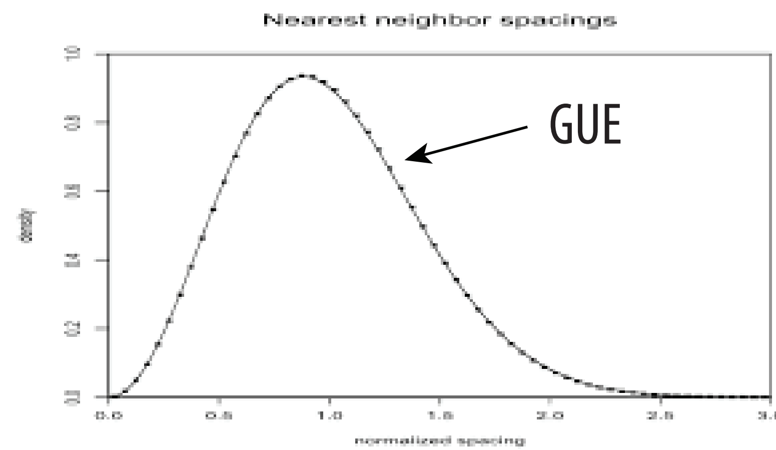
$[\mathbf{N}]_{ij} \sim N(0,1)+iN(0,1)$, $\quad \mathbf{A} = (\mathbf{N}+\mathbf{N}^\dagger)/2$ ***Gaussian unitary ensemble (GUE)***

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



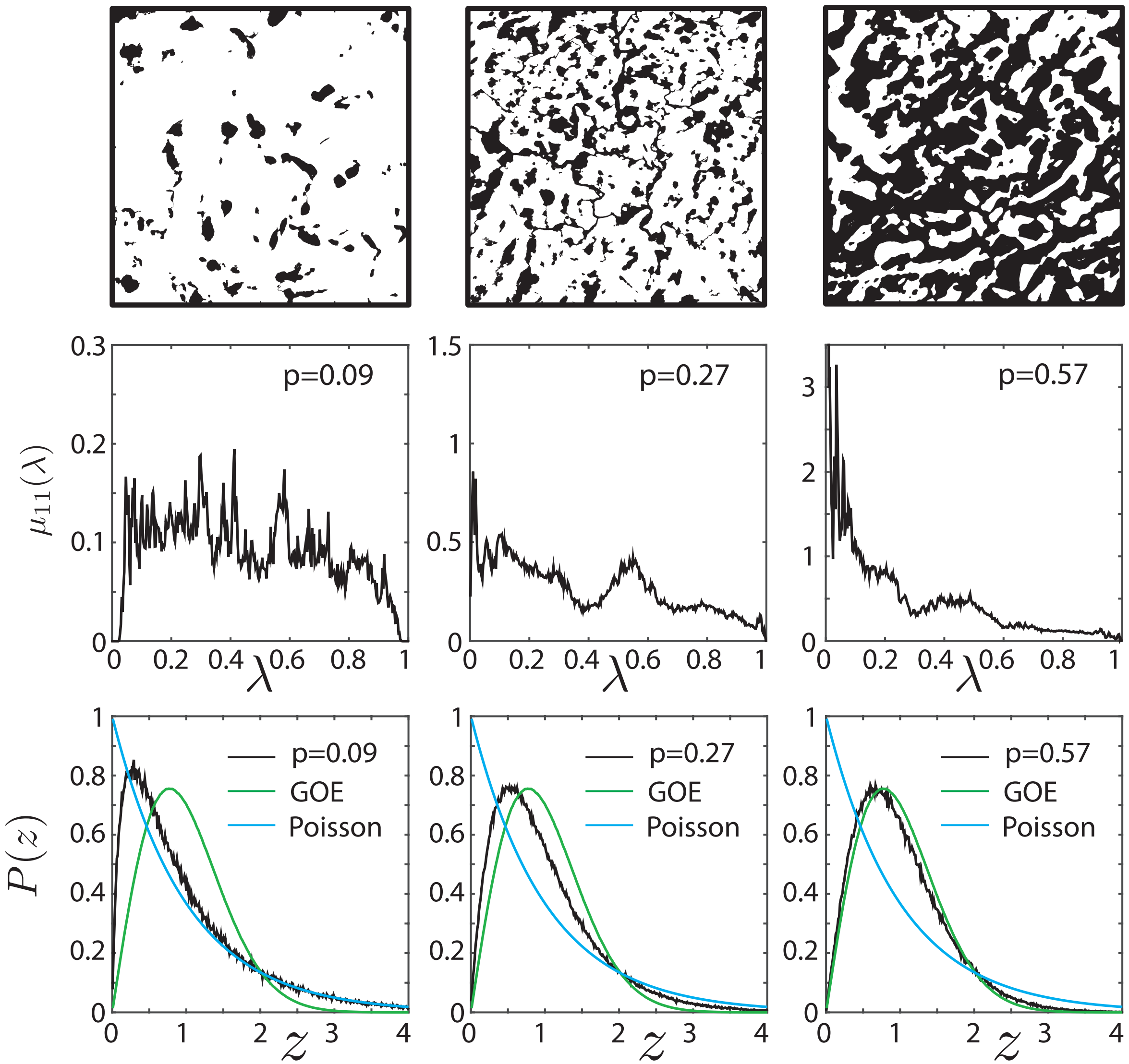
RMT used to characterize disorder-driven transitions in mesoscopic conductors, neural networks, random graph theory, etc.

Phase transitions ~ transitions in universal eigenvalue statistics.

