From Quasiperiodic Composites to Percolation Transitions and Applied Statistics

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Early Career Data Scientist - AI/ML

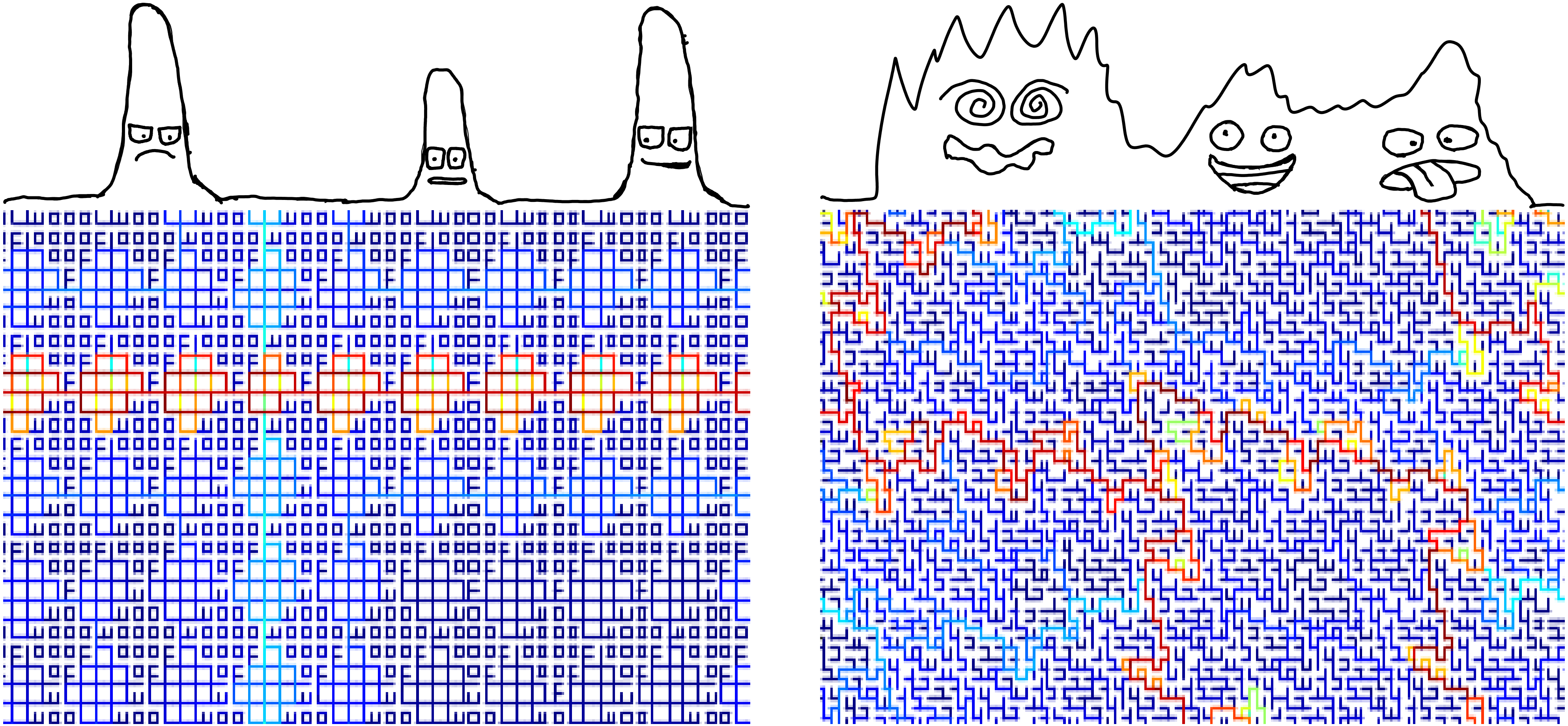
Oct 20, 2021

Physics @BERKELEY

Applied Physics Laboratory
UNIVERSITY of WASHINGTON

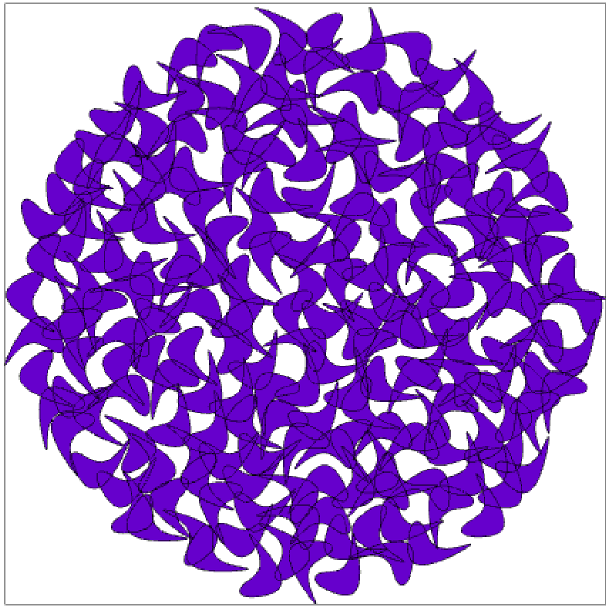
THE UNIVERSITY OF UTAH
Physics & Astronomy

Order to Disorder in Quasiperiodic Composites



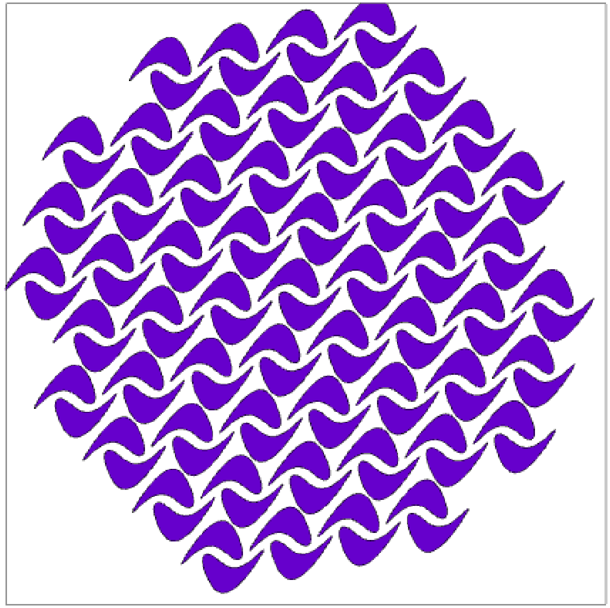
Materials Science Before the 80’s

Disordered



Amorphous, Glass Like

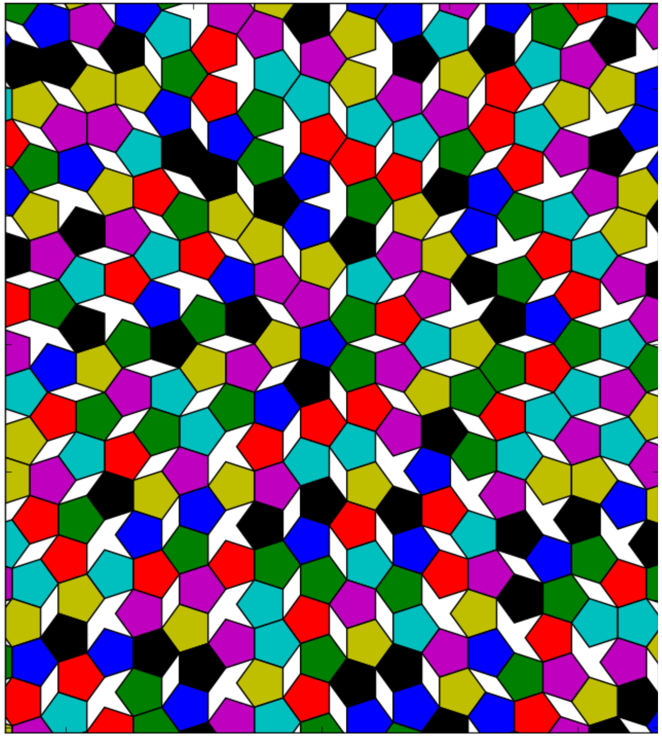
Periodic



Crystalline, Translational Symmetry

Quasiperiodic Tilings are for Art and Math, Not for Materials Science?

Green Mosque in Bursa, Turkey



2D tiling with pentagons and gaps

Roger Penrose

Girih tiles in the early 13th century

Present Day

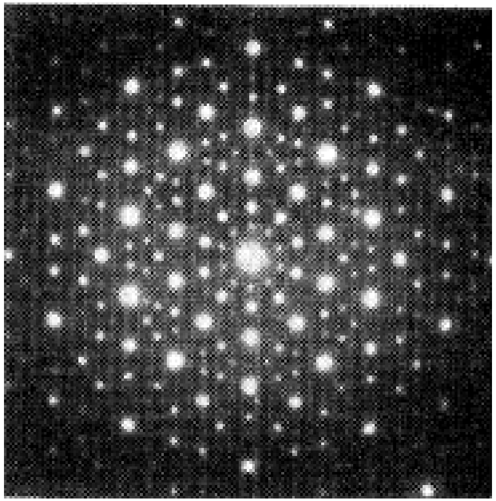
Experimental Discovery

VOLUME 53, NUMBER 20 PHYSICAL REVIEW LETTERS 12 NOVEMBER 1984

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

D. Shechtman and I. Blech

Department of Materials Engineering, Israel Institute of Technology–Technion, 3200 Haifa, Israel



TEM Diffraction pattern
for an AlMg alloy
notice ten fold symmetry

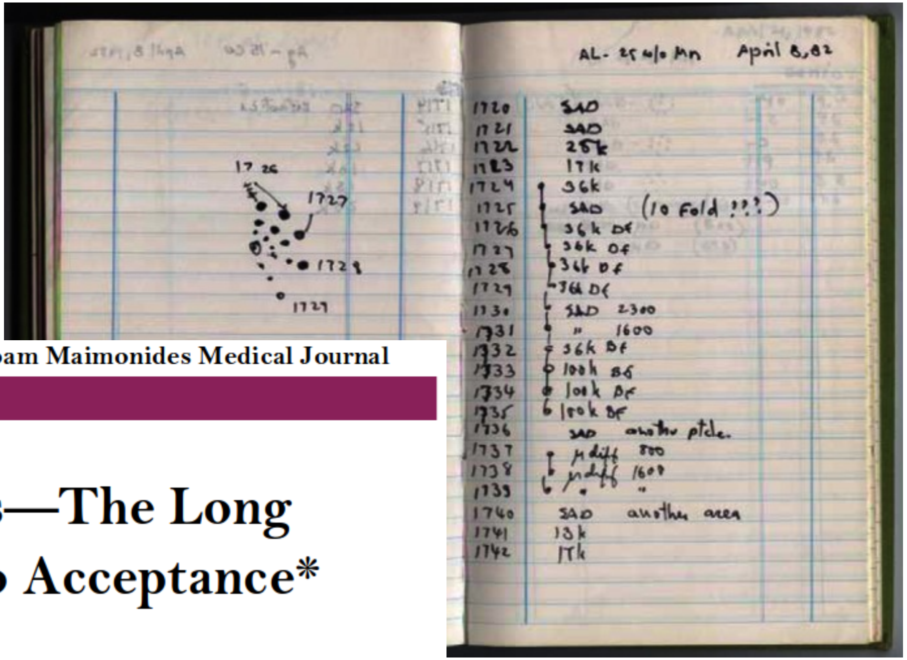
Open Access **Rambam Maimonides Medical Journal**

