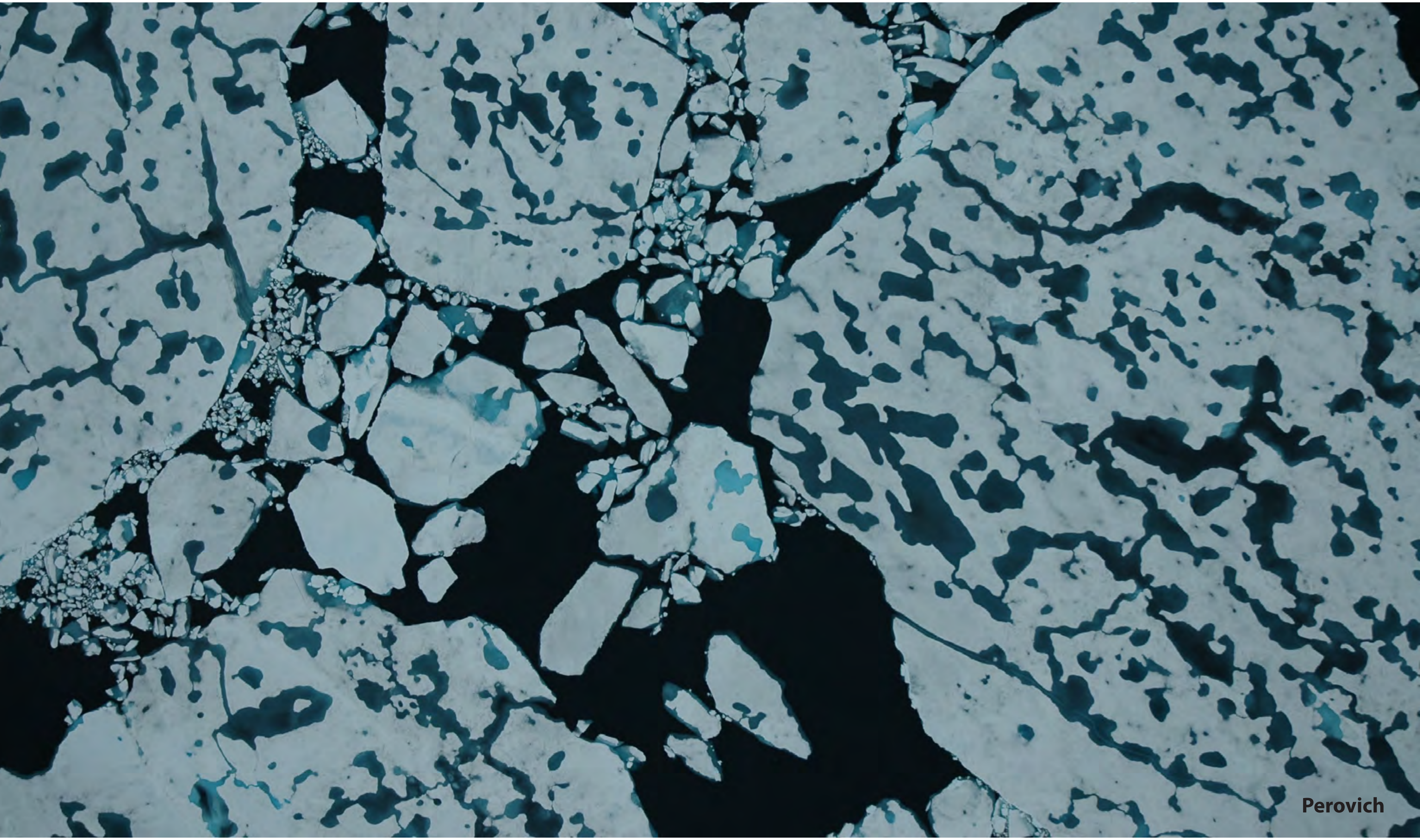
Multiscale homogenization for sea ice and other composite materials

Kenneth M. Golden University of Utah



ICIAM 2019, Valencia

SEA ICE covers ~12% of Earth's ocean surface

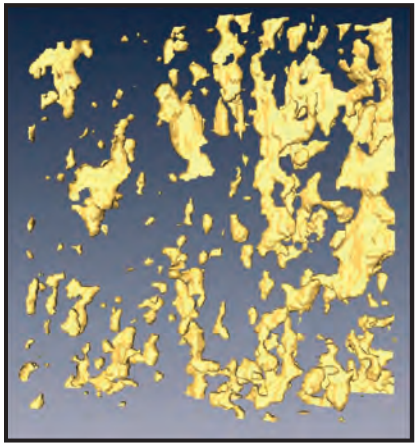
- **boundary between ocean and atmosphere**
- **mediates exchange of heat, gases, momentum**
- **global ocean circulation**
- **hosts rich ecosystem**
- **indicator of climate change**

Sea Ice is a Multiscale Composite Material

sea ice microstructure

brine inclusions

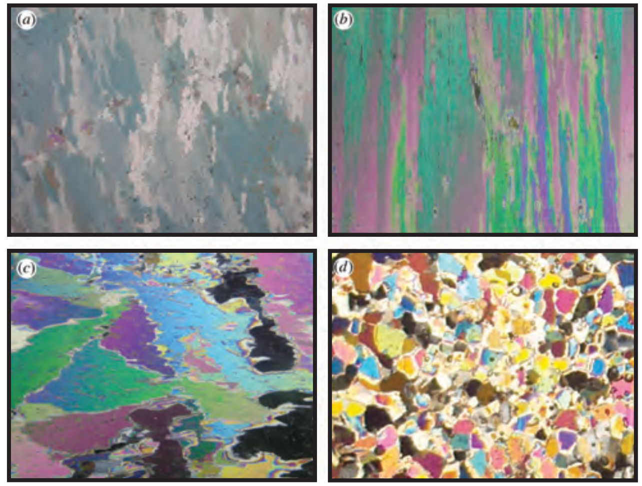
Weeks & Assur 1969



H. Eicken

Golden *et al. GRL* 2007

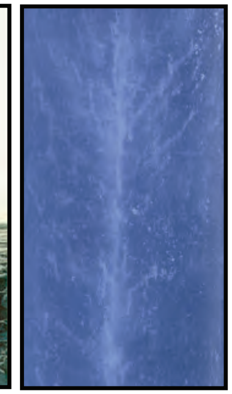
polycrystals



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

brine channels

D. Cole



K. Golden

millimeters

centimeters

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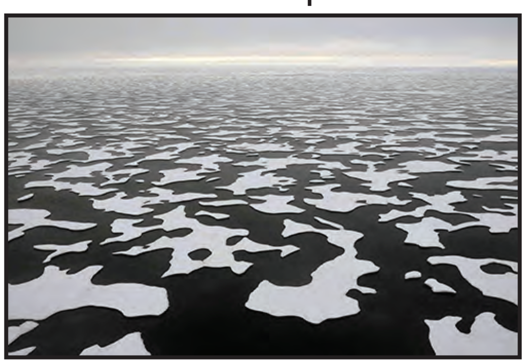
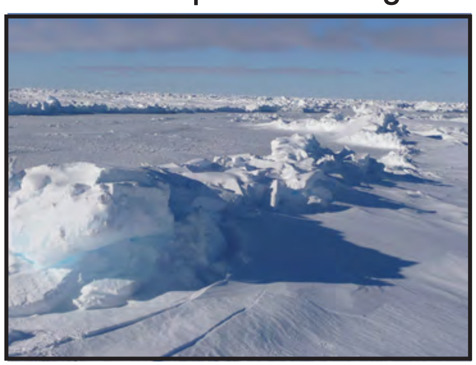
sea ice mesostructure

Arctic melt ponds



K. Frey

Antarctic pressure ridges



K. Golden

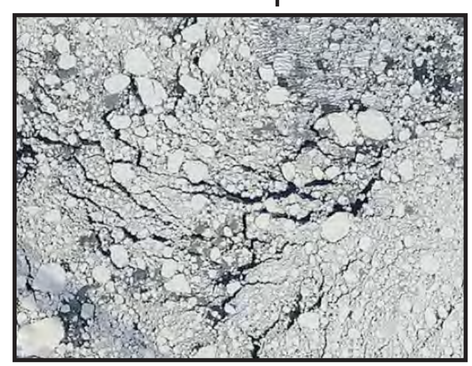
meters

sea ice macrostructure

sea ice floes

J. Weller

sea ice pack



NASA

kilometers

What is this talk about? HOMOGENIZATION

What is the role of microstructure in determining effective properties?

Using methods of statistical physics and homogenization to **LINK SCALES** ***in the sea ice system ... rigorously compute effective behavior and improve climate models.***

1. Sea ice microphysics and fluid transport

2. Analytic Continuation Method, integral representations

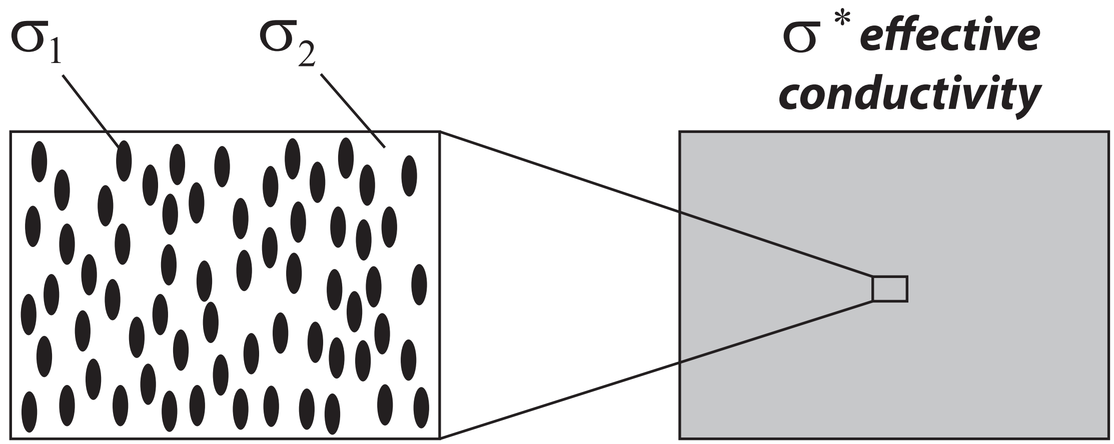
3. Extension of ACM to advection diffusion, waves in sea ice

4. Fractal geometry of melt pond evolution

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

cross - pollination

HOMOGENIZATION - Linking Scales in Composites



inhomogeneous medium

homogeneous medium

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

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

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

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

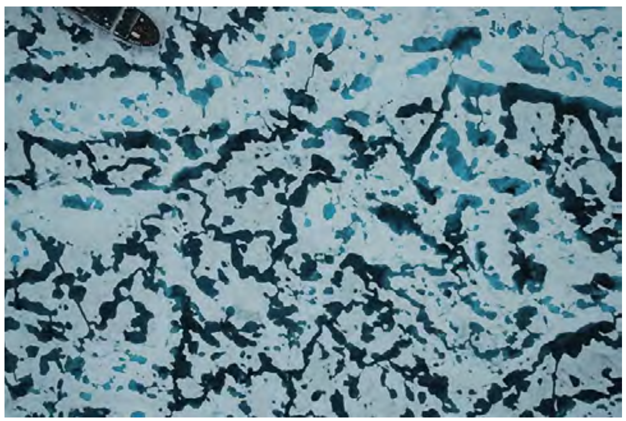
How do scales interact in the sea ice system?

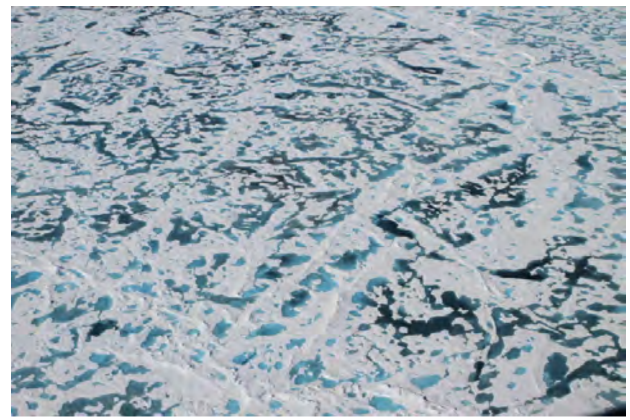

NASA

basin scale - grid scale albedo

Linking Scales

km scale melt ponds

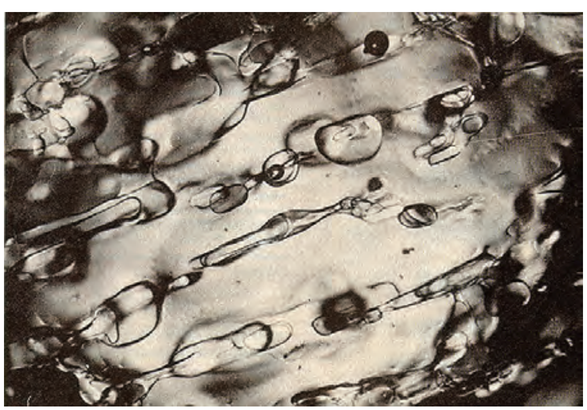



Perovich

km scale melt ponds

Linking Scales

mm scale brine inclusions



meter scale snow topography

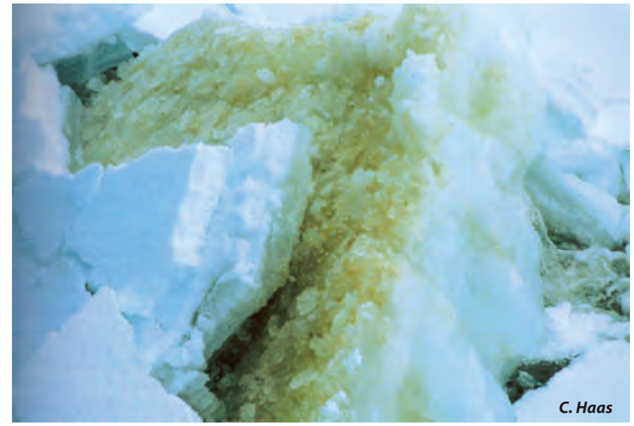
sea ice microphysics

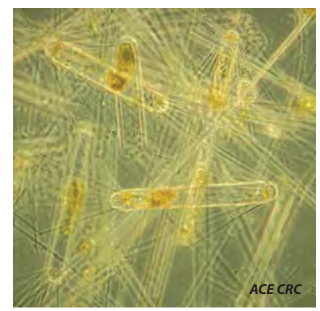
fluid transport

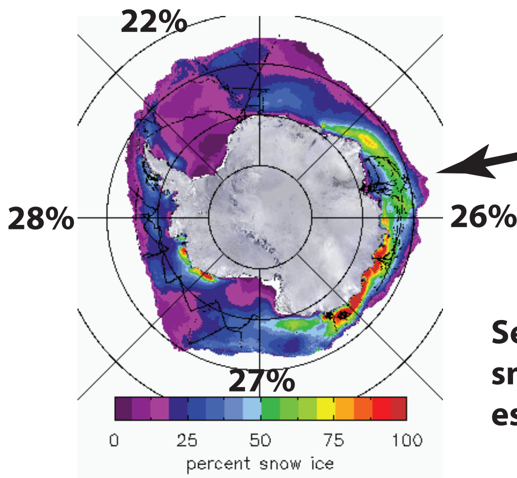
fluid flow through the porous microstructure of sea ice governs key processes in polar climate and ecosystems