Spectral computations for Arctic melt ponds

spectral measures

eigenvalue spacing distributions



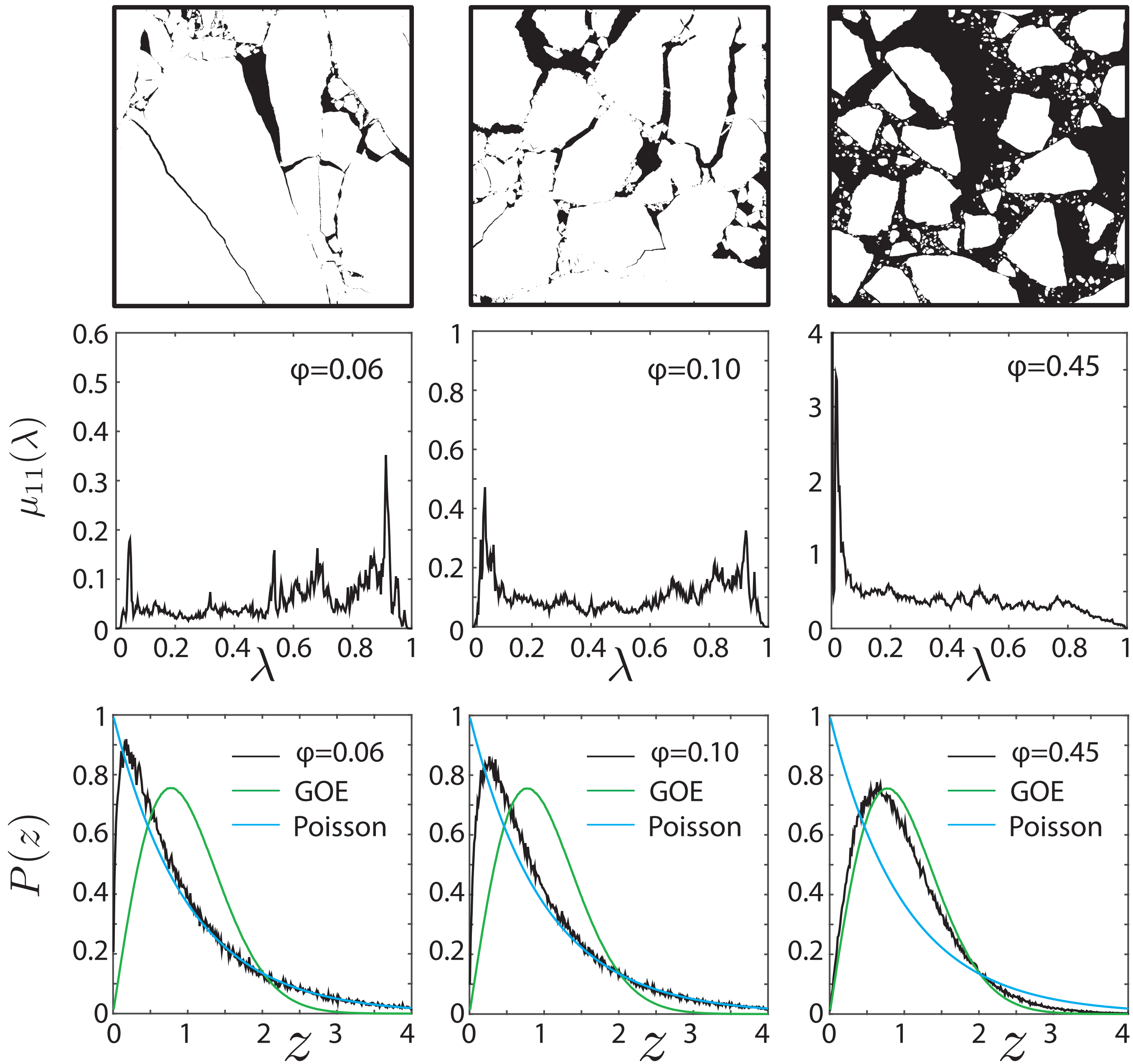
uncorrelated → **level repulsion**

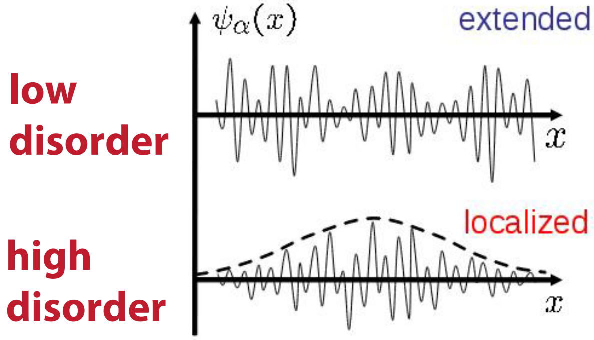
TRANSITION

Ben Murphy
Elena Cherkaev
Ken Golden
2017

eigenvalue statistics for transport tend toward the UNIVERSAL Wigner-Dyson distribution as the "conducting" phase percolates