NOBEL LAUREATE PERSPECTIVE

Quasi-Periodic Crystals—The Long Road from Discovery to Acceptance*

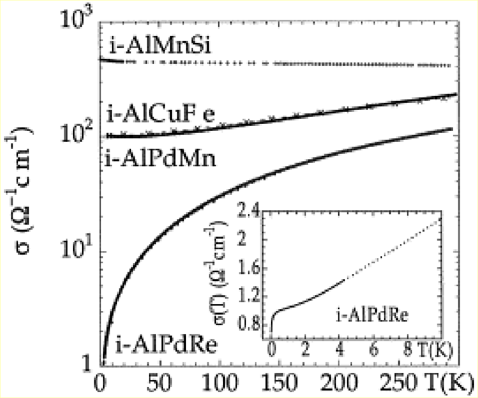
Daniel Shechtman, Ph.D.**

Nobel Prize Laureate in Chemistry, 2011. Philip Tobias Professor of Materials Science, Department of Materials Science and Engineering, Technion–Israel Institute of Technology, Haifa, Israel



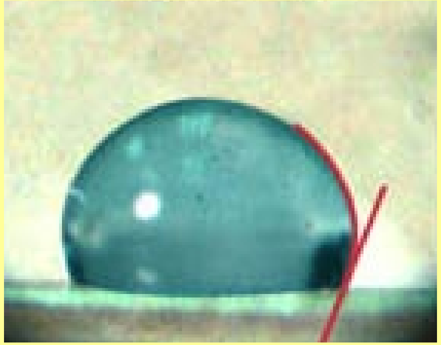
Discovery of Novel Properties in Molecular Quasicrystals

- low electrical conductivity
- low thermal conductivity
- mechanically hard
- small coefficient of friction



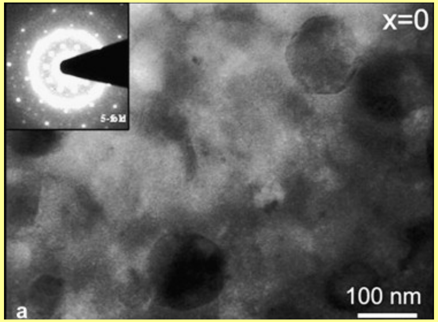
an insulating aluminum alloy

Berger, *et al*.
Physica B Condens.
(2000)



water beading more strongly on a quasicrystal coating than on Teflon

Made by Professor Orest Symko



hard alloy quasicrystal inclusions

Singh, *et al*.
Intermetallics
(2010)

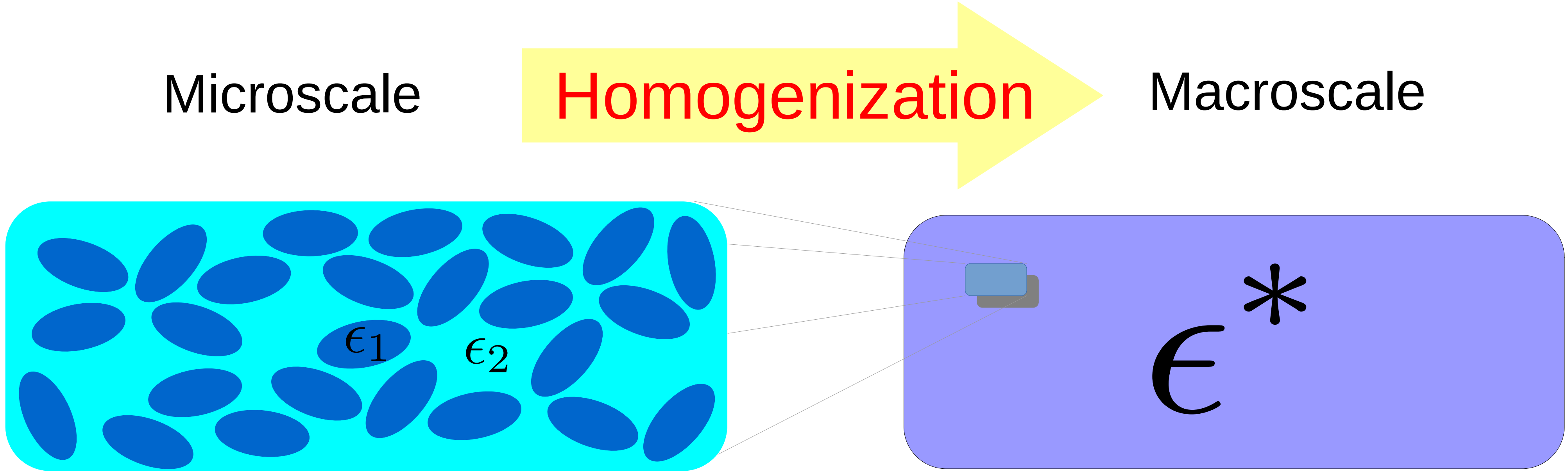
Is there a connection between quasiperiodic geometry and these interesting material properties?

Material Properties are Represented by Coefficients in Constitutive Equations

- Electric Conduction $\vec{J} = \sigma \vec{E}$
- Heat Conduction $\vec{Q} = -k \nabla T$
- Volume Polarization $\vec{P} = \epsilon_0 \chi_e \vec{E}$

Permittivity

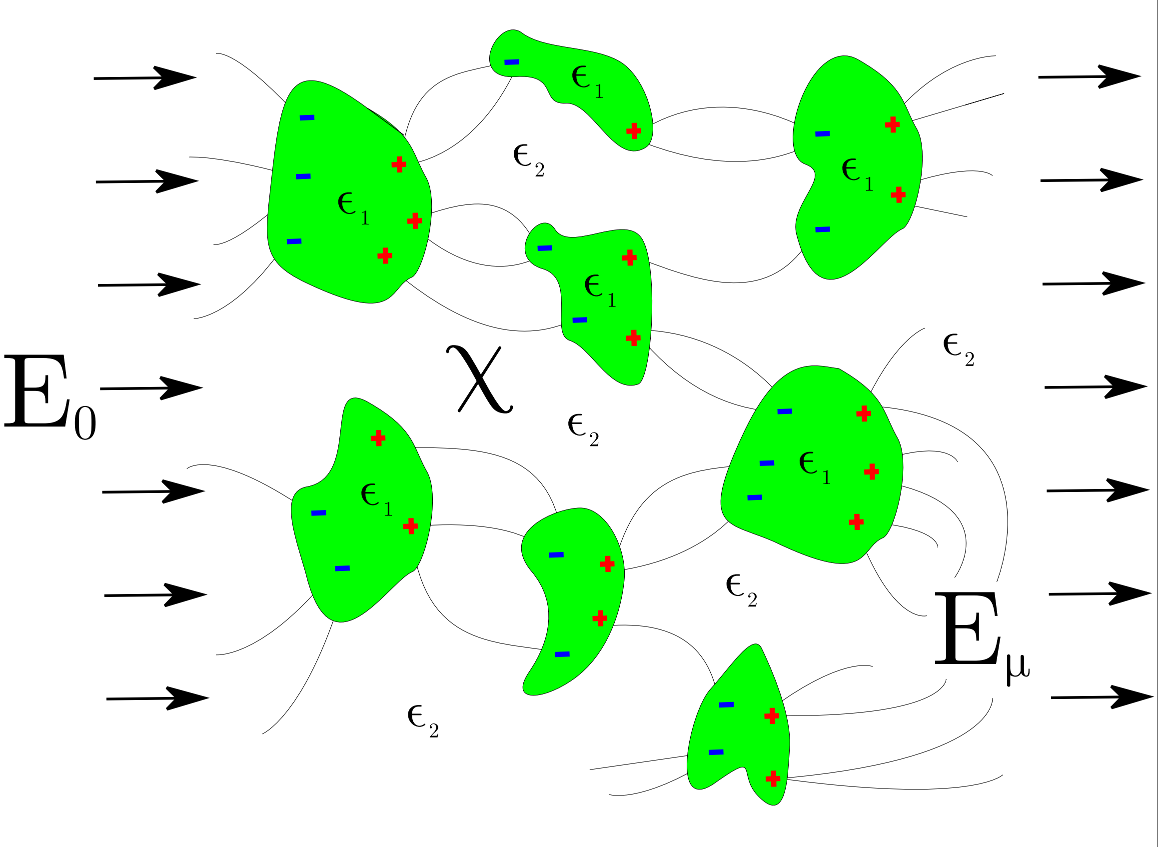
$$\vec{D} = \epsilon \vec{E} = \epsilon_0 \vec{E} + \vec{P}$$



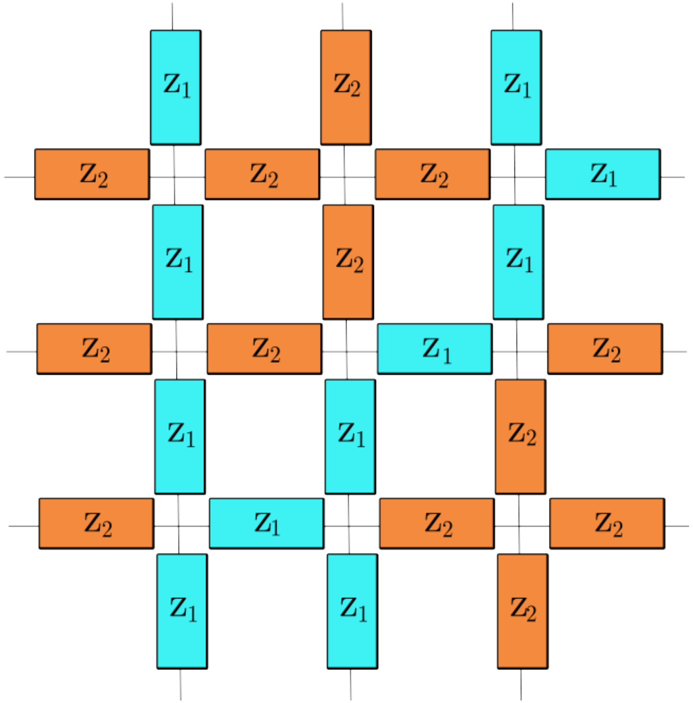
$$\langle D \rangle = \langle \epsilon E \rangle = \boldsymbol{\epsilon}^* \langle E \rangle = \boldsymbol{\epsilon}^* E_0$$