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

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

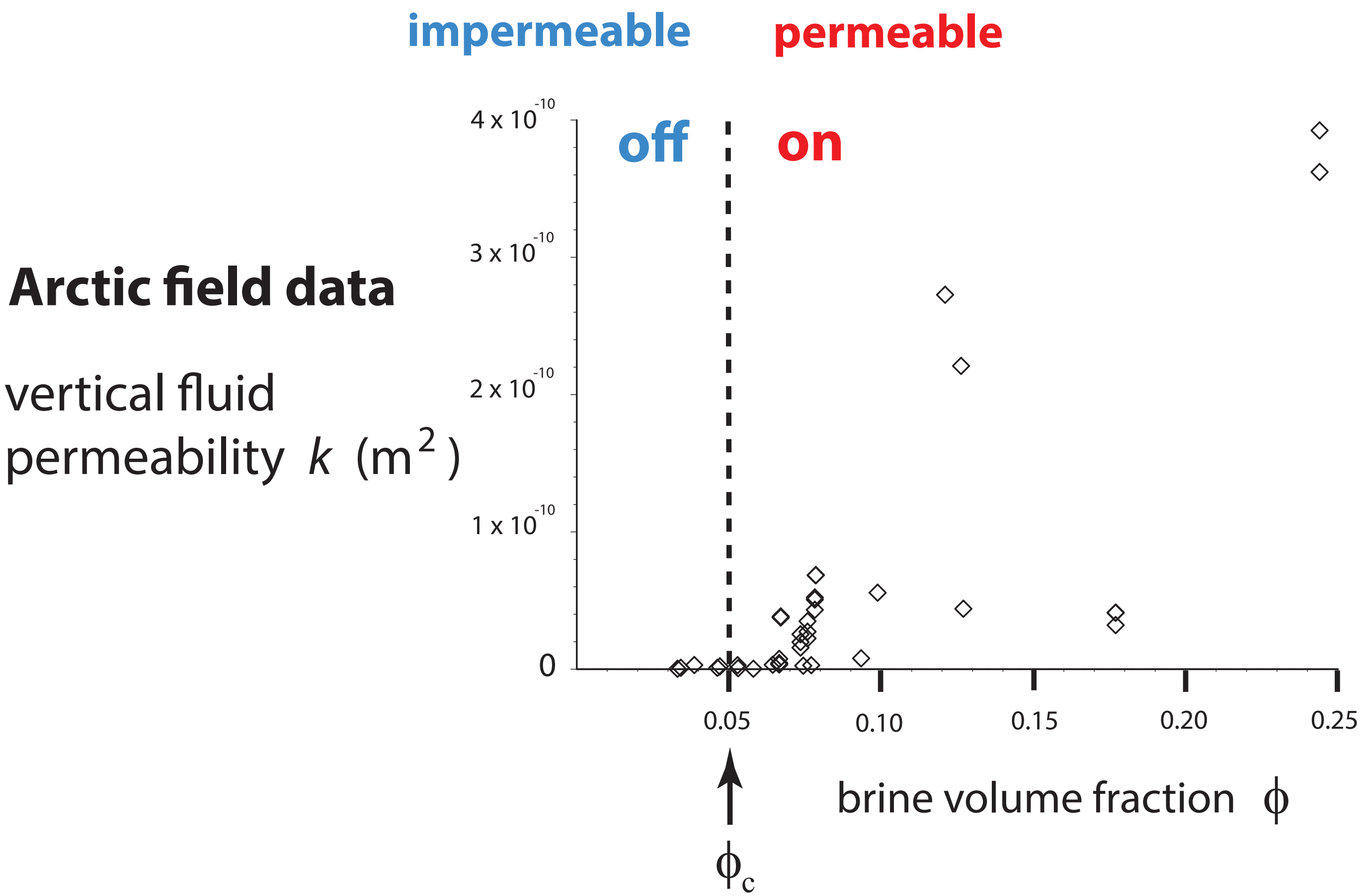
viscosity

$\mathbf{k}$ = fluid permeability tensor

HOMOGENIZATION

mathematics for analyzing effective behavior of heterogeneous systems

Critical behavior of fluid transport in sea ice



"on - off" switch for fluid flow

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

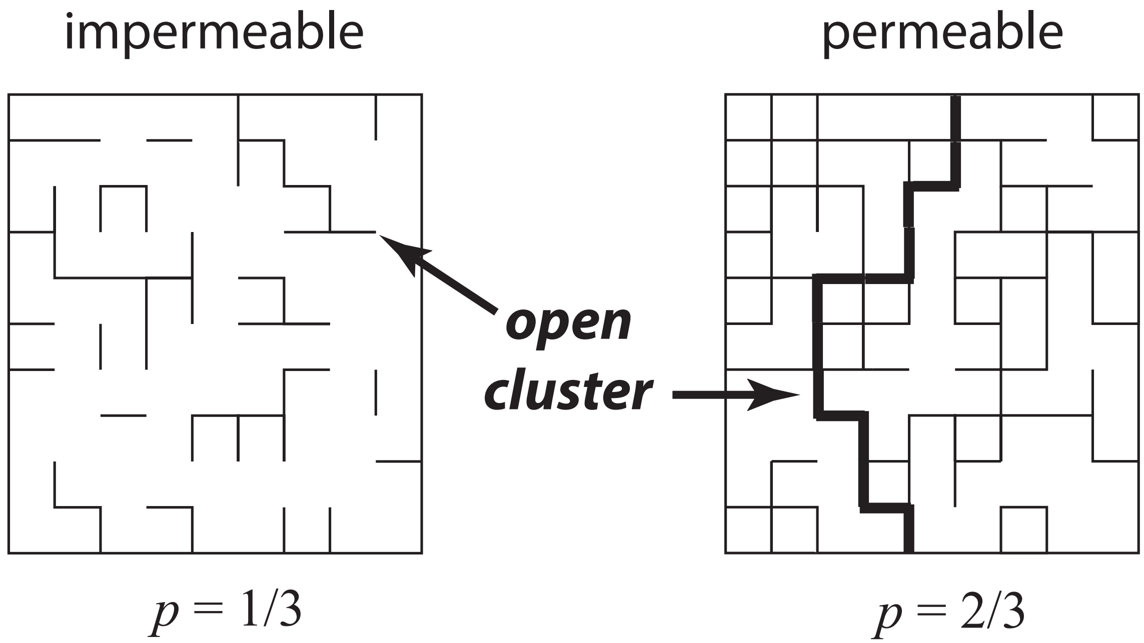
RULE OF FIVES

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

Why is the rule of fives true?

percolation theory

probabilistic theory of connectedness



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

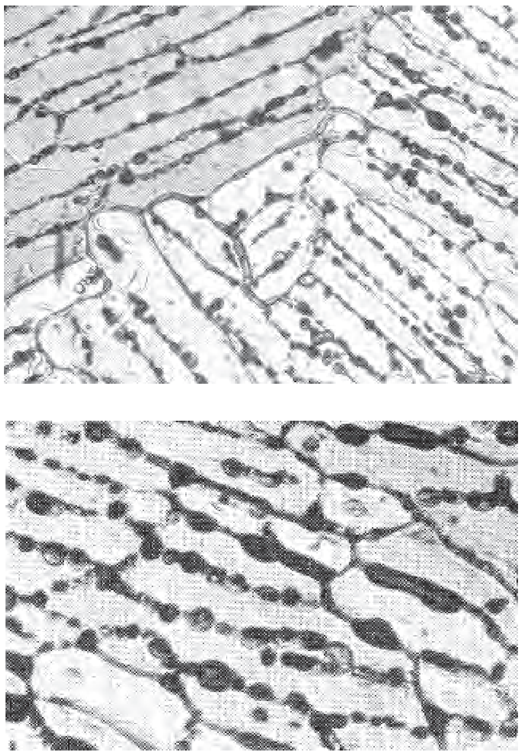
percolation threshold

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

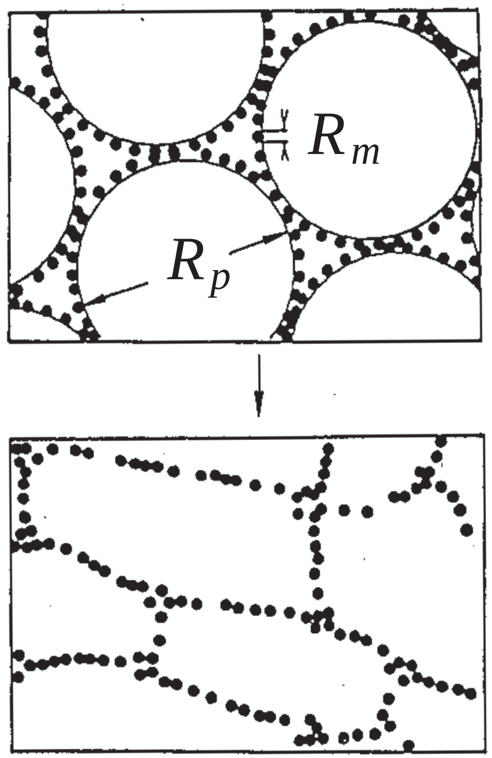
smallest *p* for which there is an infinite open cluster

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

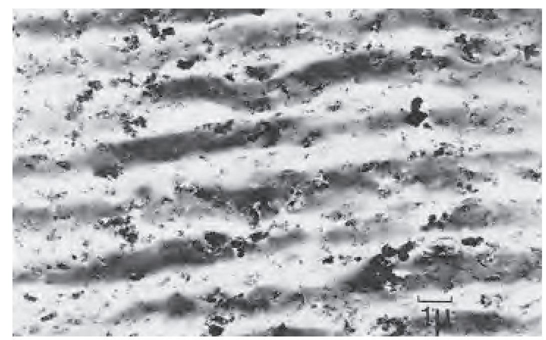
$\phi_c \approx 5\ \%$ Golden, Ackley, Lytle, *Science*, 1998