Spectral computations for Arctic sea ice pack





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**

SPR

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

eigenvector localization and mobility edges

Inverse Participation Ratio: $$I(\vec{v}_n) = \sum_{i=1}^{N} |(\vec{v}_n)_i|^4$$

Completely Localized: $$I(\vec{e}_n) = 1$$

Completely Extended: $$I\left(\frac{1}{\sqrt{N}}\vec{1}\right) = \frac{1}{N}$$

Anderson Model

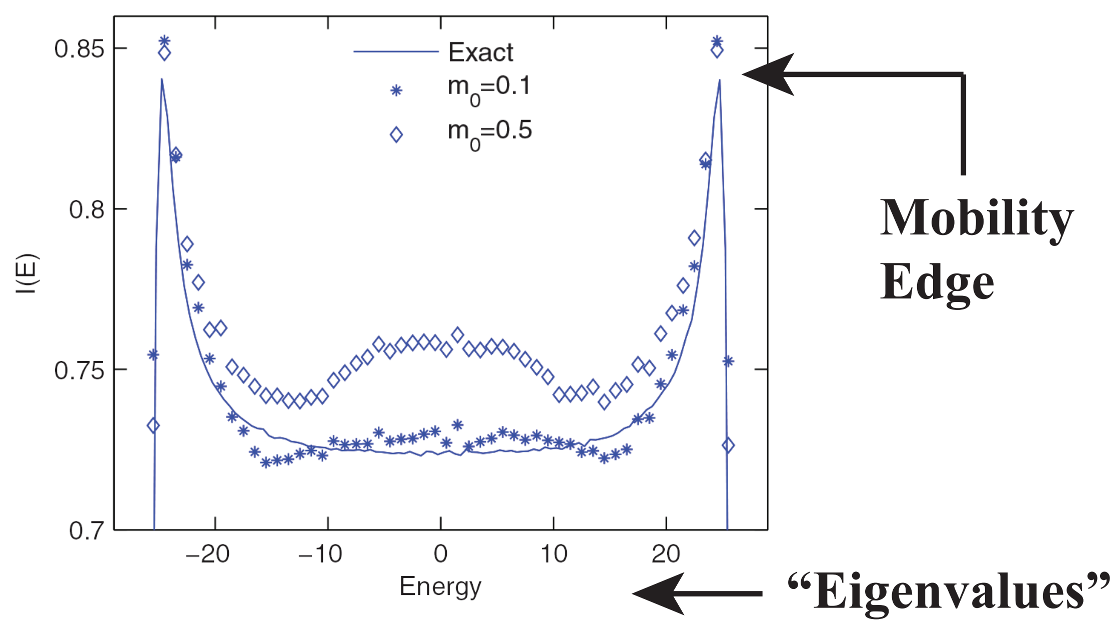
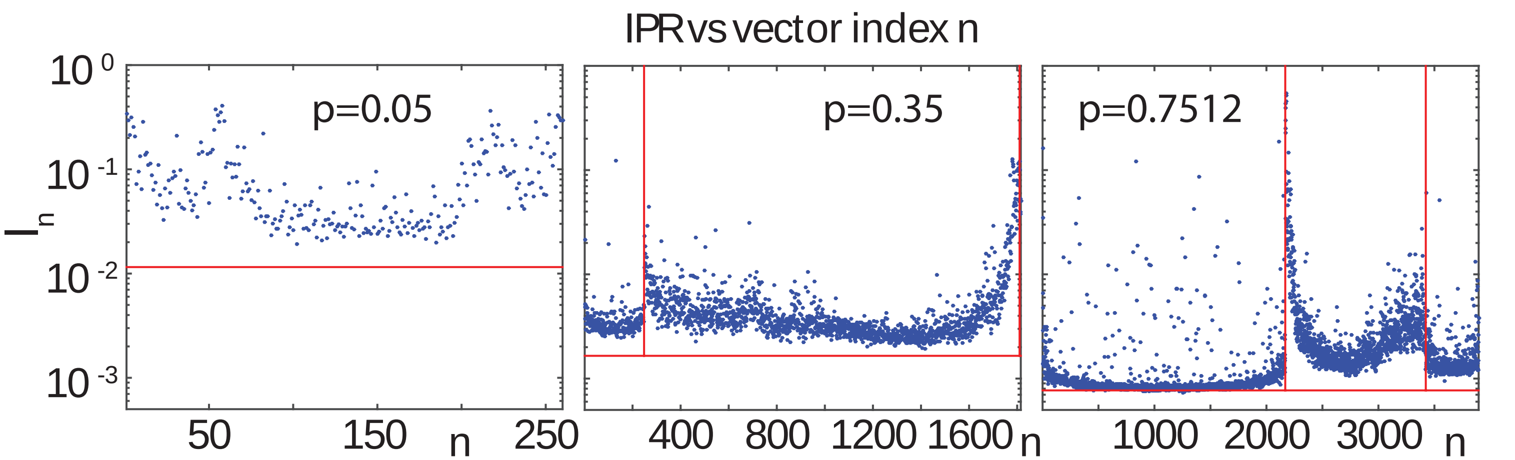
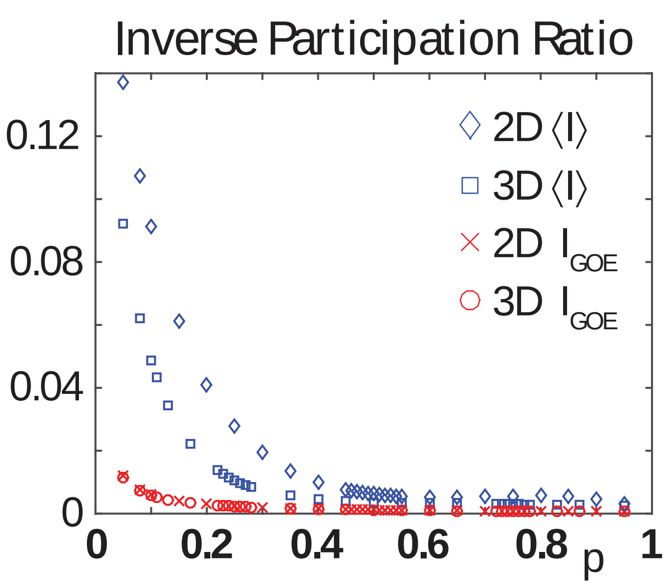


FIG. 4. (Color online) IPR for Anderson model in two dimensions with $x = 6.25$ ($w = 50$) from exact diagonalization (solid line) and from LDRG with different values of the cutoff m_0. LDRG data are averaged over 100 runs of systems with 100×100 sites.

PHYSICAL REVIEW B 90, 060205(R) (2014)

Localization properties of eigenvectors in random resistor networks





$$I_n = \sum_i (\vec{v}_n)_i^4$$

Murphy, Cherkaev, Golden, 2017

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**

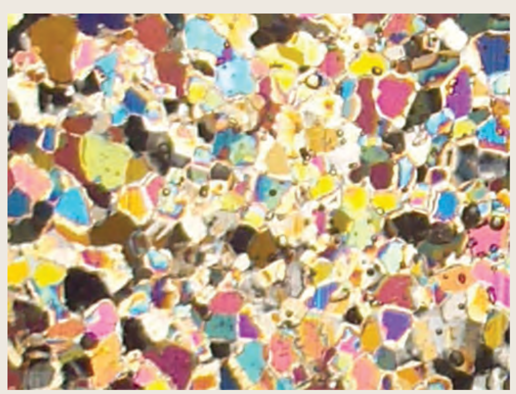
  Milton (1981, 2002), Barabash and Stroud (1999), ...

- **Forward and inverse bounds**

  orientation statistics

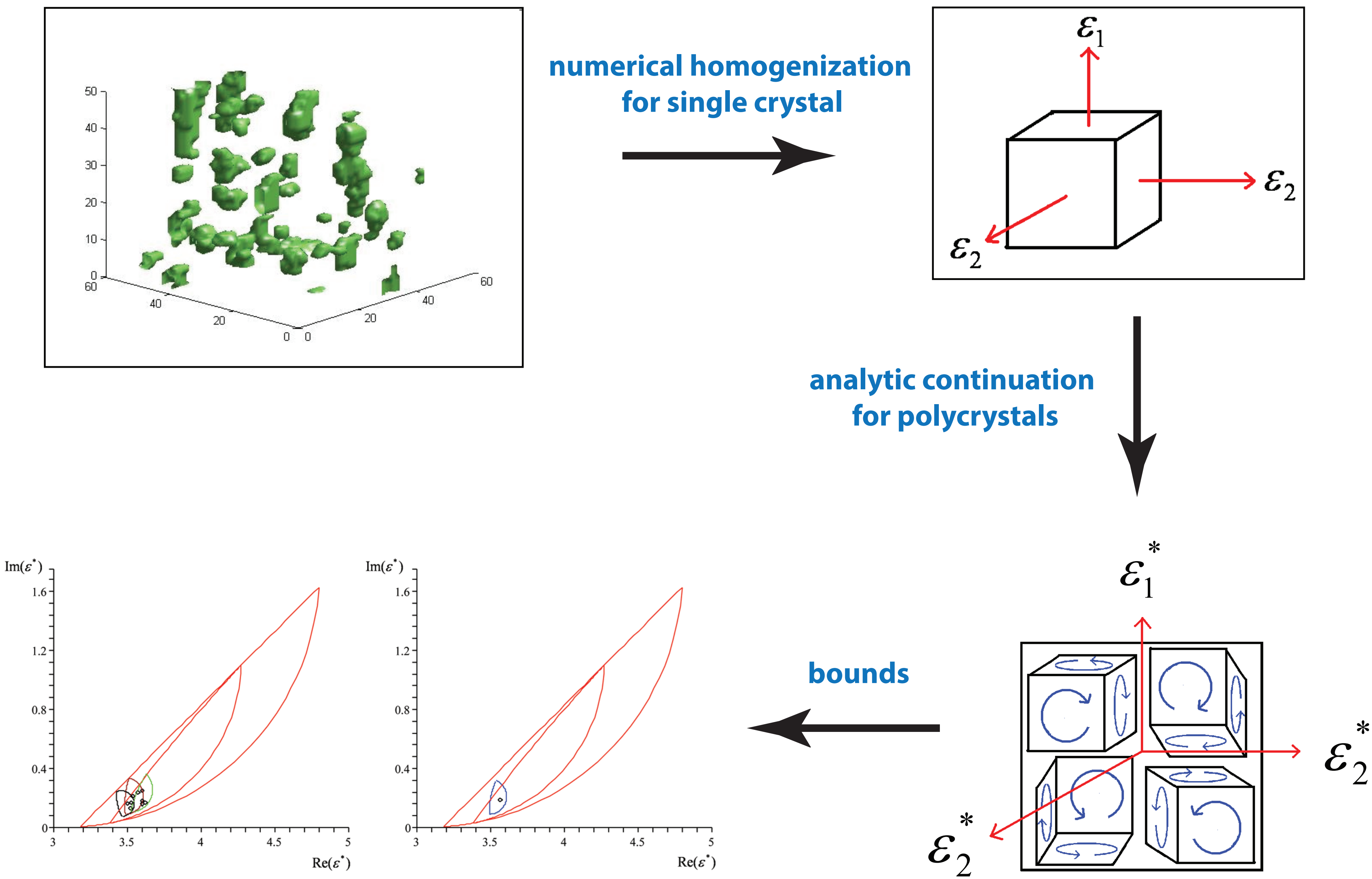
- **Applied to sea ice using two-scale homogenization**