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

Binary Composite or Network

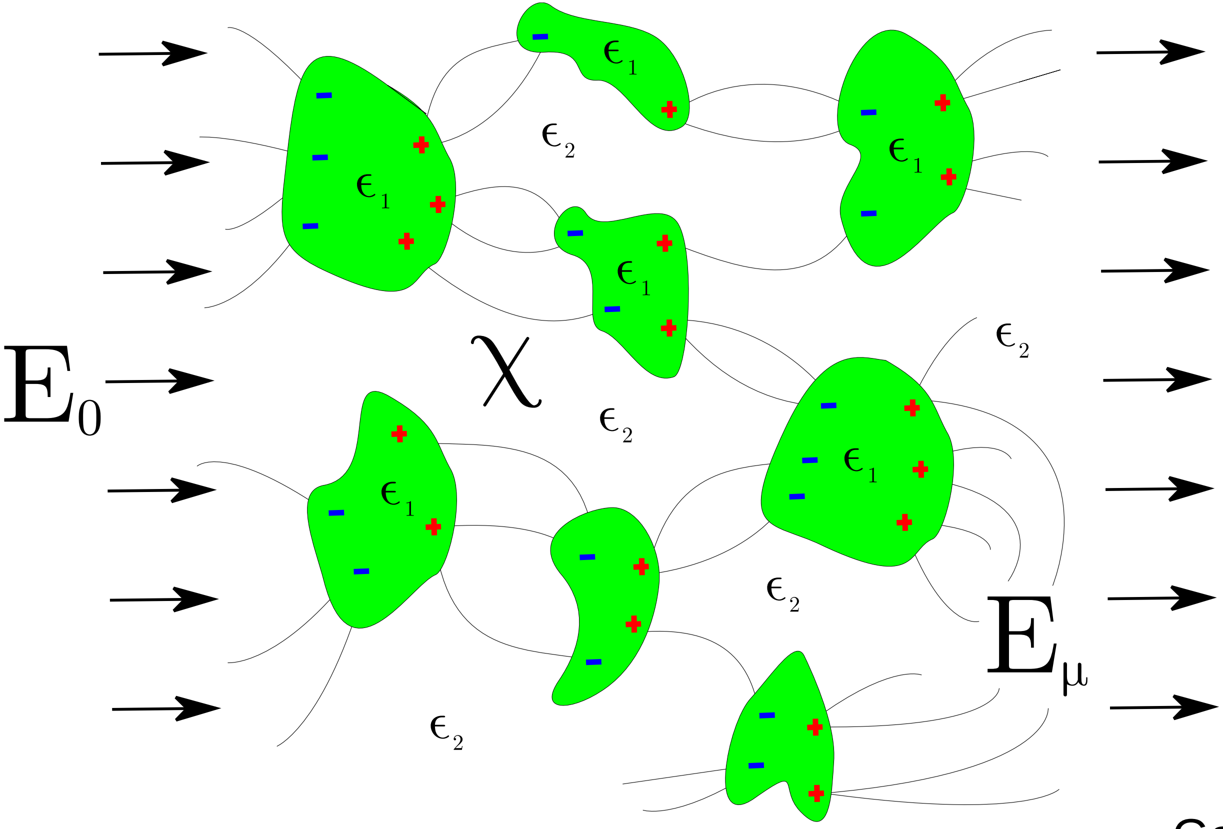


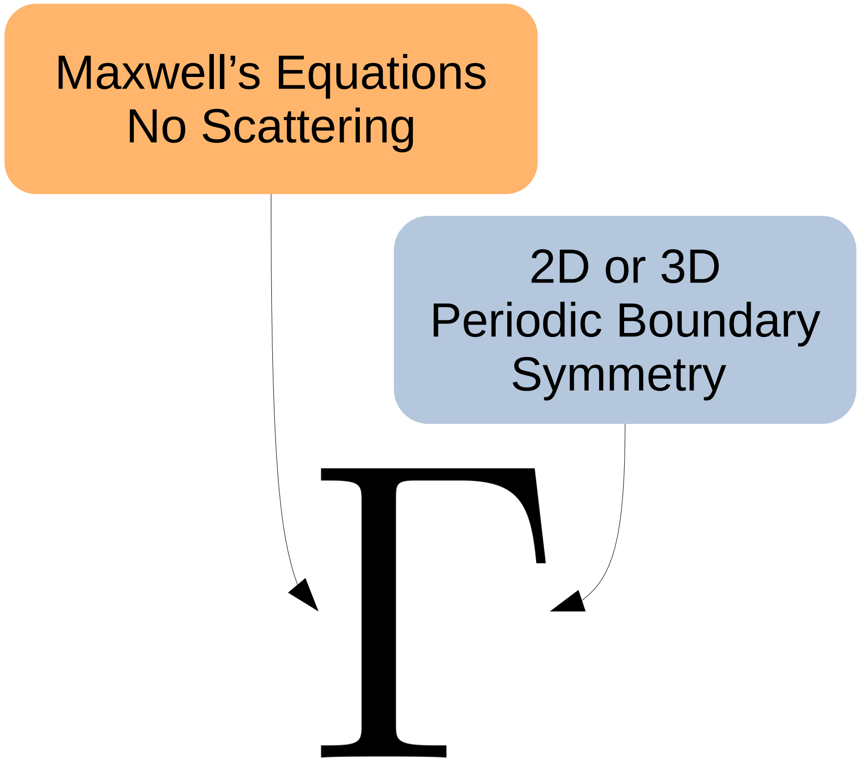
$$\epsilon(x) = \epsilon_1 \chi(x) + \epsilon_2 (1 - \chi(x))$$



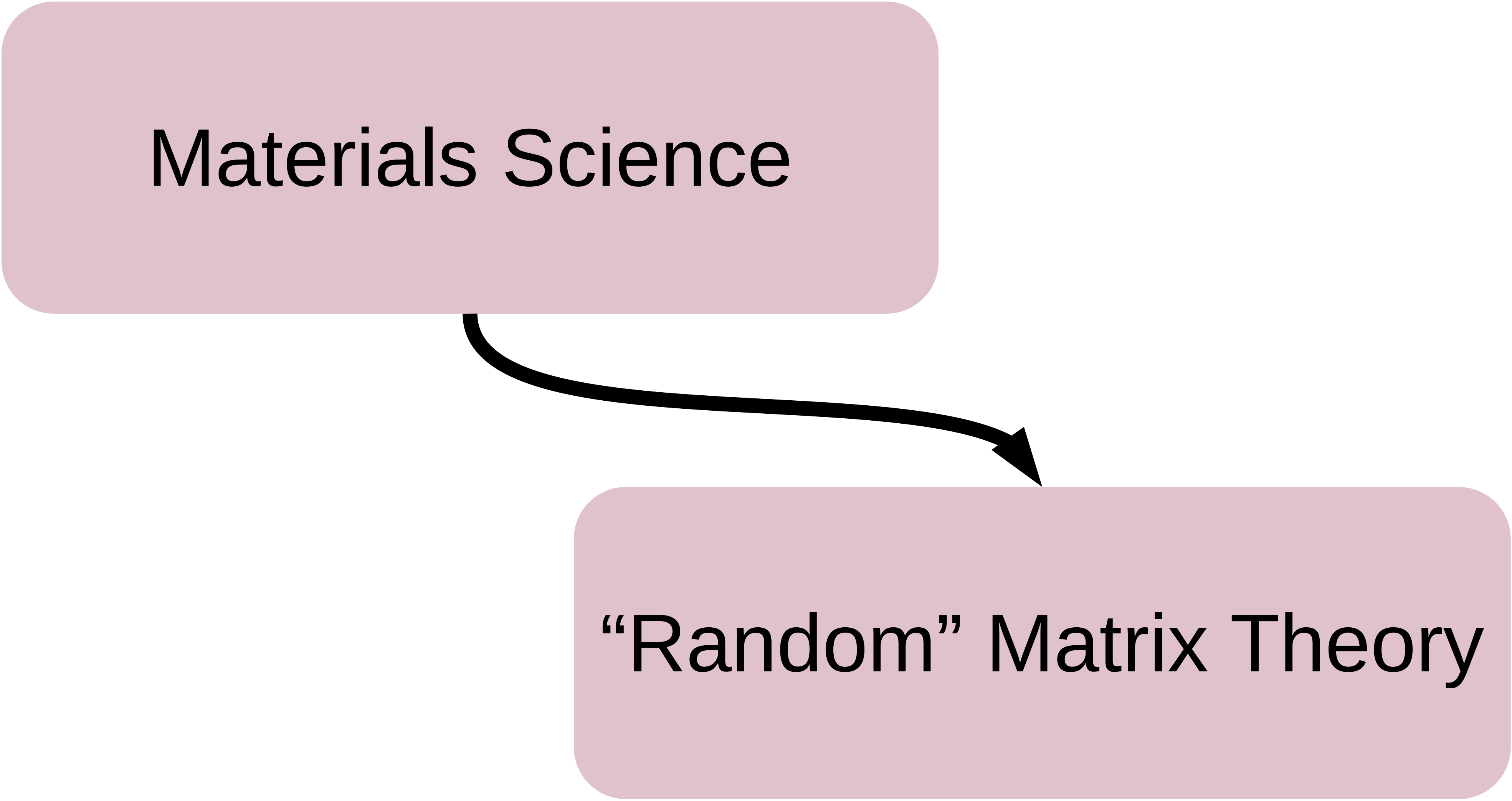
$$z = z_1 \chi + z_2 (\mathbb{1} - \chi)$$

Physics and Boundary Conditions





Gamma takes the curl-free or acyclic part.


Materials Science
“Random” Matrix Theory

Physics

$$\Gamma$$

Microgeometry

$$\chi$$

Material Properties

$$\epsilon_1 \qquad \epsilon_2$$

$$\boxed{\chi\Gamma\chi}$$

Geometric information relevant to material properties is distilled into the weighted eigenvalues of this matrix.

$$\boxed{s}$$

Think of this as the independent variable.

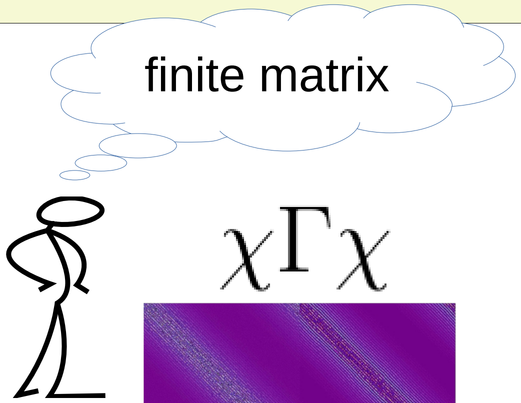
Stieltjes Integral Representation

Bergman (1980) Milton (1980) Golden and Papanicolaou (1983)

$$\frac{w_1}{s-\lambda_1}+\frac{w_2}{s-\lambda_2}+\cdots \quad \Longrightarrow$$

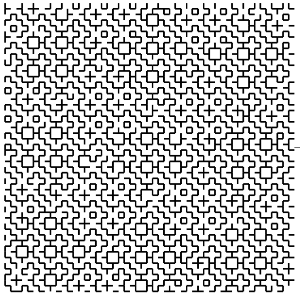
Material Properties

$$\epsilon^*$$



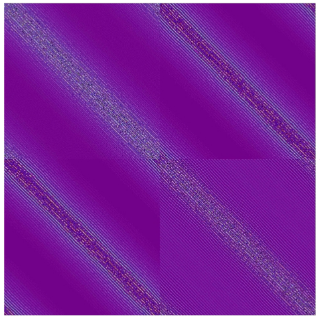
Direct Calculation

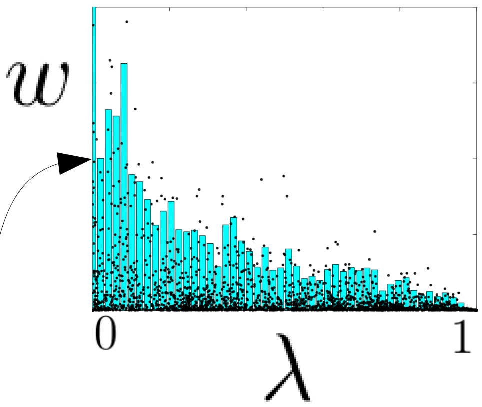
χ



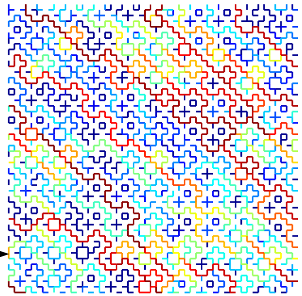
Murphy, Hohenegger, Cherkaev, Golden, Comm. Math. Sci. 2015

$\chi\Gamma\chi$





χE



Morison, Murphy, Cherkaev, Golden 2021

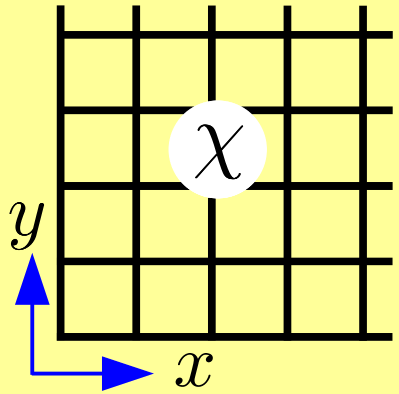
I designed representative quasiperiodic microgeometry.