sea ice



compressed powder



radar absorbing composite

sea ice is radar absorbing

Thermal evolution of permeability and microstructure in sea ice

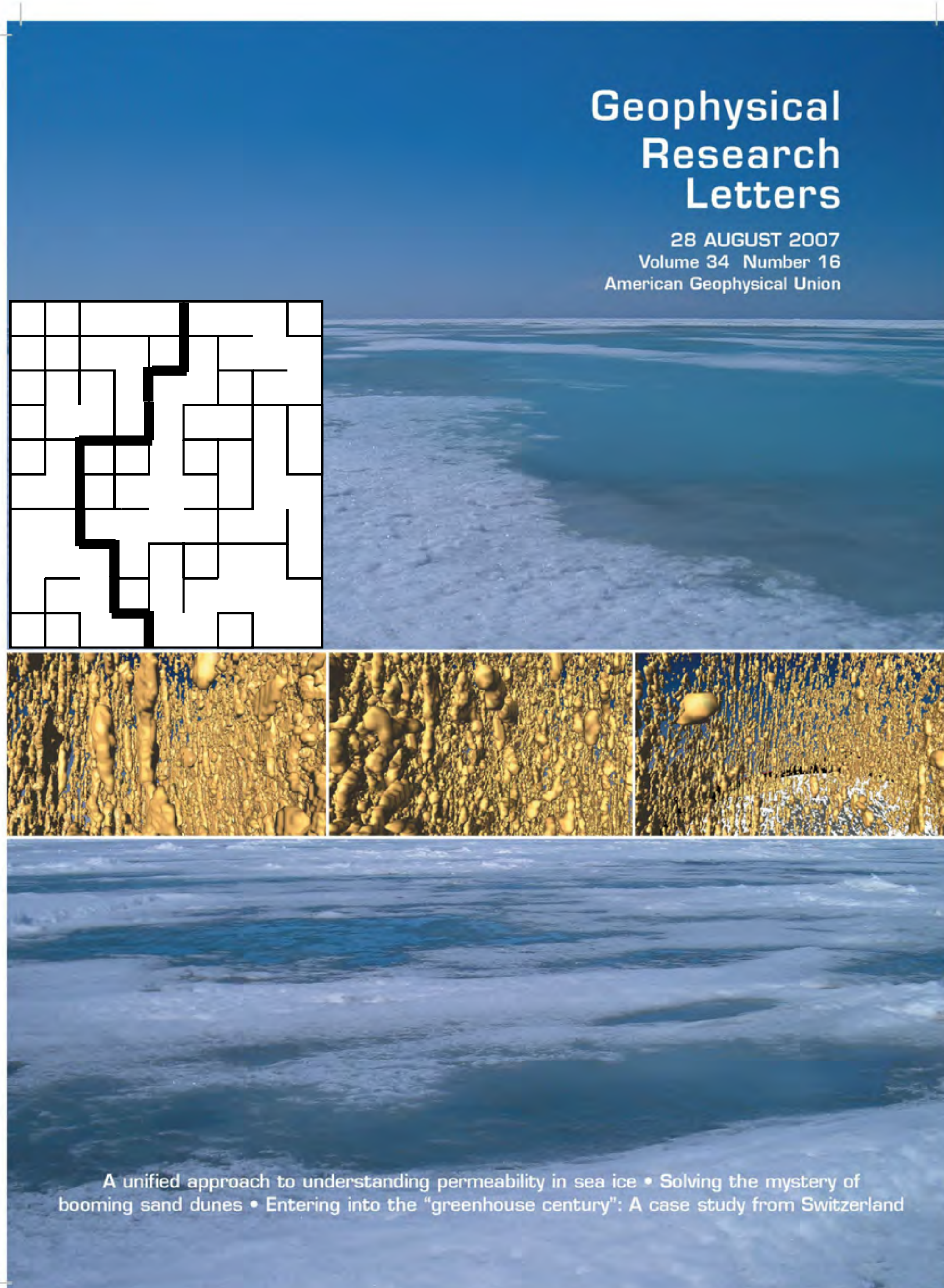
Golden, Eicken, Heaton, Miner, Pringle, Zhu, Geophysical Research Letters 2007

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

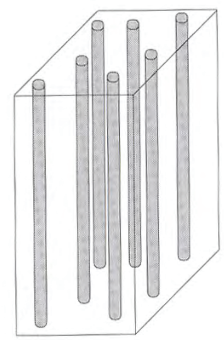
confirms rule of fives

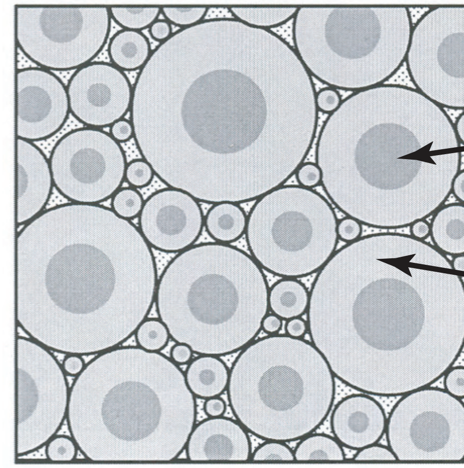
Pringle, Miner, Eicken, Golden J. Geophys. Res. 2009

PIPE BOUNDS on vertical fluid permeability k

Golden, Heaton, Eicken, Lytle, Mech. Materials 2006
Golden, Eicken, Heaton, Miner, Pringle, Zhu, Geophys. Res. Lett. 2007

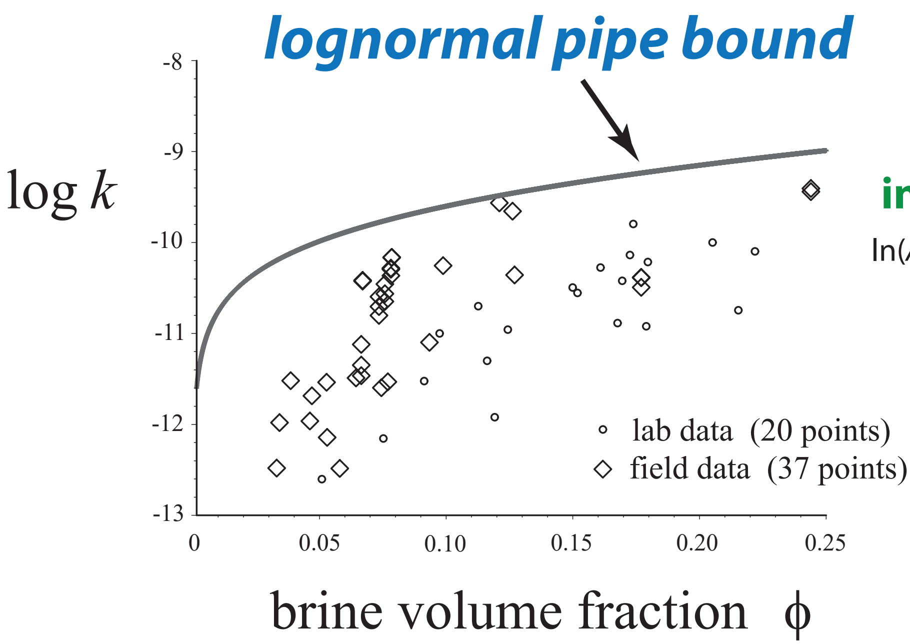
vertical pipes
with appropriate radii
maximize k





optimal coated cylinder geometry

fluid analog of arithmetic mean upper bound for effective conductivity of composites (Wiener 1912)



Golden et al., Geophys. Res. Lett. 2007

$$k \;\leq\; \frac{\phi\langle R^4\rangle}{8\langle R^2\rangle} \;=\; \frac{\phi}{8}\langle R^2\rangle e^{\sigma^2}$$

inclusion cross sectional areas A lognormally distributed

ln(A) normally distributed, mean μ (increases with T) variance σ^2 (Gow and Perovich 96)

get bounds through variational analyis of ***trapping constant*** γ for diffusion process in pore space with absorbing BC

Torquato and Pham, *PRL* 2004

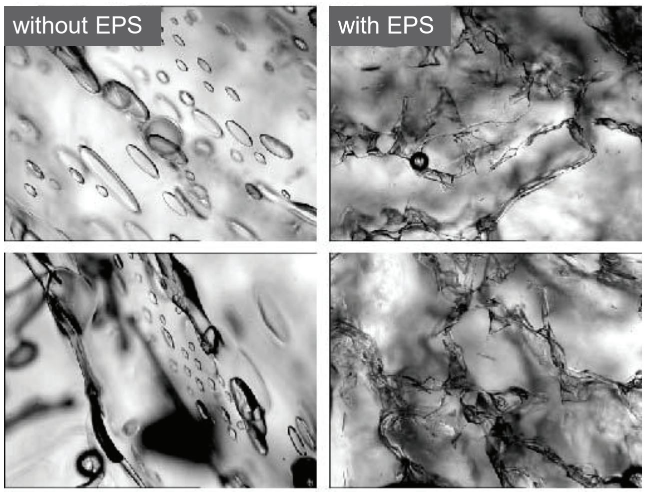
$$\mathbf{k} \;\leq\; \gamma^{-1}\mathbf{I}$$

for any ergodic porous medium (Torquato 2002, 2004)

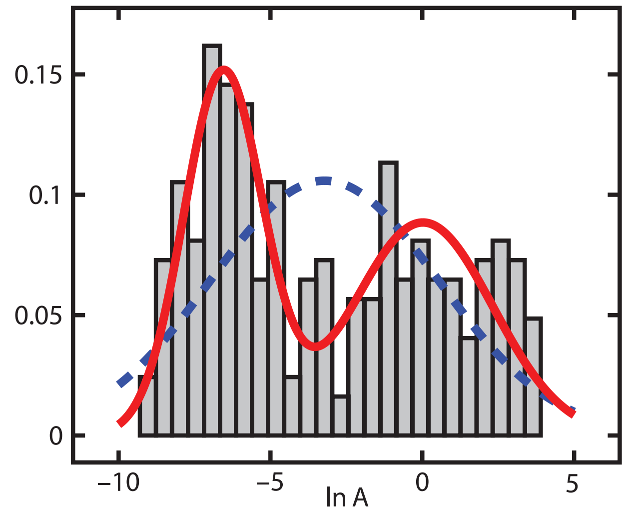
BACTERIAL FORAGING

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

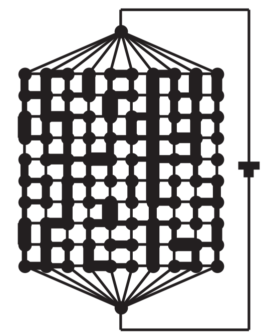
How does EPS affect fluid transport?

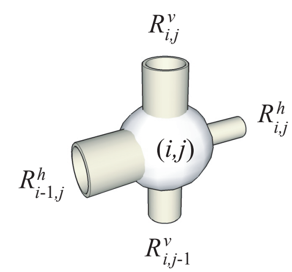


Krembs, Eicken, Deming, PNAS 2011



RANDOM PIPE MODEL





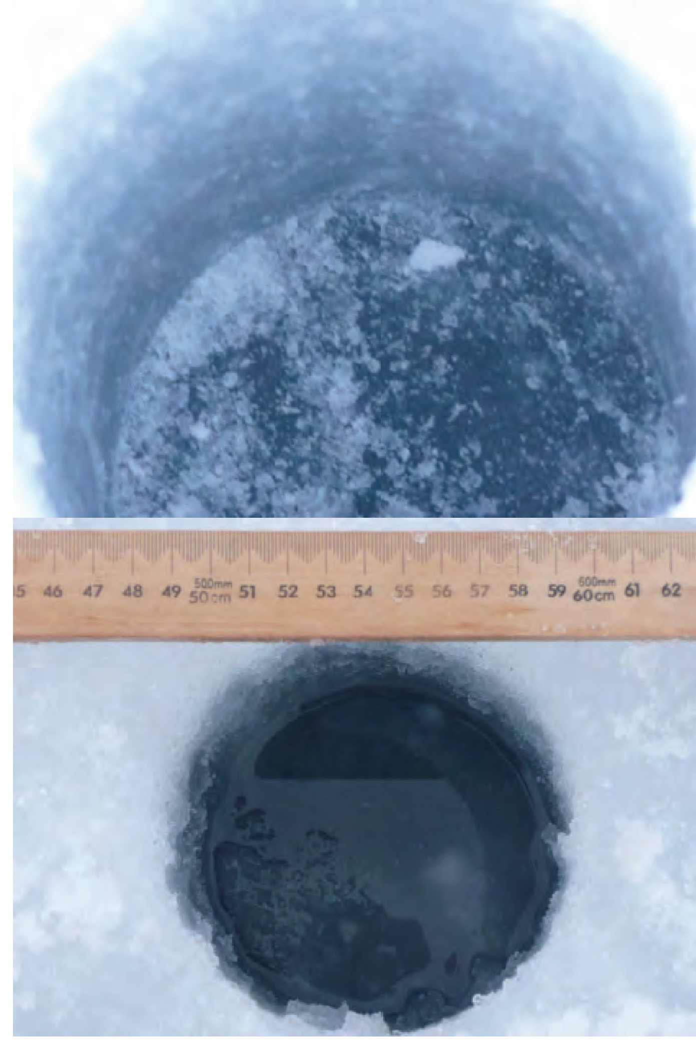
Zhu, Jabini, Golden, Eicken, Morris *Ann. Glac.* 2006

- **Bimodal** lognormal distribution for brine inclusions
- Develop random pipe network model with bimodal distribution; Use numerical methods that can handle larger variances in sizes.
- Results predict observed drop in fluid permeability *k*.
- **Rigorous bound on *k* for bimodal distribution of pore sizes**

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

How does the biology affect the physics?