- **Inverse bounds give method for distinguishing ice types using remote sensing techniques**



Proc. Roy. Soc. A 8 Feb 2015

two scale homogenization for polycrystalline sea ice

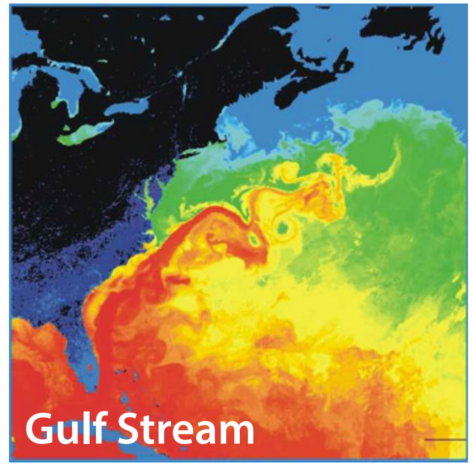


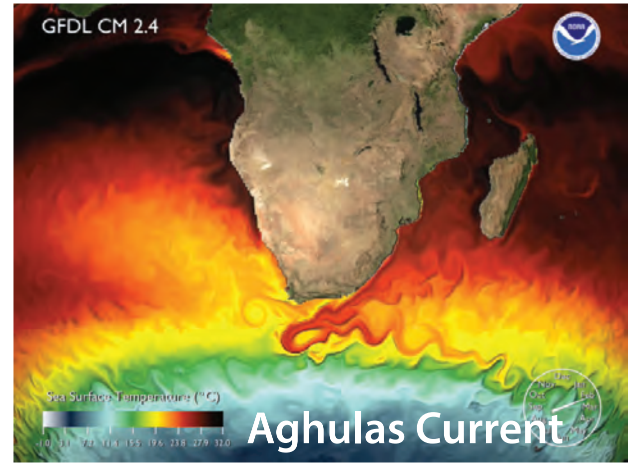
Gully, Lin, Cherkaev, Golden, Proc. Roy. Soc. A (and cover) 2015

advection enhanced diffusion

effective diffusivity

sea ice floes diffusing in ocean currents
diffusion of pollutants in atmosphere
salt and heat transport in ocean
heat transport in sea ice with convection





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

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

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

homogenize

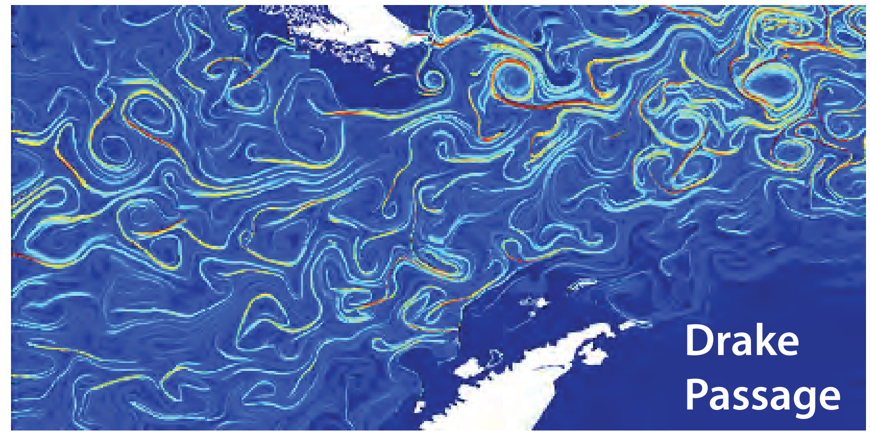
$$\frac{\partial \overline{T}}{\partial t} = \kappa^* \Delta \overline{T}$$

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, 2018



Stieltjes Integral Representation for Advection Diffusion

[Murphy, Cherkaev, Zhu, Xin & Golden 2018]

[Murphy, Cherkaev, Xin, Zhu & Golden 2017]

$$\kappa^* = \kappa \left(1 + \int_{-\infty}^{\infty} \frac{d\mu(\tau)}{\kappa^2 + \tau^2} \right), \quad F(\kappa) \ = \int_{-\infty}^{\infty} \frac{d\mu(\tau)}{\kappa^2 + \tau^2}$$