Quasiperiodic in Materials Science

"...any solid having an essentially discrete diffraction diagram."
International Union of Crystallography

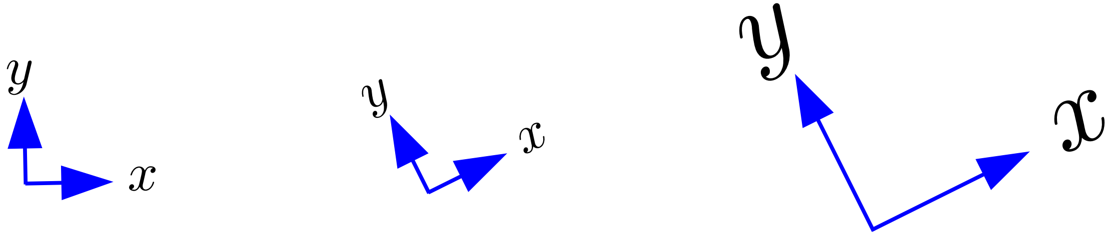
The term "quasicrystal" should simply be regarded as an abbreviation for "quasiperiodic crystal,"
Ron Lifshitz arXiv 2000

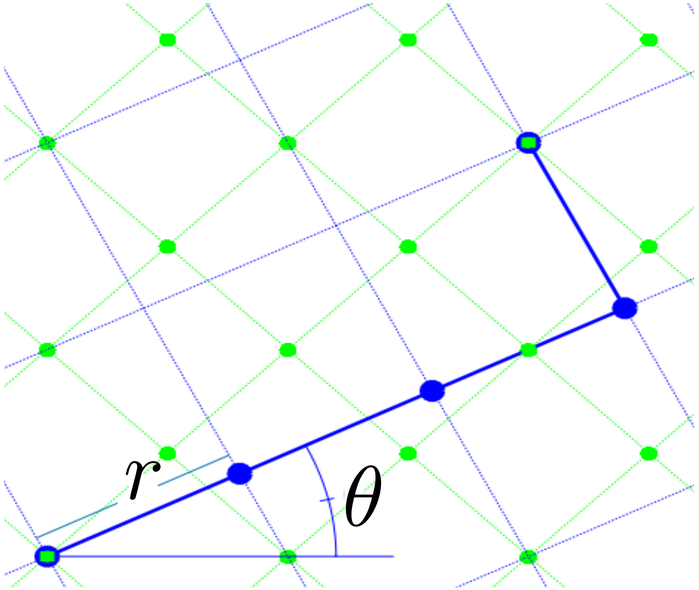
Trial Microgeometry



- Deterministic
- Non-periodic
- Repeated Building Blocks

A Moiré Pattern



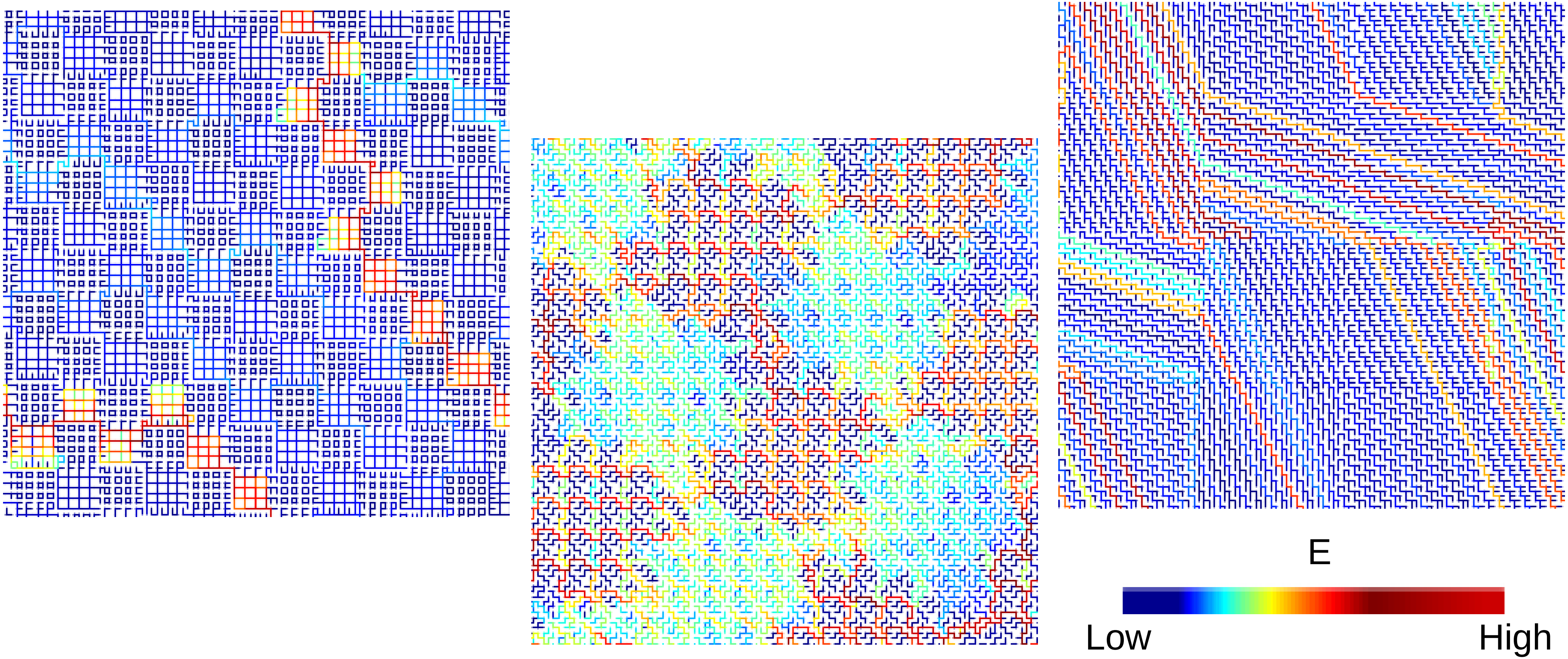


$$\begin{pmatrix} x' \\ y' \end{pmatrix} = r \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

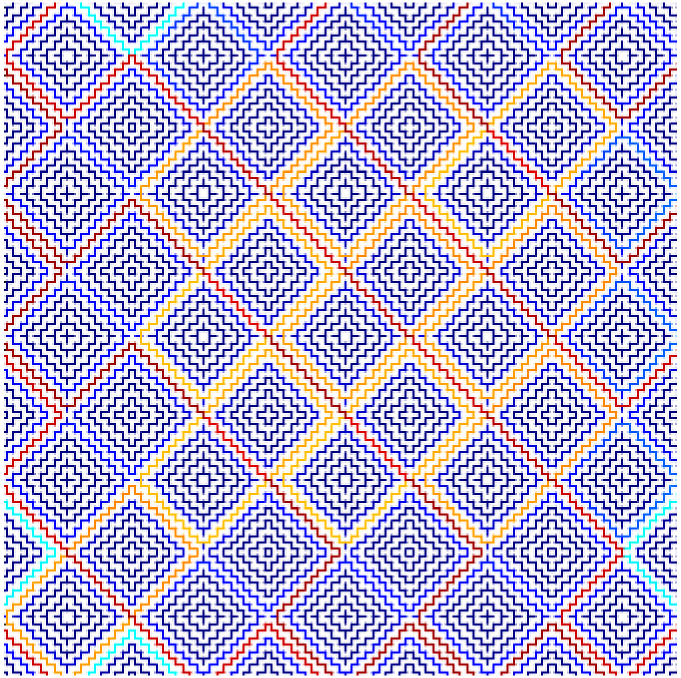
$$\psi\left(x', y'\right) = \cos 2\pi x' \cos 2\pi y'$$

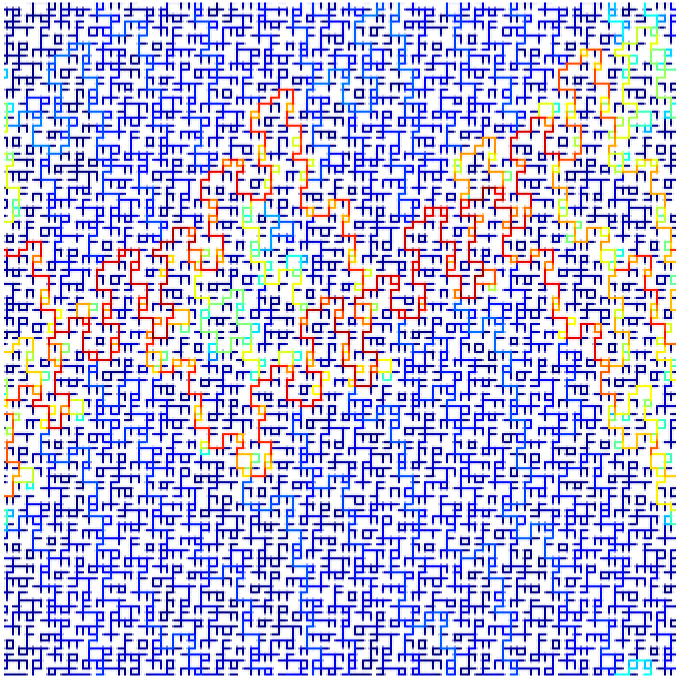
$$\chi = \begin{cases} 1, & \psi \geq 0 \\ 0, & \psi < 0 \end{cases}$$

