Stieltjes Functions and their Integral Representations in Sea Ice Modeling

Kenneth M. Golden Dept. of Mathematics, Univ. of Utah

> CIRM Conference on Herglotz-Nevanlinna functions and their applications to dispersive systems and composite materials 26 May 2022



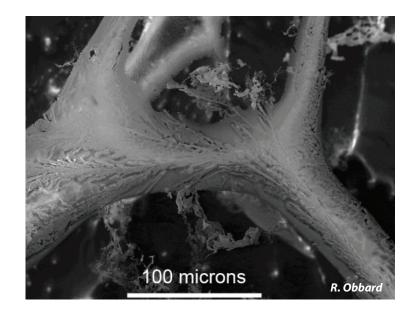


sea ice may appear to be a barren, impermeable cap ...

Golden



brine inclusions in sea ice (mm)



micro - brine channel (SEM)

brine channels (cm)

sea ice is a porous composite

pure ice with brine, air, and salt inclusions





horizontal section

vertical section

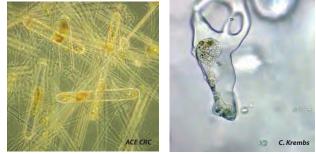
fluid flow through the porous microstructure of sea ice governs key processes in polar climate and ecosystems

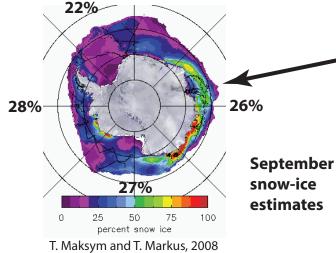
evolution of Arctic melt ponds and sea ice albedo



nutrient flux for algal communities







Antarctic surface flooding and snow-ice formation

- evolution of salinity profiles - ocean-ice-air exchanges of heat, CO₂

Sea Ice is a Multiscale Composite Material *microscale*

brine inclusions



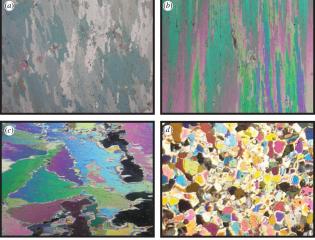
H. Eicken

Golden et al. GRL 2007

Weeks & Assur 1969

millimeters

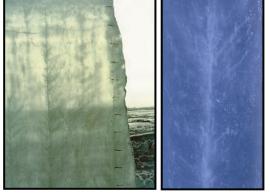
polycrystals



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

centimeters

brine channels



D. Cole

K. Golden

mesoscale

macroscale

Arctic melt ponds



Antarctic pressure ridges





sea ice floes

sea ice pack





K. Golden

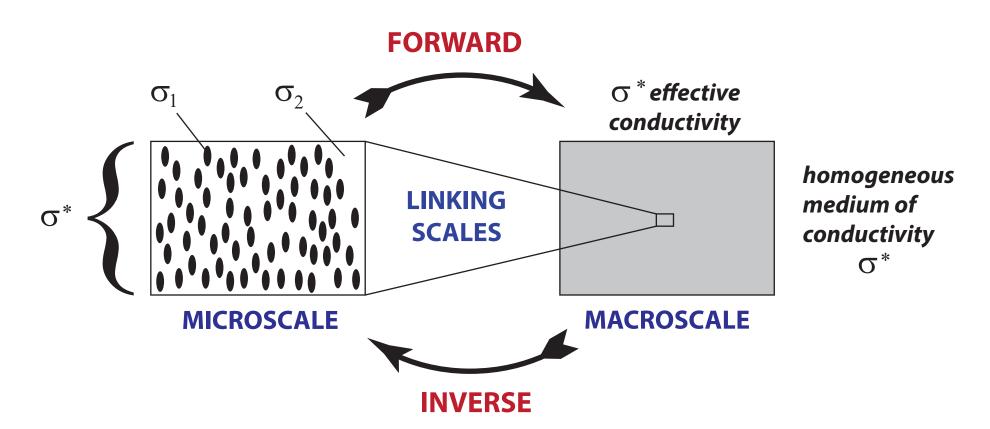
J. Weller

kilometers

NASA

meters

HOMOGENIZATION for Composite Materials



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

What is this talk about?

the role of "microstructure" in determining sea ice effective properties

Using homogenization and statistical physics to compute effective behavior on scales relevant to coarse-grained sea ice and climate models, process studies, ...

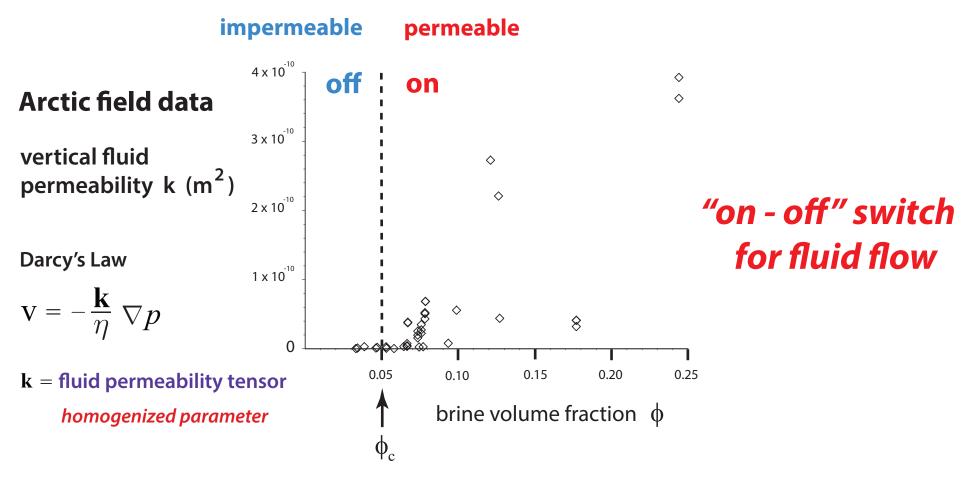
MICROSCALE: brine + polycrystalline microstructure; EM, fluid transport MESOSCALE: advection diffusion, thermal transport, ocean waves

A tour of Stieltjes functions in the study of sea ice and its role in climate.