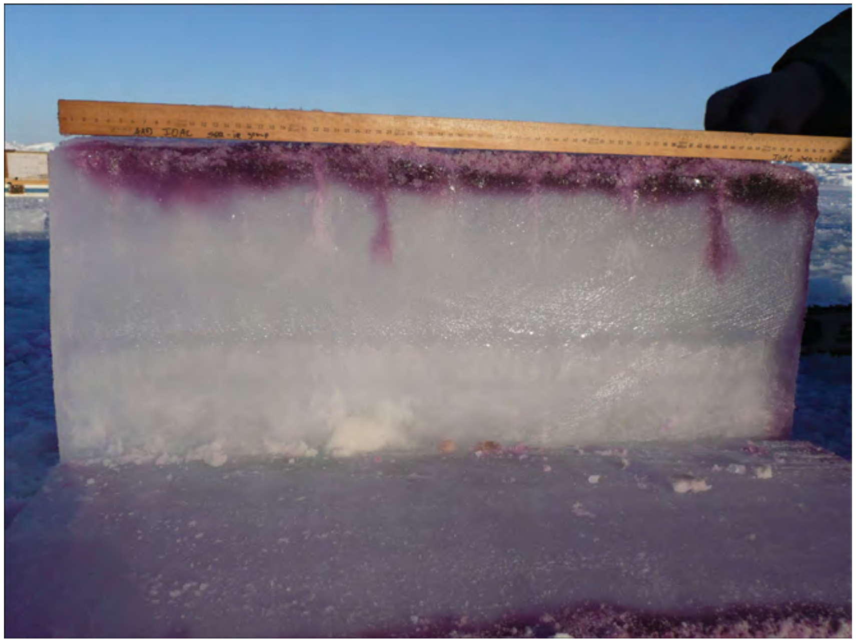
photo by Jan Lieser

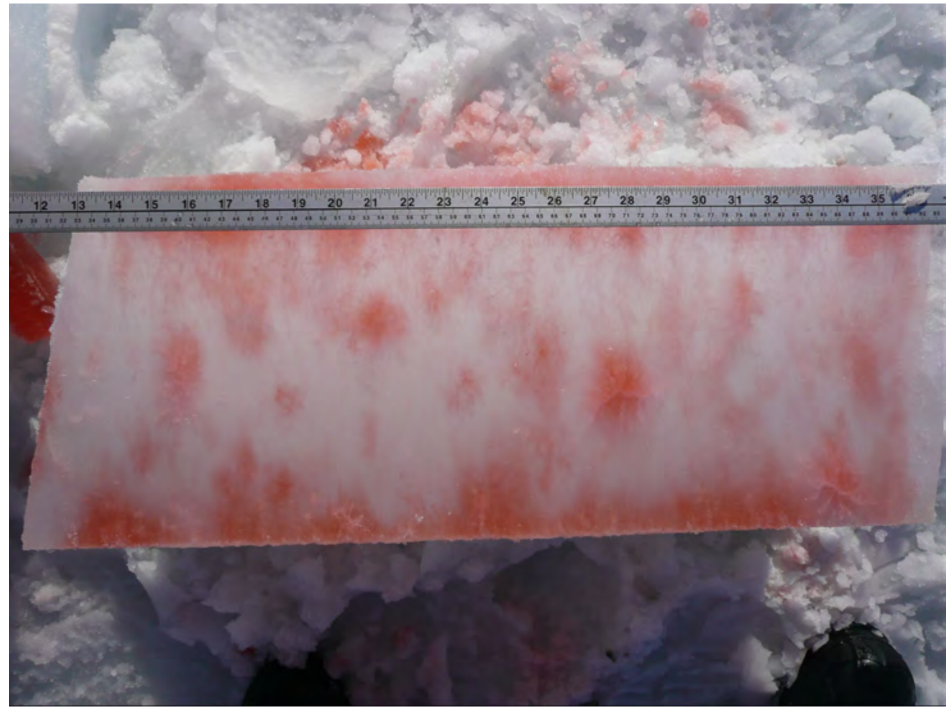


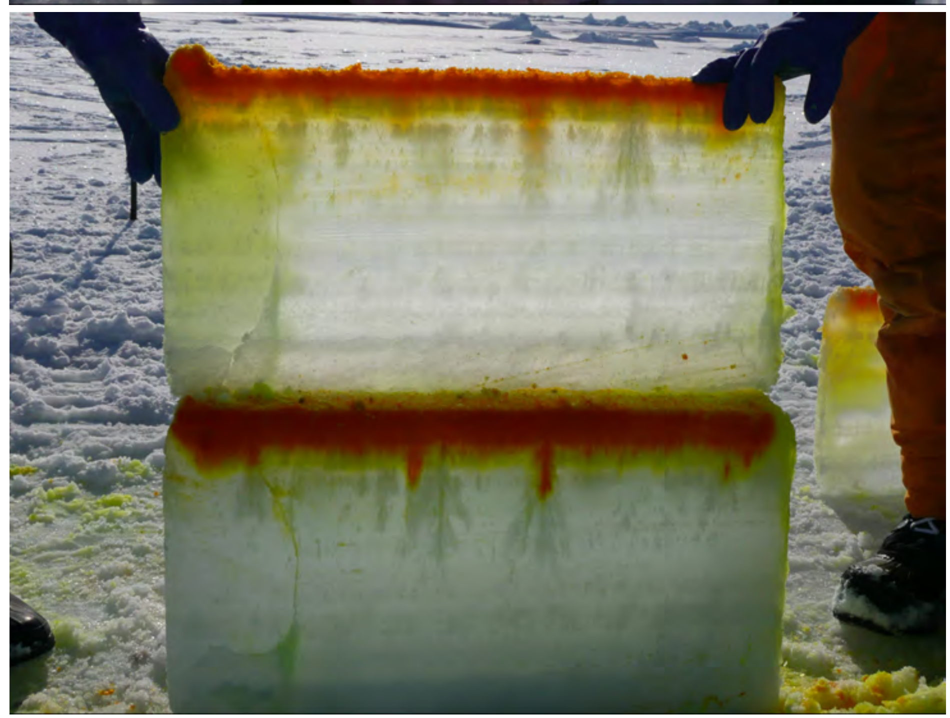
measuring fluid permeability of Antarctic sea ice

SIPEX 2007

tracers flowing through inverted sea ice blocks







Remote sensing of sea ice

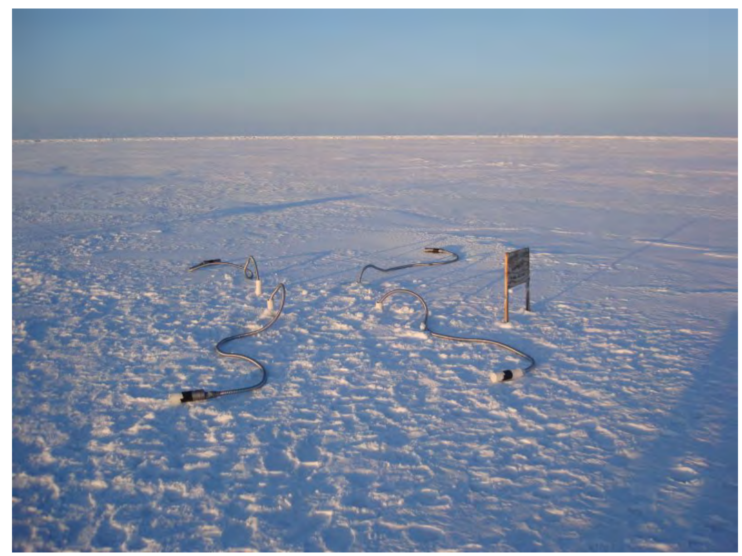
sea ice thickness
ice concentration

INVERSE PROBLEM

Recover sea ice properties from electromagnetic (EM) data

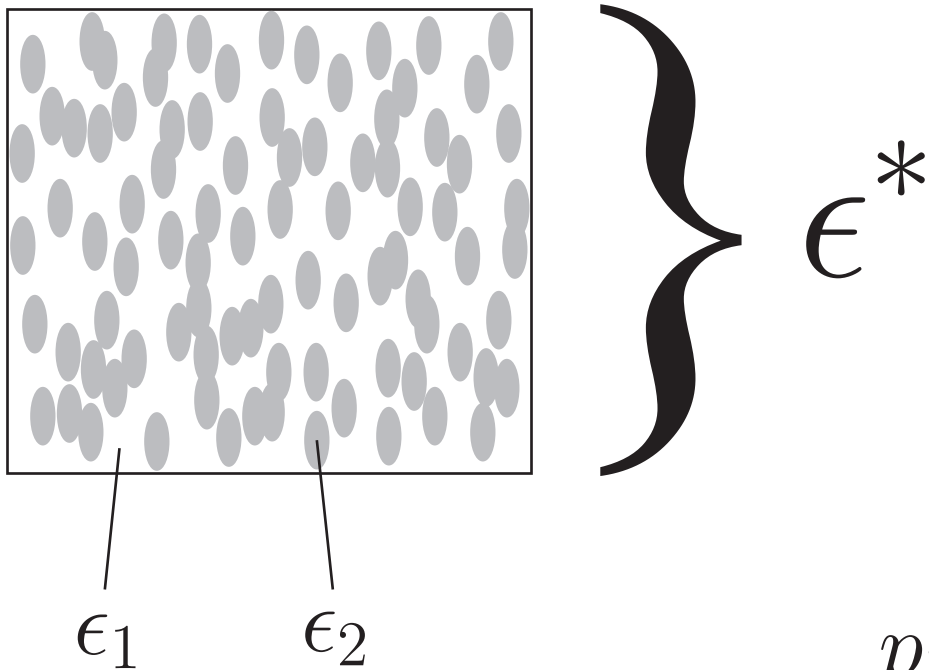
$$\varepsilon^*$$

effective complex permittivity
(dielectric constant, conductivity)



brine volume fraction
brine inclusion connectivity

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



$$D = \epsilon E$$

$$\nabla \cdot D = 0$$

$$\nabla \times E = 0$$

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

p_1 , p_2 = volume fractions of the components

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

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

Analytic Continuation Method for Homogenization

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

Stieltjes integral representation for homogenized parameter

separates geometry from parameters

geometry

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

material parameters

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

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

$\chi =$ characteristic function of the brine phase

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

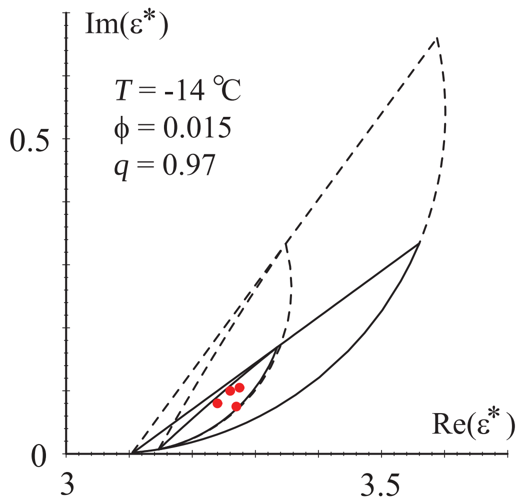
$\Gamma\chi$: microscale $\longrightarrow$ macroscale

$\Gamma\chi$ *links scales*

Golden and Papanicolaou, Comm. Math. Phys. 1983

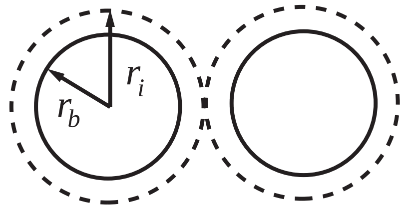
forward and inverse bounds on the complex permittivity of sea ice