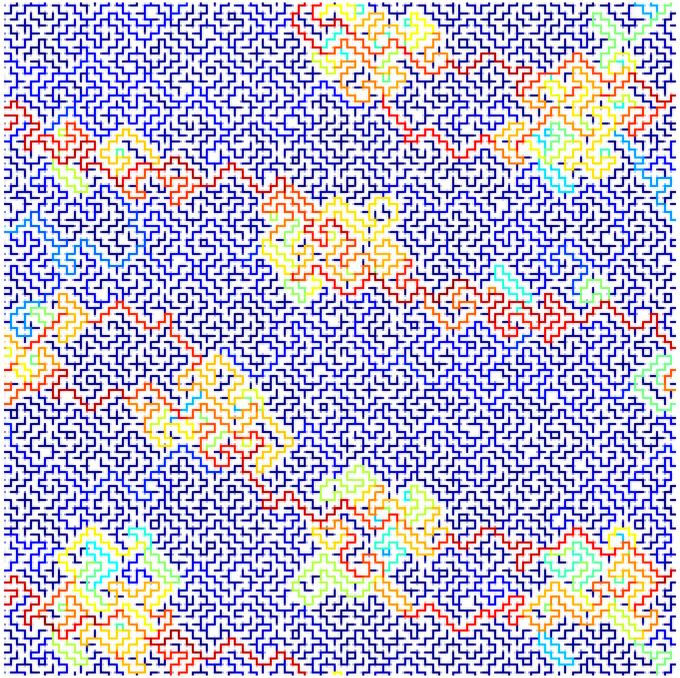
Wide Variety of Microgeometry



Wide Variety of Microgeometry





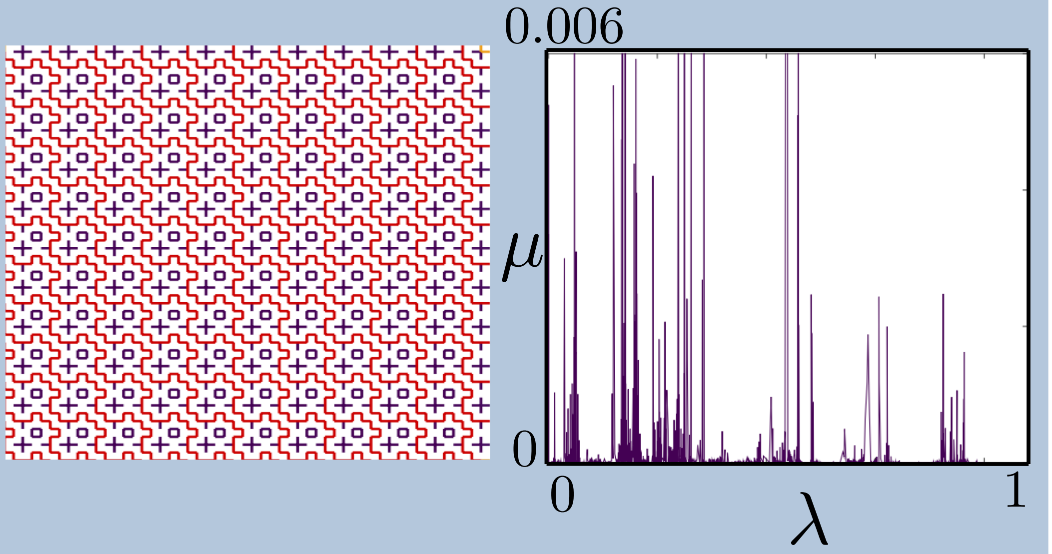


Small Difference in Moiré Parameters

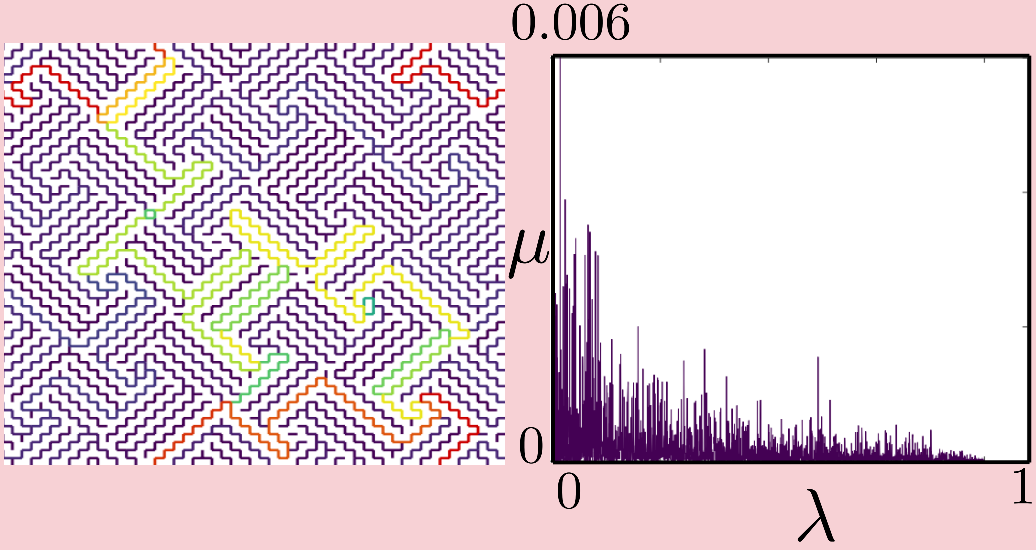
Big Difference in Material Properties

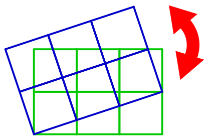
Dramatically Different!