Solving problems in the physics of sea ice drives advances in theory of composite materials.

microscale

Critical behavior of fluid transport in sea ice



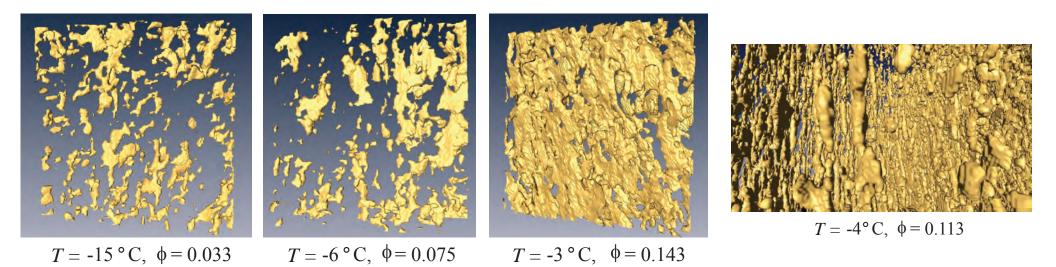
critical brine volume fraction $\phi_c \approx 5\%$ \checkmark $T_c \approx -5^{\circ}C, S \approx 5$ ppt

RULE OF FIVES

Golden, Ackley, Lytle Science 1998 Golden, Eicken, Heaton, Miner, Pringle, Zhu GRL 2007 Pringle, Miner, Eicken, Golden J. Geophys. Res. 2009

sea ice ~ compressed powder in stealthy composites

brine volume fraction and *connectivity* increase with temperature

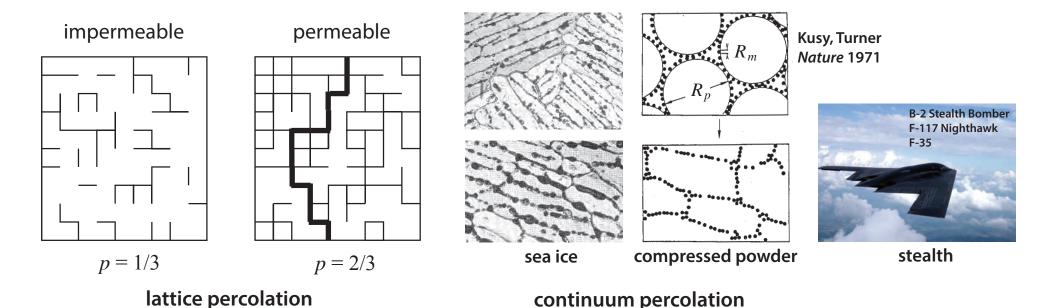


X-ray tomography for brine phase in sea ice

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

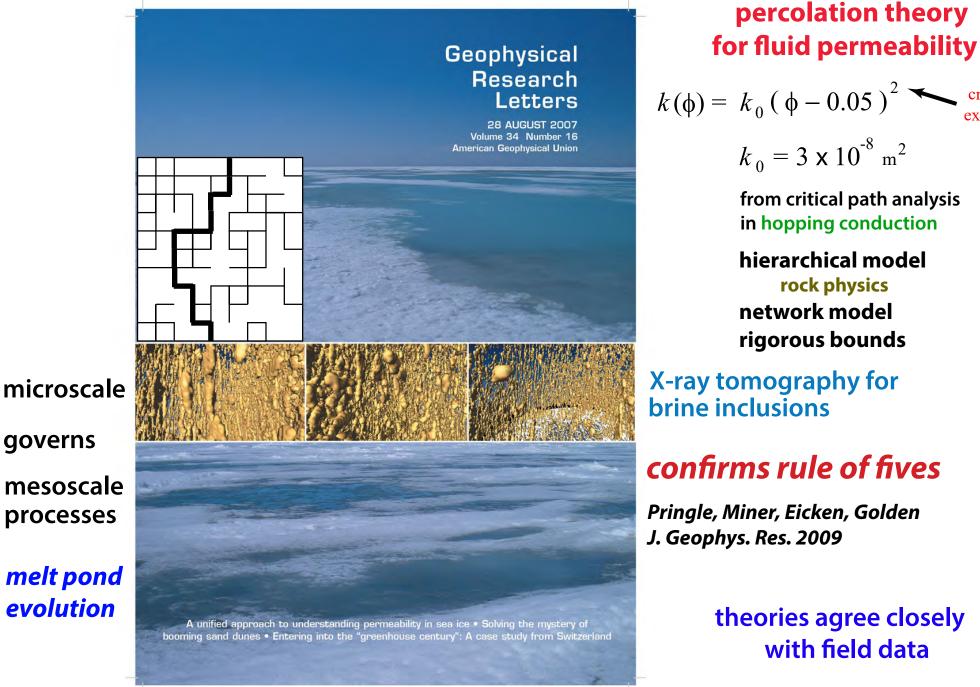
PERCOLATION THRESHOLD $\phi_c \approx 5 \%$

Golden, Ackley, Lytle, *Science* 1998



Thermal evolution of permeability and microstructure in sea ice

Golden, Eicken, Heaton^{*}, Miner, Pringle, Zhu, Geophysical Research Letters 2007



from critical path analysis in hopping conduction

critical

exponent

hierarchical model rock physics network model rigorous bounds

X-ray tomography for

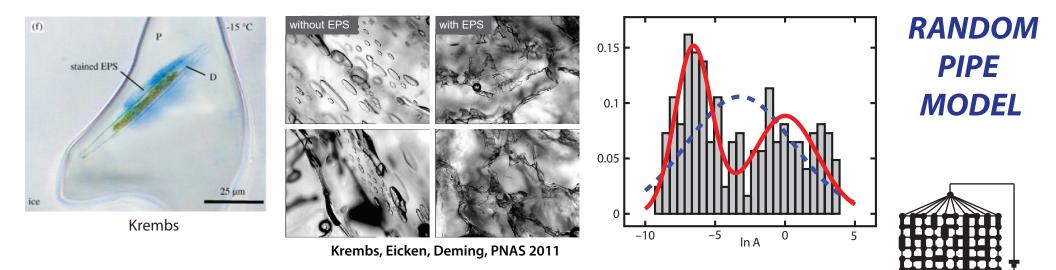
confirms rule of fives

Pringle, Miner, Eicken, Golden

theories agree closely with field data

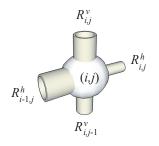
Sea ice algae secrete extracellular polymeric substances (EPS) affecting evolution of brine microstructure.

How does EPS affect fluid transport? How does the biology affect the physics?



