Random matrices, spectral measures, and composite media

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SIAM Conference on Mathematics of Materials
MS1: Stochastic Homogenization
Philadelphia, 9 June 2013

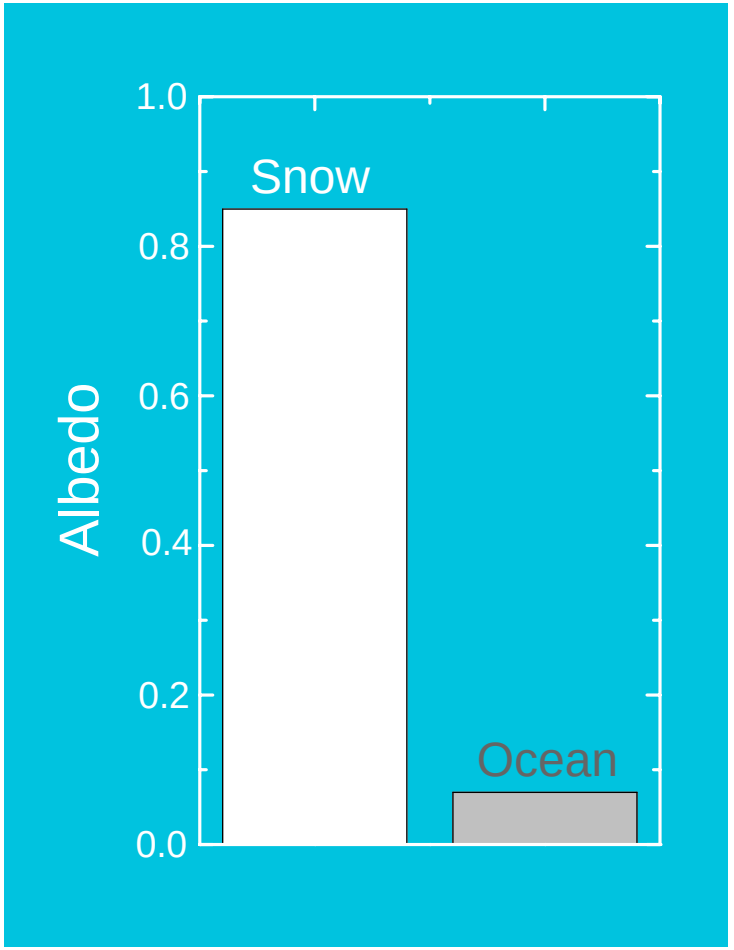
Frey

SEA ICE covers 7 - 10% of earth's ocean surface

- boundary between ocean and atmosphere
- mediates exchange of heat, gases, momentum
- indicator and agent of climate change

polar ice caps critical to global climate in reflecting incoming solar radiation

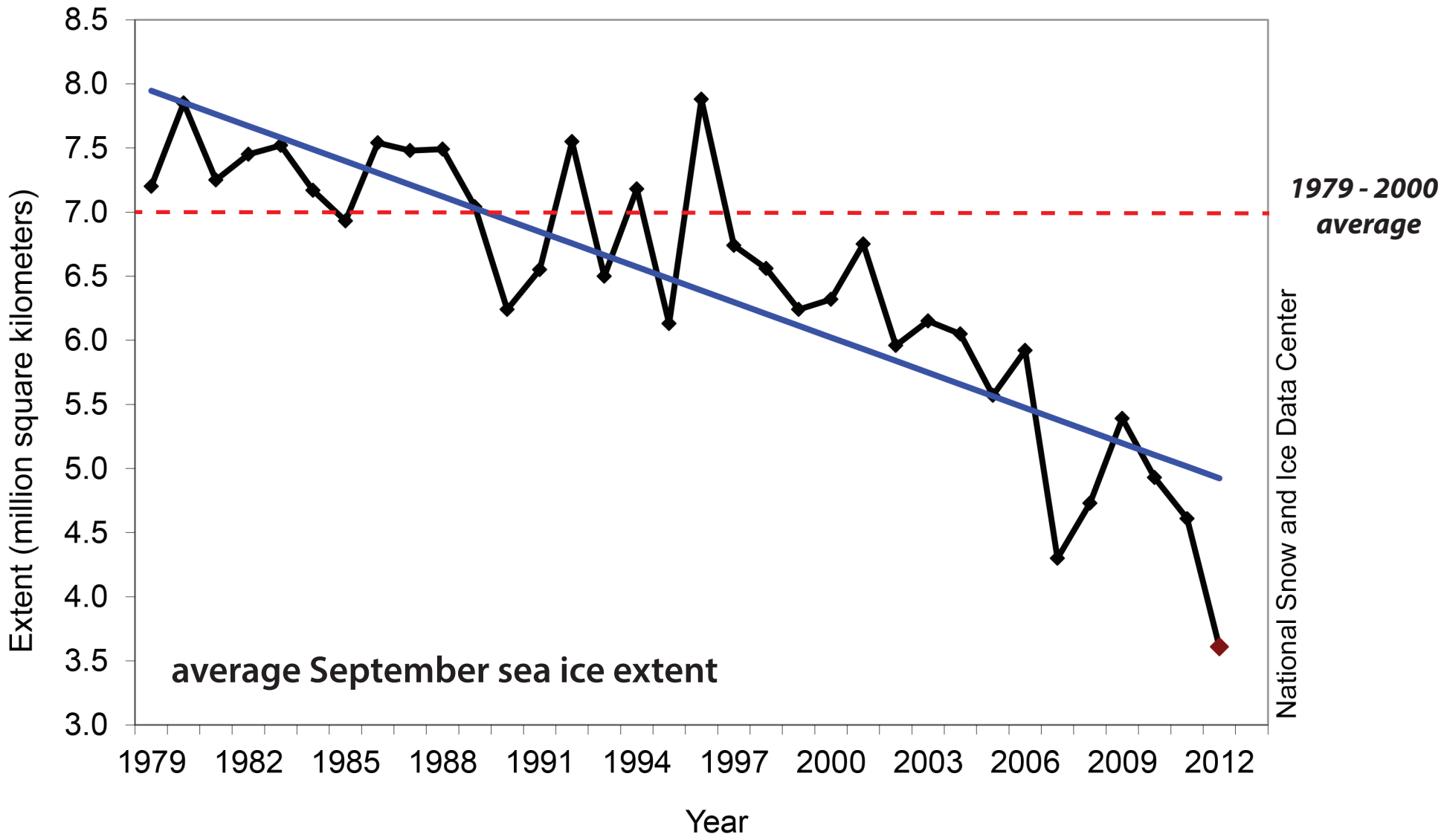
white snow and ice reflect



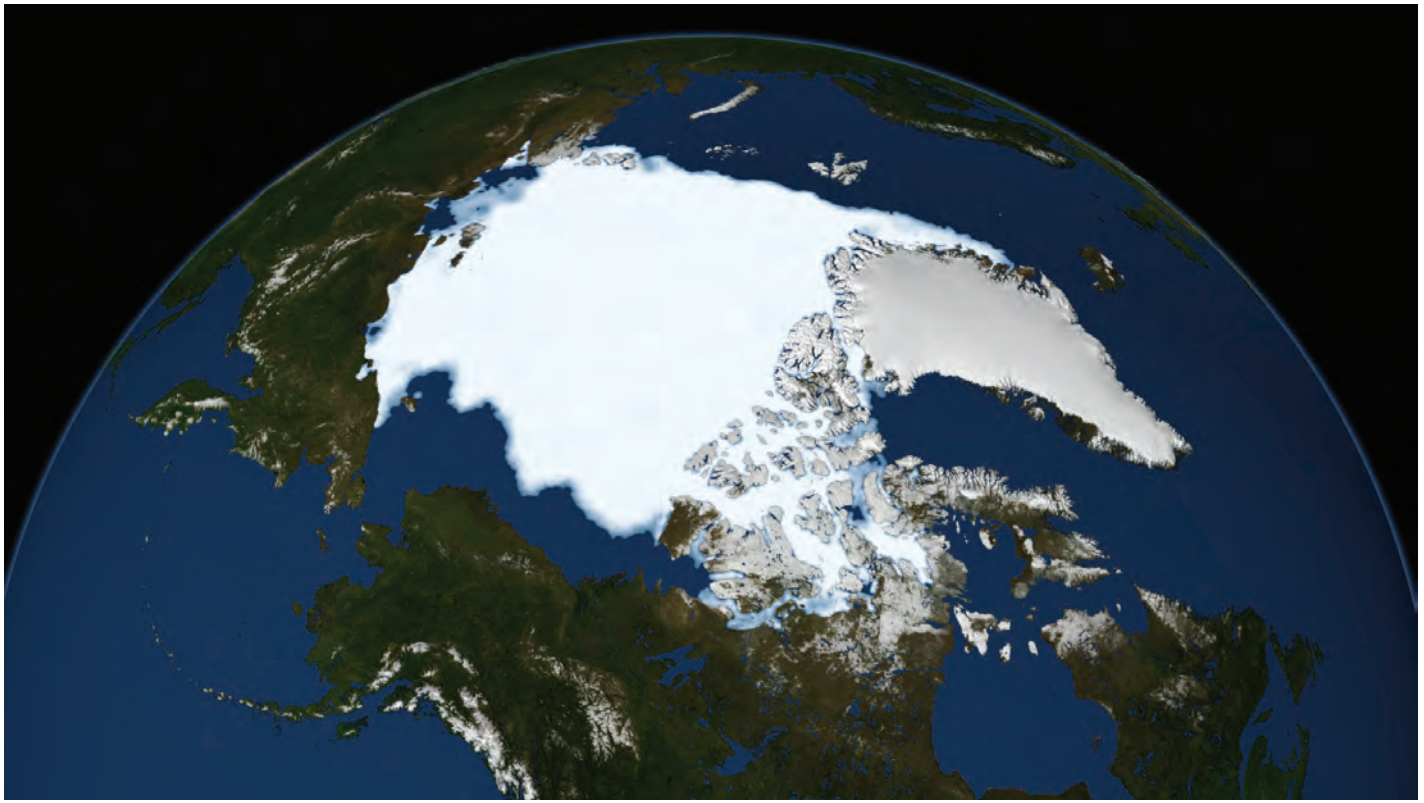
dark water and land absorb

$$\textit{albedo}\ \alpha = \frac{\text{reflected sunlight}}{\text{incident sunlight}}$$

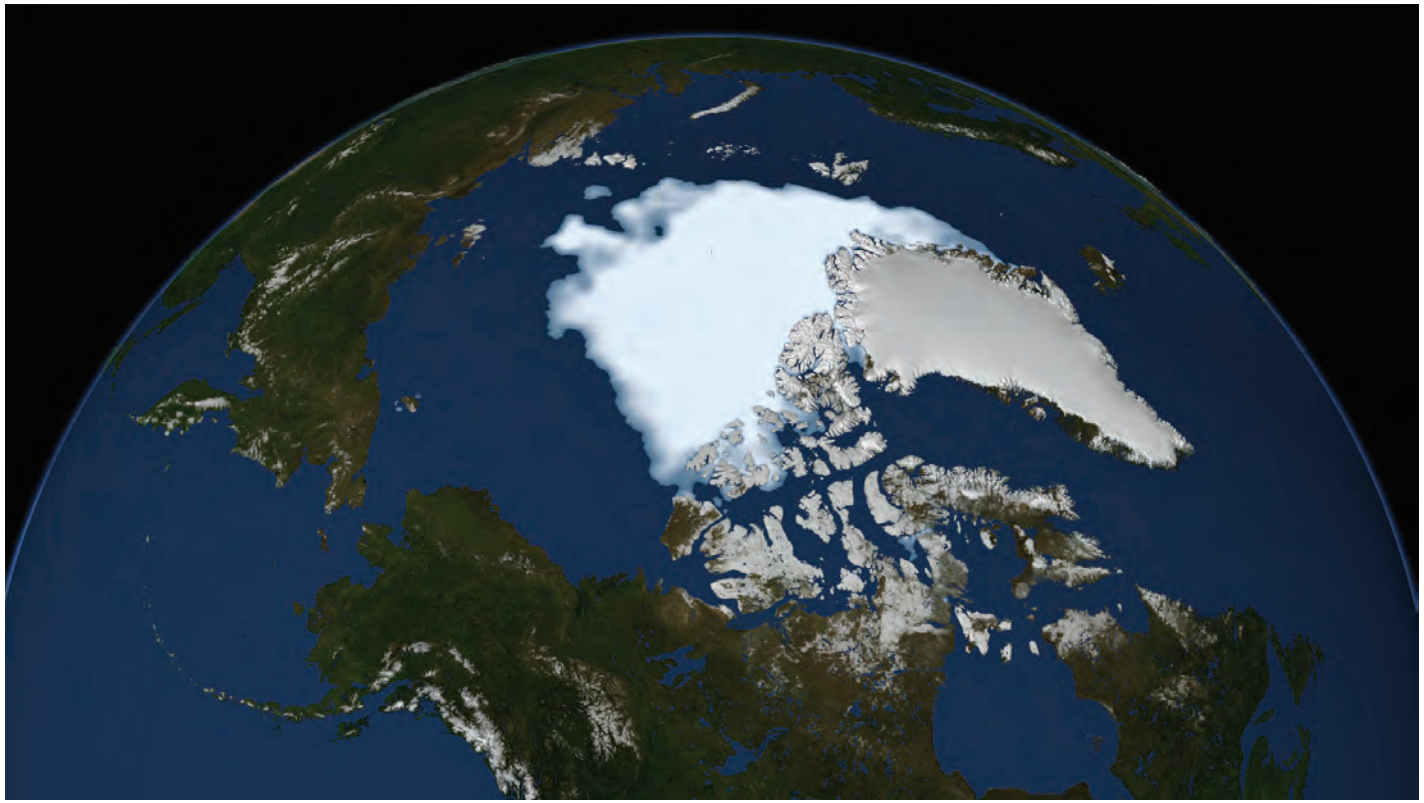
the summer Arctic sea ice pack is melting



21 September 1979

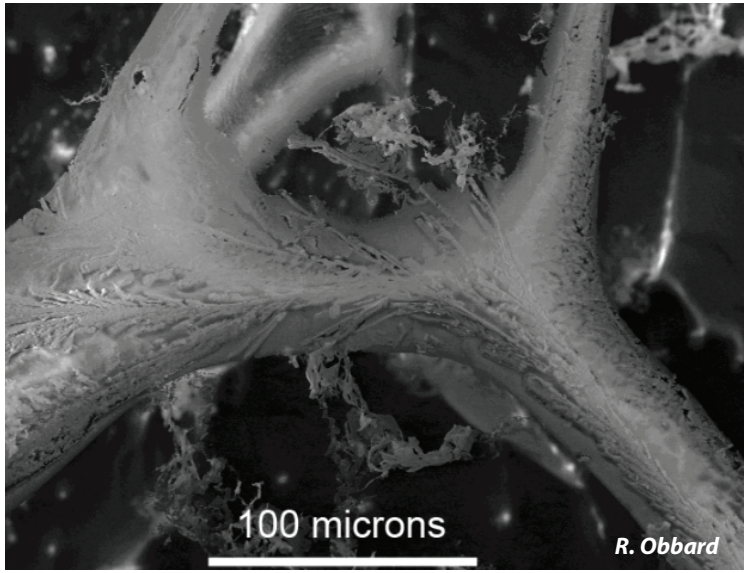


13 September 2012



sea ice may appear to be a barren, impermeable cap ...

brine inclusions in sea ice (mm)

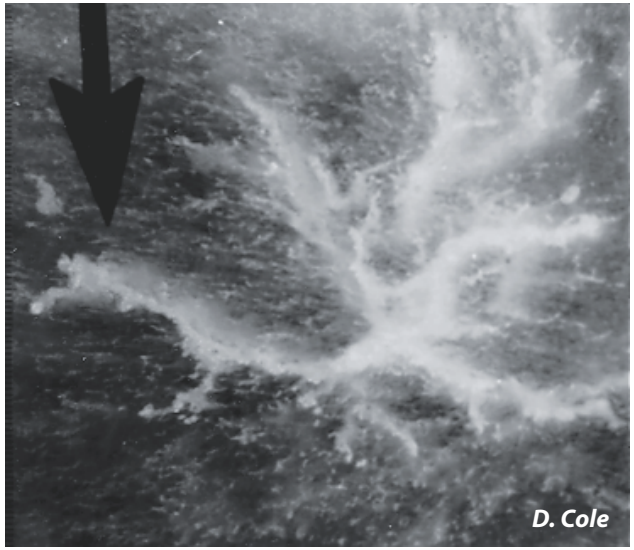


micro - brine channel (SEM)

sea ice is a porous composite

pure ice with brine, air, and salt inclusions

brine channels (cm)



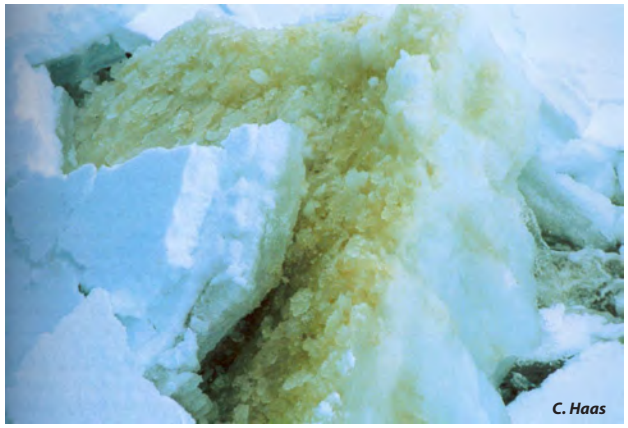
horizontal section

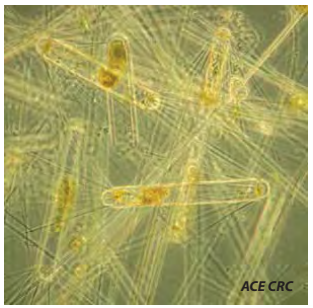
vertical section

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

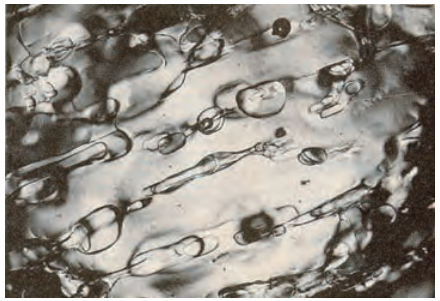
nutrient flux for algal communities





- drainage of brine and melt water
- ocean-ice-air exchanges of heat, CO_2

linkage of scales



What is this talk about? (+ preview of afternoon lecture)

Using the mathematics of composite materials and statistical physics to study sea ice structures and processes ... to improve projections of climate change.