Periodic

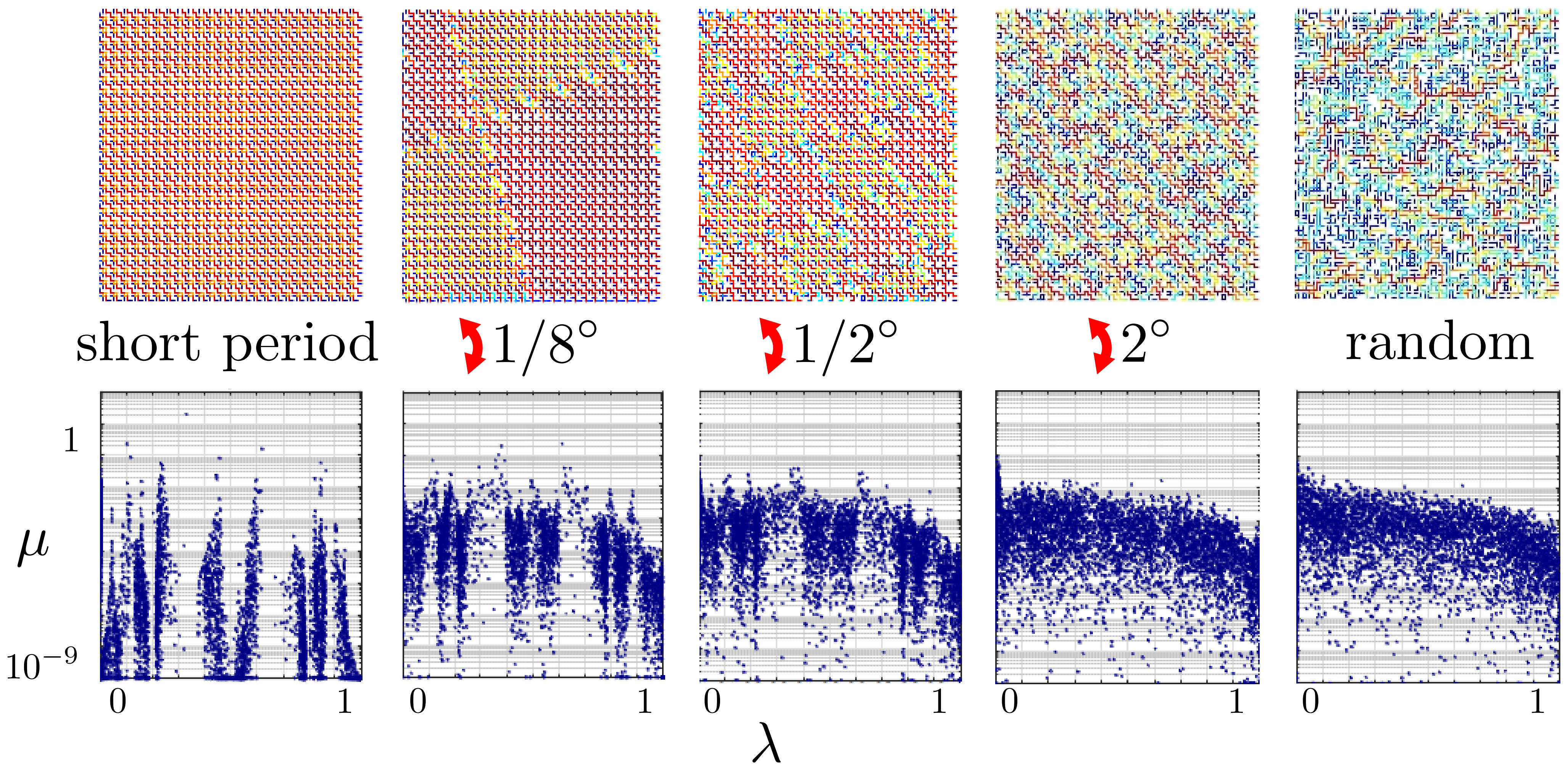


Aperiodic

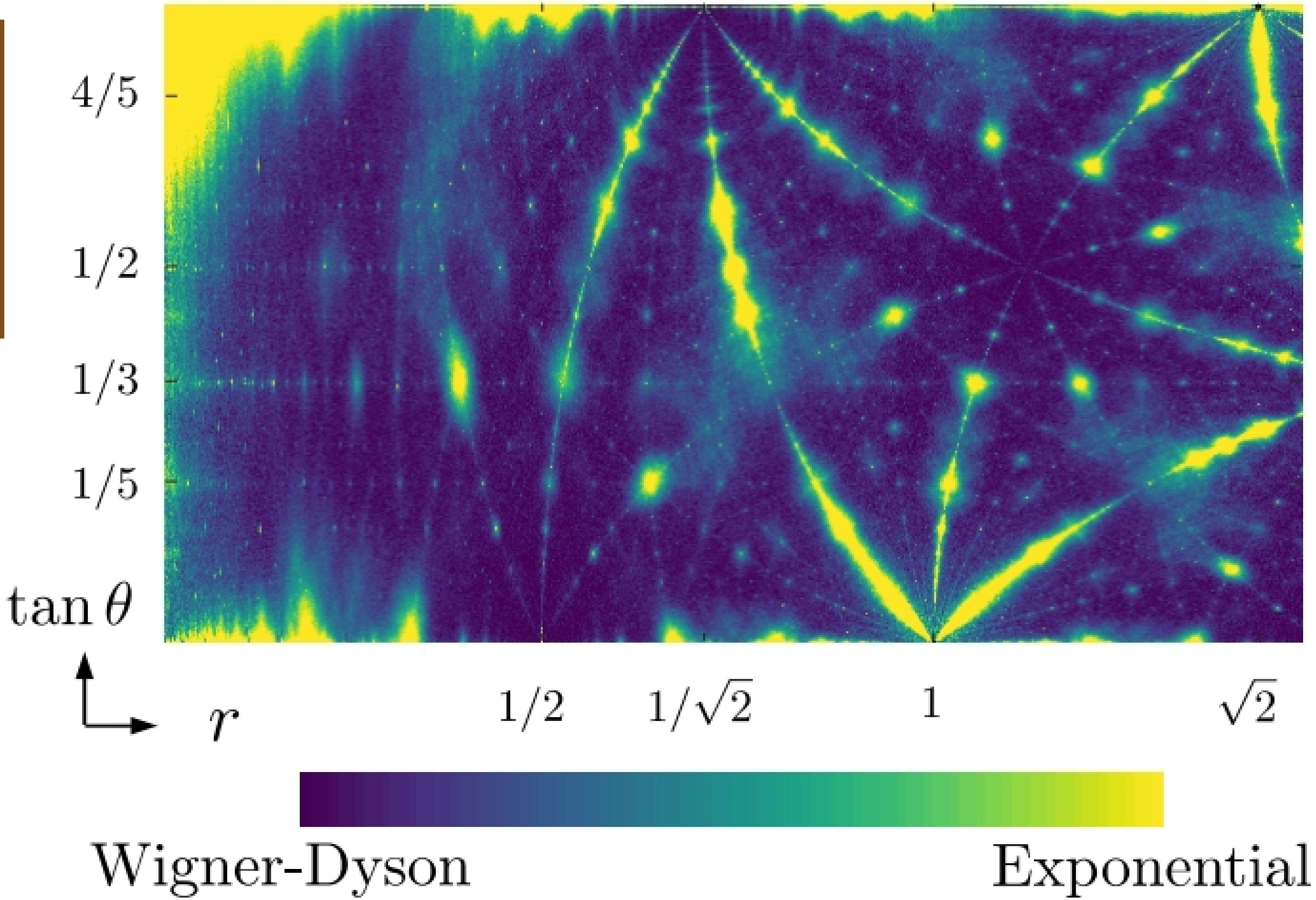




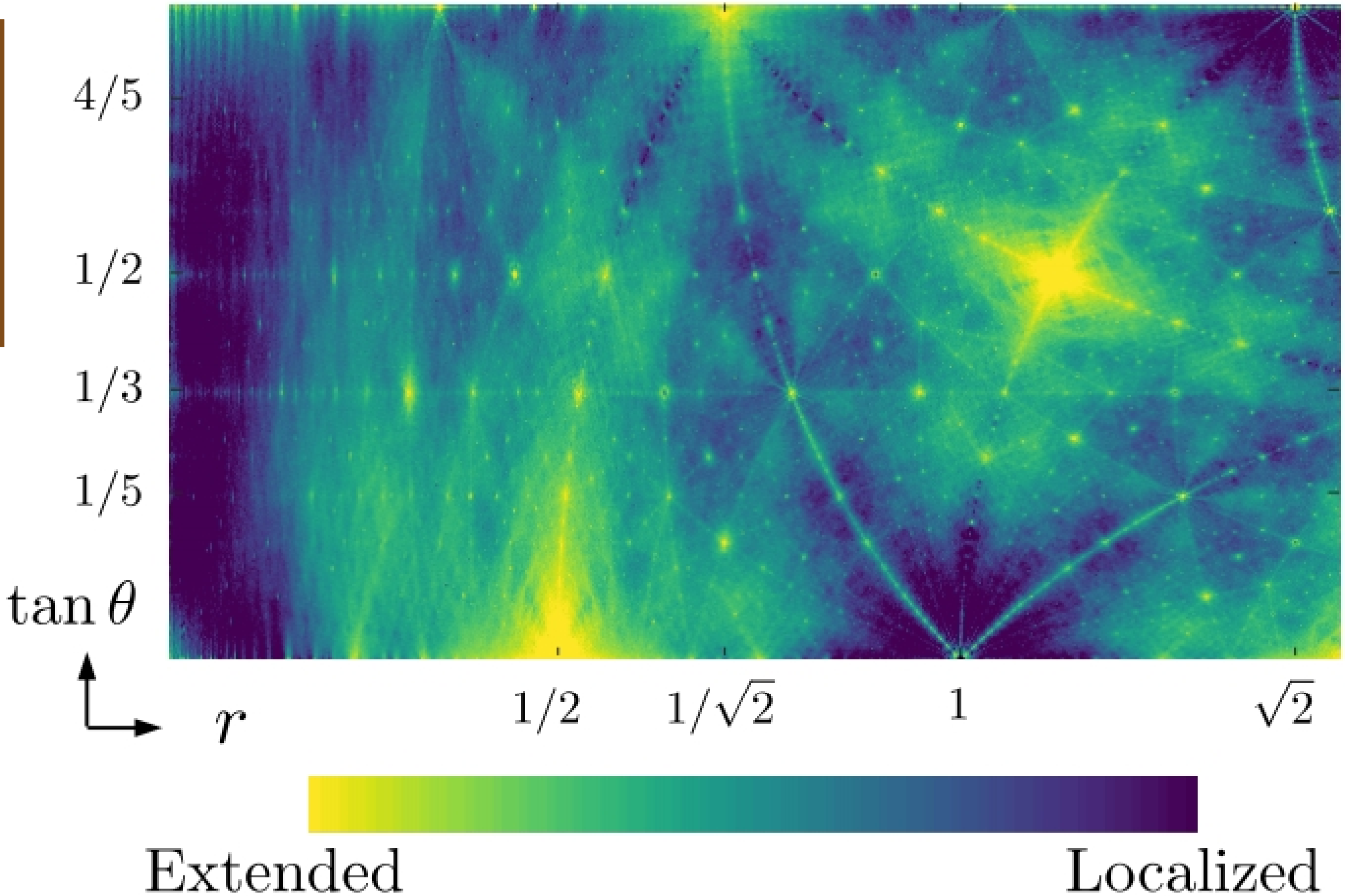
A Parameterized Transition



constellation of ordered eigenvalue statistics within a sea of randomness



constellation of extremely extended states within a sea of moderate localization



Is this real?

Can it be measured?

Is the resonant structure physical?

Plasmon Resonances

material properties approach eigenvalues

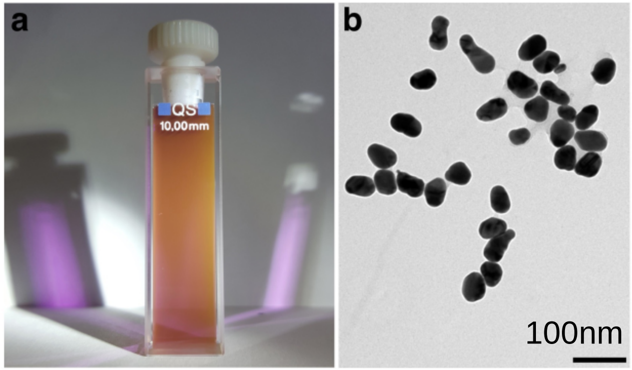
$$\frac{w_1}{s-\lambda_1} + \frac{w_2}{s-\lambda_2} + \cdots \Rightarrow \text{Material Properties } \epsilon^*$$