- 2D random pipe model with bimodal distribution of pipe radii
- Rigorous bound on permeability k; results predict observed drop in k

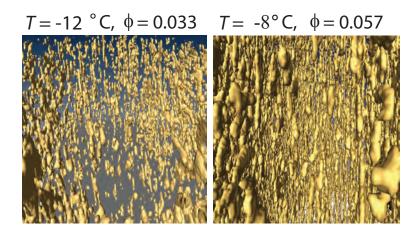
Steffen, Epshteyn, Zhu, Bowler, Deming, Golden Multiscale Modeling and Simulation, 2018

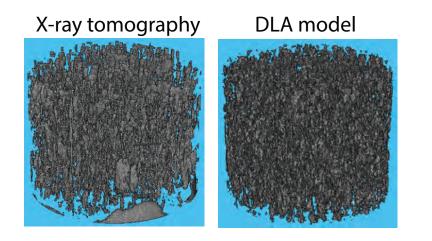


Zhu, Jabini, Golden, Eicken, Morris *Ann. Glac.* 2006

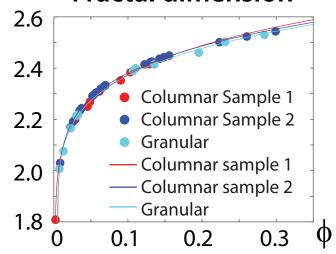
Thermal evolution of the fractal geometry of the brine microstructure in sea ice

N. Ward, D. Hallman, J. Reimer, H. Eicken, M. Oggier and K. M. Golden, 2022





+ implications for brine phase as a habitat



Fractal dimension

brine volume fraction (porosity)

theory of porosity as a function of fractal dimension

invert

excellent correspondence with data

Katz and Thompson, PRL, 1985

Arctic and Antarctic field experiments

develop electromagnetic methods of monitoring fluid transport and microstructural transitions

extensive measurements of fluid and electrical transport properties of sea ice:

2007 Antarctic SIPEX	
2010 Antarctic McMu	urdo Sound
2011 Arctic Barro	w AK
2012 Arctic Barro	w AK
2012 Antarctic SIPEX	
2013 Arctic Barro	w AK
2014 Arctic Chuke	chi Sea



Notices Notes Series

of the American Mathematical Society

May 2009

Volume 56, Number 5

Climate Change and the Mathematics of Transport in Sea Ice

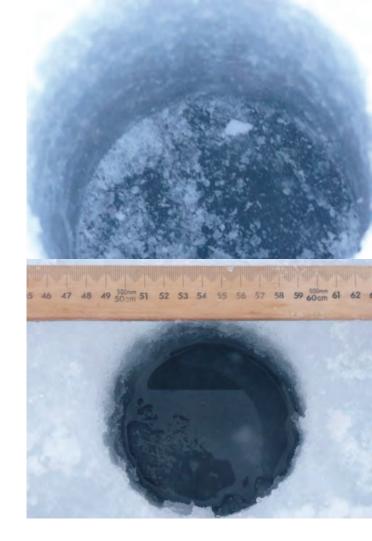
page 562

Mathematics and the Internet: A Source of Enormous Confusion and Great Potential

page 586

photo by Jan Lieser

Real analysis in polar coordinates (see page 613)



measuring fluid permeability of Antarctic sea ice

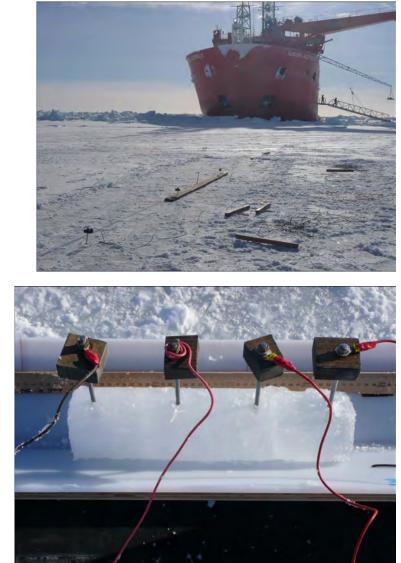
SIPEX 2007

electrical measurements



Section 12

Wenner array



vertical conductivity

Zhu, Golden, Gully, Sampson *Physica B* 2010 Sampson, Golden, Gully, Worby *Deep Sea Research* 2011

cross borehole tomography



Ingham, Jones, Buchanan Victoria University, Wellington, NZ

Measuring sea ice thickness











Remote sensing of sea ice



sea ice thickness ice concentration

INVERSE PROBLEM

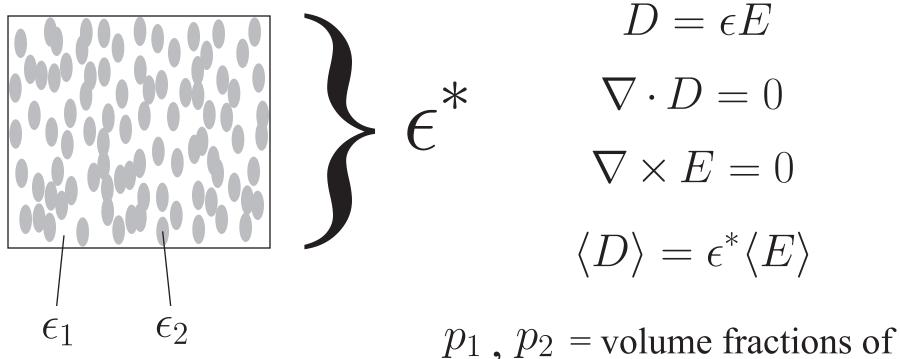
Recover sea ice properties from electromagnetic (EM) data

8*

effective complex permittivity (dielectric constant, conductivity)