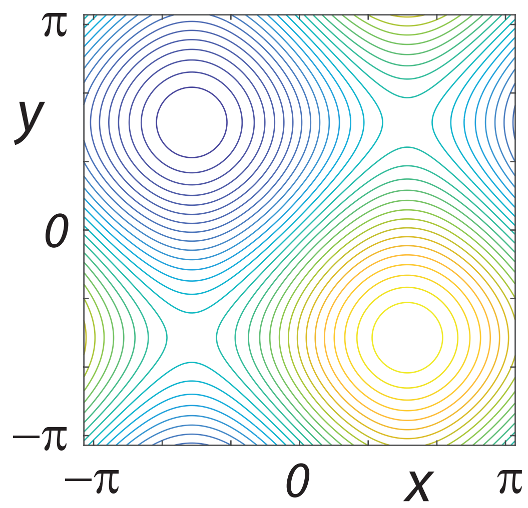
- μ is a positive definite measure corresponding to the spectral resolution of the self-adjoint operator $i\Gamma H\Gamma$
- $H =$ stream matrix , $\kappa =$ local diffusivity
- $\Gamma := -\nabla(-\Delta)^{-1}\nabla\cdot$, Δ is the Laplace operator
- $i\Gamma H\Gamma$ is bounded for time independent flows
- $F(\kappa)$ is analytic off the spectral interval in the κ-plane

separation of material properties and flow field

spectral measure calculations

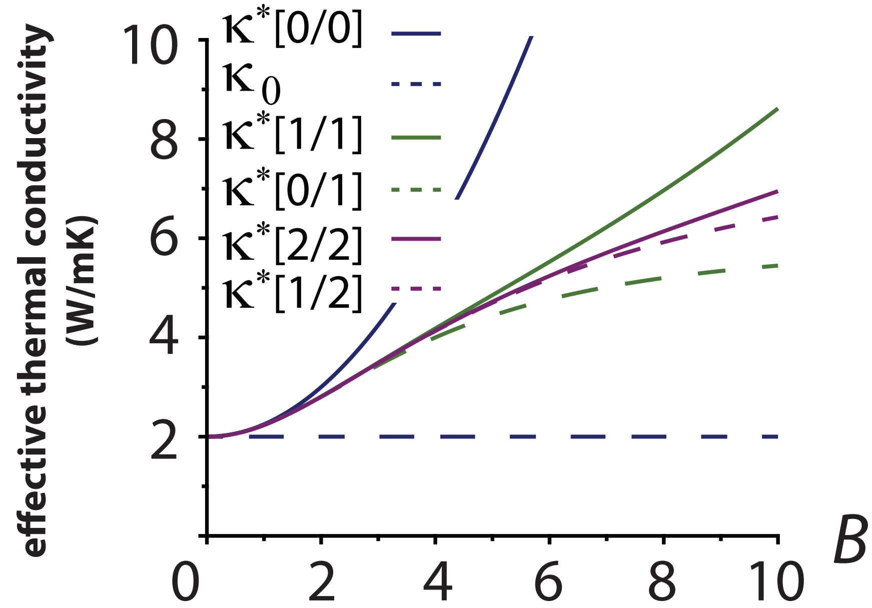
RIGOROUS BOUNDS on convection - enhanced thermal conductivity of sea ice