→ 1. ***Fluid flow through sea ice*** - percolation, flow in porous media

2. ***Arctic and Antarctic experiments*** on fluid and electrical transport

3. ***Fractal structure*** - floe and melt pond configurations

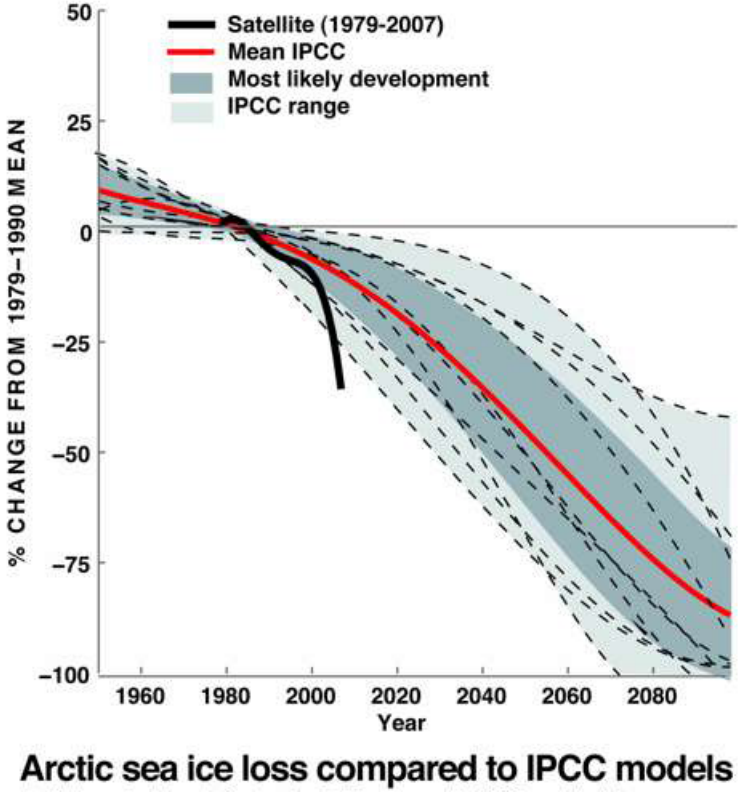
→ 4. ***Multiscale Homogenization*** - spectral upscaling, random matrices

critical behavior ***linkage of scales***

.... and to suggest a path forward for more rigorously and efficiently representing sea ice in climate models.

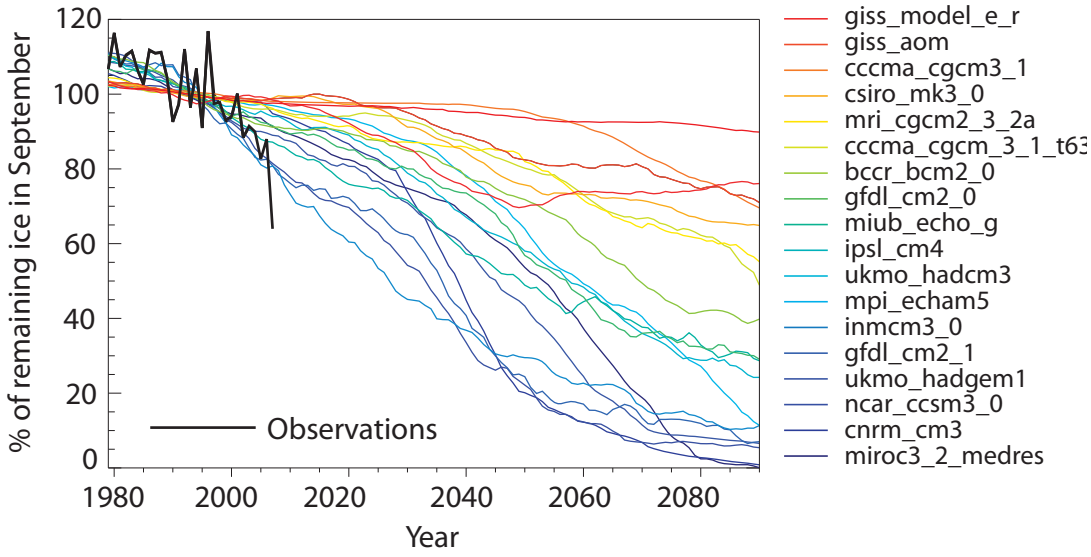
Intergovernmental Panel on Climate Change (IPCC) 2007 projections

observed decline in summer Arctic sea ice outpacing global climate models



Arctic sea ice loss compared to IPCC models

September 2007



March 2009

Boé, Hall, Qu 2009

sea ice microphysics

fluid transport

Darcy's Law for slow viscous flow in a porous medium

averaged fluid velocity

pressure gradient

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

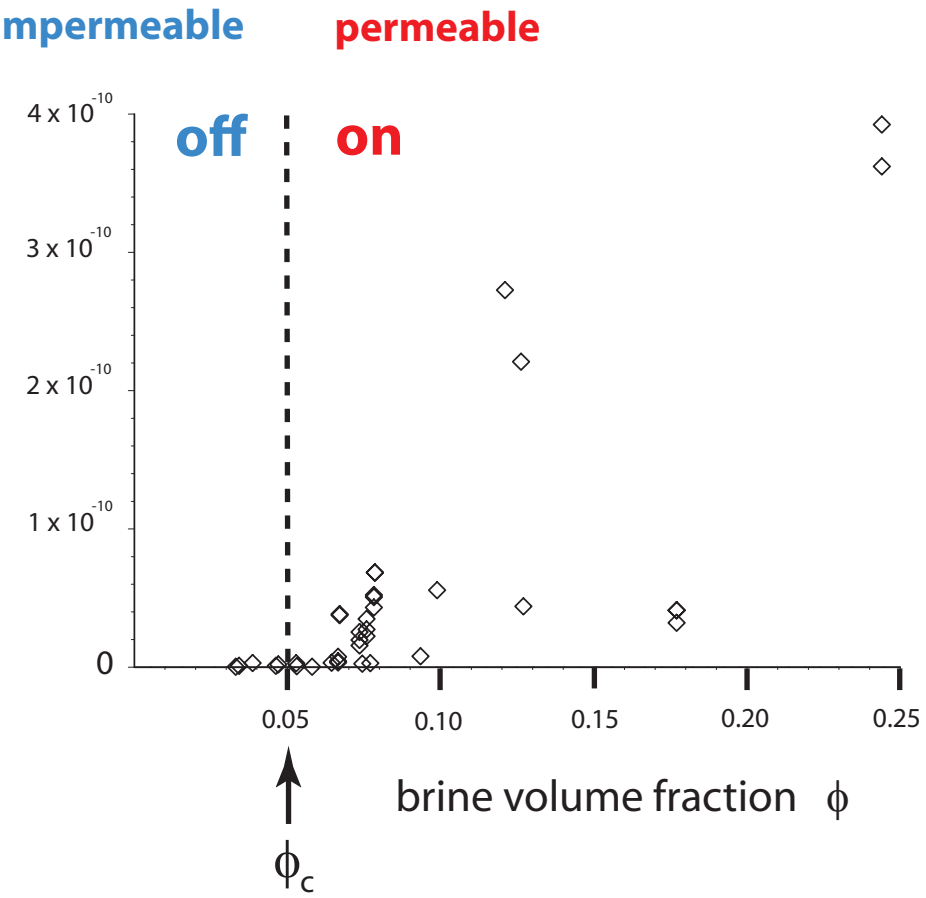
viscosity

$\mathbf{k}$ = fluid permeability tensor

example of *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

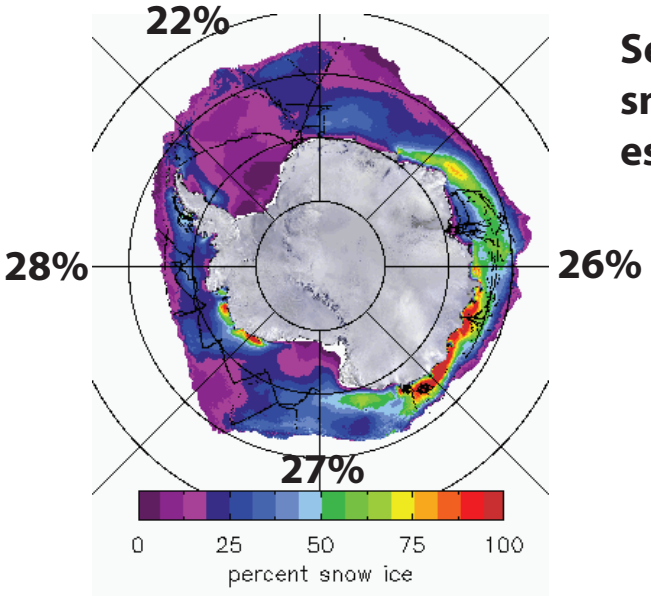
Golden, Ackley, Lytle *Science* 1998

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

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

rule of fives constrains:

Antarctic surface flooding and snow-ice formation

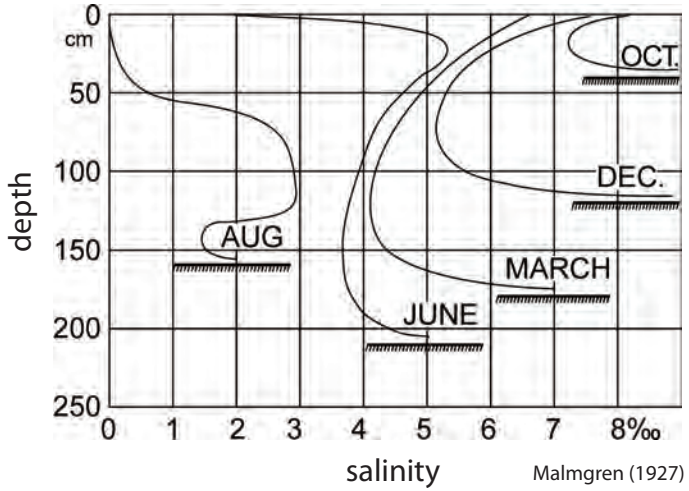


September snow-ice estimates

Antarctic snow-to-ice conversion from passive microwave imagery

T. Maksym and T. Markus, 2008

evolution of salinity profiles



Malmgren (1927)

currently assumed constant in climate models

convection - enhanced thermal conductivity

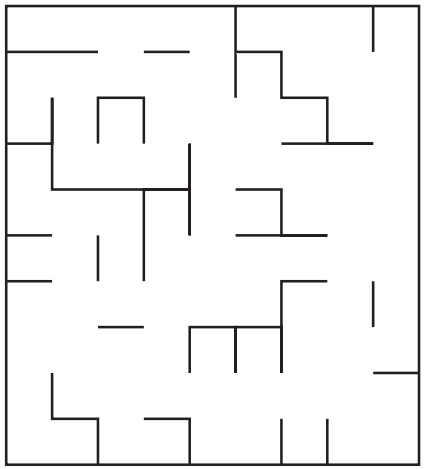
Lytle and Ackley, 1996
Trodahl, et. al., 2000, 2001
Wang, Zhu, Golden, 2012

theoretical models explaining the *rule of fives* and fluid flow properties

percolation theory

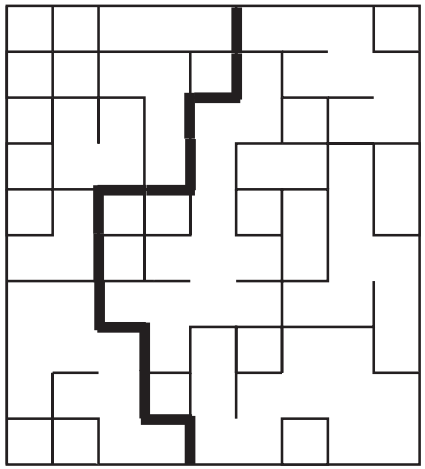
mathematical theory of connectedness

impermeable



$p = 1/3$

permeable



$p = 2/3$

bond → *open* *with probability p*
closed with probability 1-p

percolation threshold

$p_c = 1/2$ for $d = 2$

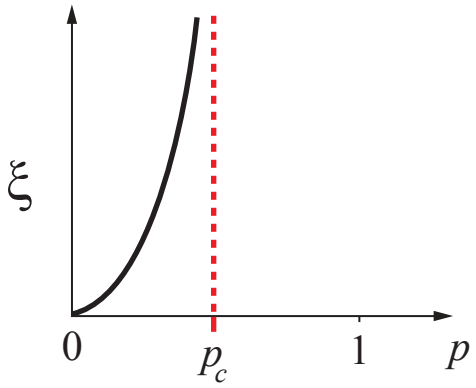
first appearance of infinite cluster ***"tipping point" for connectivity***

order parameters in percolation theory

geometry ***transport***

correlation length

characteristic scale of connectedness

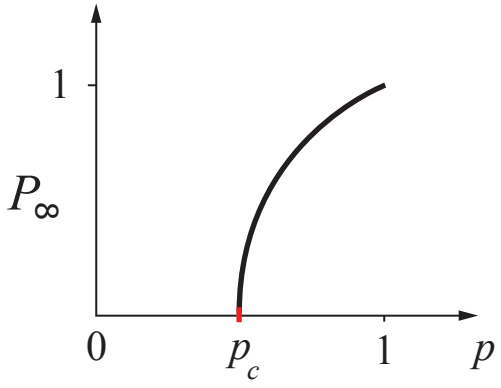


$$\xi(p) \sim |p - p_c|^{-\nu}$$

$$p \to p_c$$

infinite cluster density

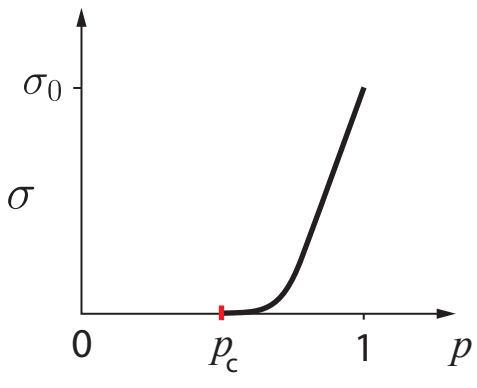
probability the origin belongs to infinte cluster



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

$$p \to p_c^+$$

effective conductivity or fluid permeability



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

$$p \to p_c^+$$

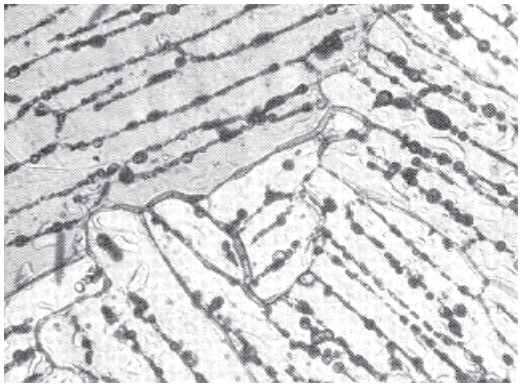
UNIVERSAL critical exponents for lattices -- depend only on dimension

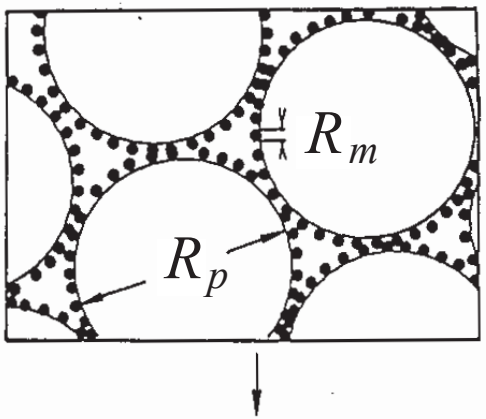
(1 ≤ *t* ≤ 2, Golden, *Phys. Rev. Lett.* 1990 **;** *Comm. Math. Phys.* 1992)

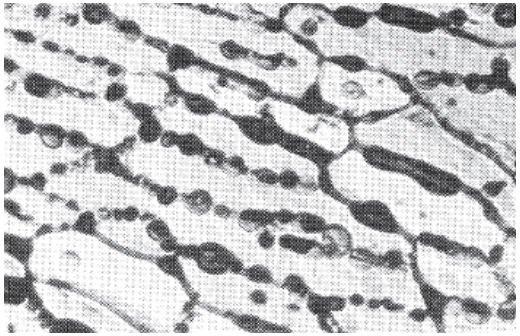
non-universal behavior in continuum

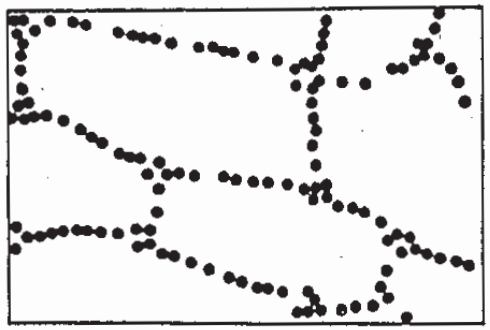
Continuum percolation model for stealthy materials applied to sea ice microstructure explains **Rule of Fives** and Antarctic data on ice production and algal growth