Composite Resonance

↓

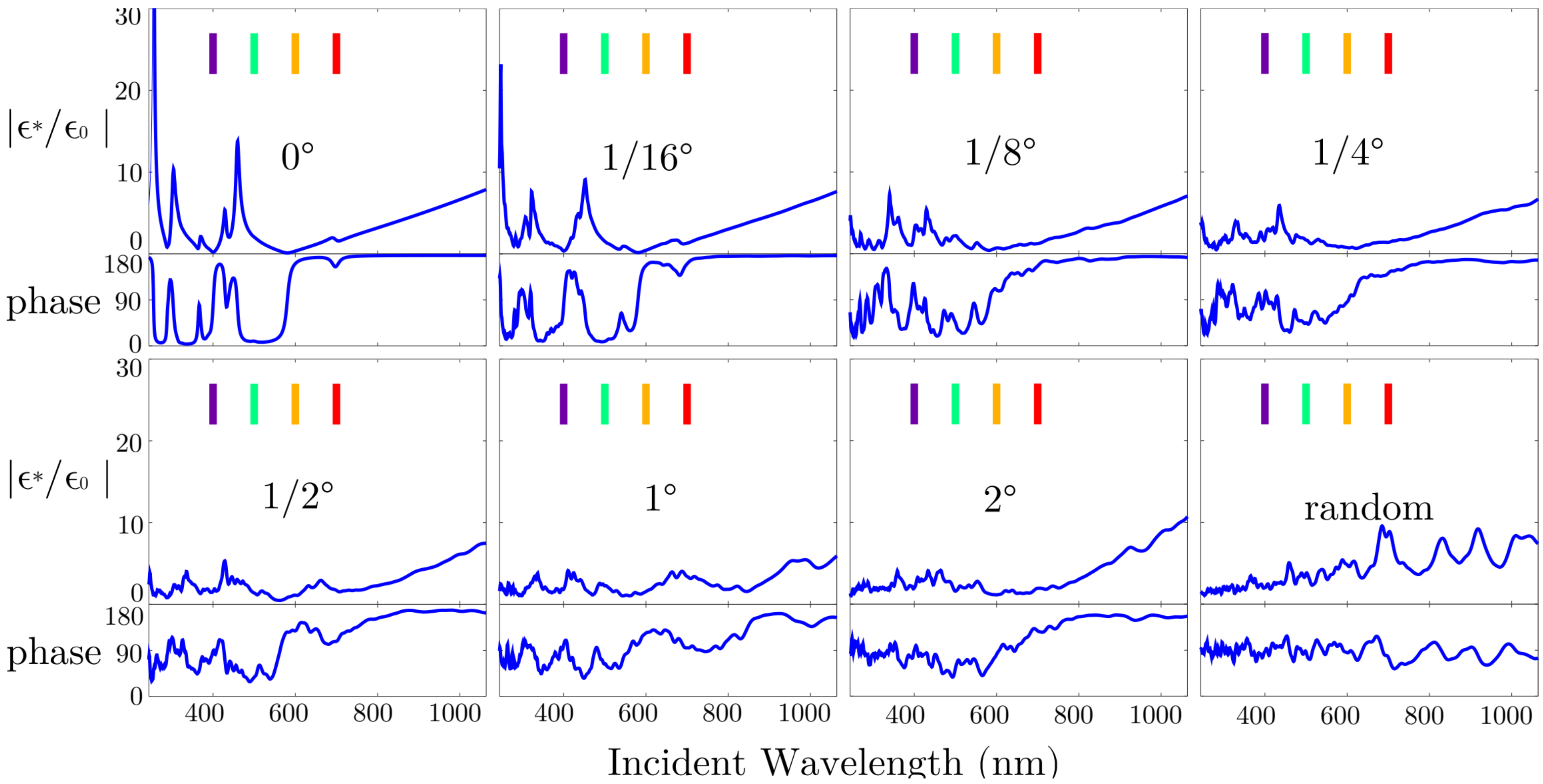
Dramatic optical properties

gold nanoparticles

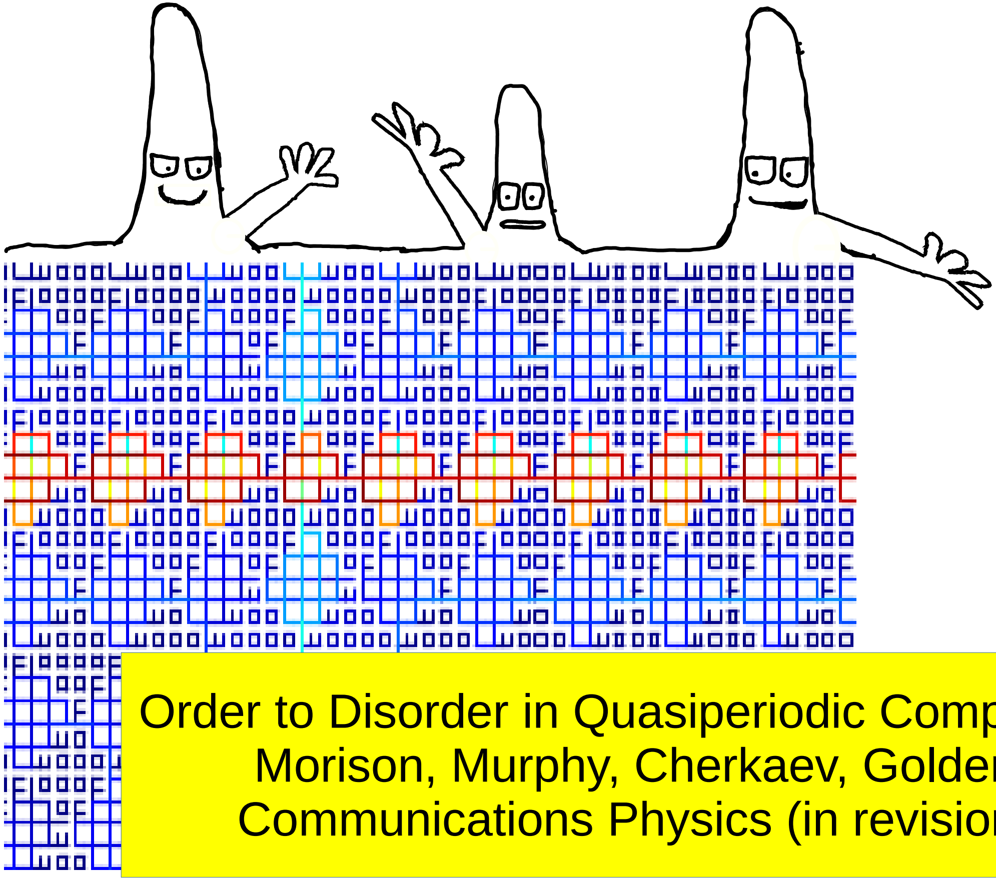


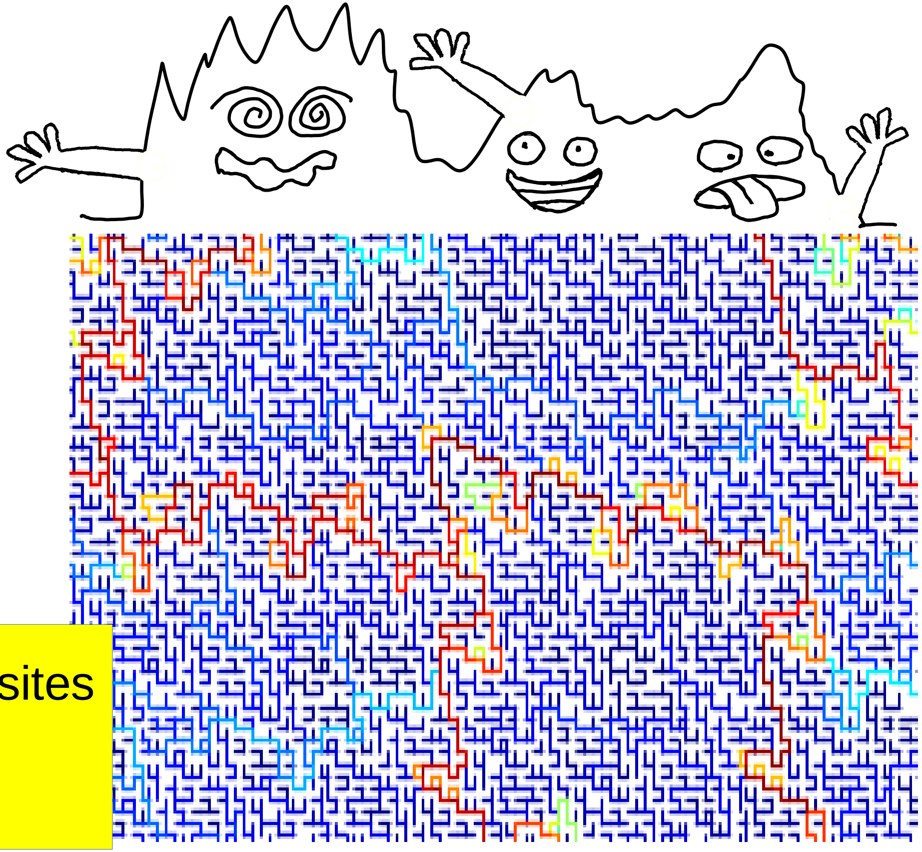
Kool, Bunschoten, Velders, and Saggiomo (2018)

From Sharp Peaks to Diffuse Absorption



Quasiperiodic geometry itself can drive an order to disorder transition!

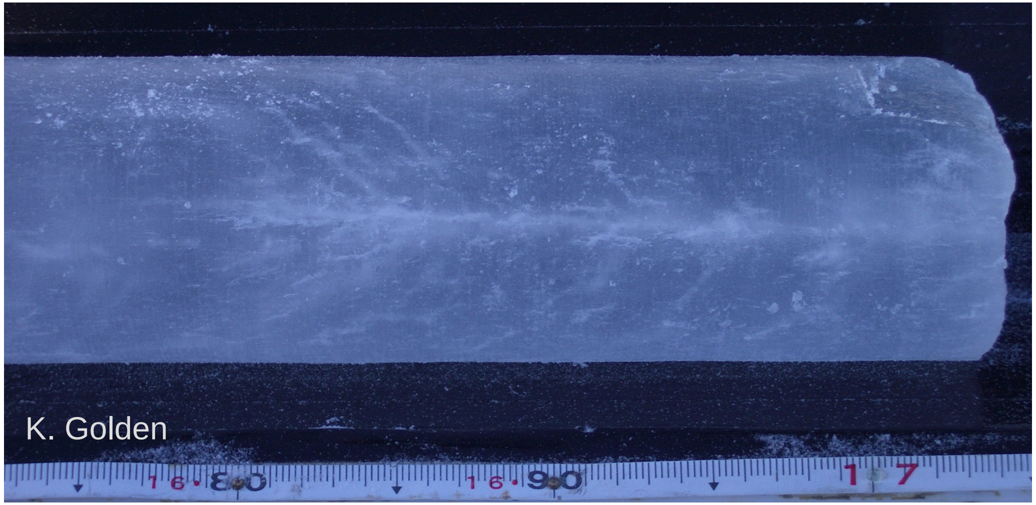


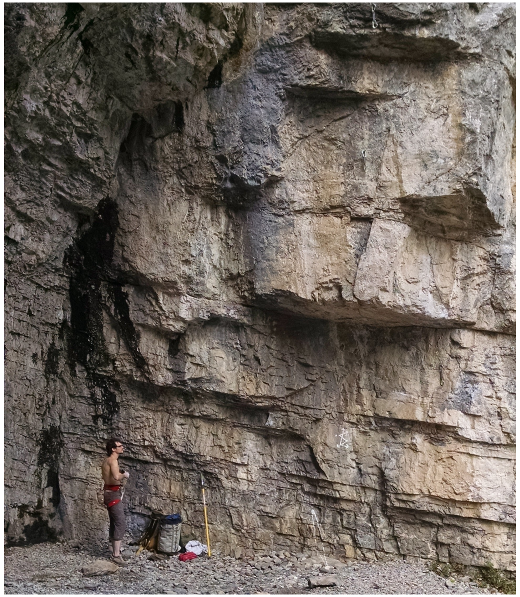


Order to Disorder in Quasiperiodic Composites
Morison, Murphy, Cherkaev, Golden
Communications Physics (in revision)

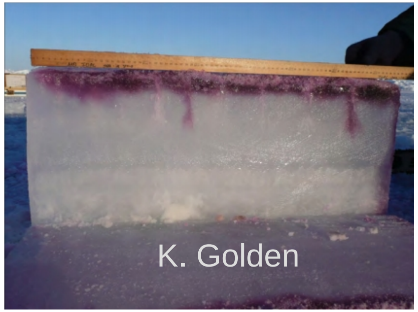
Two Perspectives on Percolation Transitions