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



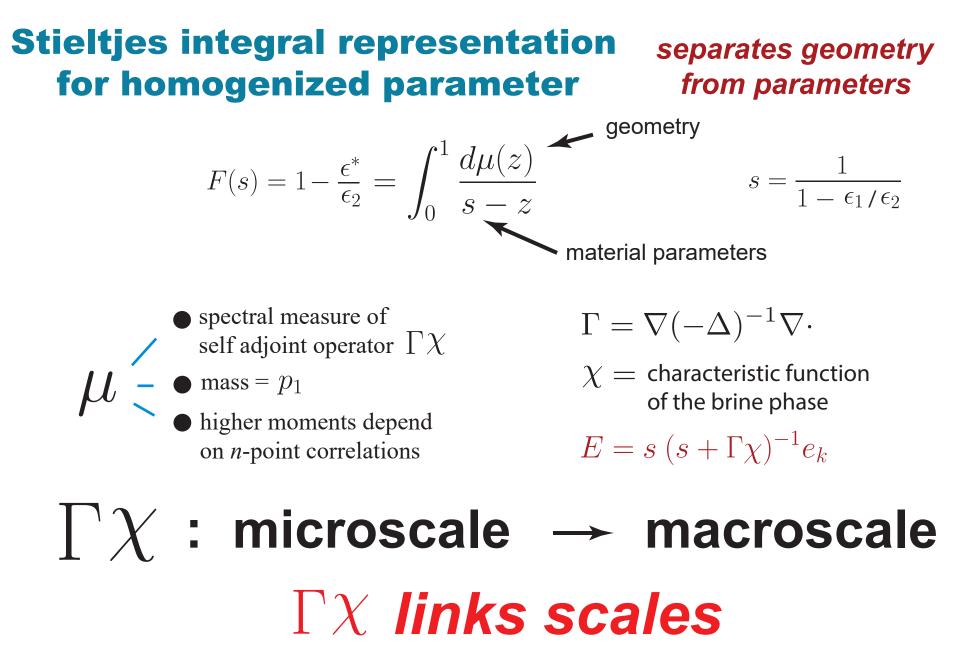
the components

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

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

Analytic Continuation Method for Homogenization

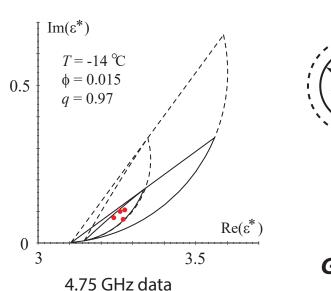
Bergman (1978), Milton (1979), Golden and Papanicolaou (1983), Theory of Composites, Milton (2002)



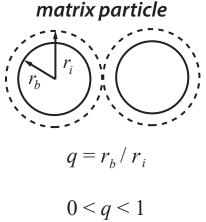
Golden and Papanicolaou, Comm. Math. Phys. 1983

This representation distills the complexities of mixture geometry into the spectral properties of an operator like the Hamiltonian in physics.

forward and inverse bounds on the complex permittivity of sea ice



forward bounds



Golden 1995, 1997

_ _ _

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



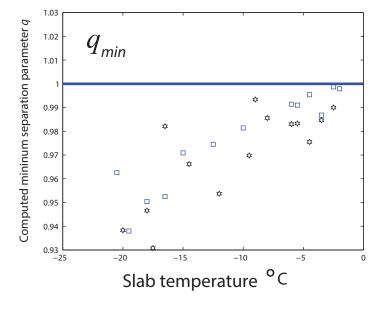
inverse bounds and recovery of brine porosity Gully, Backstrom, Eicken, Golden Physica B, 2007 inversion for brine inclusion separations in sea ice from measurements of effective complex permittivity ϵ^*

rigorous inverse bound on spectral gap

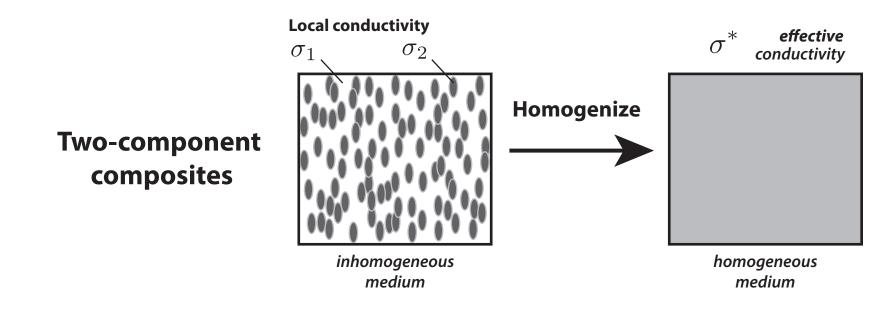
construct algebraic curves which bound admissible region in (p,q)-space

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

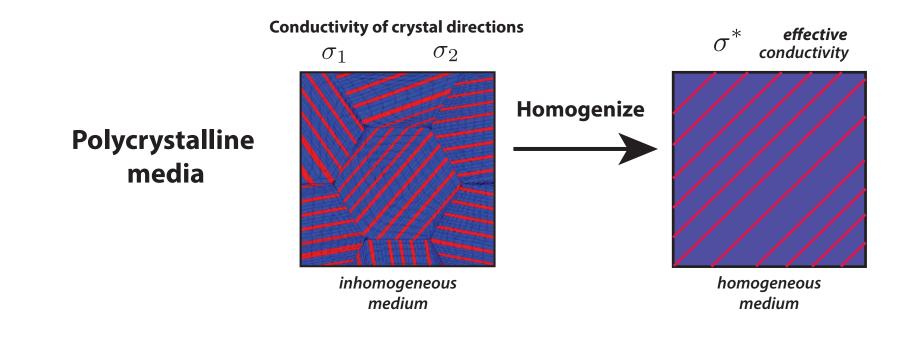
inverse bounds



Homogenization for polycrystalline materials



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

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

PROCEEDINGS A



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

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



higher threshold for fluid flow in granular sea ice

granular

microscale details impact "mesoscale" processes

5%

columnar

nutrient fluxes for microbes melt pond drainage snow-ice formation

10%

Golden, Sampson, Gully, Lubbers, Tison 2022

electromagnetically distinguishing ice types Kitsel Lusted, Elena Cherkaev, Ken Golden

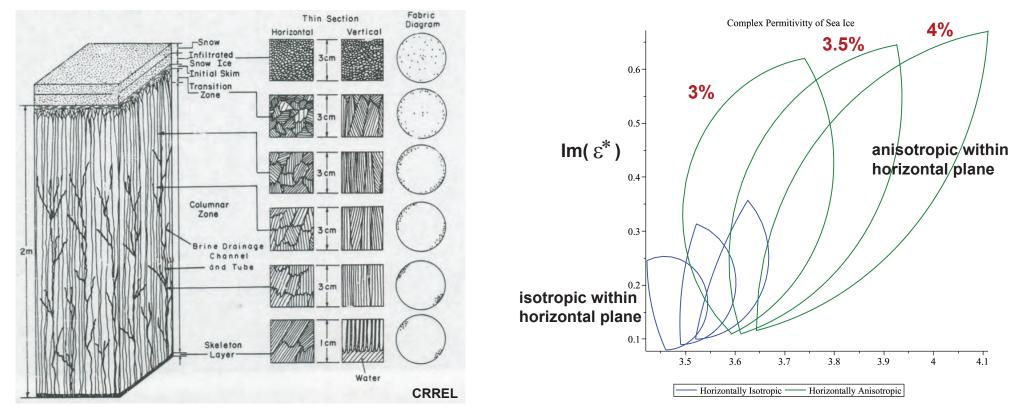
Rigorous bounds on the complex permittivity tensor of sea ice with polycrystalline anisotropy in the horizontal plane