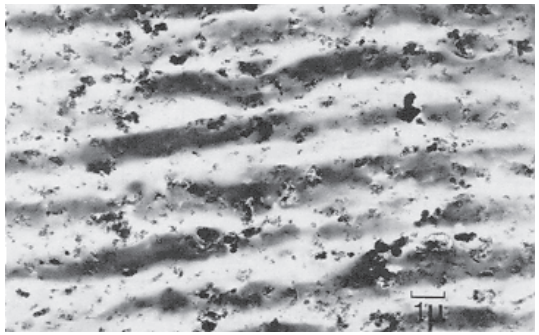
$\phi_c \approx 5\ \%$ Golden, Ackley, Lytle, *Science,* 1998











sea ice

compressed powder

radar absorbing composite

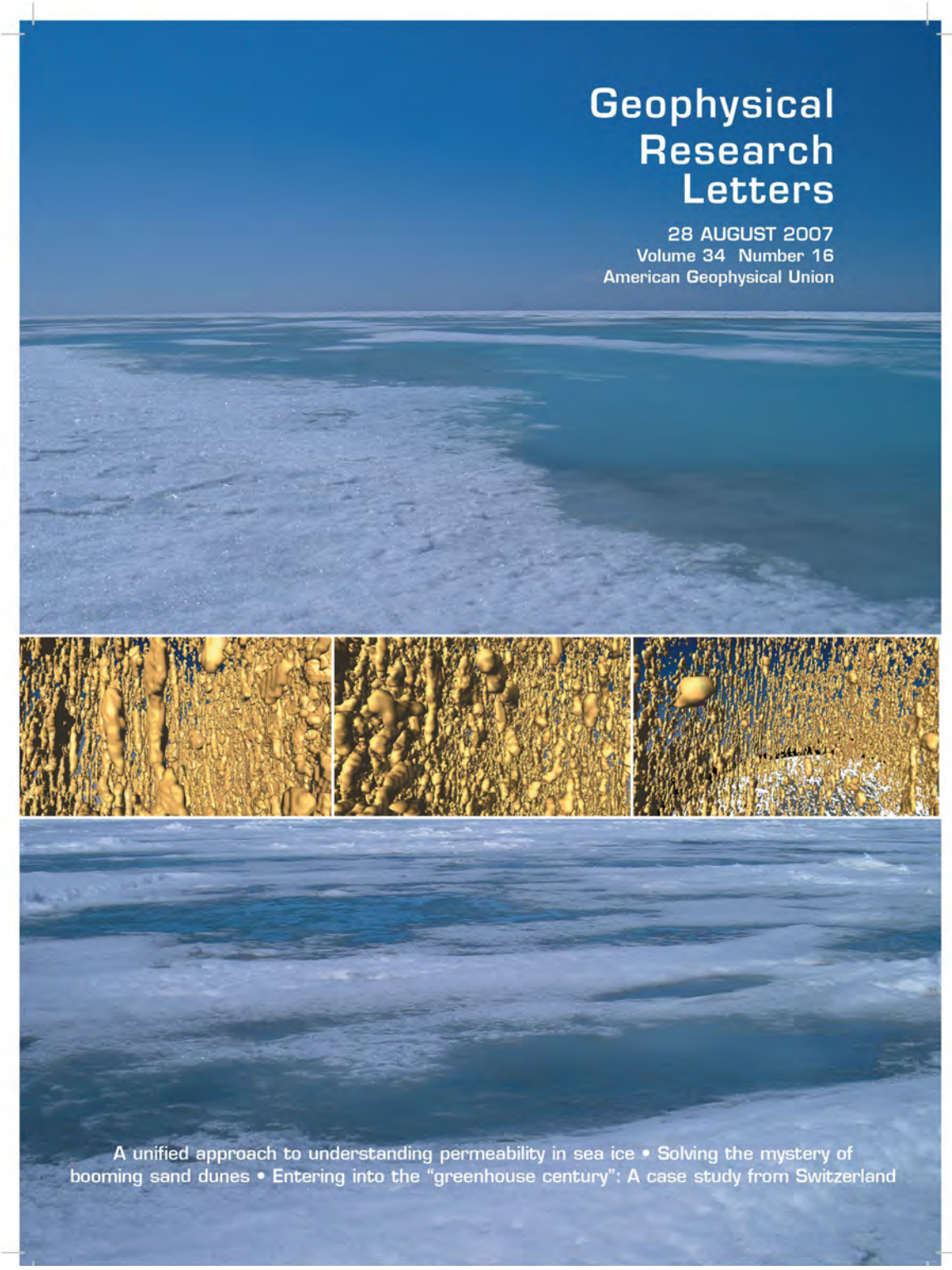
sea ice is radar absorbing

Thermal evolution of permeability and microstructure in sea ice ***Golden, Eicken, Heaton, Miner, Pringle, Zhu***

micro-scale

controls

macro-scale processes



rigorous bounds
percolation theory
hierarchical model
network model

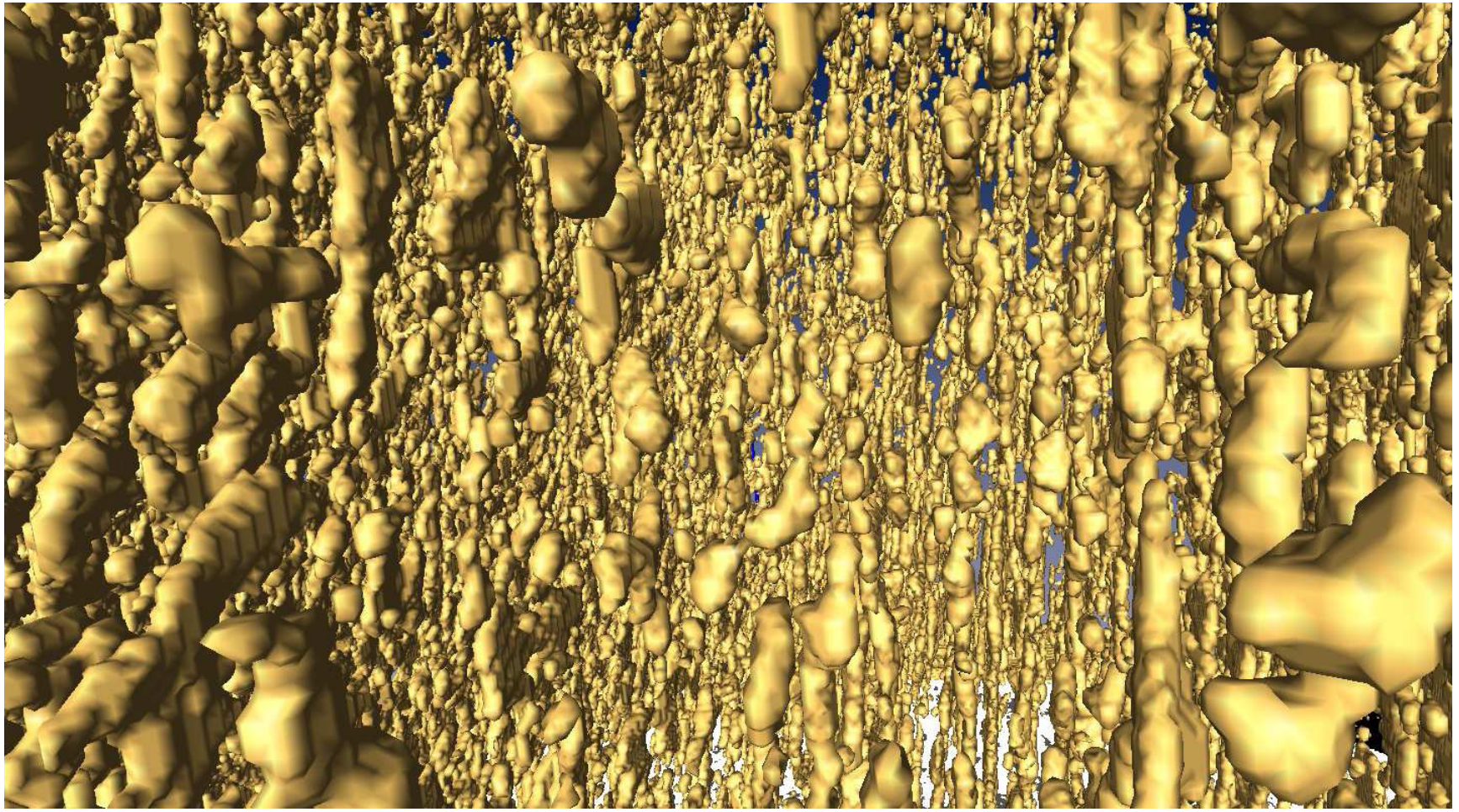
field data

X-ray tomography for brine inclusions

unprecedented look at thermal evolution of brine phase and its connectivity

X-ray computed tomography of brine inclusions in sea ice

~ 1 cm across

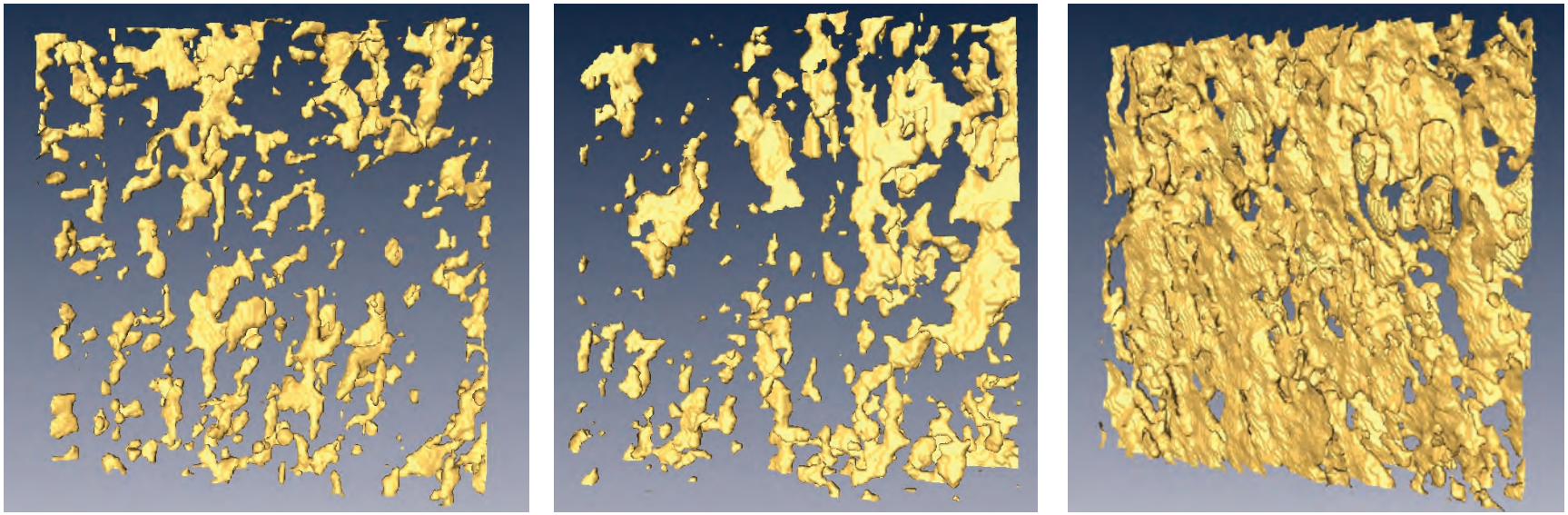


brine volume fraction $\phi = 5.7\ \%$ $\quad T = -8^{\circ}C$

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

brine connectivity (over cm scale)

8 x 8 x 2 mm



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

X-ray tomography confirms percolation threshold

3-D images
pores and throats

3-D graph
nodes and edges

analyze graph connectivity as function of temperature and sample size

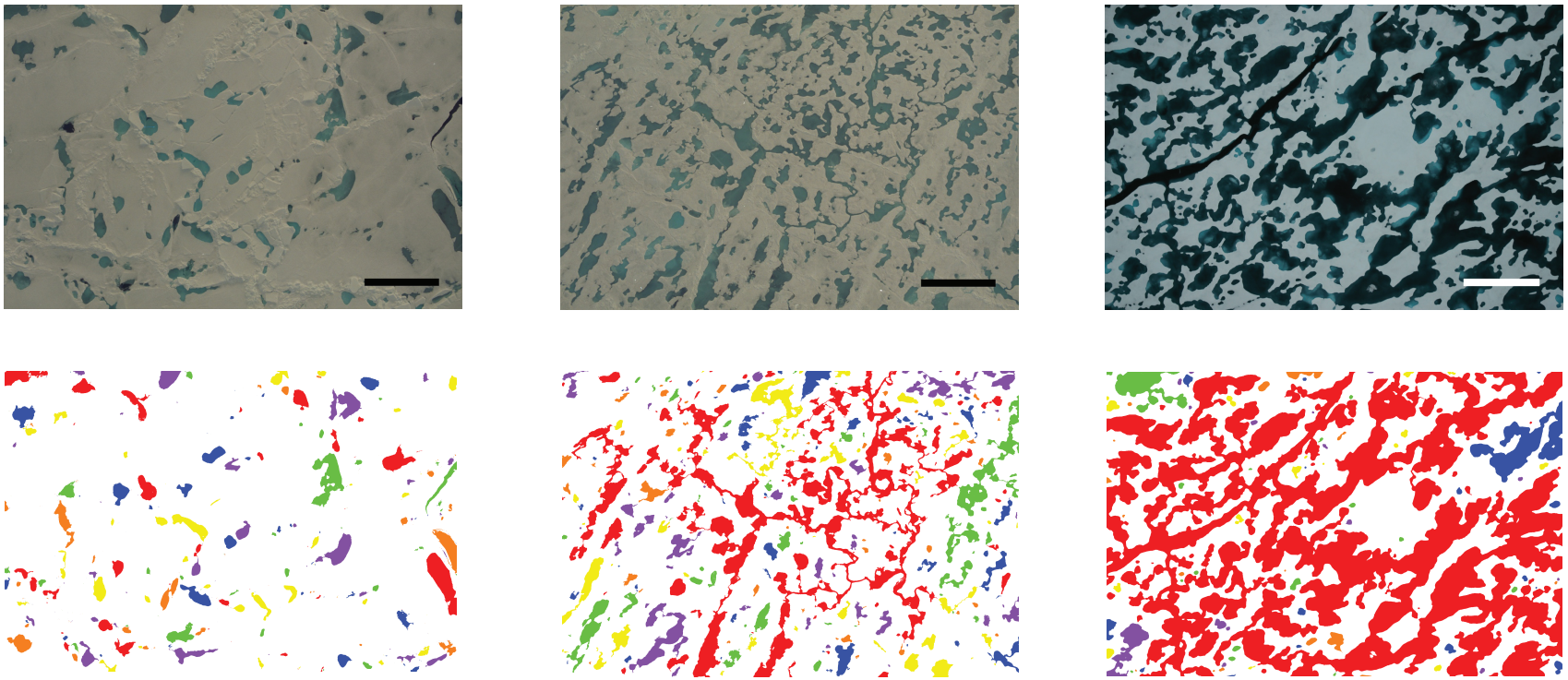
- ***use finite size scaling techniques to confirm rule of fives***
- ***order parameter data from a natural material***

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

melt ponds on the surface of Arctic sea ice

Frey

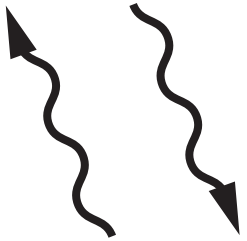
small simple ponds coalesce to form
large connected structures with complex boundaries

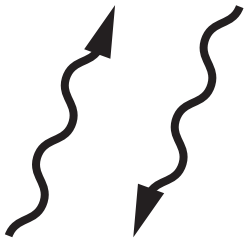


melt pond percolation

multiscale homogenization

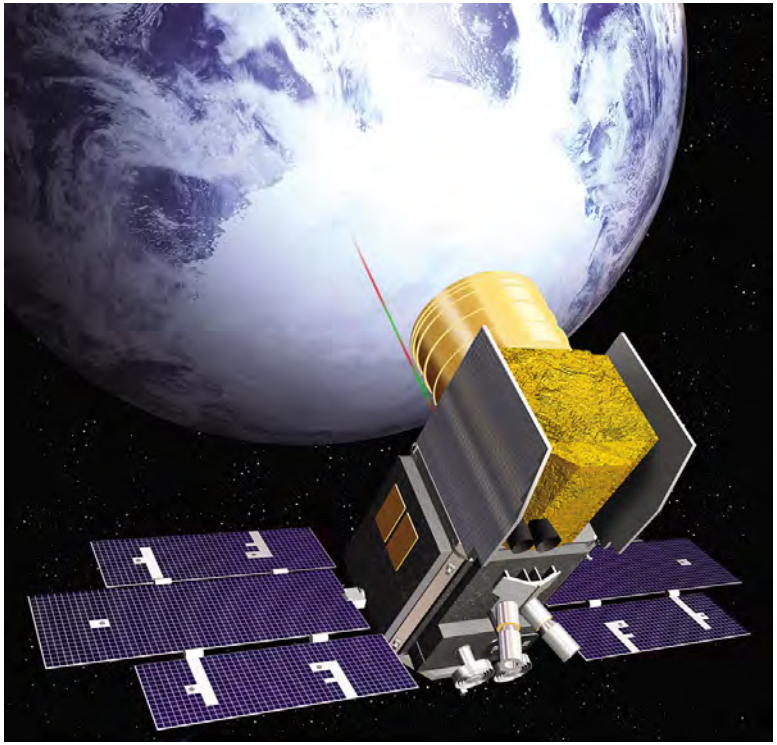
Remote sensing of sea ice





Recover sea ice properties from electromagnetic (EM) data

INVERSE PROBLEM



NASA's Ice, Cloud and Land Elevation Satellite (ICESat)