Kraitzman, Hardenbrook, Murphy, Zhu, Cherkaev, Golden 2018

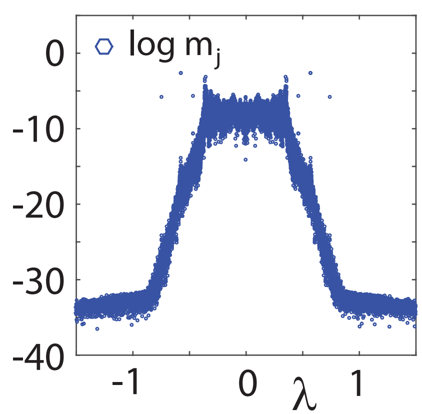


***BC* - flow streamlines**

$H = B \sin x - C \sin y \quad B = C$



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

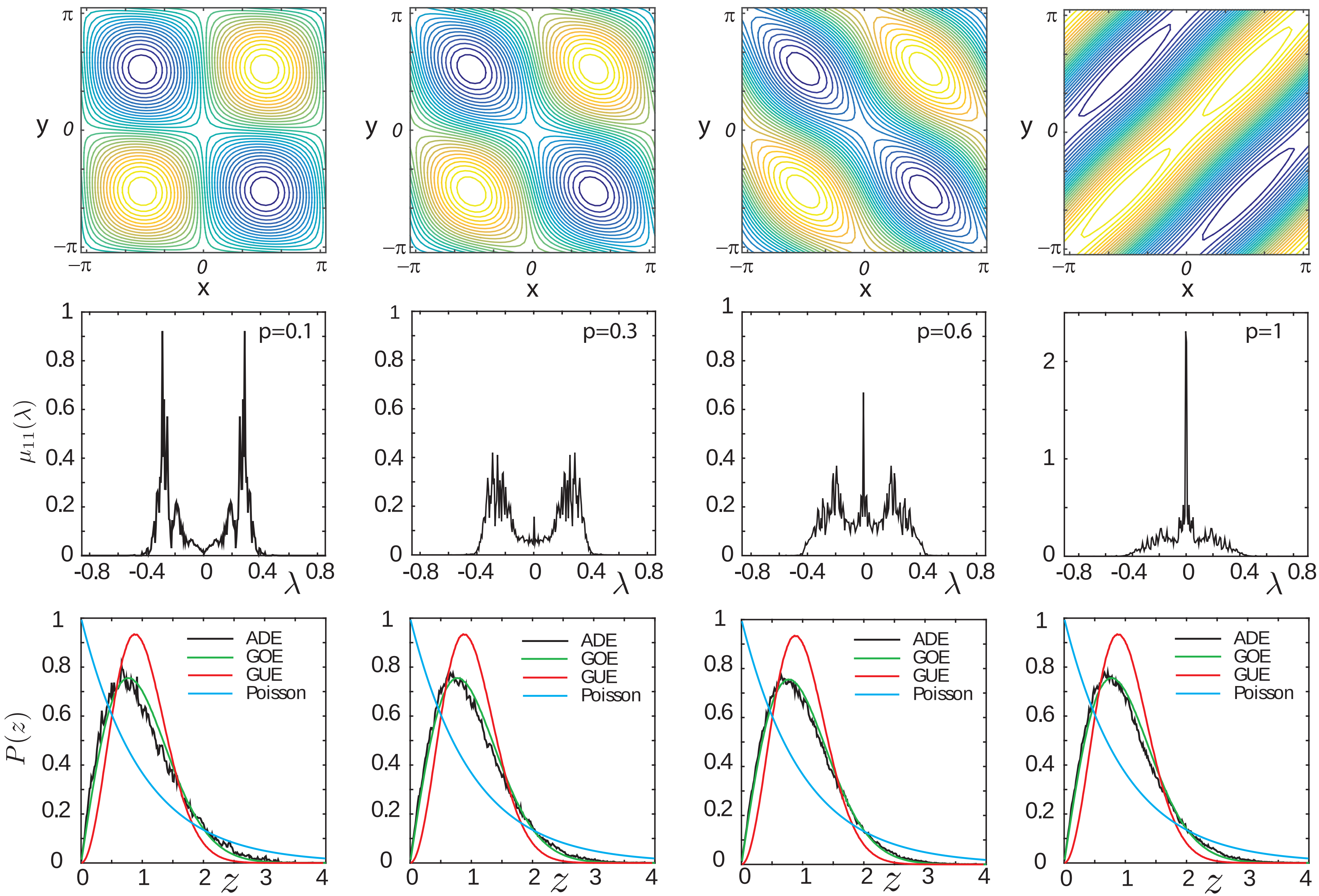


spectral masses

Murphy, Cherkaev, Zhu, Xin, Golden 2018

Spectral measures and eigenvalue spacings for cat's eye flow

$$H(x,y) = \sin(x)\sin(y) + A\cos(x)\cos(y), \qquad A \sim U(-p,p)$$

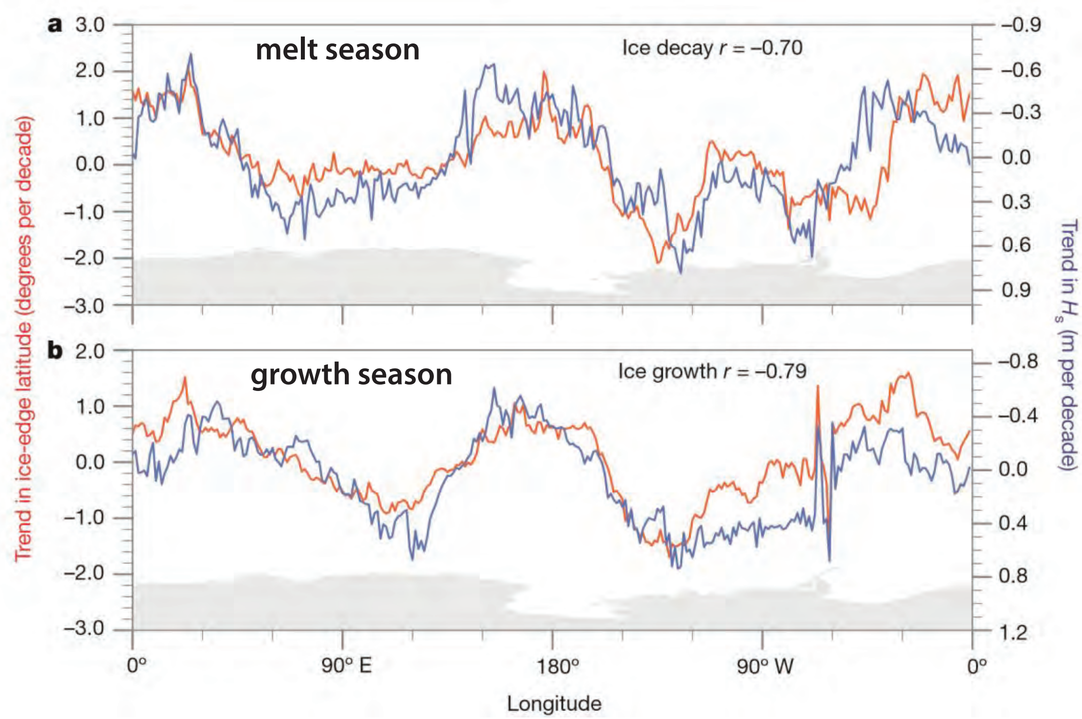


Murphy, Cherkaev, Zhu, Xin, Golden

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

Kohout et al., *Nature* 2014

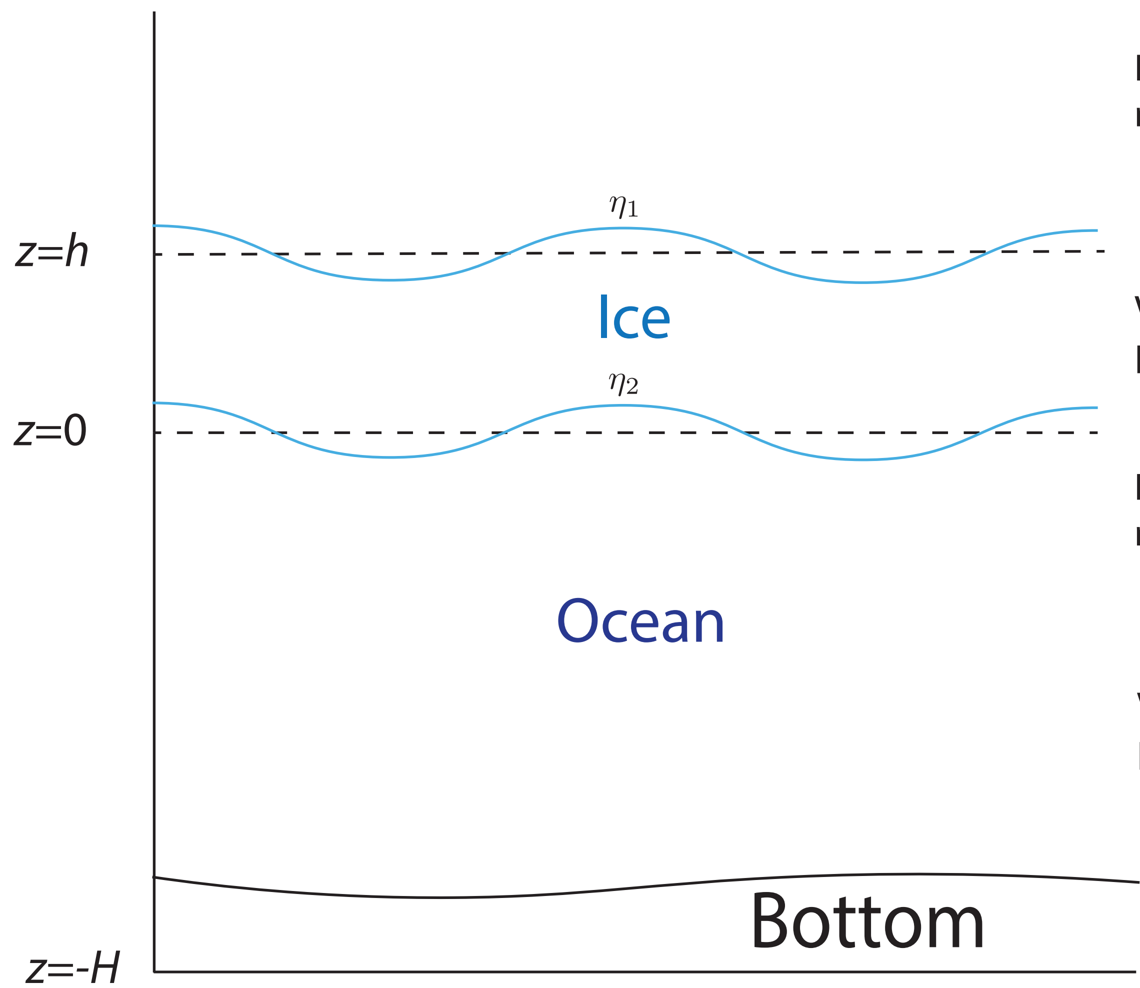
- during three large-wave events, significant wave heights did not decay exponentially, enabling large waves to persist deep into the pack ice.
- large waves break sea ice much farther from the ice edge than would be predicted by the commonly assumed exponential decay