Kenzie McLean, Elena Cherkaev, Ken Golden 2022

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

input: orientation statistics

output: bounds



Re(ϵ^*)

mesoscale

wave propagation in the marginal ice zone (MIZ)



Sampson, Murphy, Cherkaev, Golden 2022

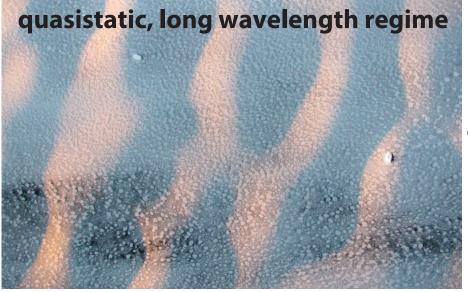


first theory of key parameter in wave-ice interactions only fitted to wave data before

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

Analytic Continuation Method

Bergman (78) - Milton (79) integral representation for ϵ^* Golden and Papanicolaou (83) Milton, *Theory of Composites* (02)



homogenized parameter depends on sea ice concentration and ice floe geometry

like EM waves

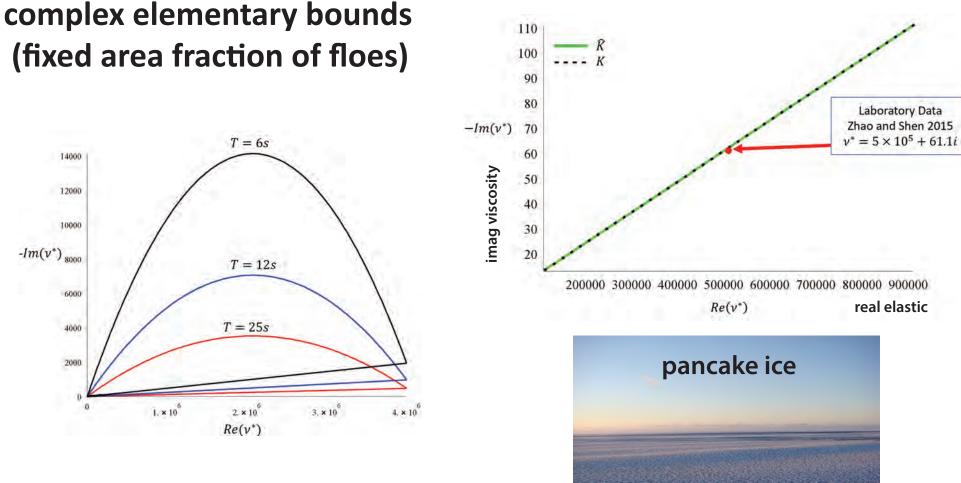


bounds on the effective complex viscoelasticity

$V_1 = 10^7 + i4875$	pancake ice
$V_2 = 5 + i 0.0975$	slush / frazil

high contrast

matrix-particle bounds



Elementary bounds for wave periods T.

Golden

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 $ec{u}$

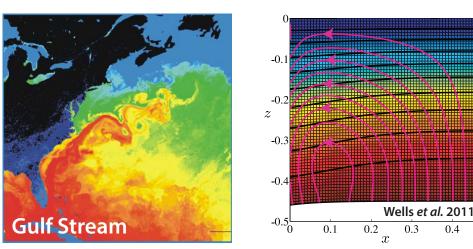
$$\frac{\partial T}{\partial t} + \vec{u} \cdot \vec{\nabla} T = \kappa_0 \Delta T$$
$$\vec{\nabla} \cdot \vec{u} = 0$$
$$homogenize$$
$$\frac{\partial \overline{T}}{\partial t} = \kappa^* \Delta \overline{T}$$

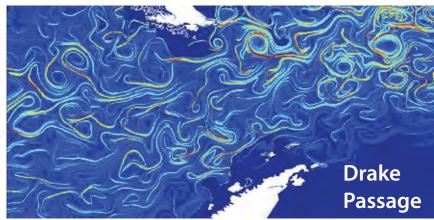
κ^* effective diffusivity

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, J. Math. Phys. 2020





-0.2

-0.4

-0.6

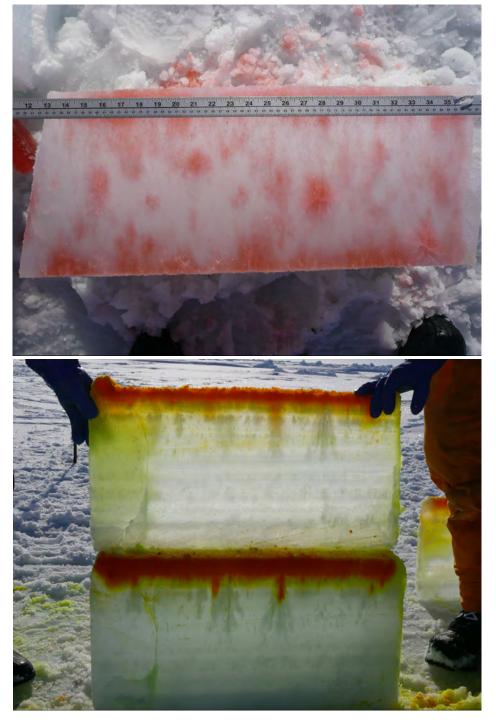
-0.8

0.4



tracers flowing through inverted sea ice blocks







Stieltjes Integral Representation for Advection Diffusion

Murphy, Cherkaev, Zhu, Xin, Golden, J. Math. Phys. 2020

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

- 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
- $\Gamma:=abla(-\Delta)^{-1}
 abla\cdot$, 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

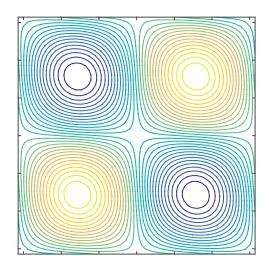
rigorous framework for numerical computations of spectral measures and effective diffusivity for model flows

new integral representations, theory of moment calculations

separation of material properties and flow field

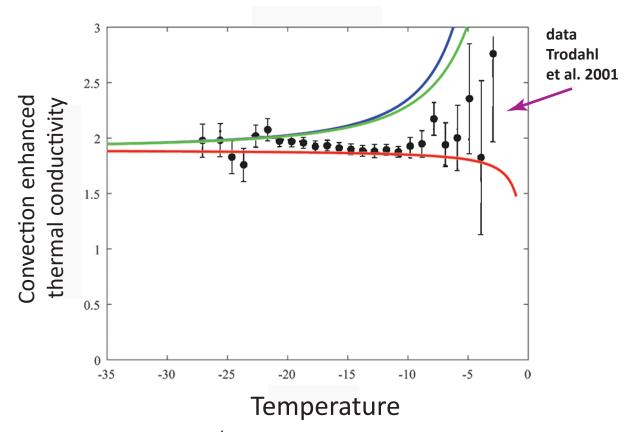
Rigorous bounds on convection enhanced thermal conductivity of sea ice