forward bounds



4.75 GHz data

matrix particle



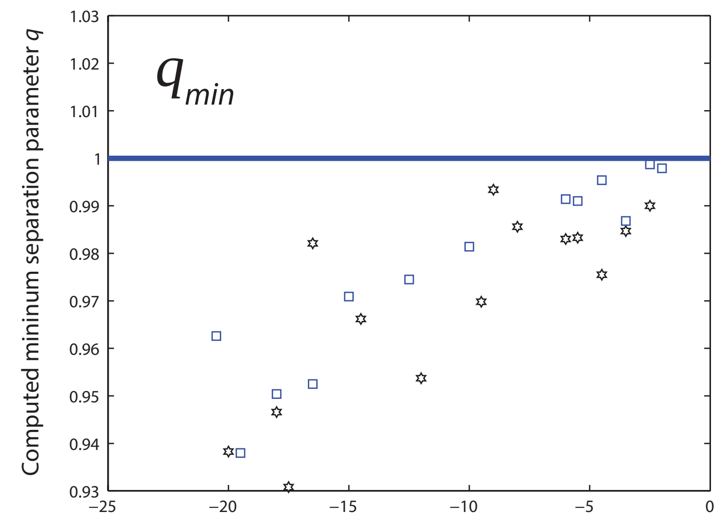
$$q = r_b / r_i$$

$$0 < q < 1$$

Golden 1995, 1997

Bruno 1991

inverse bounds



Slab temperature °C

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

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

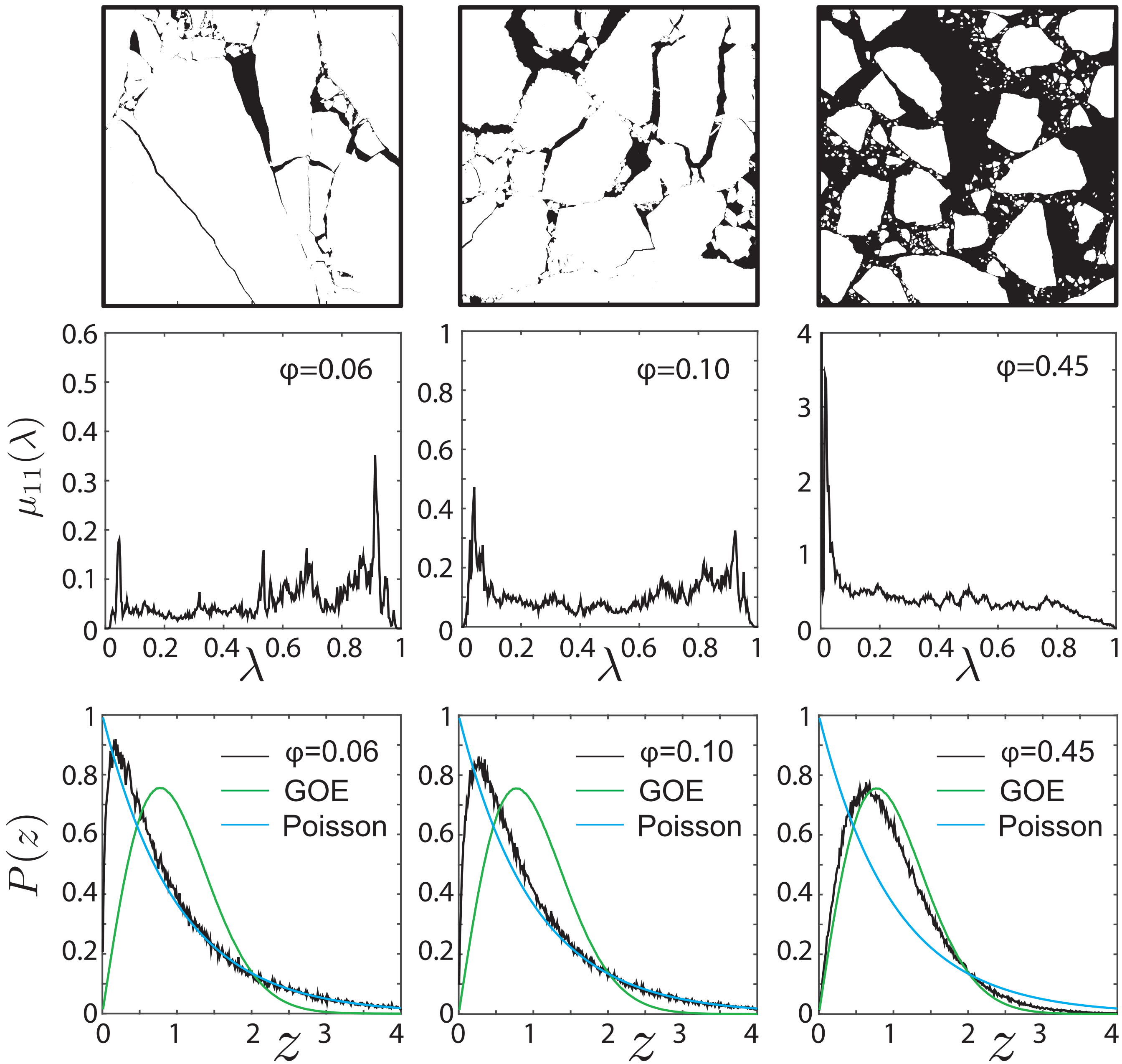
earlier studies of spectral measures

Day and Thorpe 1996
Helsing, McPhedran, Milton 2011

Spectral computations for sea ice floe configurations

spectral measures

eigenvalue spacing distributions

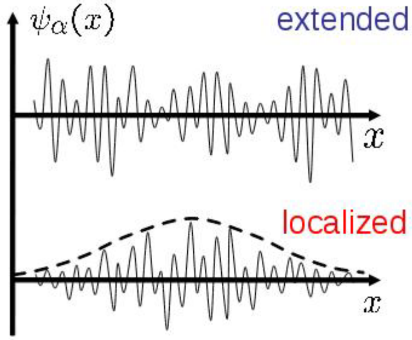


UNIVERSAL Wigner-Dyson distribution

uncorrelated → **level repulsion**

ANDERSON TRANSITION

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



metal / insulator transition

localization

Anderson 1958
Mott 1949
Shklovshii et al 1993
Evangelou 1992

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

we find a surprising analog

Anderson transition for classical transport in composites

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

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

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

Bounds on the complex permittivity of polycrystalline materials by analytic continuation

Proc. Roy. Soc. A 8 Feb 2015

Adam Gully, Joyce Lin,
Elena Cherkaev, Ken Golden

- **Stieltjes integral representation for effective complex permittivity**

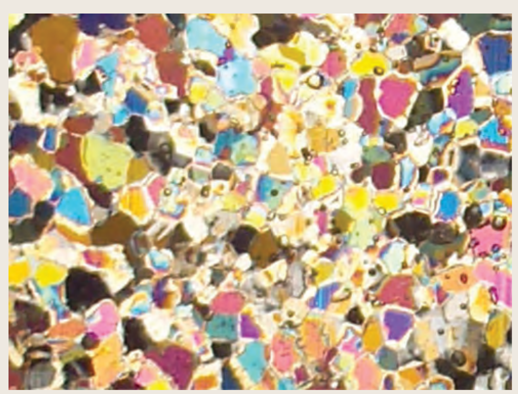
  Milton (1981, 2002), Barabash and Stroud (1999), ...

- **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**



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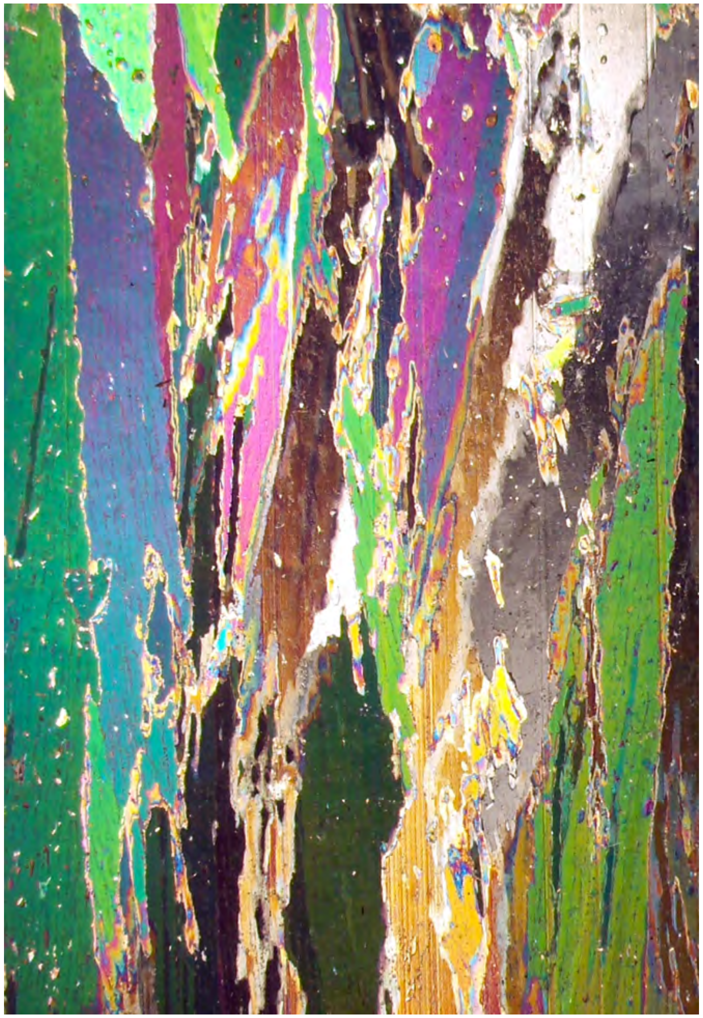
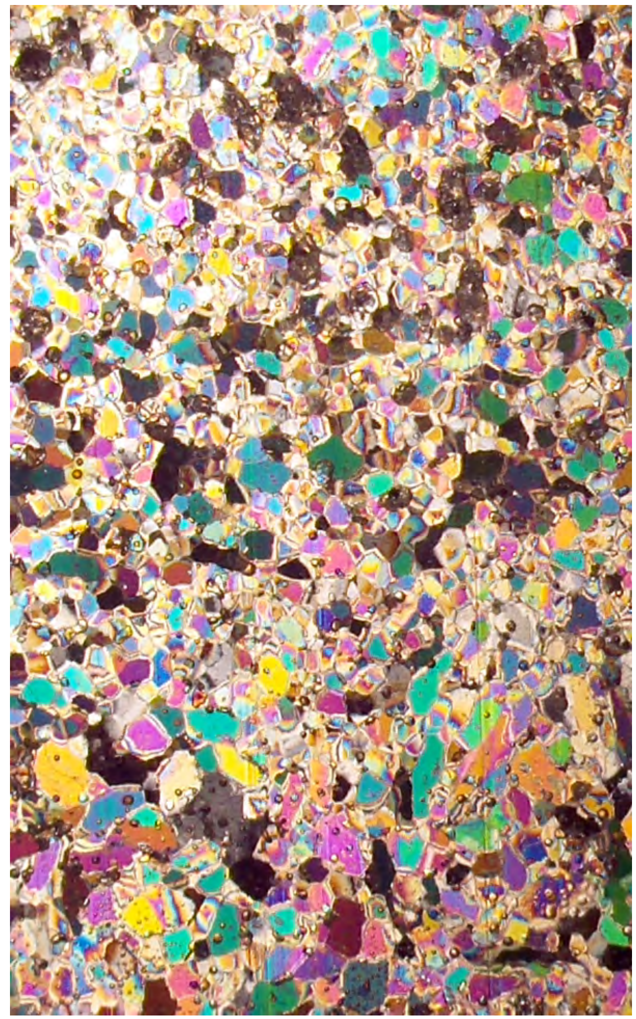
higher threshold for fluid flow in Antarctic granular sea ice

columnar

granular

5%





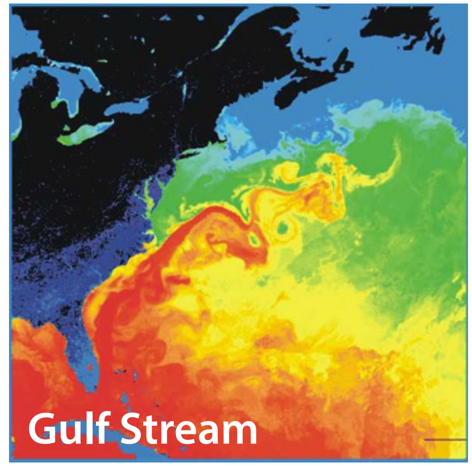
10%

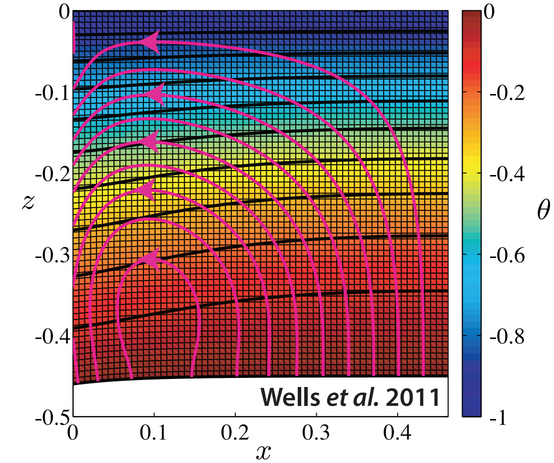
Golden, Sampson, Gully, Lubbers, Tison 2019

advection enhanced diffusion

effective diffusivity

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





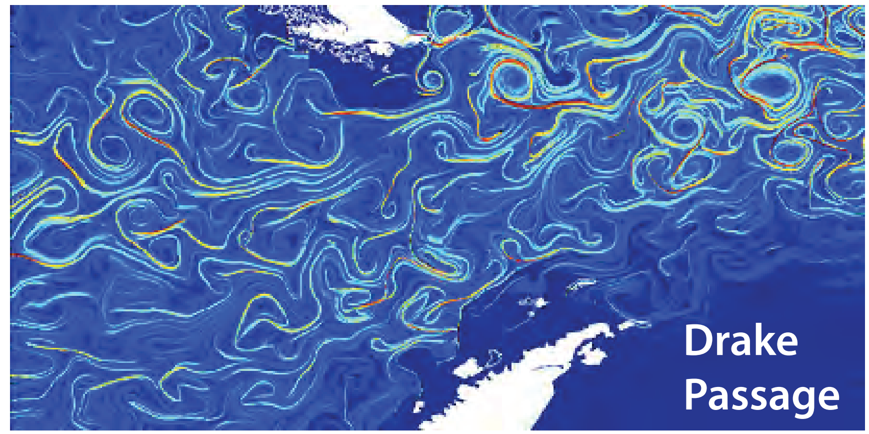
advection diffusion equation with a velocity field $\vec{u}$

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

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

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.* 2019

Stieltjes Integral Representation for Advection Diffusion

Murphy, Cherkaev, Zhu, Xin, Golden, *J. Math. Phys.* 2019

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

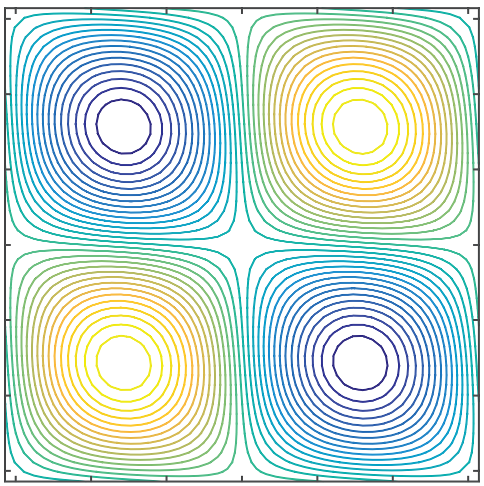
- μ is a positive definite measure corresponding to the spectral resolution of the self-adjoint operator $i\Gamma H\Gamma$
- $H =$ stream matrix , $\kappa =$ local diffusivity
- $\Gamma := -\nabla(-\Delta)^{-1}\nabla\cdot$, Δ is the Laplace operator
- $i\Gamma H\Gamma$ is bounded for time independent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