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



G shear modulus
P pressure
ω angular frequency
U velocity field
ν viscosity
λ Poission ratio
ρ density
g gravity

Viscous fluid layer (Keller 1998)

Effective Viscosity $\boxed{\nu}$

Equations of motion:

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

Viscoelastic fluid layer (Wang-Shen 2010)

Effective Complex Viscosity $\boxed{\nu_e = \nu + iG/\rho\omega}$

Equations of motion

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

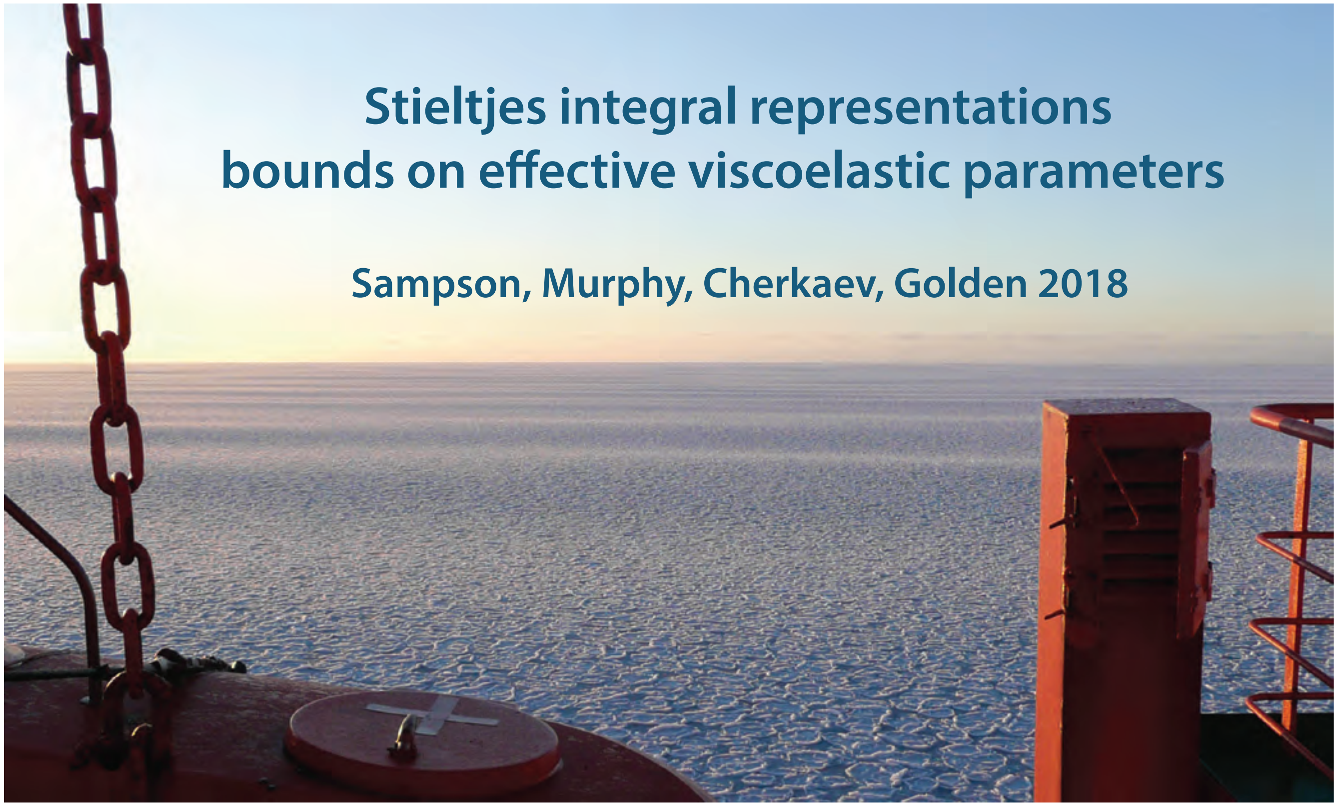
Viscoelastic thin beam (Mosig *et al.* 2015)

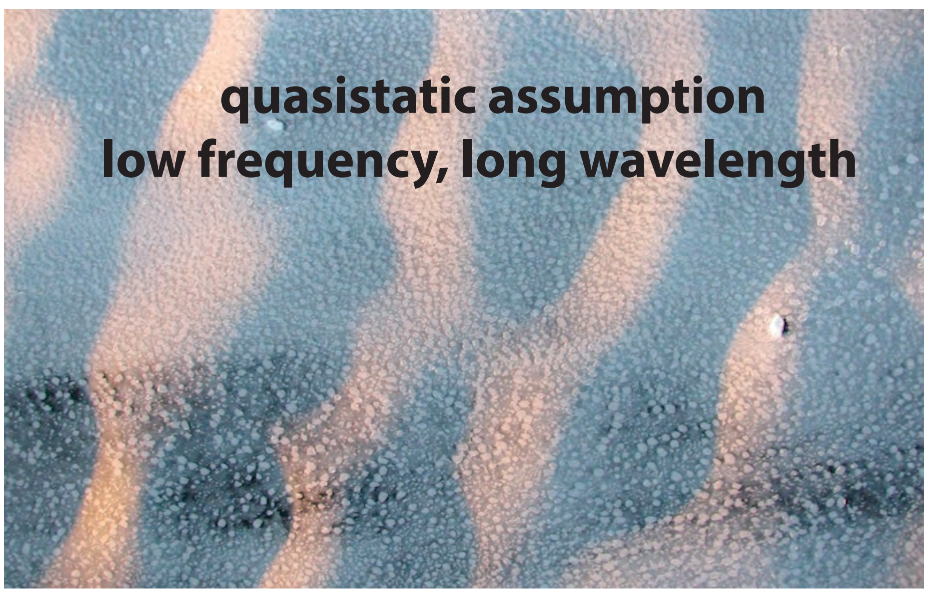
Effective Complex Shear Modulus $\boxed{G_v = G - i\omega\rho\nu}$