Kraitzman, Hardenbrook, Dinh, Murphy, Zhu, Cherkaev, Golden 2022



cat's eye flow model for brine convection cells

similar bounds for shear flows



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

direct calculation of spectral measures

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

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

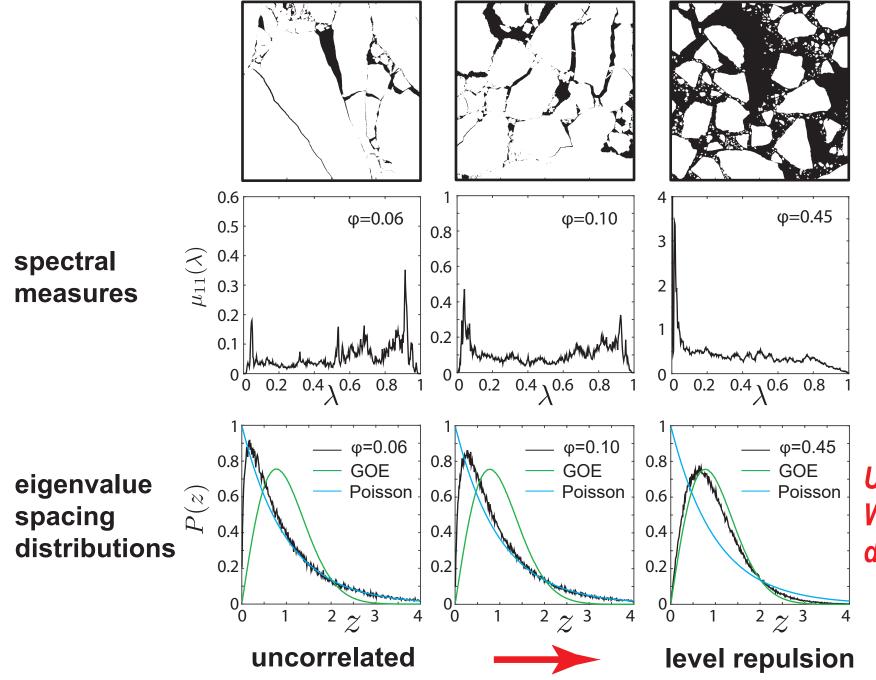
once we have the spectral measure μ it can be used in Stieltjes integrals for other transport coefficients:

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

earlier studies of spectral measures

Day and Thorpe 1996 Helsing, McPhedran, Milton 2011

Spectral computations for sea ice floe configurations



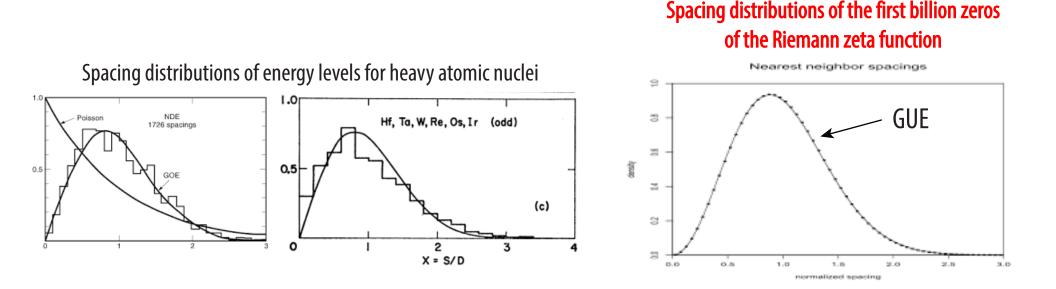
UNIVERSAL Wigner-Dyson distribution

Eigenvalue Statistics of Random Matrix Theory

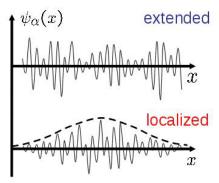
Wigner (1951) and Dyson (1953) first used random matrix theory (RMT) to describe quantized energy levels of heavy atomic nuclei.

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

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



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



electronic transport in semiconductors

metal / insulator transition localization Anderson 1958 Mott 1949 Shklovshii et al 1993 Evangelou 1992

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

from analysis of spectral measures for brine, melt ponds, ice floes

we find percolation-driven

Anderson transition for classical transport in composites

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



-- but with NO wave interference or scattering effects ! --

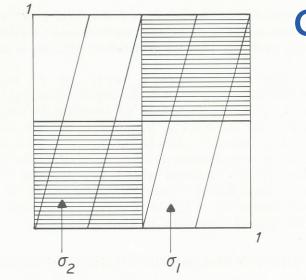
local conductivity in 1D inhomogeneous material

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

effective conductivity

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

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



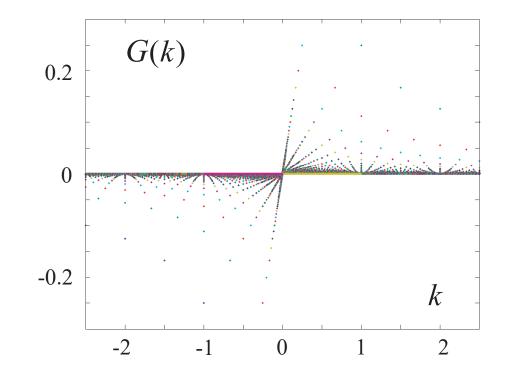
Classical transport in quasiperiodic media

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

line of slope k through an infinite checkerboard effective conductivity $\sigma^*(k)$ effective resistivity $1/\sigma^*(k) = 1 - G(k)$

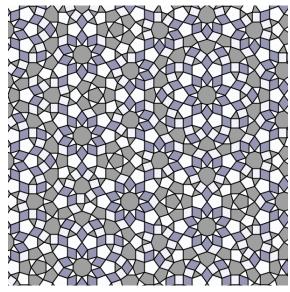
$$G(k) = \begin{cases} 0, & k \text{ irrational} \\ 1/pq, & k = p/q \text{ rational} \end{cases}$$