The Worbot - a low frequency EM induction instrument for measuring sea ice thickness

The key parameter in modeling the response of sea ice to an EM field is its

complex *permittivity* or *dielectric constant* ε^*

which depends strongly on the brine microstructure

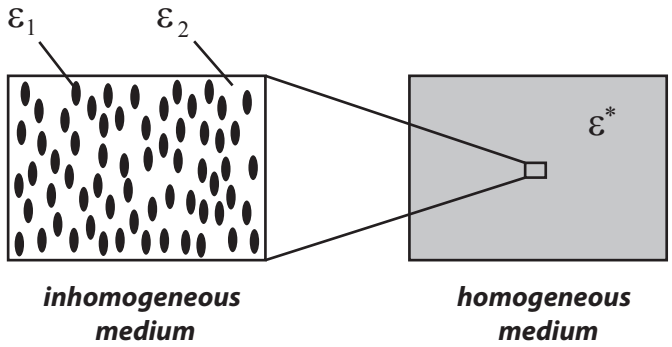
e.g., interpretation of EM thickness data depends on knowledge of ε^*

ocean swells propagating through a vast field of pancake ice

HOMOGENIZATION: long wave sees an effective medium, not individual floes

Theory of Effective Electromagnetic Behavior of Composites

analytic continuation method



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

composite geometry **(spectral measure μ)** $\longrightarrow$ ε^*

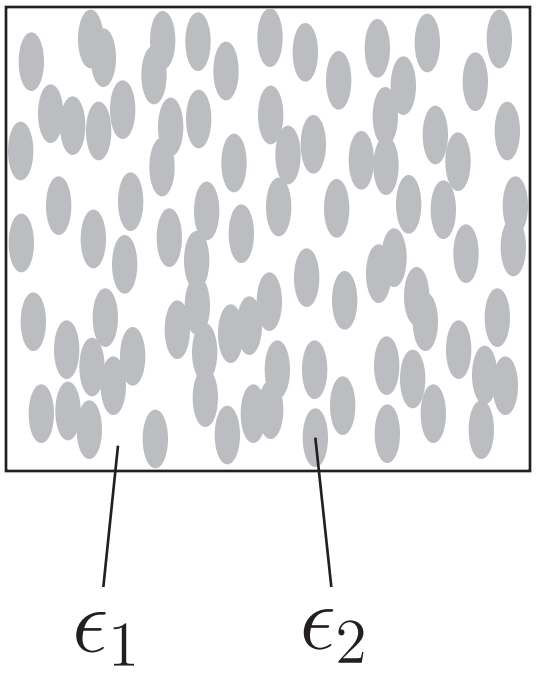
integral representations, rigorous bounds, approximations, etc.

Inverse Homogenization Cherkaev and Golden (1998), Day and Thorpe (1999), Cherkaev (2001) (McPhedran, McKenzie, and Milton, 1982)

ε^* $\longrightarrow$ ***composite geometry*** **(spectral measure μ)**

recover brine volume fraction, connectivity, etc.

Effective complex permittivity of a two phase composite in the quasistatic (long wavelength) limit



ϵ^*

$$D = \epsilon E$$

$$\nabla \cdot D = 0$$

$$\nabla \times E = 0$$

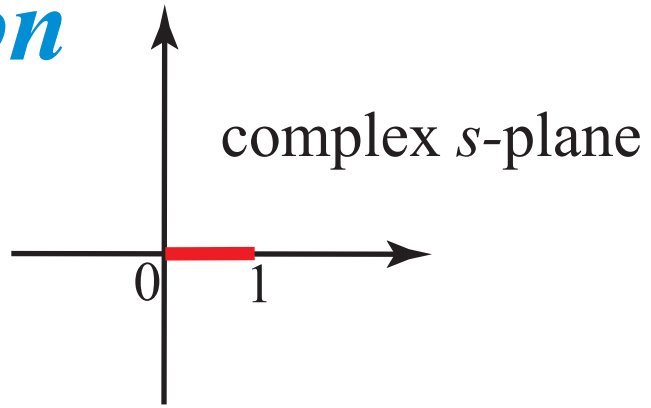
$$\langle D \rangle = \epsilon^* \langle E \rangle$$

p_1 , p_2 = volume fractions of the components

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

Stieltjes integral representation

$$F(s) = 1 - \frac{\epsilon^*}{\epsilon_2}\,, \qquad s = \frac{1}{1 - \epsilon_1 / \epsilon_2}$$



$$F(s) = \int_0^1 \frac{d\mu(z)}{s - z}\,, \qquad \mu$$

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

representation ***separates***

GEOMETRY μ from

medium parameters in S

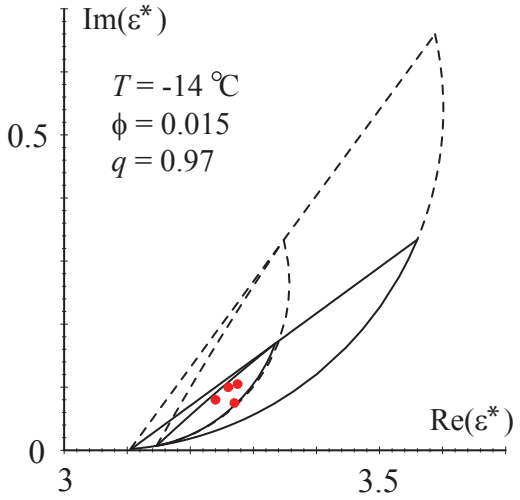
$$E = (s + \Gamma\chi)^{-1} e_k$$

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

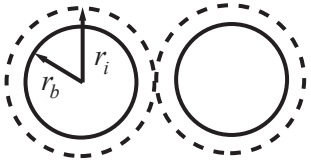
χ = indicator function of medium 1

forward and inverse bounds for sea ice

matrix particle bounds



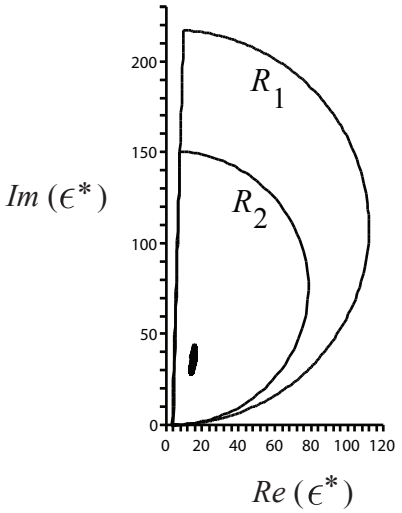
4.75 GHz data



$q = r_b / r_i$

$0 < q < 1$

Golden 1997



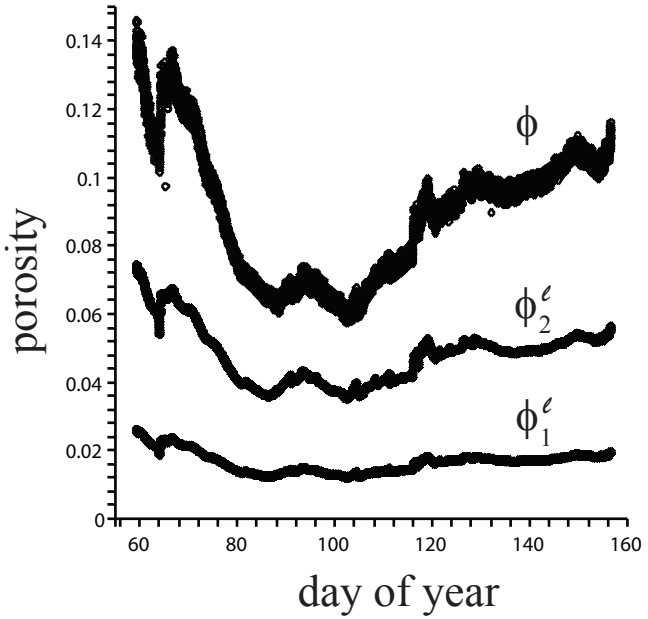
50 MHz capacitance probe
data taken near Barrow, AK

inverse bounds and
microstructural recovery

Gully, Backstrom, Eicken, Golden, Physica B, 2007

polycrystalline bounds

Gully, Lin, Cherkaev, Golden, 2012

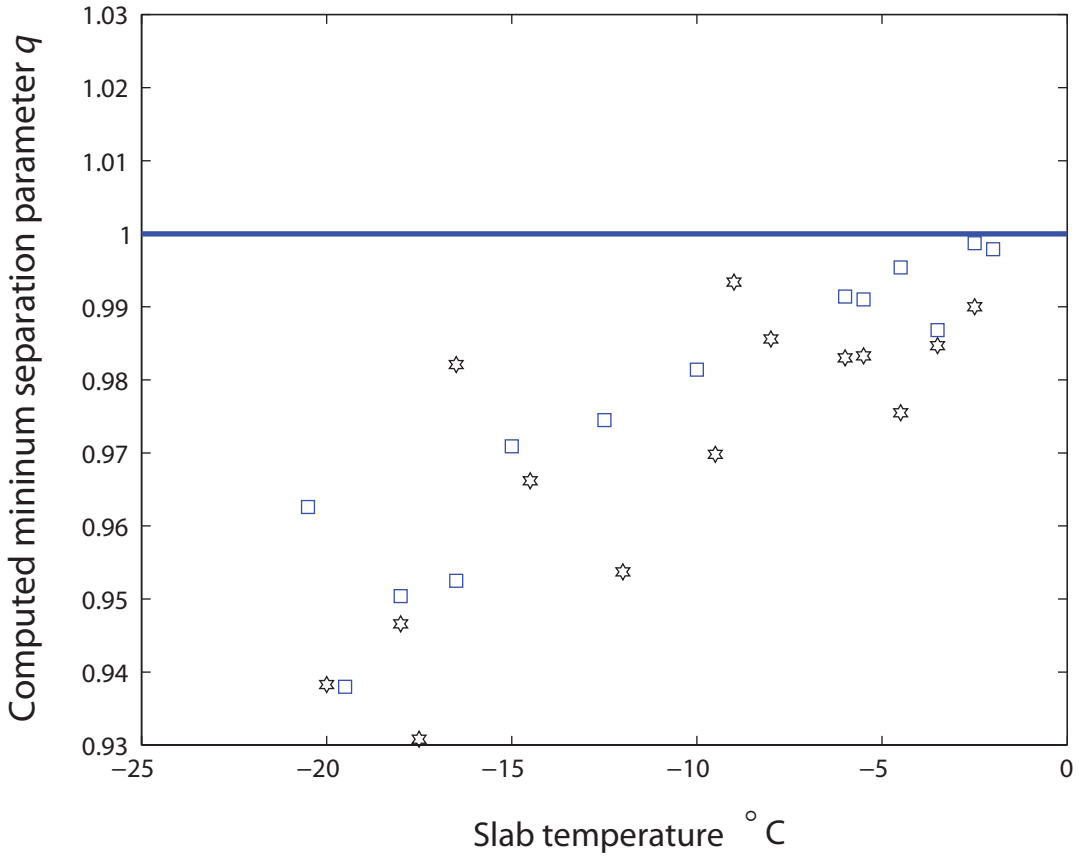


Recovery of inclusion separations in strongly heterogeneous composites from effective property measurements

Chris Orum, Elena Cherkaev, Ken Golden, Proc. Roy. Soc. A, 2012

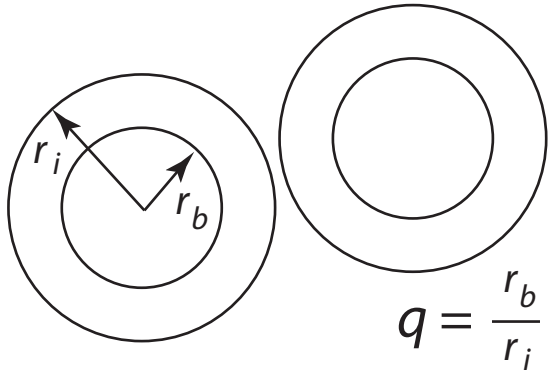
matrix particle composites (O. Bruno, 1991)

reduced spectral inversion -- construct algebraic curves which bound admissible region in (p,q)-space, q = separation parameter <1

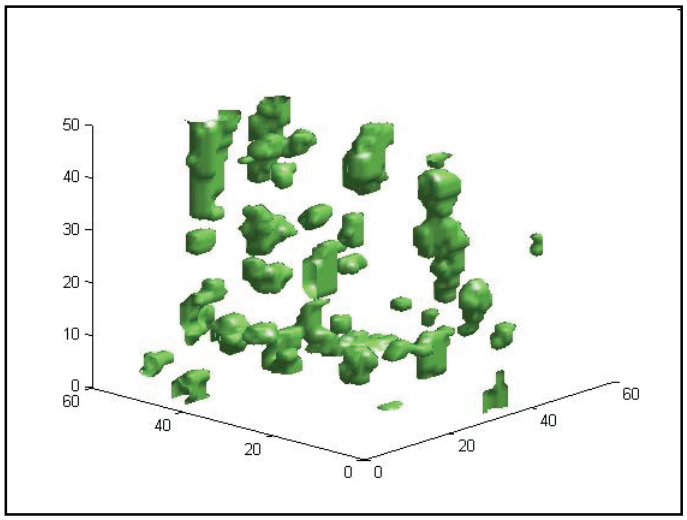


rigorous inverse bound on spectral gap

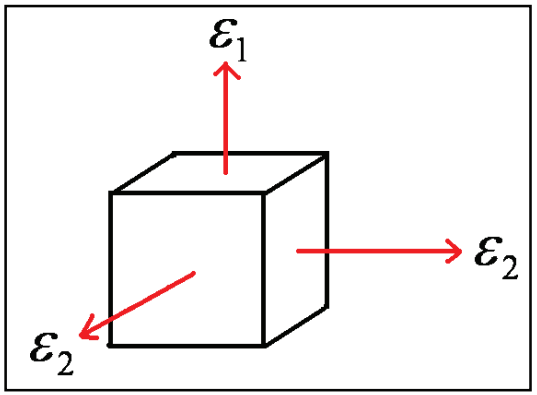
inversion for brine inclusion separations in sea ice from measurements of effective complex permittivity



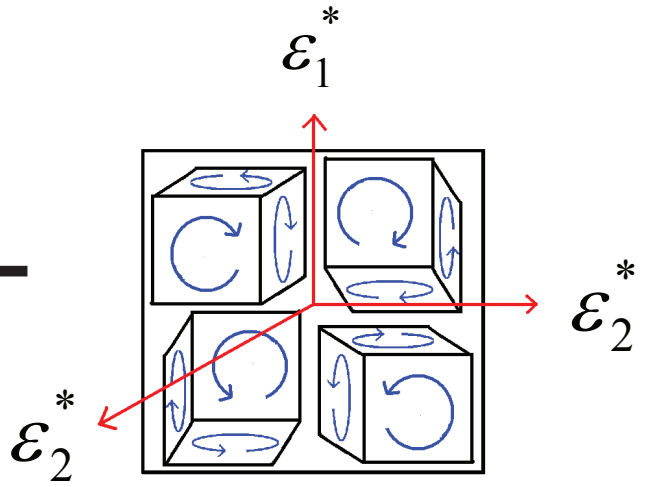
two scale homogenization for polycrystalline sea ice