separation of material properties and flow field

spectral measure calculations

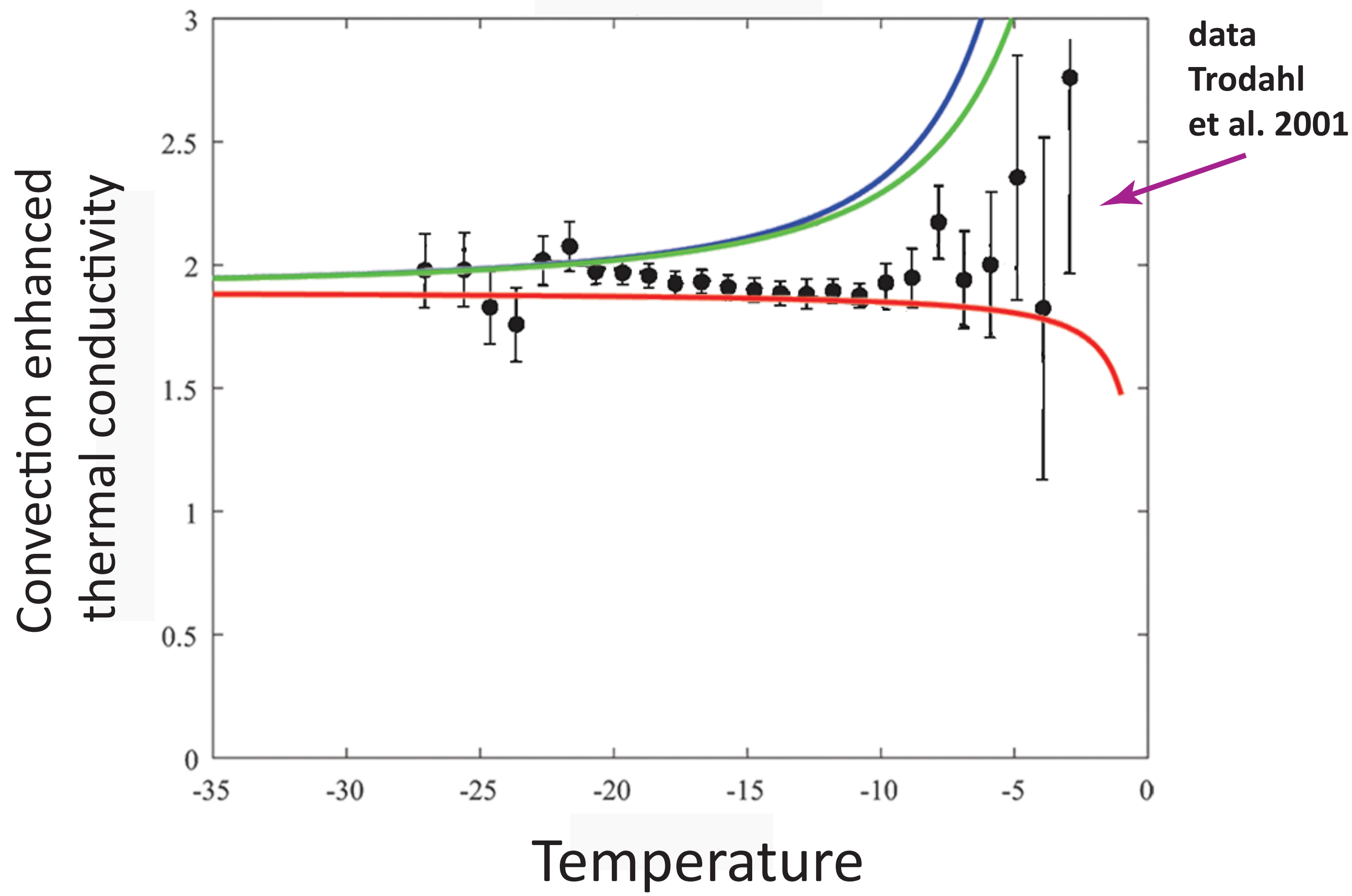
Rigorous bounds on convection enhanced thermal conductivity of sea ice

Kraitzman, Hardenbrook, Murphy, Zhu, Cherkaev, Strong, Golden 2019



cat's eye flow model for
brine convection cells

similar bounds
for shear flows

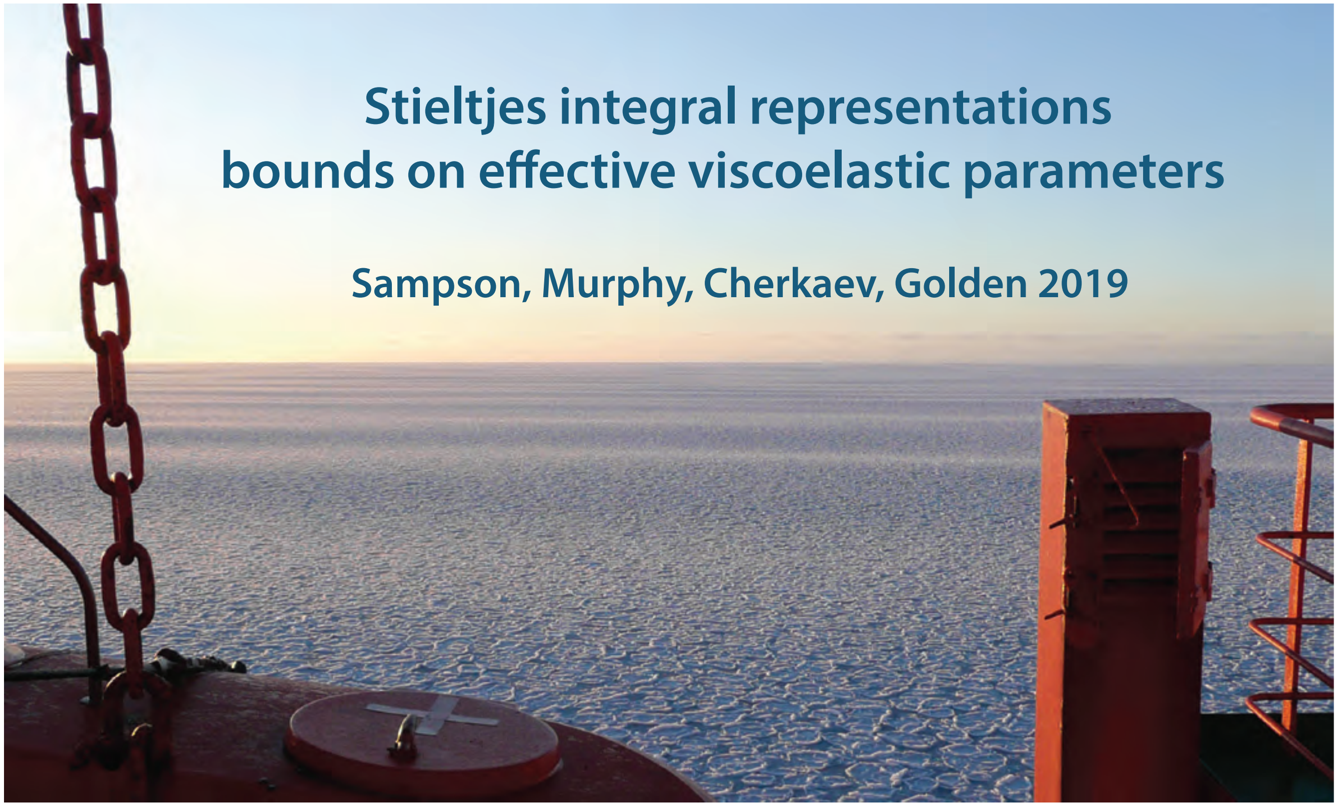


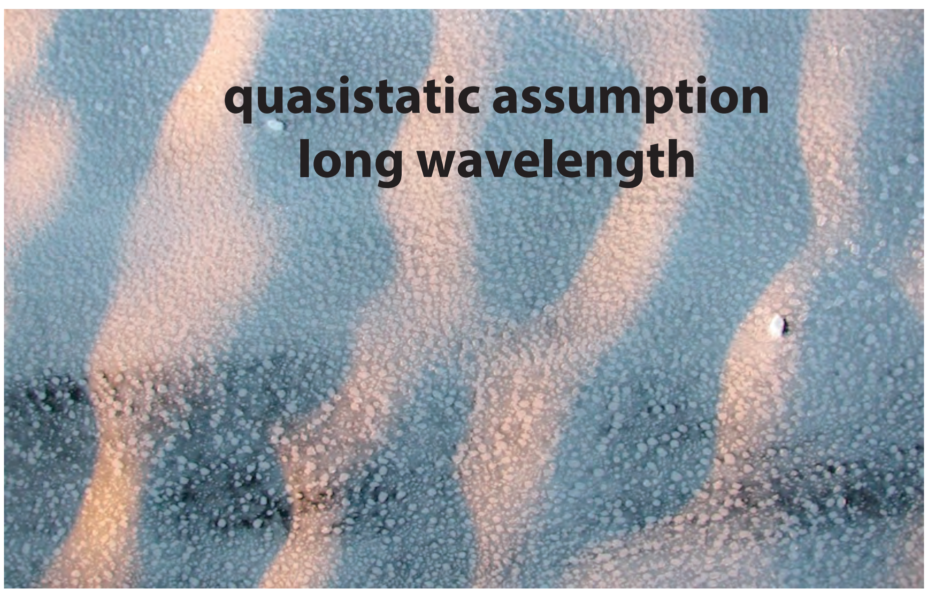
rigorous Padé bounds from Stieltjes integral +
analytical calculations of moments of measure

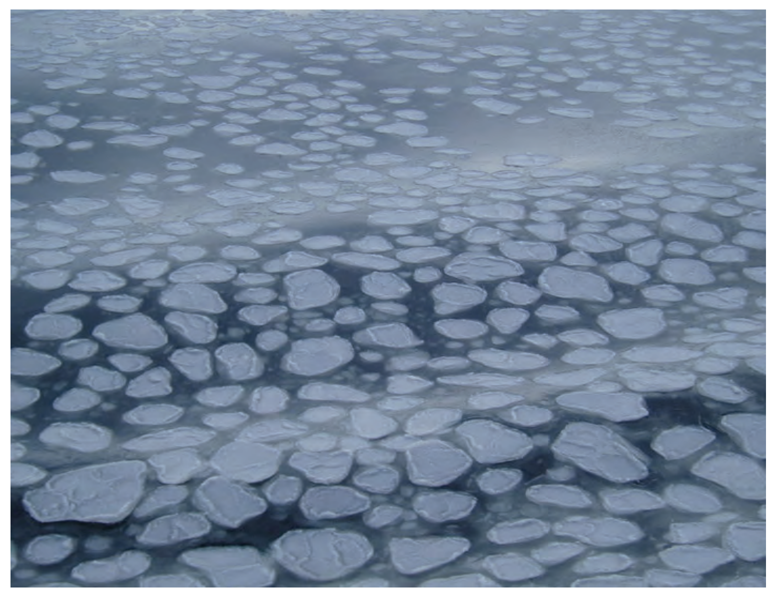
rigorous bounds assuming information on flow field INSIDE inclusions

Kraitzman, Cherkaev, Golden
SIAM J. Appl. Math (in revision), 2019

wave propagation in the marginal ice zone







melt pond formation and albedo evolution:

- ***major drivers in polar climate***
- ***key challenge for global climate models***

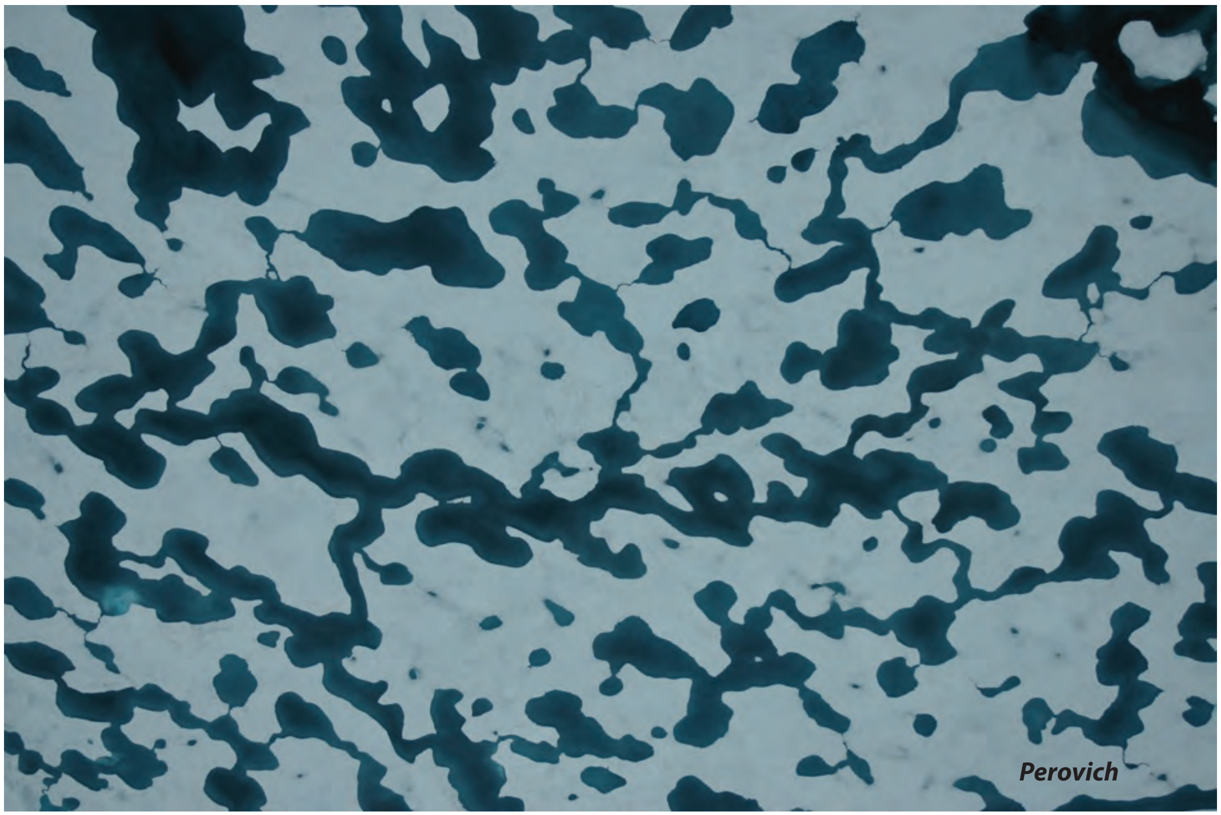
numerical models of melt pond evolution, including topography, drainage (permeability), etc.