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

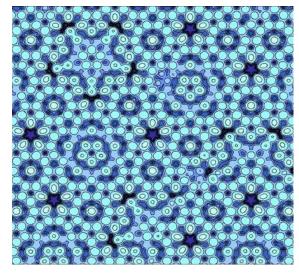


Order to Disorder in Quasiperiodic Composites

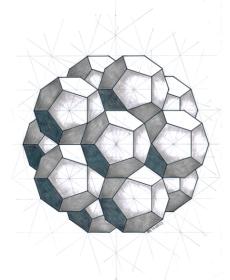
D. Morison (Physics), N. B. Murphy, E. Cherkaev, K. M. Golden, Communications Physics 2022



quasiperiodic checkerboard _{Stampfli}, 2013



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



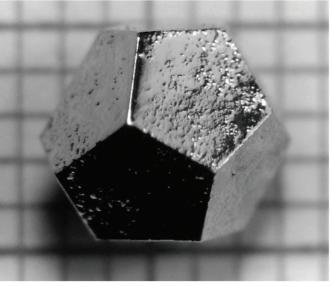
dense packing of dodecahedra 3D Penrose tiling Tripkovic, 2019

quasiperiodic crystal quasicrystal

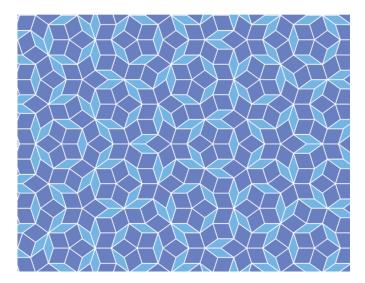
ordered but aperiodic

lacks translational symmetry

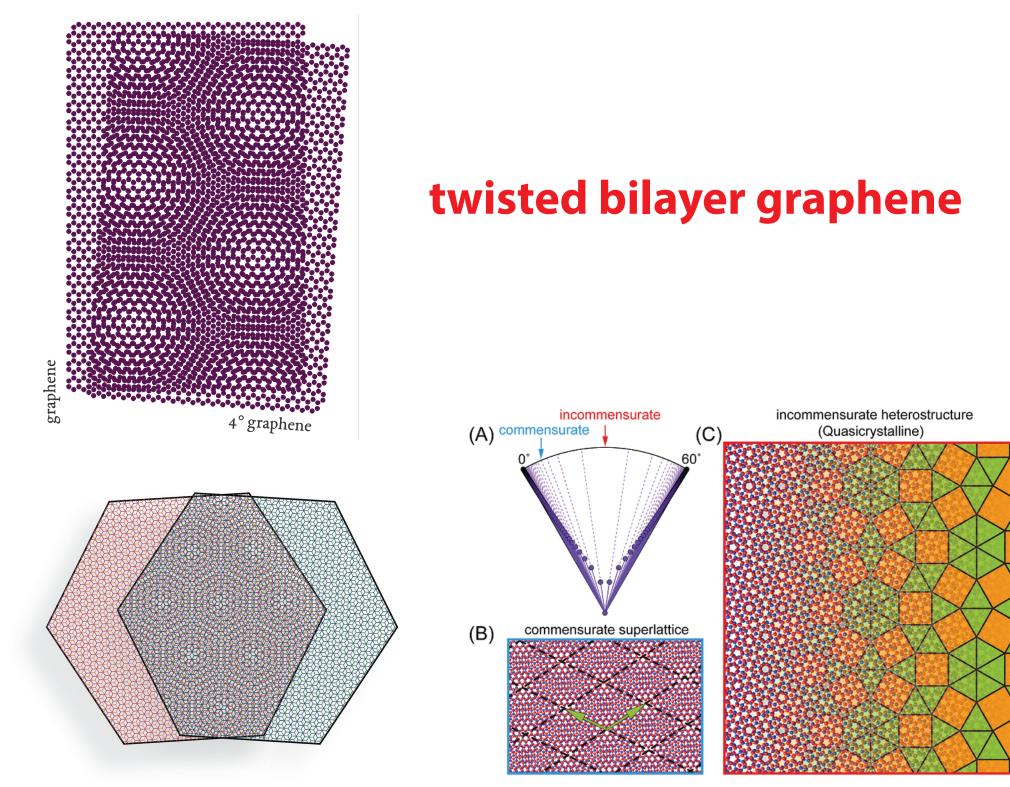
Schechtman et al., 1984 Levine & Steinhardt, 1984