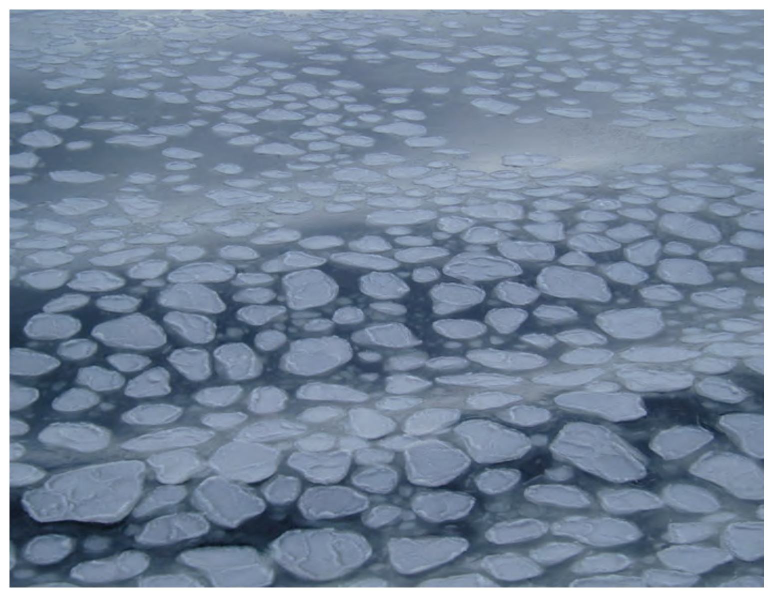
Stieltjes integral representation for effective complex viscoelastic parameter; bounds

Sampson, Murphy, Cherkaev, Golden 2018

wave propagation in the marginal ice zone







Stieltjes Integral Representation for Complex Viscoelasticity

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

local $\nabla \cdot \sigma = 0$ $\sigma_{ij} = C_{ijkl}\epsilon_{kl}$

$$C_{ijkl} = (\nu_1 \chi + (1-\chi)\nu_2)\lambda_s$$

$$\nabla \cdot \big((\nu_1 \chi + (1-\chi)\nu_2)\lambda_s : \epsilon\big) = 0$$

$$s = \frac{1}{1 - \frac{\nu_1}{\nu_2}}$$

Strain Field

$$\epsilon = \frac{1}{2}[\nabla u + (\nabla u)^T] = \nabla^s u$$

$$\epsilon = \epsilon_0 + \epsilon_f \text{ where } \epsilon_f = \nabla^s \phi$$

Elasticity Tensor

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

RESOLVENT $\epsilon = \left(1 - \frac{1}{s}\Gamma\chi\right)^{-1}\epsilon_0$ $\Gamma = \nabla^s(\nabla \cdot \nabla^s)^{-1}\nabla \cdot$ ϵ_0 **avg strain**

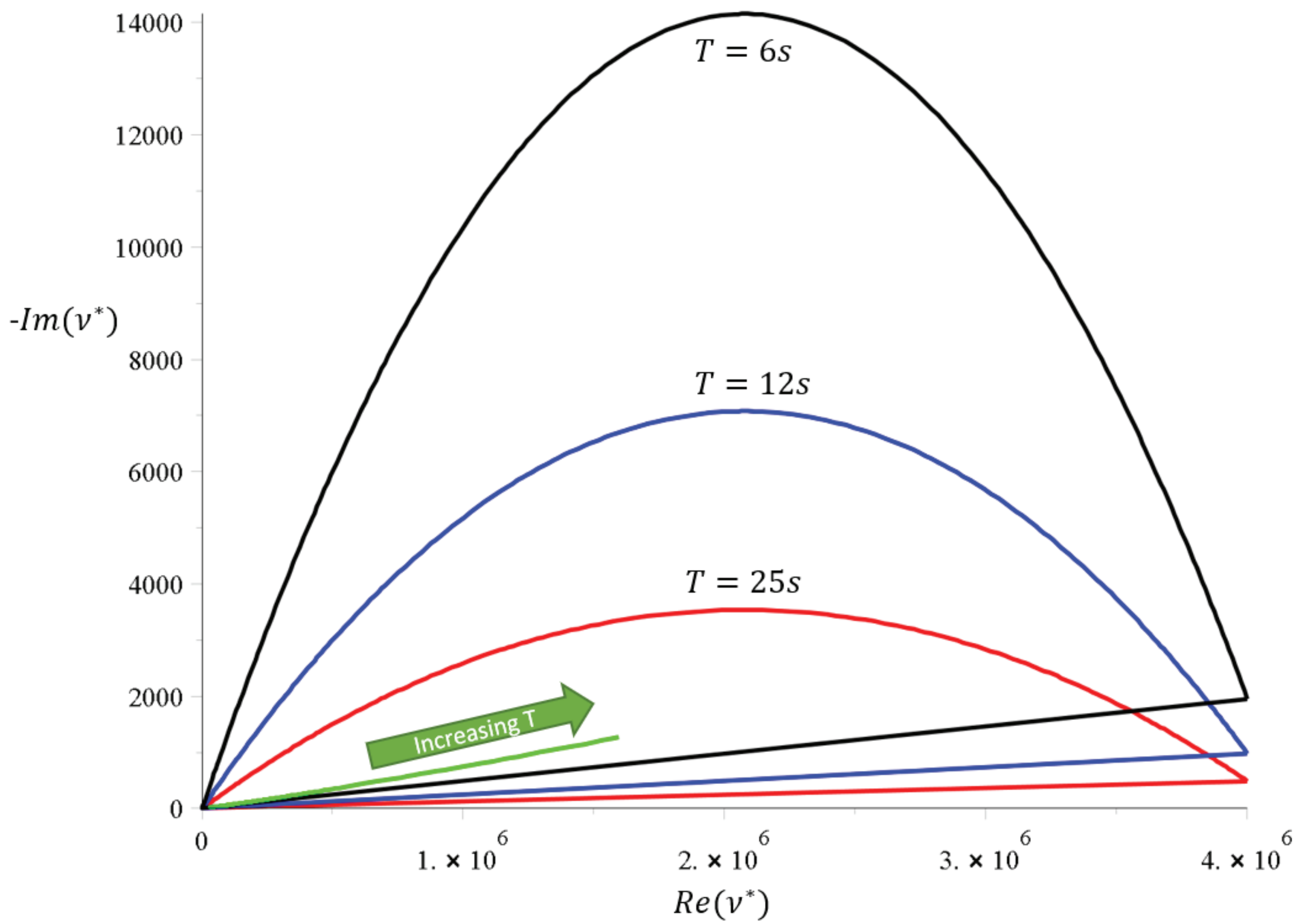
$$F(s) = 1 - \frac{\nu^*}{\nu_2} \qquad F(s) = ||\epsilon_0||^{-2} \int_\Sigma \frac{d\mu(\lambda)}{s - \lambda}$$

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



Sampson, Murphy, Cherkaev, Golden 2018

Conclusions

1. Summer Arctic sea ice is melting rapidly, and melt ponds and other processes must be accounted for in order to predict melting rates.

2. Fluid flow through sea ice mediates melt pond evolution and many processes important to climate change and polar ecosystems.

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

4. Random matrix theory and an unexpected Anderson transition arises in our studies of percolation in sea ice structures.

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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Buchanan Bay, Antarctica   Mertz Glacier Polynya Experiment   July 1999