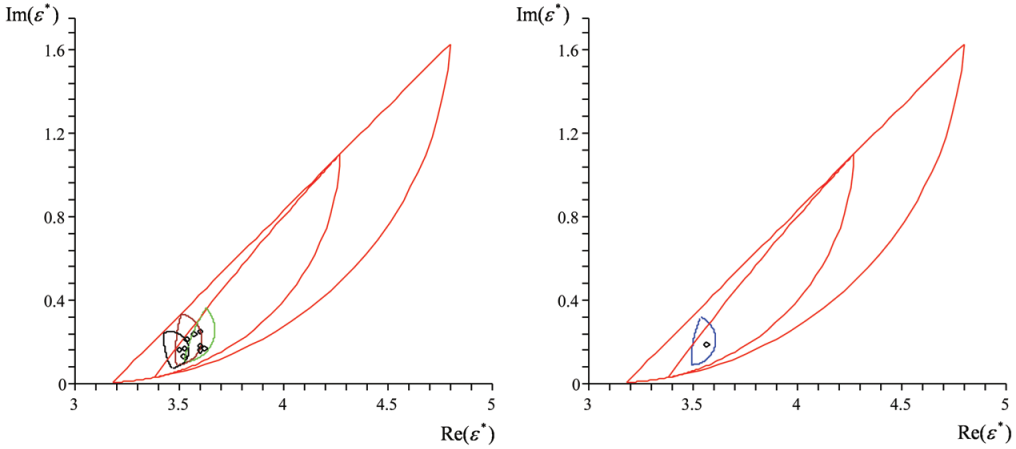
numerical homogenization for single crystal



analytic continuation for polycrystals



bounds



Gully, Lin, Cherkaev, Golden 2013

Spectral analysis of multiscale sea ice structures

homogenization for brine inclusions, melt ponds, and sea ice pack

how to upscale information on "microstructure"
into effective behavior for larger scales

numerical computation of spectral measure μ

N. B. Murphy, C. Hohenegger, C. S. Sampson, B. Alali, K. Steffen, D. K. Perovich, H. Eicken, and K. M. Golden 2012

direct calculation of spectral measure

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

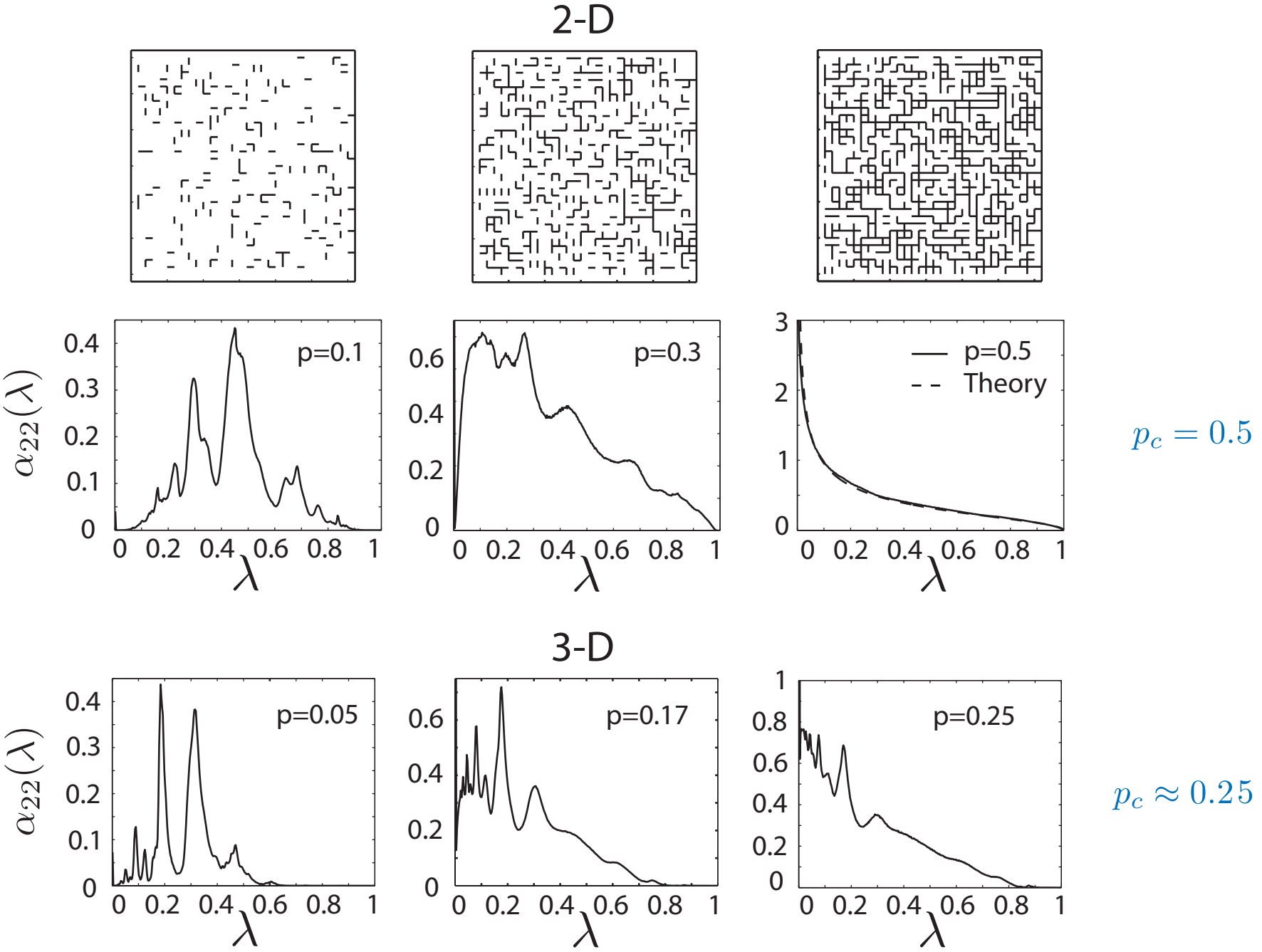
2. The fundamental operator $\Gamma\chi$ becomes a random matrix depending only on the composite geometry.

3. Compute the eigenvalues λ_i and eigenvectors of $\Gamma\chi$ with $(\text{length})^2 = \alpha_i$

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

Dirac point measure (Dirac delta)

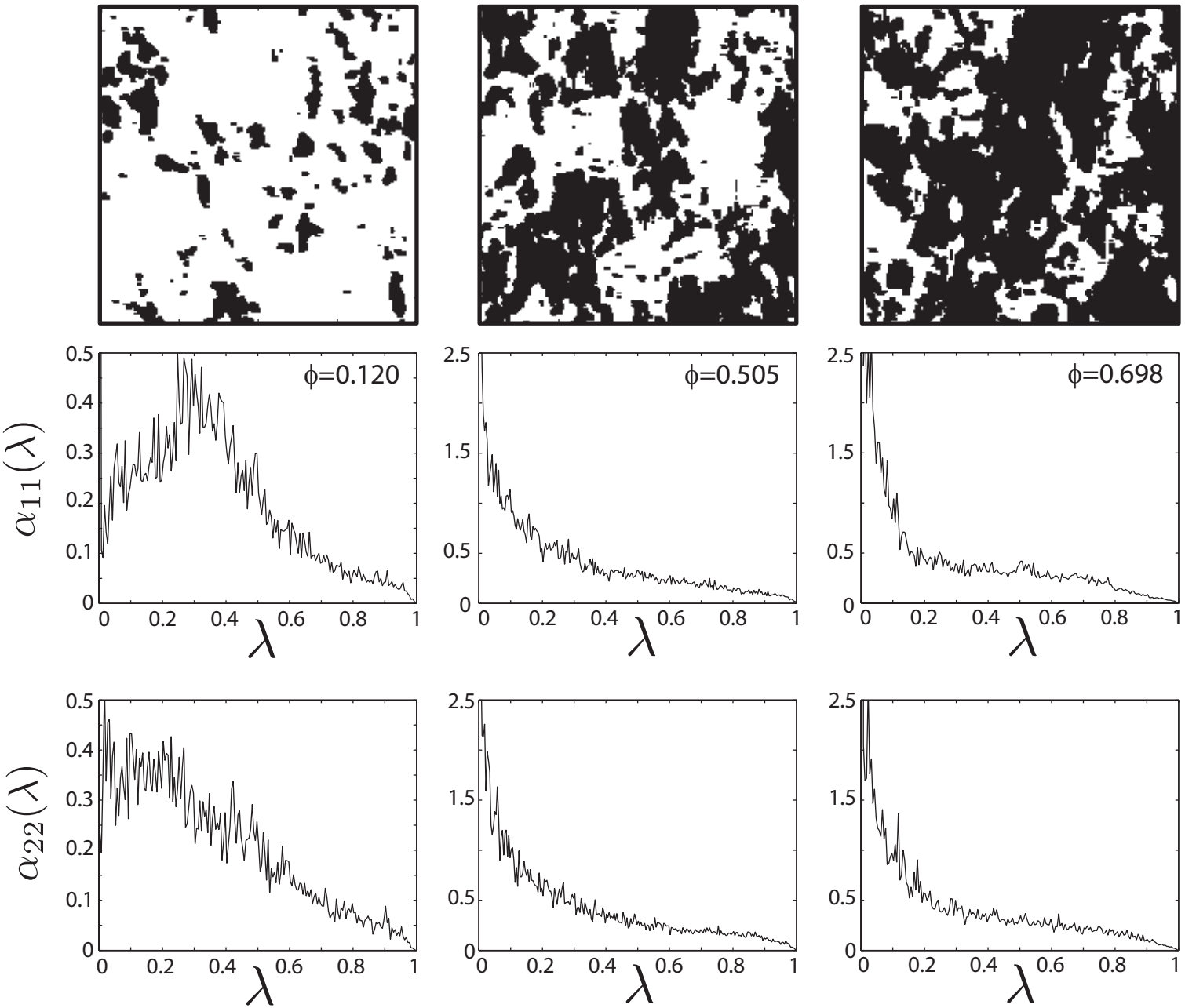
The Spectral Measures for Random Resistor Networks



spectral gaps collapse at the percolation transitions

Murphy and Golden, J. Math. Phys. (2012)

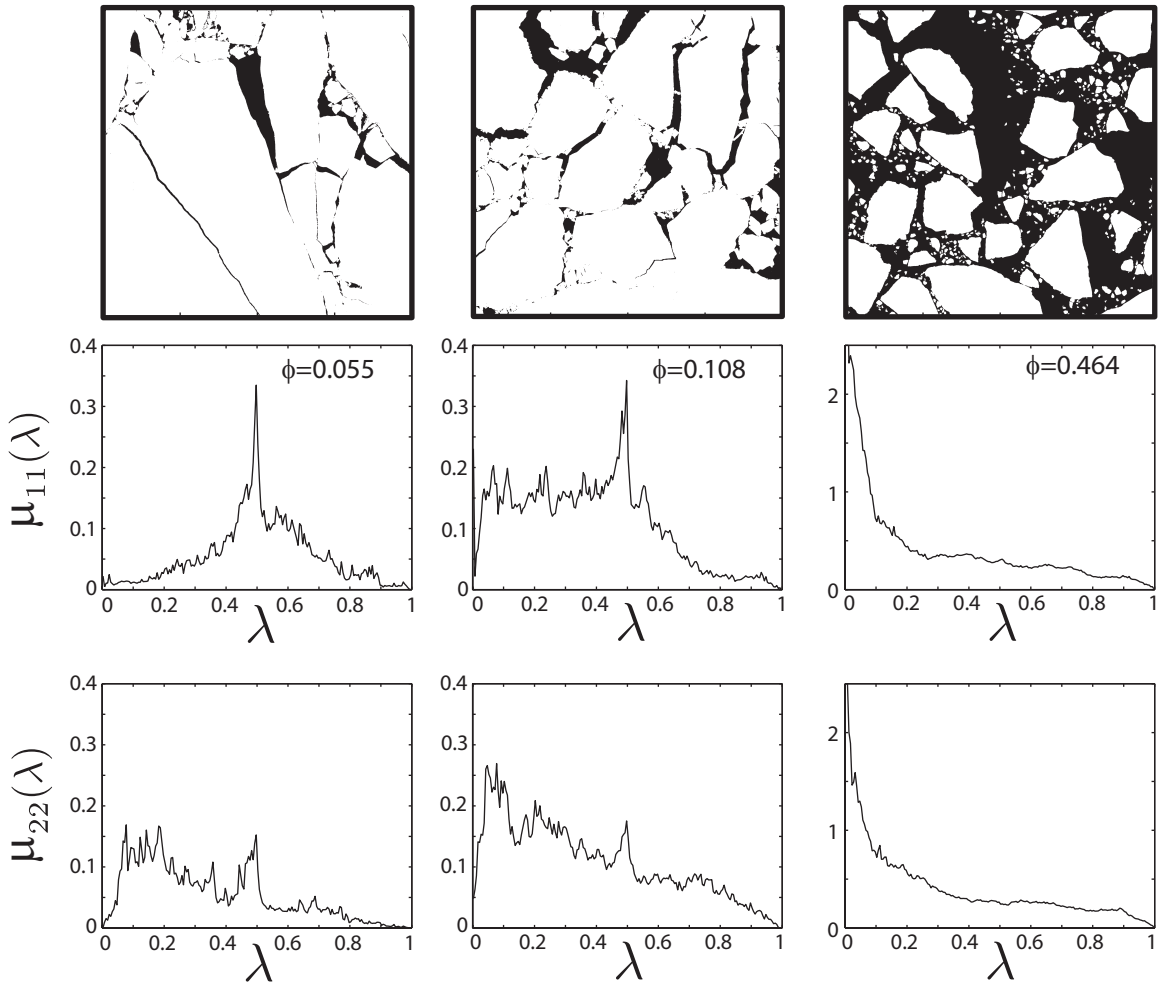
Spectral Measures for Sea Ice Structures: Brine Inclusions



N. B. Murphy, C. Hohenegger, C. S. Sampson, D. K. Perovich, H. Eicken, E. Cherkaev, B. Alali, and K. M. Golden, 2013

spectral measures provide a path toward rigorously incorporating "composite microstructure" into calculations of effective behavior on larger scales

spectral measures for the Arctic sea ice pack



area under curve = φ = open water fraction

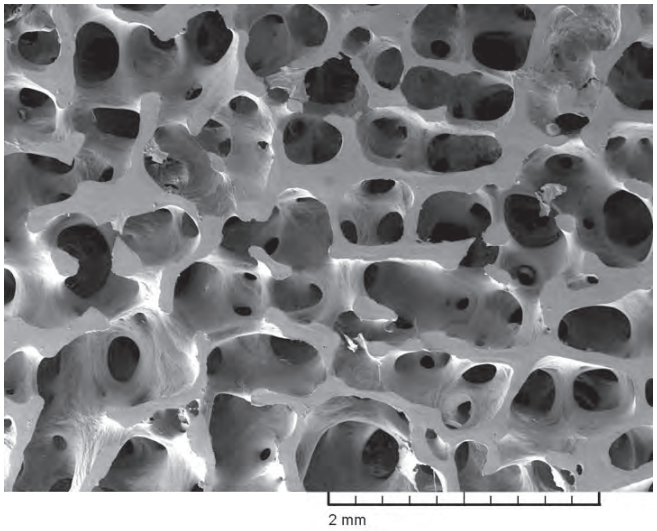
spectral gap closes as ocean phase becomes connected

N. B. Murphy, C. Hohenegger, C. S. Sampson, D. K. Perovich, H. Eicken, E. Cherkaev, B. Alali, and K. M. Golden, 2013

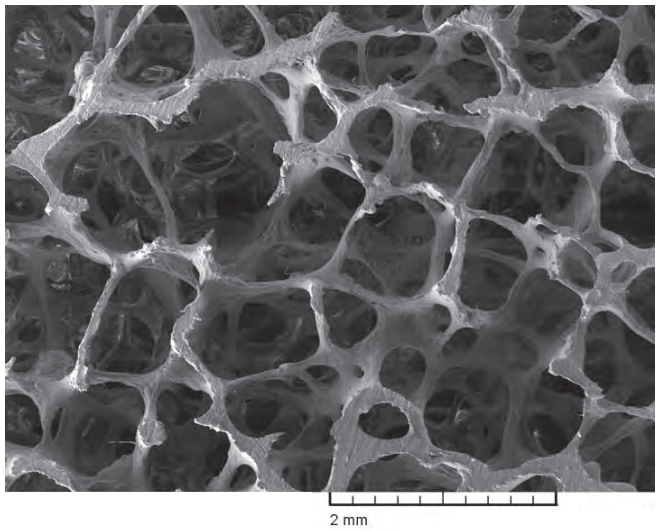
spectral characterization of porous microstructures in bone