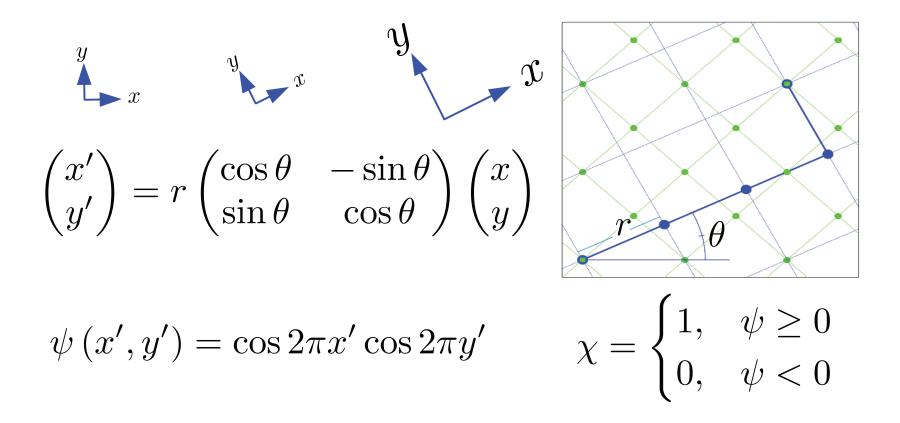
Holmium-magnesium-zinc quasicrystal



aperiodic tiling of the plane - R. Penrose 1970s



Moiré patterns generate two component composites

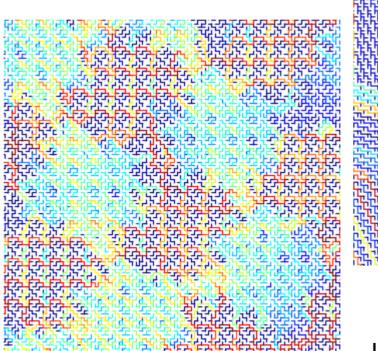


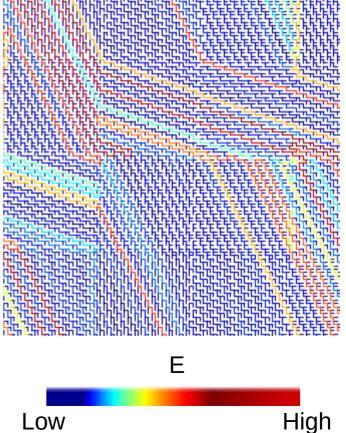
rotation and dilation

Small Difference in Moiré Parameters

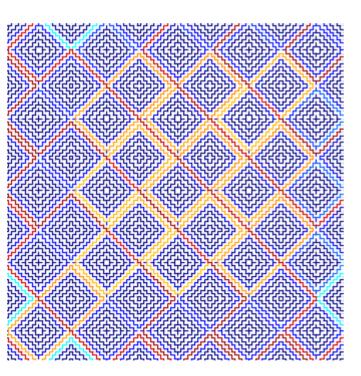
Big Difference in Material Properties

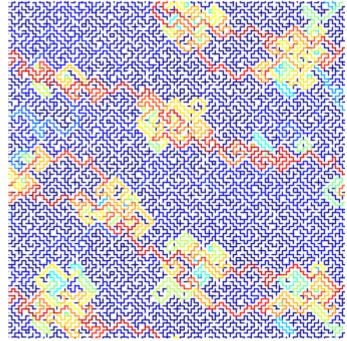
Wide Variety of Microgeometries





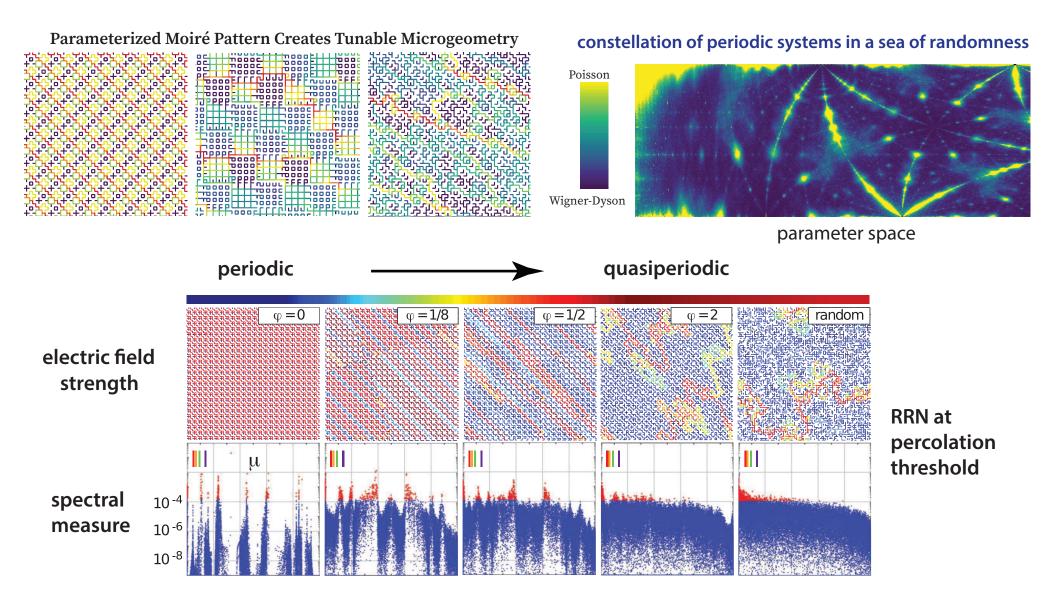
Wide Variety of Microgeometries





Order to disorder in quasiperiodic composites

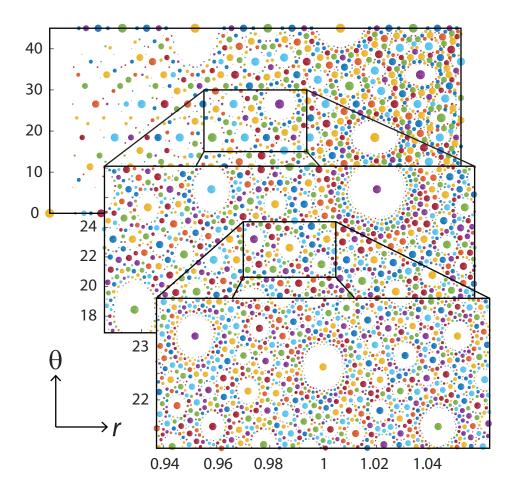
Morison, Murphy, Cherkaev, Golden, Commun. Phys. 2022



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

photonic crystals and quasicrystals

Fractal arrangement of periodic systems



Sequential insets zooming into smaller regions of parameter space.

size of the dots ~ length of period

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

Conclusions

- 1. Sea ice is a fascinating multiscale composite with structure similar to many other natural and man-made materials.
- 2. Homogenization and statistical physics help *link scales in the sea ice system*; provide rigorous methods for finding effective behavior; advance sea ice representations in climate models.
- 3. Stieltjes functions and their integral representations provide powerful methods of homogenization for EM waves, advection diffusion, polycrystalline media, and ocean surface waves in the ice cover.
- 4. Mathematical methods developed for sea ice advance the theory of composites, and quasiperiodic media in particular.
- 5. Our research is helping to improve projections of climate change, the fate of Earth's sea ice packs, and the ecosystems they support.

University of Utah Sea Ice Modeling Group (2017-2021)

Senior Personnel: Ken Golden, Distinguished Professor of Mathematics Elena Cherkaev, Professor of Mathematics Court Strong, Associate Professor of Atmospheric Sciences Ben Murphy, Adjunct Assistant Professor of Mathematics

Postdoctoral Researchers: Noa Kraitzman (now at ANU), Jody Reimer

Graduate Students: Kyle Steffen (now at UT Austin with Clint Dawson)

Christian Sampson (now at UNC Chapel Hill with Chris Jones) Huy Dinh (now a sea ice MURI Postdoc at NYU/Courant) Rebecca Hardenbrook David Morison (Physics Department) Ryleigh Moore Delaney Mosier Daniel Hallman

Undergraduate Students: Kenzie McLean, Jacqueline Cinella Rich,

Dane Gollero, Samir Suthar, Anna Hyde, Kitsel Lusted, Ruby Bowers, Kimball Johnston, Jerry Zhang, Nash Ward, David Gluckman

High School Students: Jeremiah Chapman, Titus Quah, Dylan Webb

Sea Ice Ecology GroupPostdoc Jody Reimer, Grad Student Julie Sherman,
Undergraduates Kayla Stewart, Nicole Forrester



of the American Mathematical Society

November 2020

Volume 67, Number 10







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

THANK YOU

Office of Naval Research

Applied and Computational Analysis Program Arctic and Global Prediction Program

National Science Foundation

Division of Mathematical Sciences Division of Polar Programs











Australian Government

Department of the Environment and Water Resources Australian Antarctic Division











Buchanan Bay, Antarctica Mertz Glacier Polynya Experiment July 1999