Lüthje, Feltham, Taylor, Worster 2006

Flocco, Feltham 2007

Skyllingstad, Paulson, Perovich 2009

Flocco, Feltham, Hunke 2012



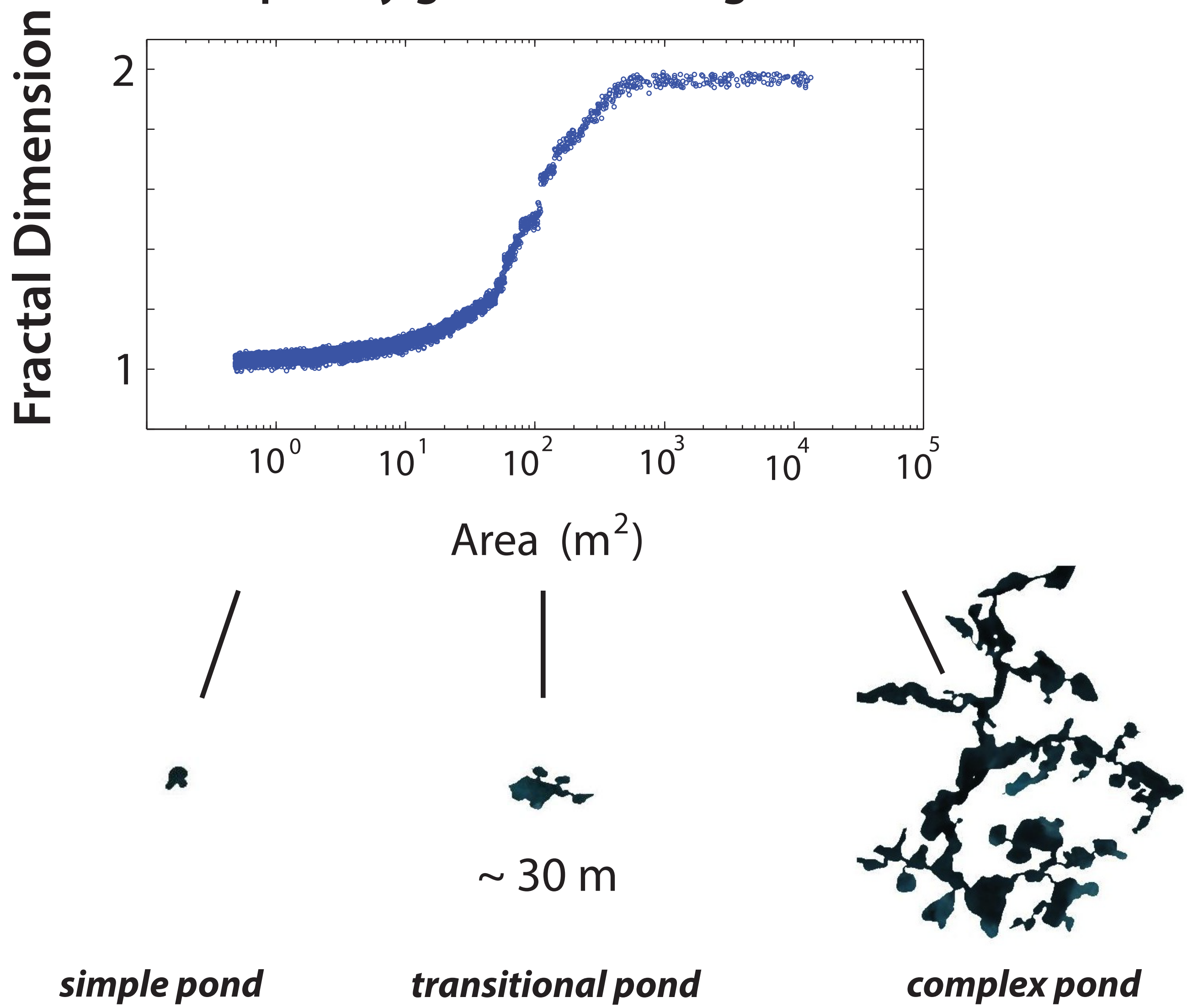
Are there universal features of the evolution similar to phase transitions in statistical physics?

Transition in the fractal geometry of Arctic melt ponds

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

The Cryosphere, 2012

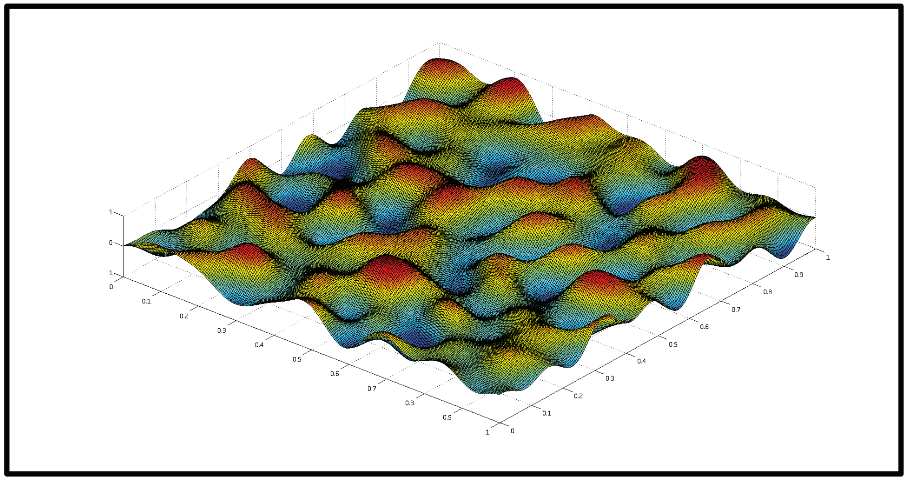
complexity grows with length scale



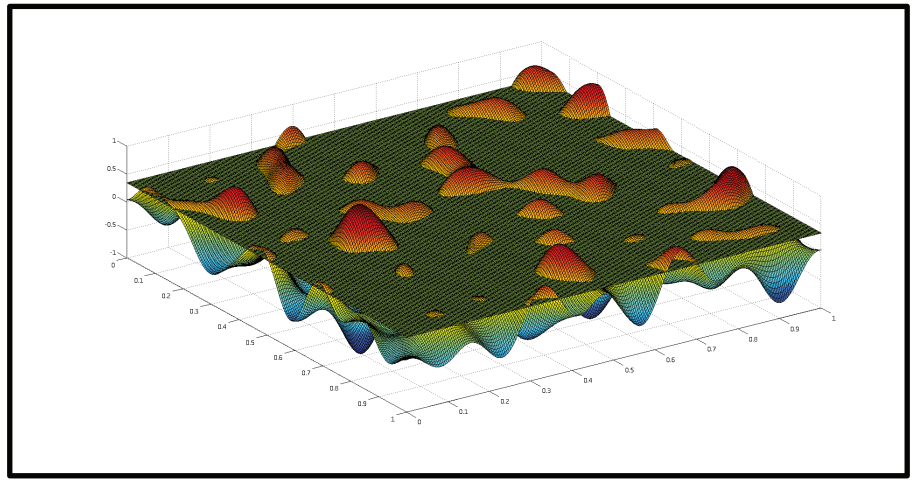
Continuum percolation model for melt pond evolution

level sets of random surfaces

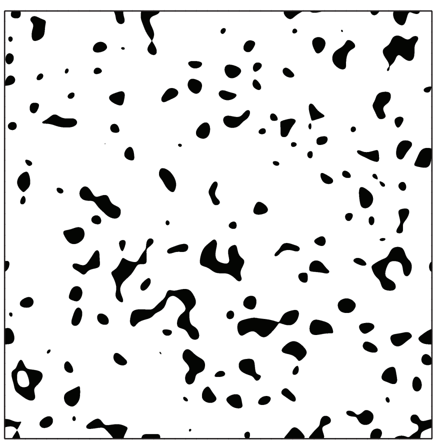
Brady Bowen, Court Strong, Ken Golden, J. Fractal Geometry 2018

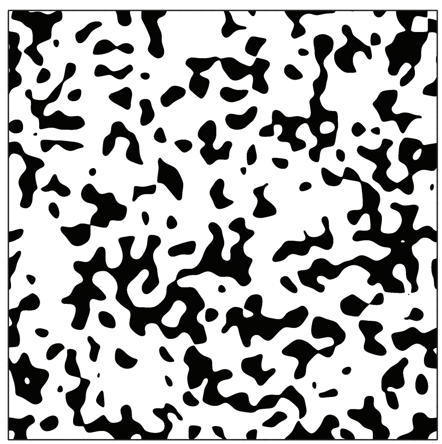


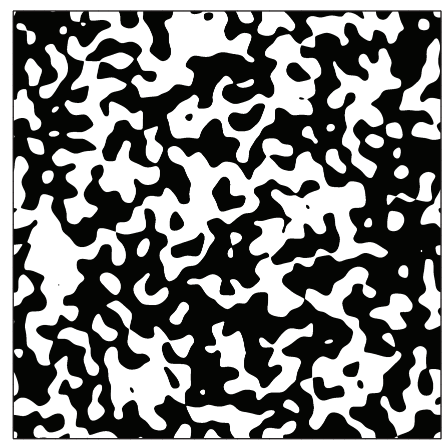
random Fourier series representation of surface topography



intersections of a plane with the surface define melt ponds

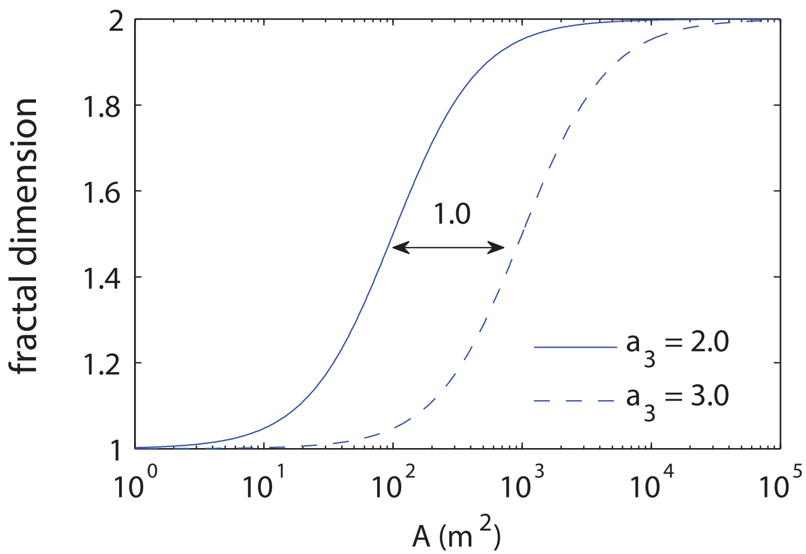


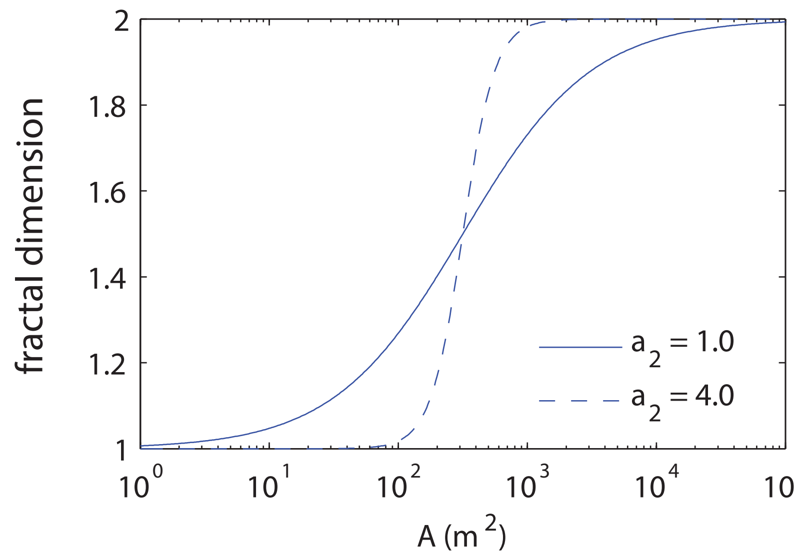




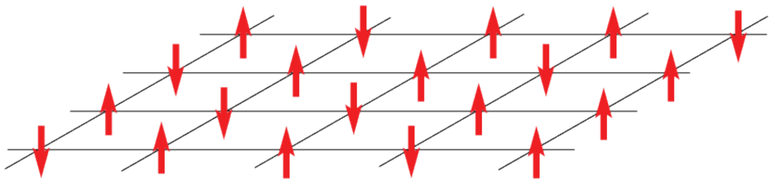
electronic transport in disordered media *diffusion in turbulent plasmas* *Isichenko, Rev. Mod. Phys., 1992*

fractal dimension curves depend on statistical parameters defining random surface