Golden, Murphy, Cherkaev, J. Biomechanics 2011

(a) young healthy trabecular bone

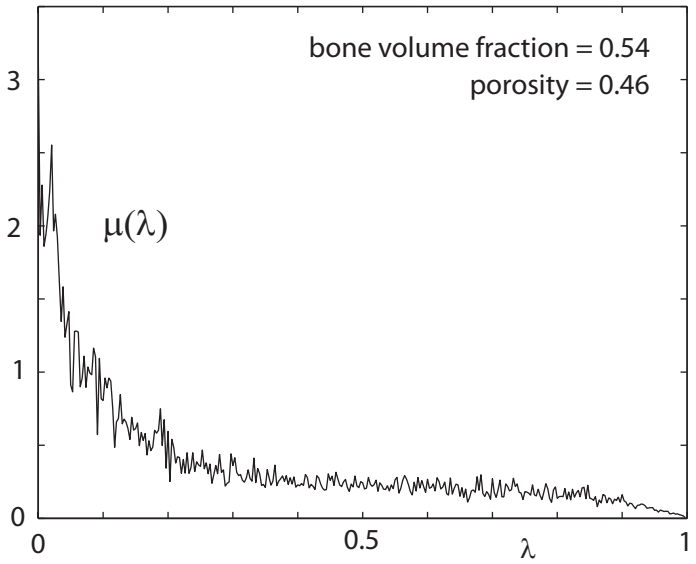


(b) old osteoporotic trabecular bone

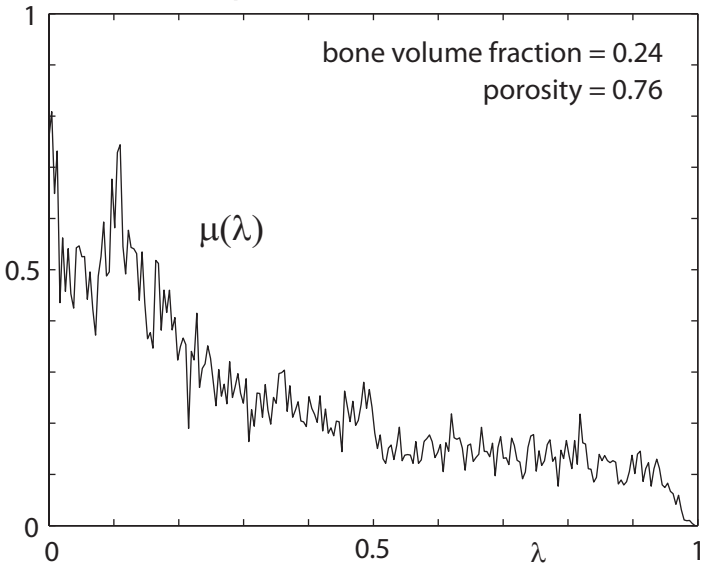


P. Hansma

(c) spectral measure - young

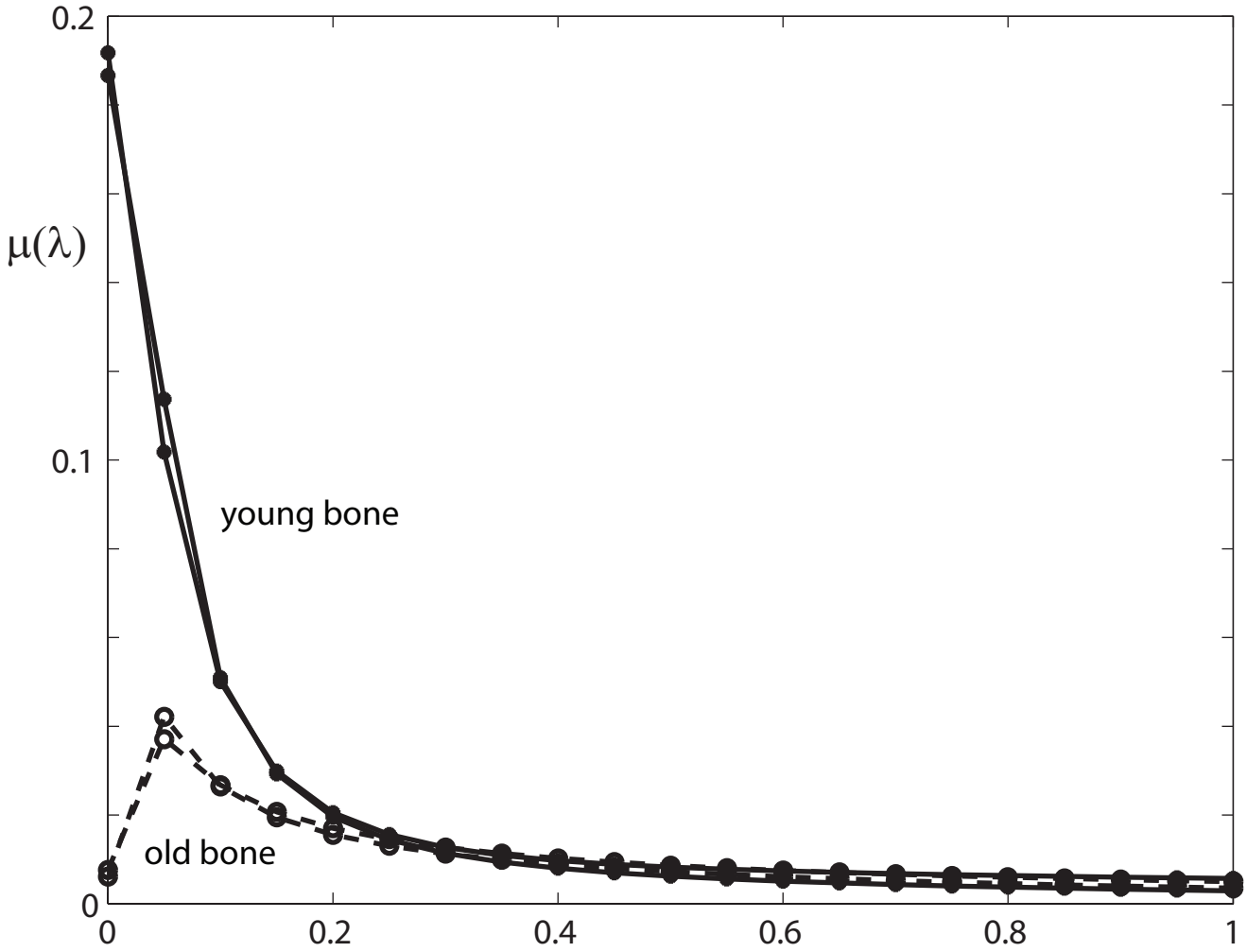


(d) spectral measure - old



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

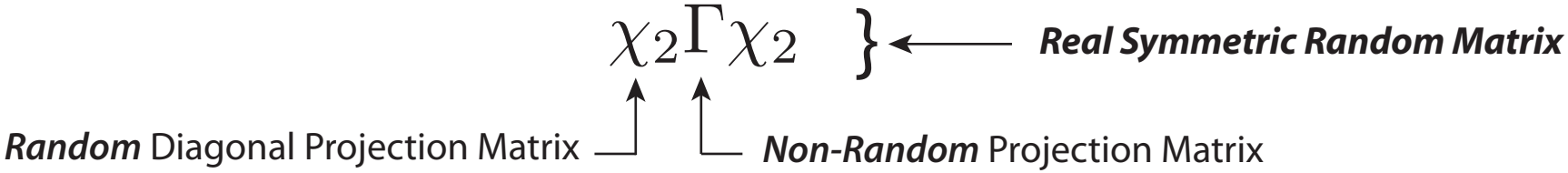
reconstruction of spectral measures from simulated complex permittivity data



regularized inversion scheme

Golden, Murphy, Cherkaev, J. Biomech. 2011

Random Matrix Theory Characterization of Phase Transitions



- The elements of a random matrix are determined by a probability law.

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

- RMT has since been used to characterize: phase transitions in disordered mesoscopic conductors, quantum chaos, neural networks, random graphs, etc.

- ***In composites***, connectedness transitions can be characterized by transitions in the short and long range correlations of eigenvalues of the matrix $\chi_2 \Gamma \chi_2$.

- The eigenvectors may be integrated out, and ***the probability distribution is exactly that of the canonical ensemble of 2-D positive charges on a line!***

$$P_N = Z_N^{-1} \exp(-\mathcal{H}_N), \qquad \mathcal{H}_N = \sum_{i=1}^{N} V(\lambda_i) - \sum_{i>j=1}^{N} \ln|\lambda_i - \lambda_j|$$

Energy Hamiltonian of Eigenvalues

Confining Potential

Logarithmic Repulsion of Eigenvalues

- The mean eigenvalue density ρ depends on the form of V, although, the ***fluctuations*** about the mean density ***are universal***.

- In order to observe the universal fluctuations of eigenvalues about the mean density, they are **unfolded** to have unit mean spacing.

Phase Transitions in Random Matrix Theory

$V(\lambda; q) \gtrsim |\lambda|$
Wigner-Dyson Eigenvalue Statistics
Strong Confinement

$\longleftrightarrow$

$V(\lambda; q) \sim \ln^2 |\lambda|$
Poissonian Eigenvalue Statistics
Weak Confinement

- ***Phase transitions*** are modeled by allowing the potential V to vary as a function of a ***disorder parameter*** q.

- When $V(\lambda; q) \gtrsim |\lambda|$ for $|\lambda| \gg 1$, highly correlated Wigner-Dyson (WD) eigenvalue statistics give rise to the phenomenon of ***level repulsion***:

$$P(z) \approx \frac{\pi z}{2} \exp(-\pi z^2/4) \qquad \text{(The Wigner Surmise)}$$

- When $V(\lambda; q) \sim \ln^2 |\lambda|$ for $|\lambda| \gg 1$, the eigenvalues are weakly correlated, giving rise to Poissonian eigenvalue statistics.

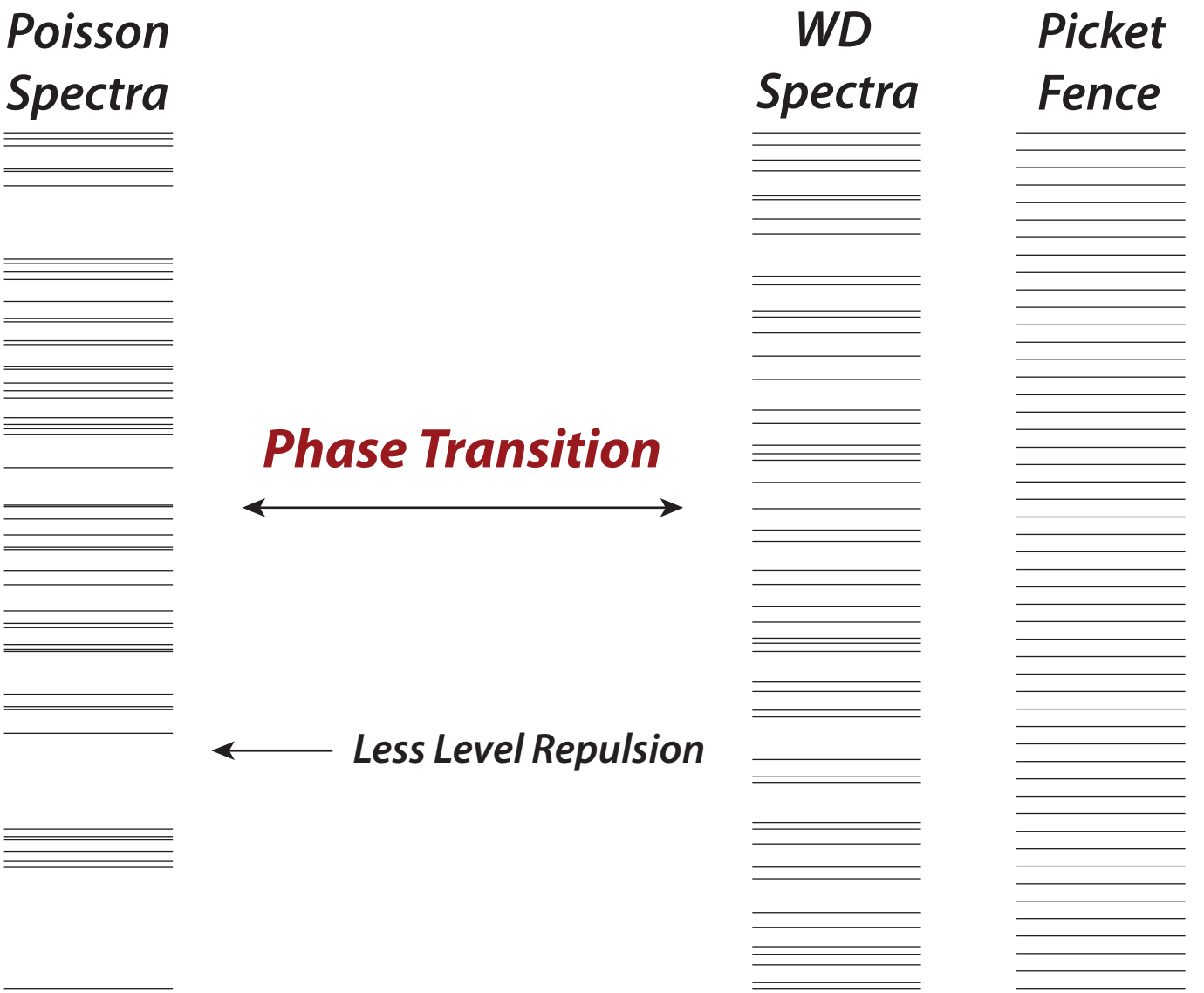
Transitions in Eigenvalue Correlations

$P(z) = \exp(-z)$

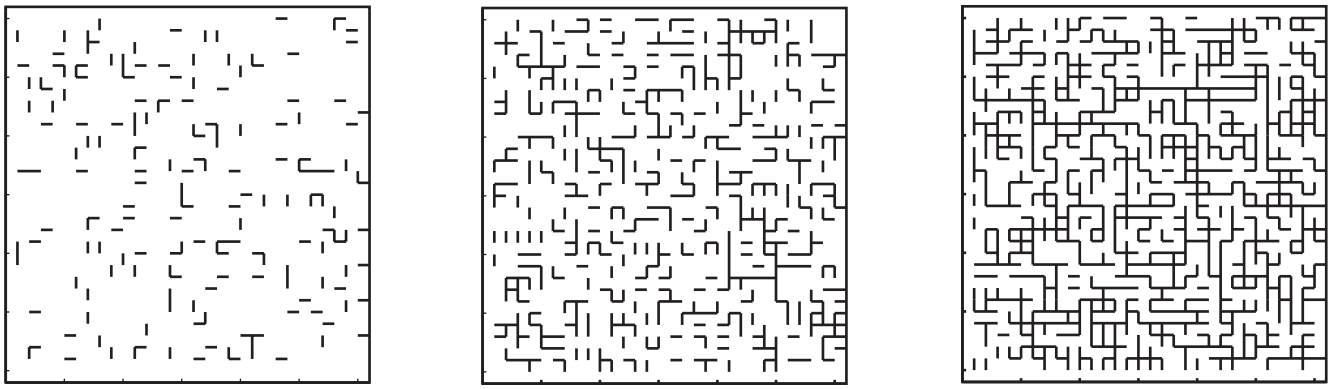
Eigenvalue Spacing Distribution

$P(z) \approx \frac{\pi z}{2} \exp(-\pi z^2/4)$

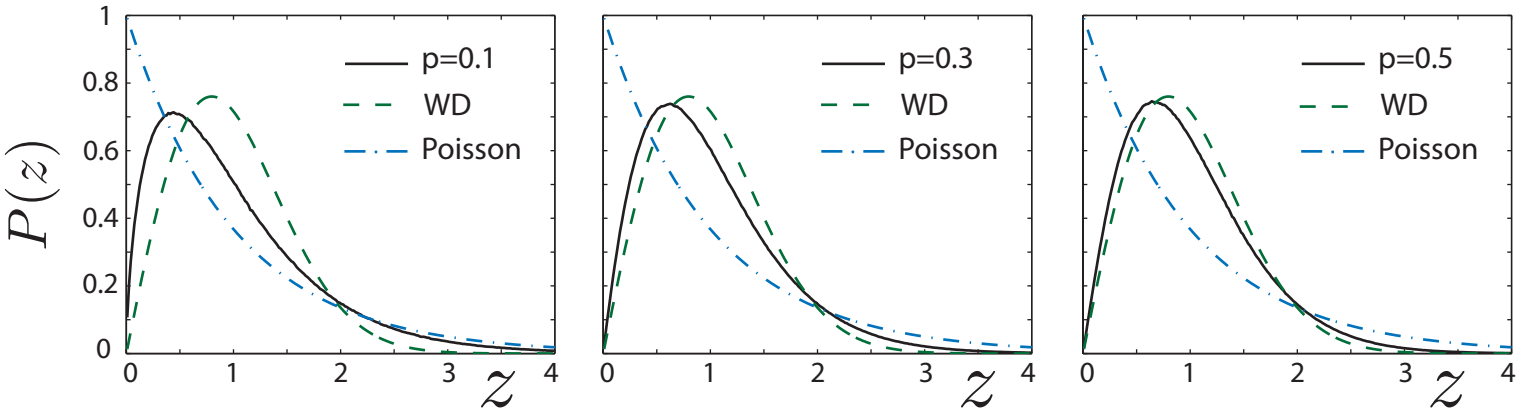
Eigenvalue Spacing Distribution



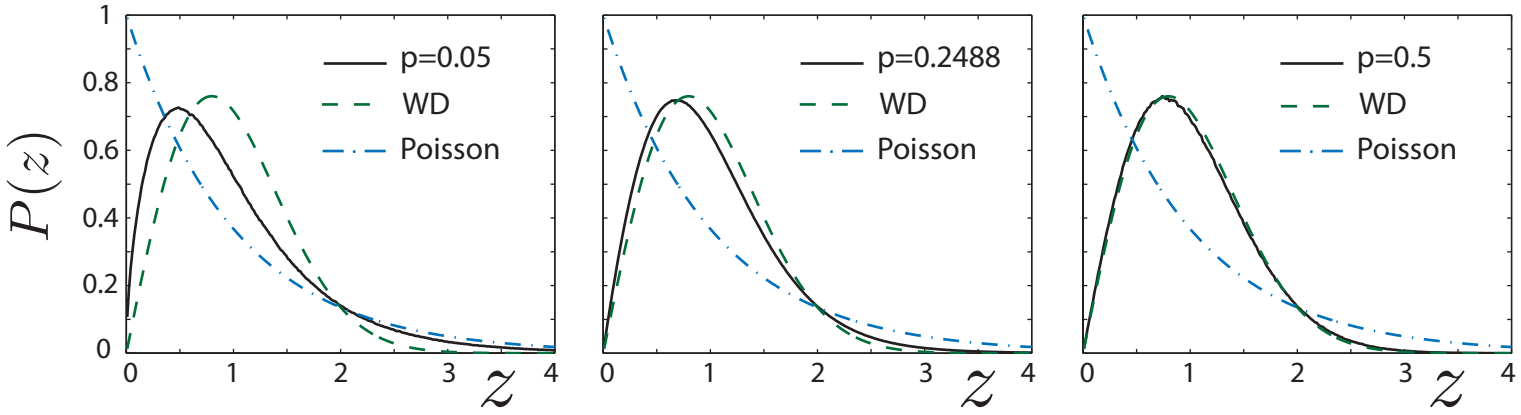
Unfolded Eigenvalue Spacing Distribution



2-d Random Resistor Network



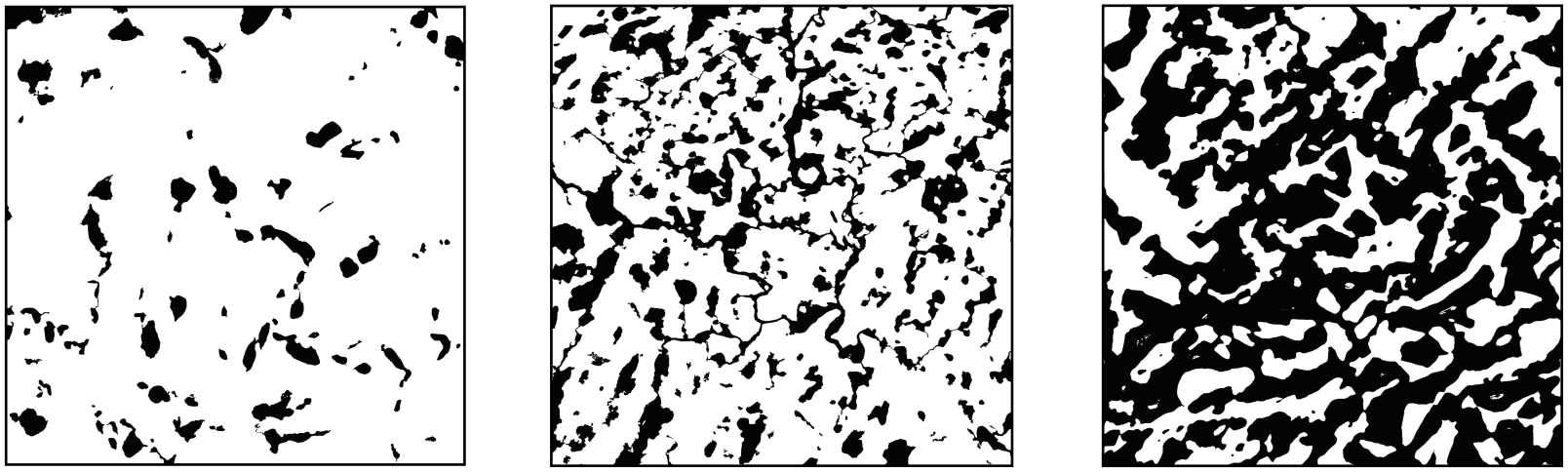
3-d Random Resistor Network

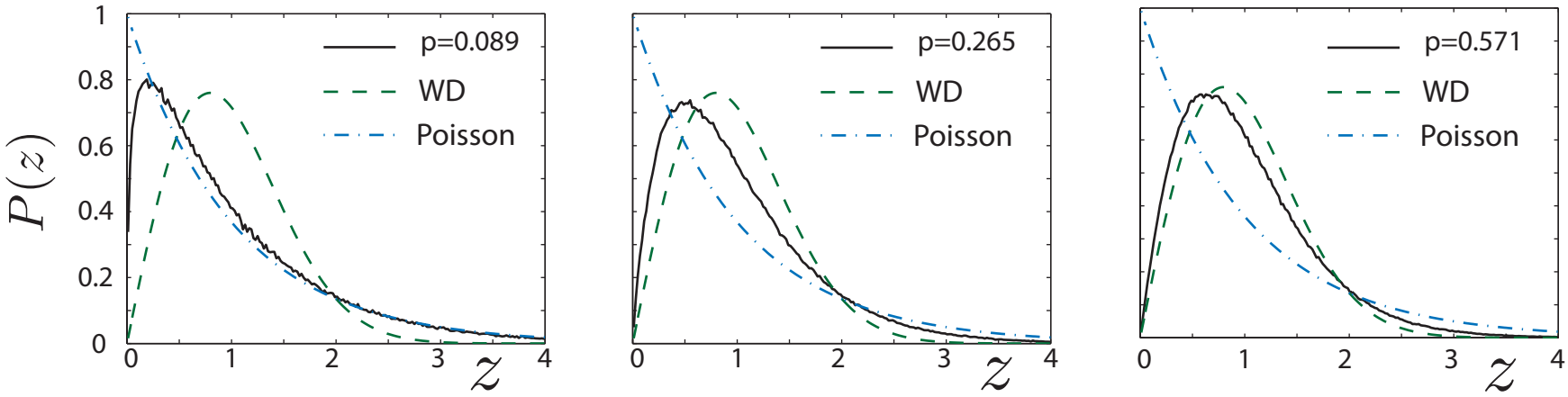


N. B. Murphy, K. M. Golden 2013

Unfolded Eigenvalue Spacing Distribution

ARCTIC MELT PONDS





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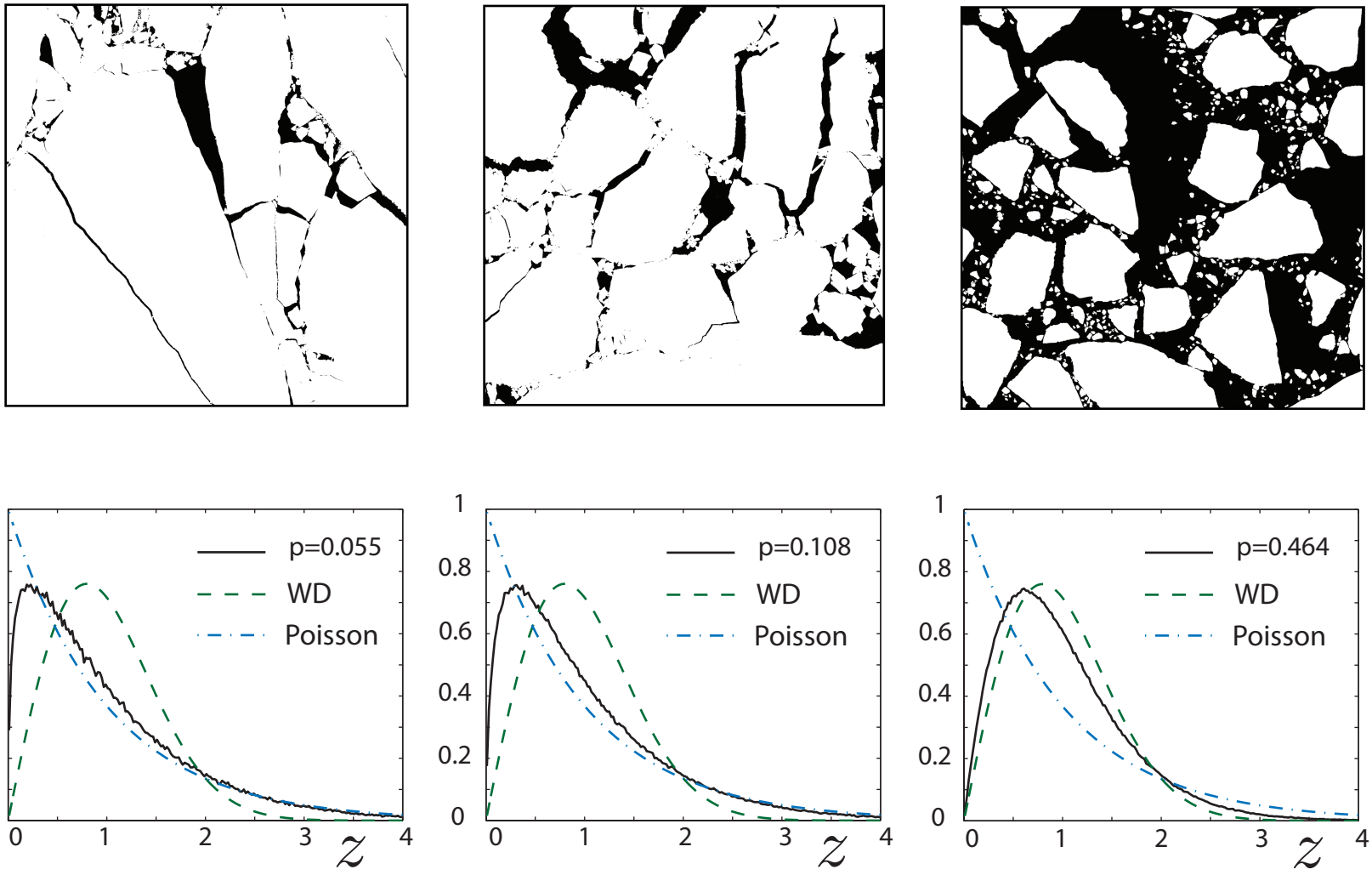
Unfolded Eigenvalue Spacing Distribution

ARCTIC SEA ICE PACK



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advection enhanced diffusion

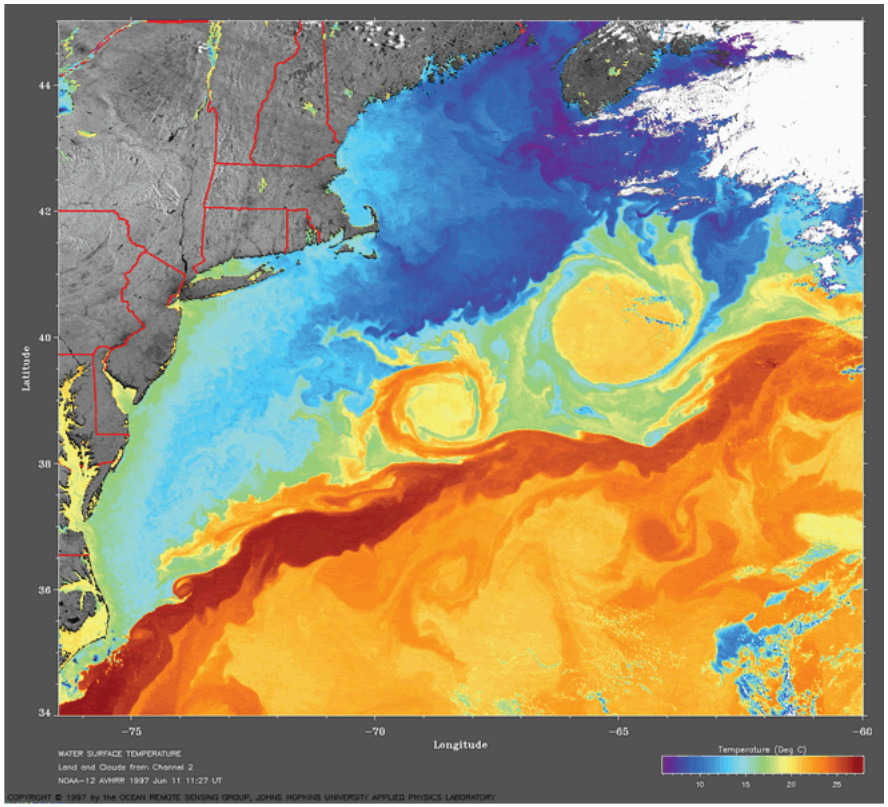
effective diffusivity

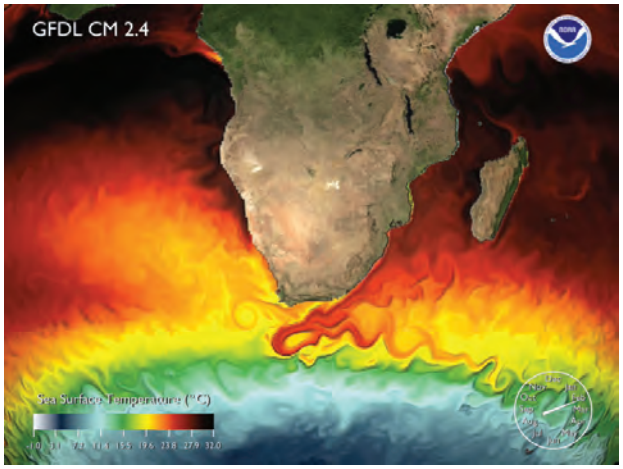
tracers, buoys diffusing in ocean eddies

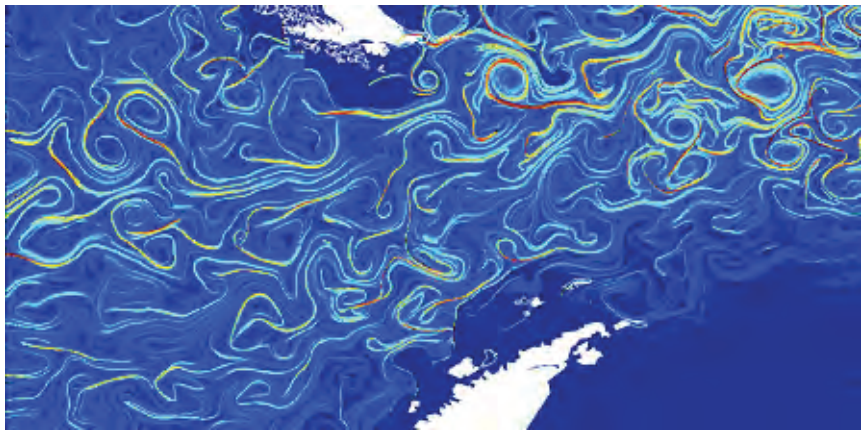
pollutants

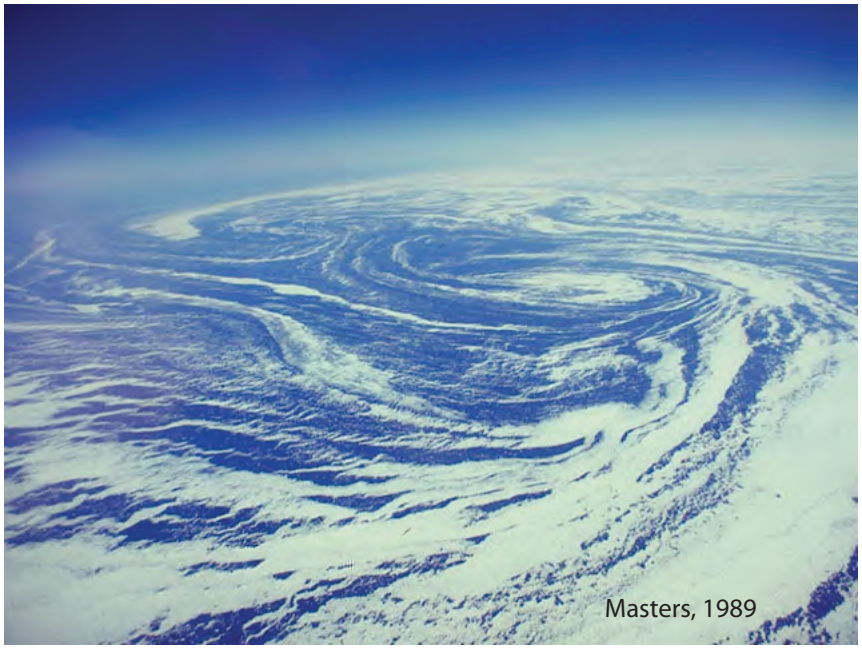
enhanced heat and salt transport

enhanced sea ice thermal conductivity









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***

composites

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

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

μ spectral measure of $\chi \mathbf{\Gamma} \chi$

advection diffusion

$$\frac{\kappa^*}{\kappa_0} = 1 + \xi^2 \int_0^\infty \frac{d\phi(\tau)}{1 + \xi^2 \tau^2}$$

ξ = Péclet number

ϕ spectral measure of $\mathrm{i}\mathbf{\Gamma H \Gamma}$

$\vec{u} = \kappa_0 \, \xi \, \vec{\nabla} \cdot \mathbf{H}$, $\mathbf{H}$ antisymmetric vector potential

Spectral Calculation of Effective Parameters

composites

Real Symmetric Random Matrix

$$\chi\Gamma\chi = \mathbf{U}\Lambda\mathbf{U}^T$$

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

$$\int_0^1 \frac{d\mu(\lambda)}{s-\lambda} = \sum_j \frac{\mu_j}{s-\lambda_j}$$

$$\mu_j = \langle(\vec{u}_j^T \vec{e}_k)^2\rangle$$

λ_j *eigenvalues of the* ***matrix*** $\chi\Gamma\chi$
with ***real*** *eigenvectors* $\vec{u}_j$

advection diffusion

Hermitian Random Matrix

$$\mathrm{i}\Gamma\mathbf{H}\Gamma = \mathbf{V}^\dagger\mathbf{T}\mathbf{V}$$

$$\frac{\kappa^*}{\kappa_0} = 1 + \xi^2 \int_0^\infty \frac{d\phi(\tau)}{1+\xi^2\tau^2}$$

$$\int_0^\infty \frac{d\phi(\tau)}{1+\xi^2\tau^2} = \sum_j \frac{\phi_j}{1+\xi^2\tau_j^2}$$

$$\phi_j = \langle|\vec{v}_j^\dagger \mathbf{\Gamma H} \vec{e}_k|^2\rangle$$

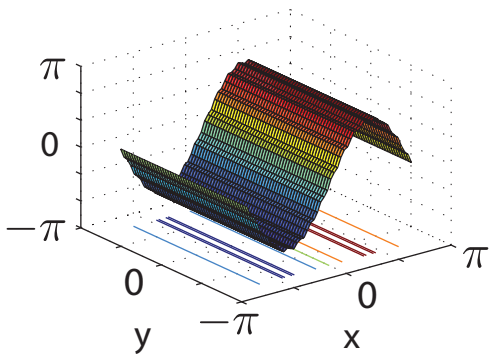
τ_j *eigenvalues of the* ***matrix*** $\mathrm{i}\Gamma\mathbf{H}\Gamma$
with ***complex*** *eigenvectors* $\vec{v}_j$

The projective nature of χ and Γ leads to an efficient way of calculating the spectral measures, which is also numerically stable and reduces roundoff error.