Ising Model for a Ferromagnet



$$s_i = \begin{cases} +1 & \text{spin up} \\ -1 & \text{spin down} \end{cases}$$

blue

white

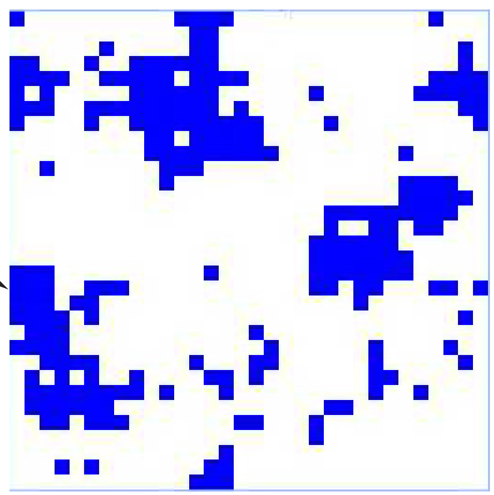
applied magnetic field H

$$\mathcal{H} = -H\sum_i s_i - J\sum_{<i,j>} s_i s_j$$

nearest neighbor Ising Hamiltonian

ferromagnetic interaction $J \geq 0$

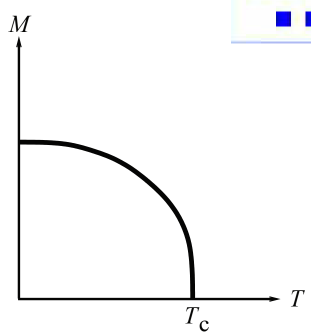
islands or ponds of like spins



magnetization

$$M(T,H) = \lim_{N\to\infty} \frac{1}{N} \left\langle \sum_j s_j \right\rangle$$

homogenized parameter like effective conductivity



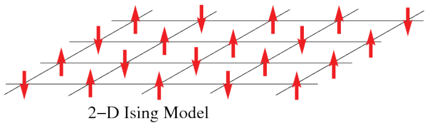
Curie point critical temperature

Stieltjes integral representation for M

Baker, PRL 1968

Ising model for ferromagnets ⟶ Ising model for melt ponds

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



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

random magnetic field represents snow topography

magnetization $M = \lim_{N \to \infty} \frac{1}{N} \left\langle \sum_j s_j \right\rangle$ **pond coverage** $\frac{(M+1)}{2}$

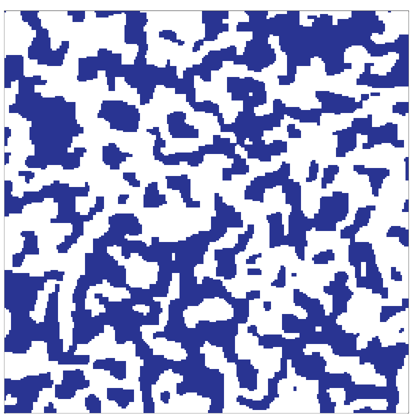
~ albedo

only nearest neighbor patches interact

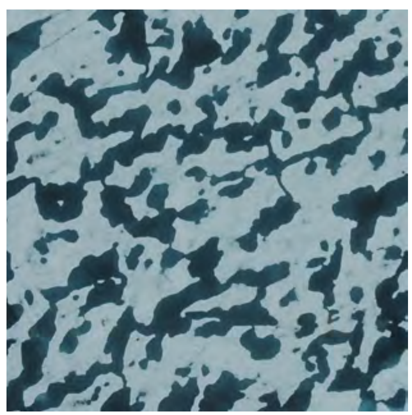
Starting with random initial configurations, as Hamiltonian energy is minimized by Glauber spin flip dynamics, system “flows” toward metastable equilibria.

Melt ponds are metastable islands of like spins.

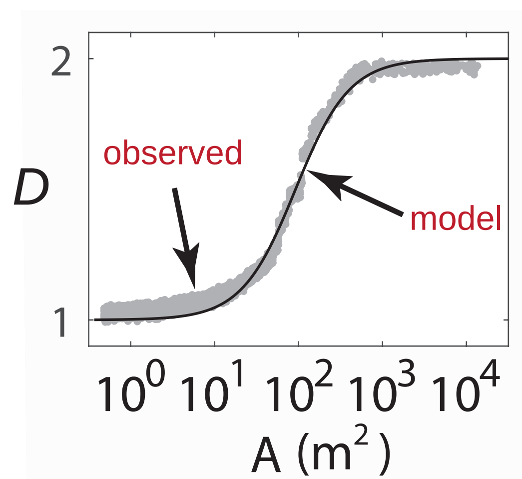
Order from Disorder



Ising model



melt pond photo (Perovich)



pond size distribution exponent

observed -1.5

(Perovich, *et al.* 2002)

model -1.58

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

The distribution of solar energy under ponded first-year sea ice

Horvat, Flocco, Rees Jones, Roach, Golden, ***in revision,*** 2019

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

Pond geometry affects the ecology of the Arctic Ocean.

The Melt Pond Conundrum:

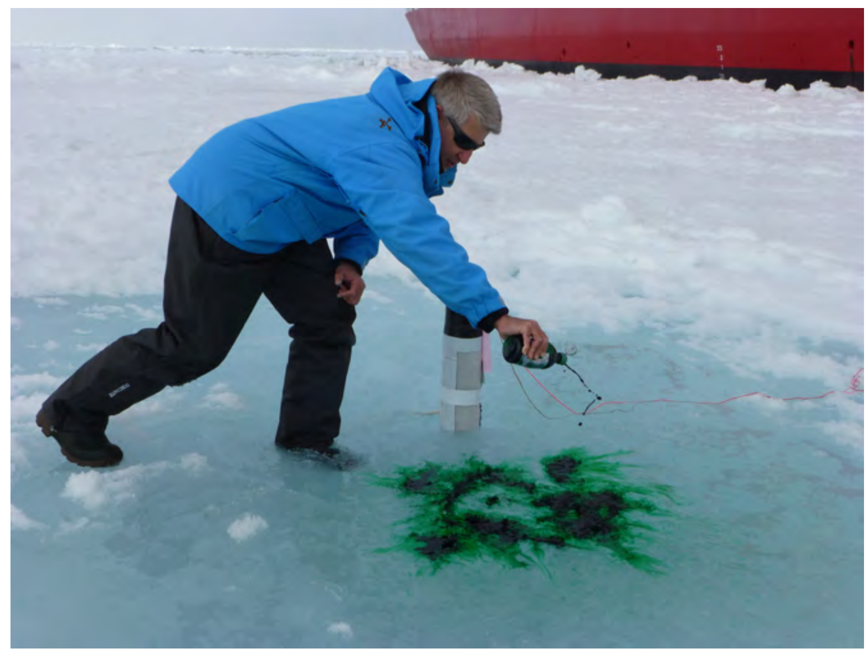
How can ponds form on top of sea ice that is highly permeable?

C. Polashenski, K. M. Golden, D. K. Perovich, E. Skyllingstad, A. Arnsten, C. Stwertka, N. Wright

Percolation Blockage: A Process that Enables Melt Pond Formation on First Year Arctic Sea Ice

J. Geophys. Res. Oceans 2017

2014 Study of Under Ice Blooms in the Chuckchi Ecosystem (SUBICE) aboard USCGC Healy



Conclusions

1. Sea ice is a fascinating multiscale composite with structure similar to many other natural and man-made materials.

2. Mathematical methods developed for sea ice advance the theory of composites in general.

2. Homogenization and statistical physics help ***link scales in sea ice and composites***; provide rigorous methods for finding effective behavior; advance sea ice representations in climate models.

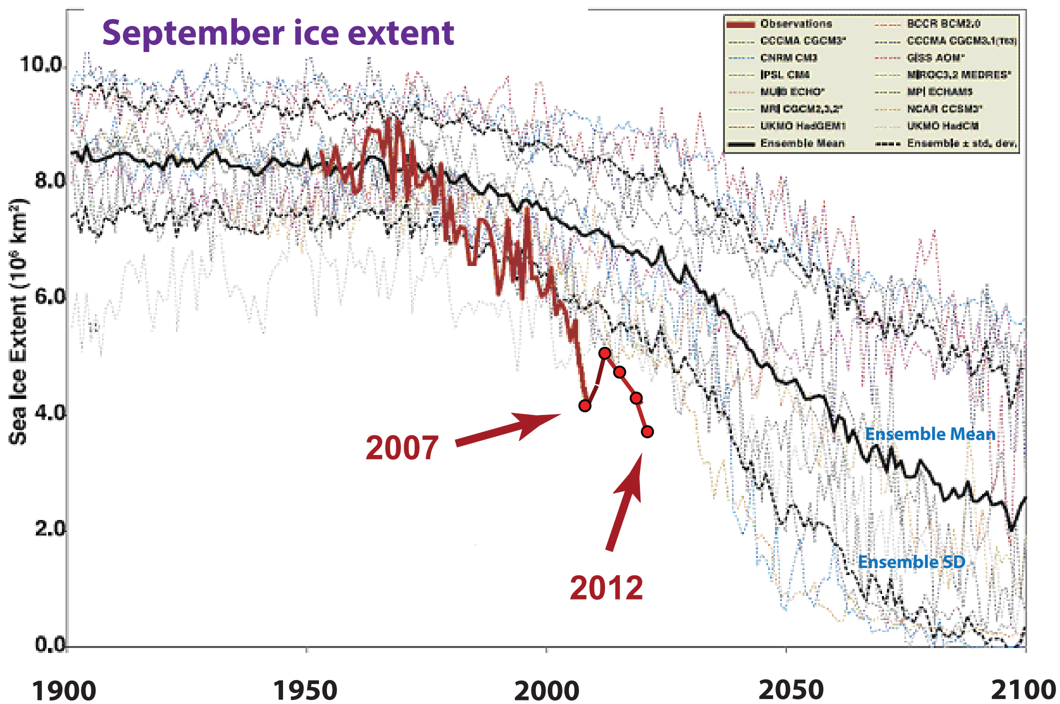
3. Fluid flow through sea ice mediates melt pond evolution and many processes important to climate change and polar ecosystems.

5. Field experiments are essential to developing relevant mathematics.

6. Our research will help to improve projections of climate change, the fate of Earth's sea ice packs, and the ecosystems they support.

Buchanan Bay, Antarctica   Mertz Glacier Polynya Experiment   July 1999

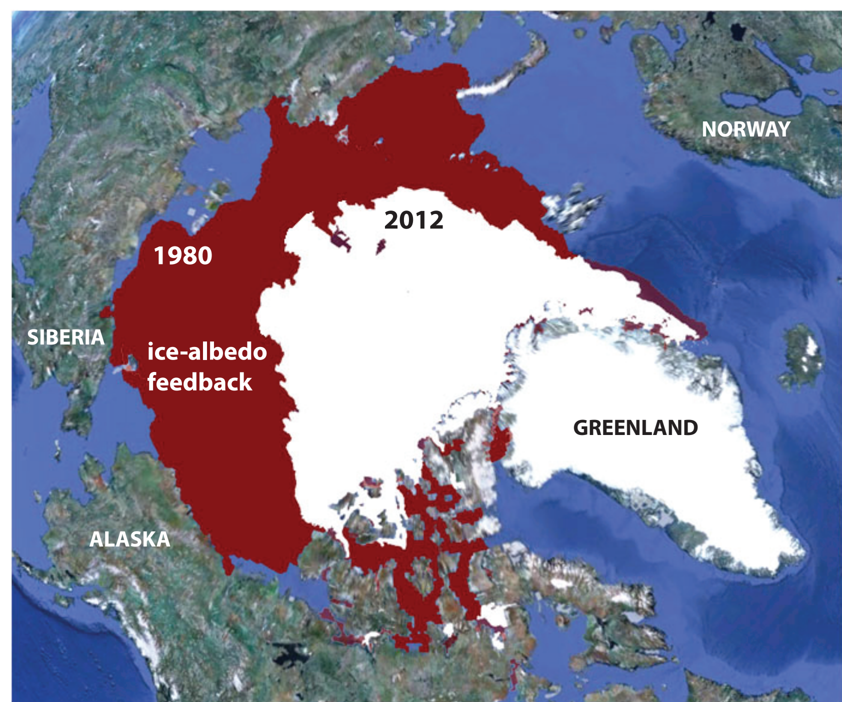
Arctic sea ice decline: faster than predicted by climate models



Stroeve et al., GRL, 2007
Stroeve et al., GRL, 2012

Change in Arctic Sea Ice Extent

September 1980 -- 7.8 million square kilometers
September 2012 -- 3.4 million square kilometers



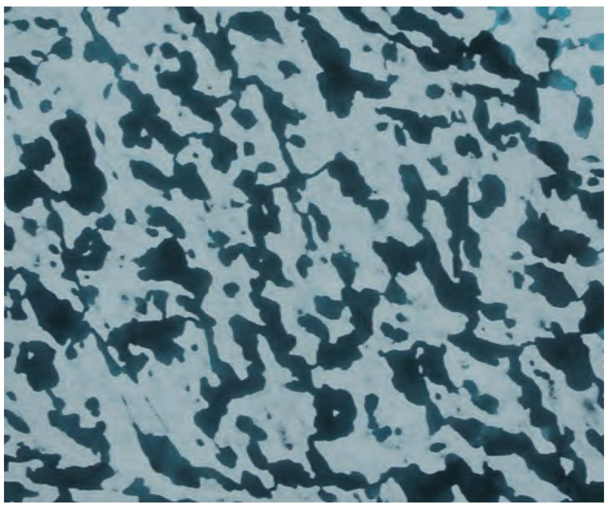
challenge

represent sea ice more realistically in climate models

account for key processes

such as melt pond evolution

How do patterns of dark and light evolve?



Impact of melt ponds on Arctic sea ice simulations from 1990 to 2007

Flocco, Schroeder, Feltham, Hunke, JGR Oceans 2012

For simulations with ponds September ice volume is nearly 40% lower.

... and other sub-grid scale structures and processes

linkage of scales