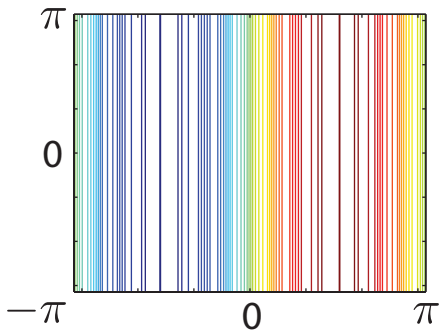
spectral measures for sample flows

Shear Flow: $H(x,y) = \sin x + (0.5+\eta)\sin(15x)/15, \quad \eta \sim U(-0.1, 0.1)$

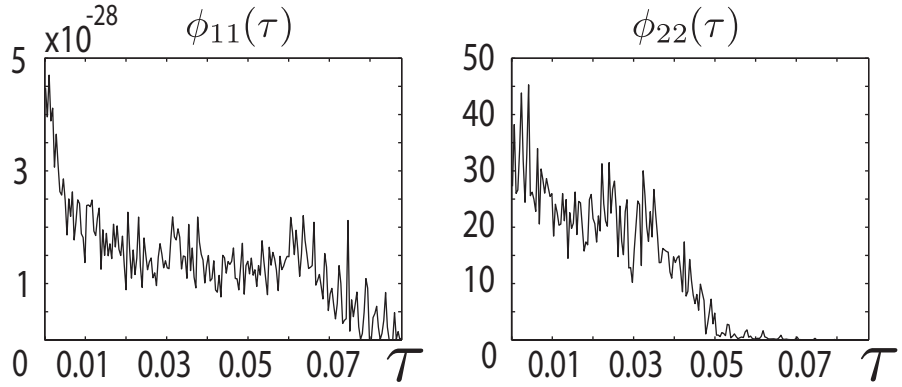
stream function



streamlines

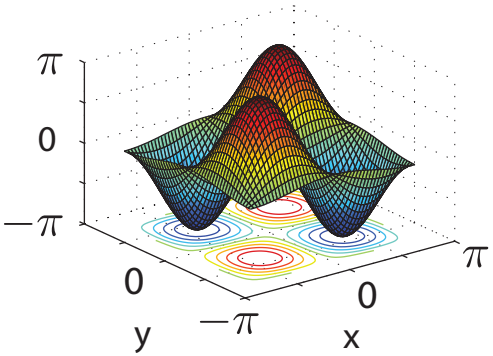


spectral functions

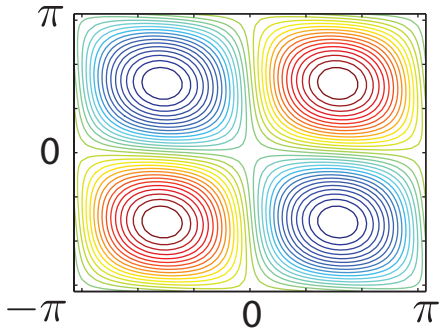


Modified Cat's Eye Flow: $H(x,y) = \sin x \sin y + \eta \cos x \cos y, \quad \eta \sim U(-0.1, 0.1)$

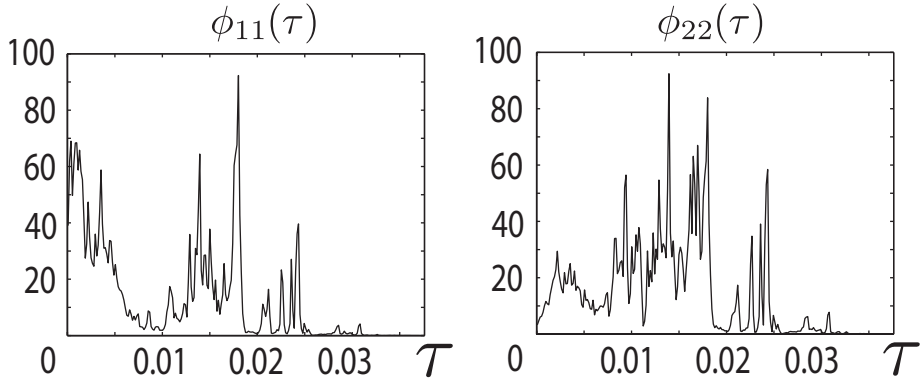
stream function



streamlines



spectral functions



Murphy, Zhu, Golden, 2012

effective diffusivities for sample flows

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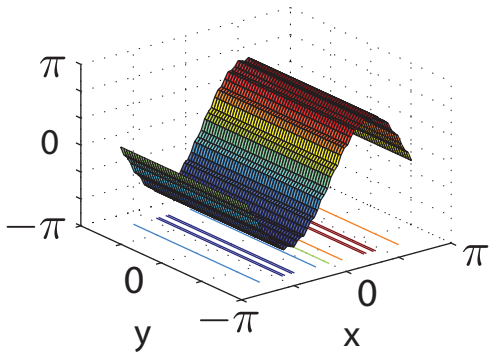
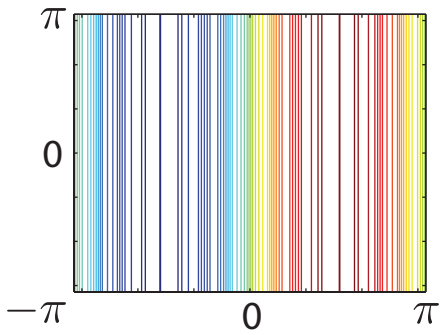
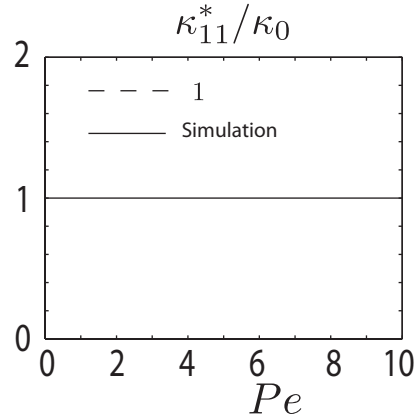
stream function

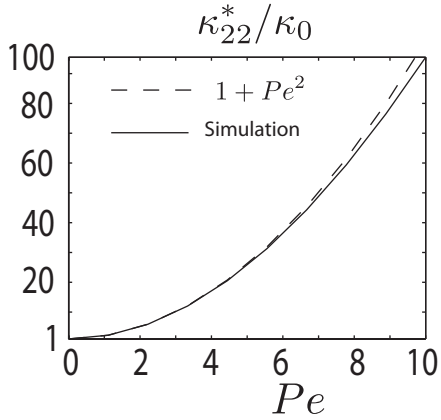


streamlines



effective diffusivities





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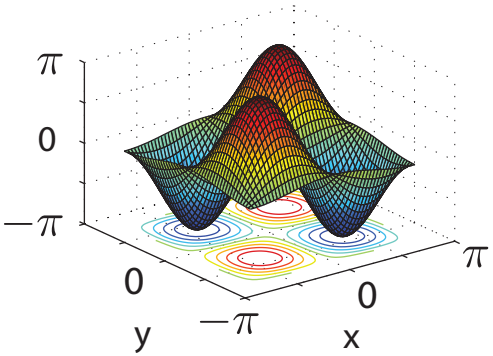
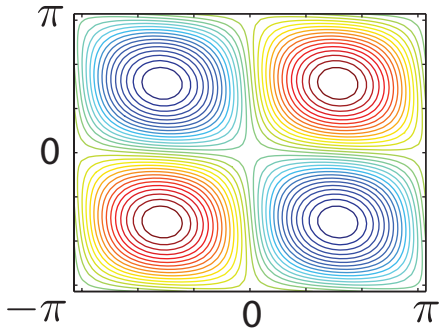
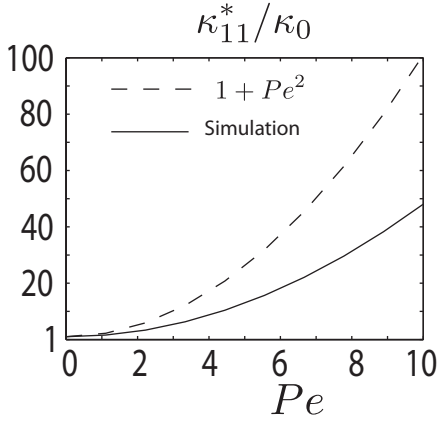
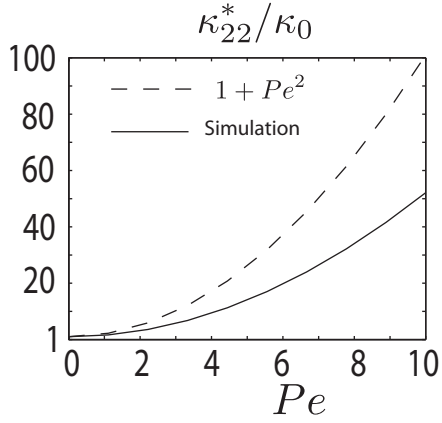


streamlines



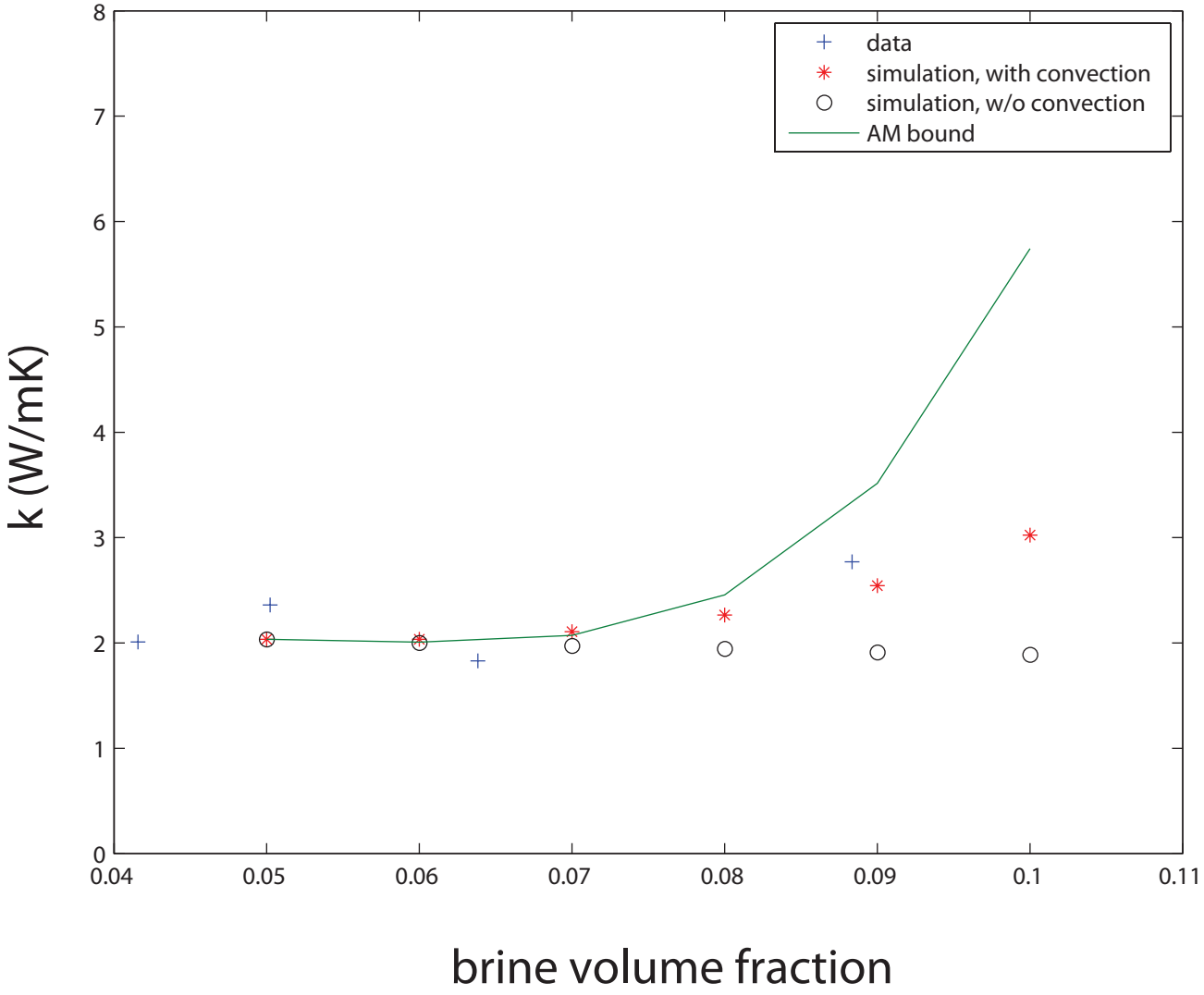
effective diffusivities





Murphy, Zhu, Golden, 2012

convection enhanced thermal conductivity of sea ice for shear flow



Wang, Zhu, Golden, 2012

Conclusions

1. Sea ice exhibits composite structure on many length scales.

2. Fluid flow through sea ice mediates many processes of importance to understanding climate change and the response of polar ecosystems.

3. Mathematical models of composite materials and statistical physics help unravel the complexities of sea ice structure and processes.

4. Homogenization theory and upscaling methods can provide a rigorous path to representing large scale effective behavior in coarse models.

5. Random matrix theory can help characterize transitions important for climate science and composite materials.

THANK YOU

National Science Foundation

Division of Mathematical Sciences

Arctic Natural Sciences

Office of Polar Programs

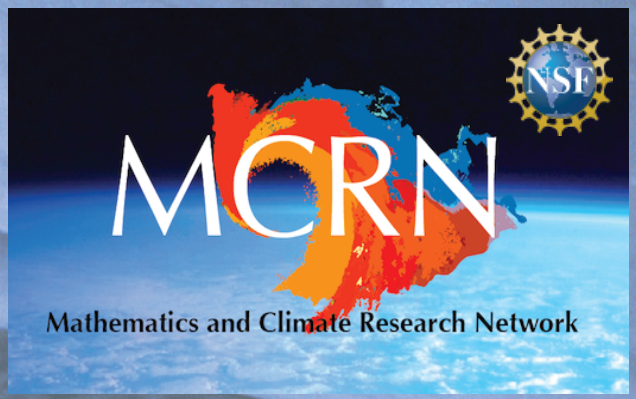
CMG Program

(Collaboration in Mathematical Geosciences)

Office of Naval Research

Applied Computational Analysis Program

Arctic and Global Prediction Program



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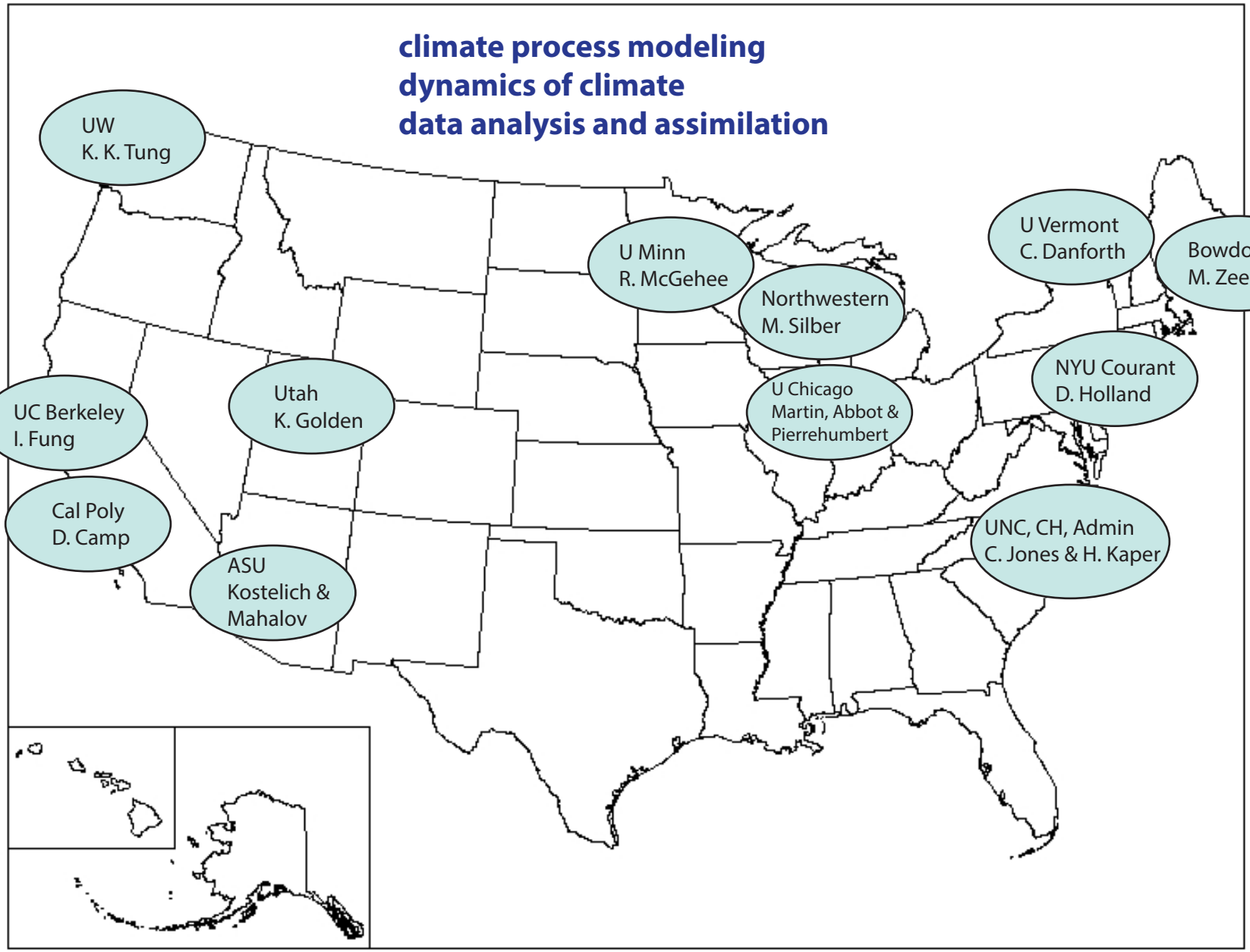
Buchanan Bay, Antarctica Mertz Glacier Polynya Experiment July 1999

Mathematics and Climate Research Network (MCRN)



NSF DMS 2010-2015, Lorenz postdocs, grad, undergrad, polar expeditions

Jones, Golden, Kaper, Zeeman