Nanometers ⟷ Kilometers





Ecology ⟷ Engineering

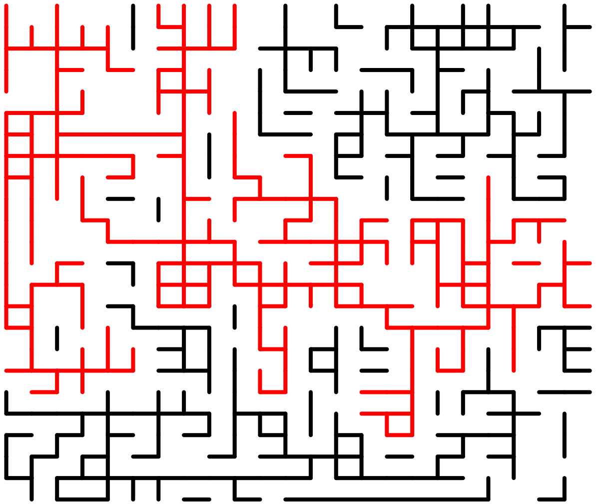


$$v = -\frac{k}{\mu}\nabla p$$

Darcy's Law

Percolation Theory

A Probabilistic Theory of Connectedness

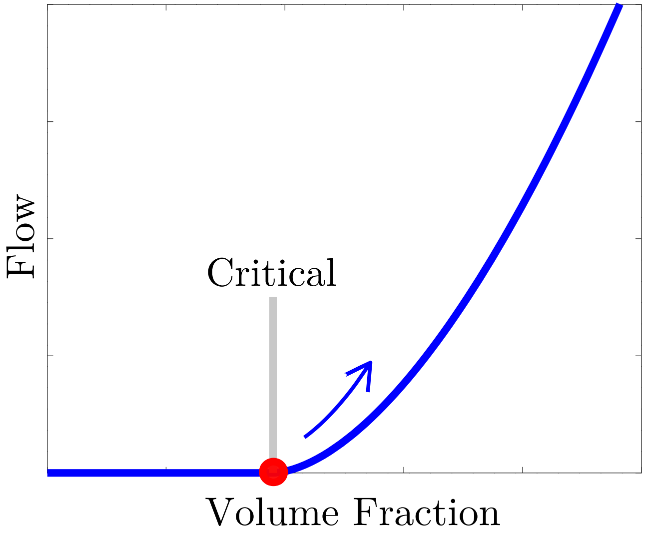


General

~~Statistical Ensemble~~

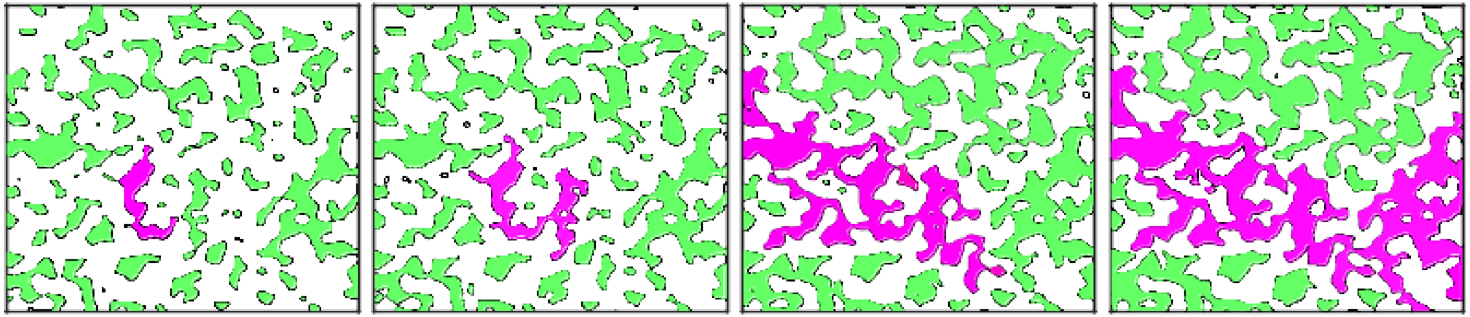
~~Infinite Open Cluster~~

~~System Size is Infinite~~



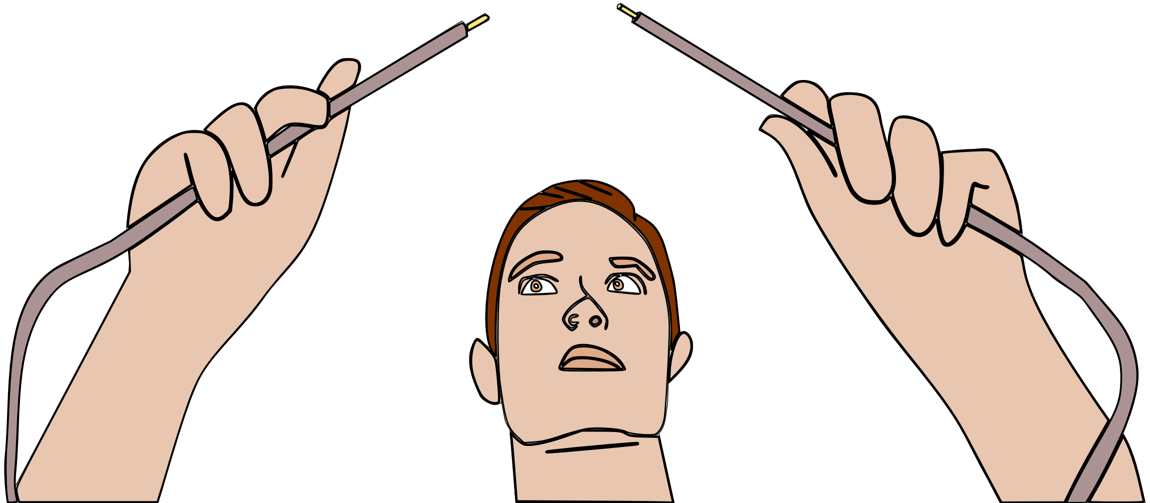
Specific

- Signal of Percolation for Specific Geometry
- Specified Boundary Conditions
- Finite System Size



$$1 - \frac{\sigma^*}{\sigma_2} = \frac{w_1}{s - \lambda_1} + \frac{w_2}{s - \lambda_2} + \dots$$

Material Properties



Bulk Transport Perspective

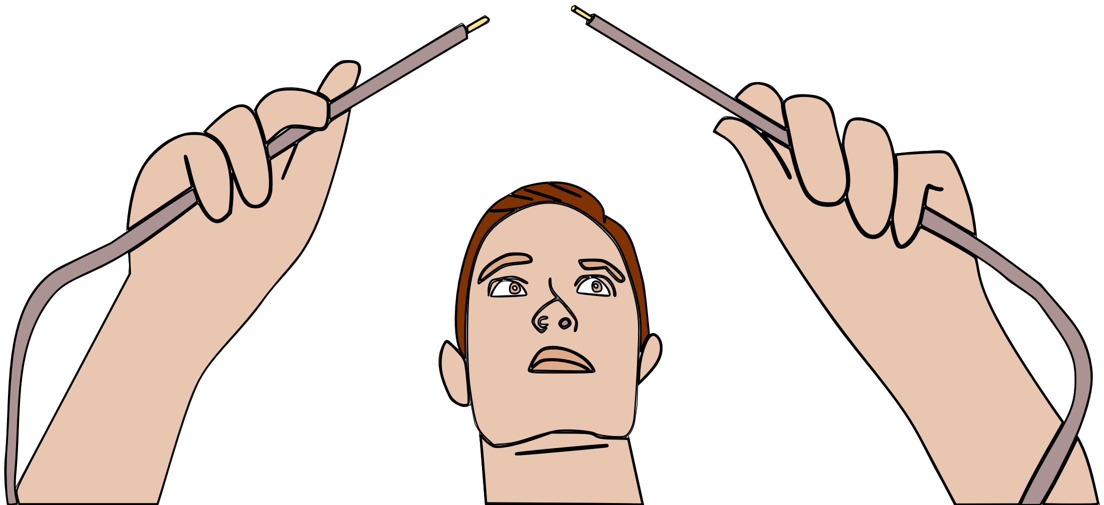
The Insulator Conductor Limit

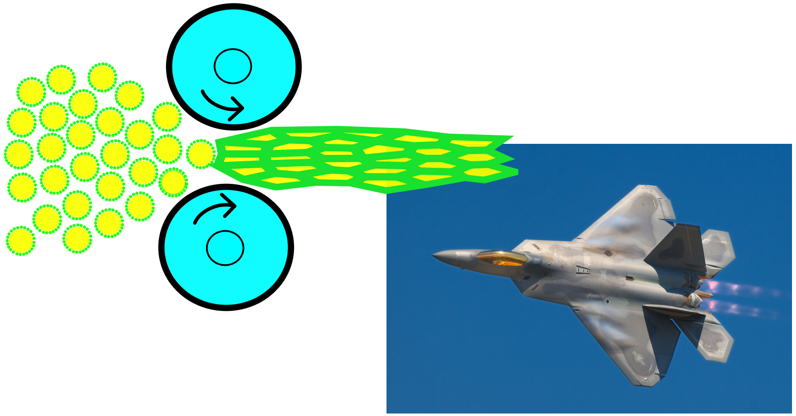
typical conductivity of:
copper $\approx 6 \times 10^{7} (S/m)$
insulator $< 10^{-14} (S/m)$

$$s = \frac{1}{1 - \sigma_1/\sigma_2}$$

$$\sigma_2 \to 0$$

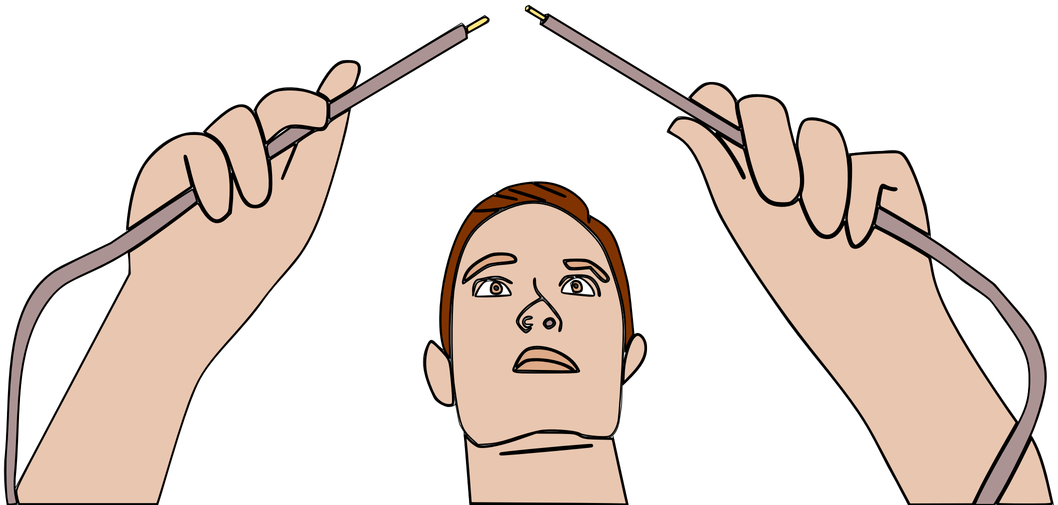
$$s \to 0$$





Jonckheere & Luck (1998)

As Geometry Shifts
Net Transport is Unchanged,
Until...



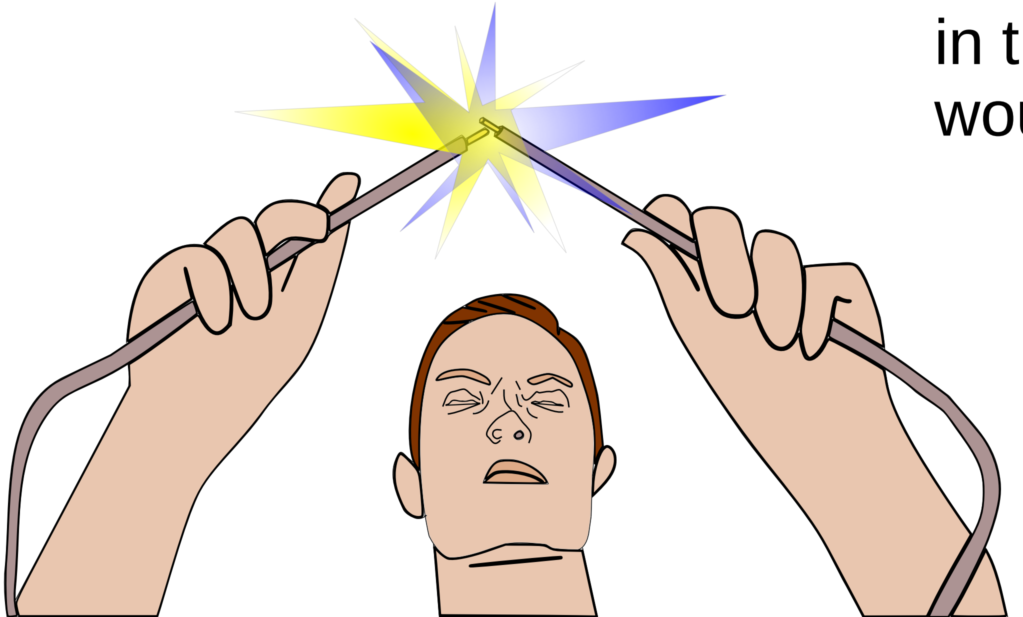
$$s \to 0$$

Material Properties

$$\chi \Gamma \chi$$

Zero Eigenvalues

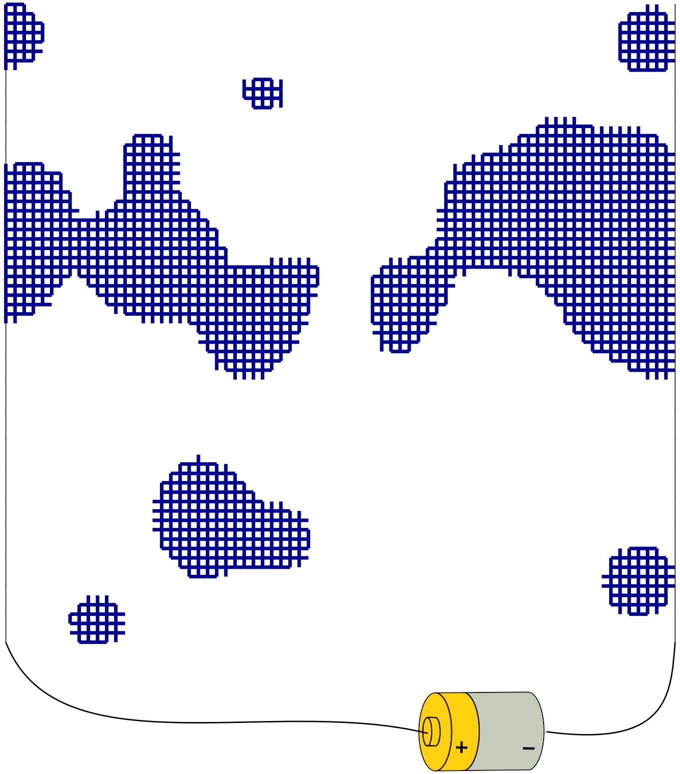
Geometric Equivalent of a Spark

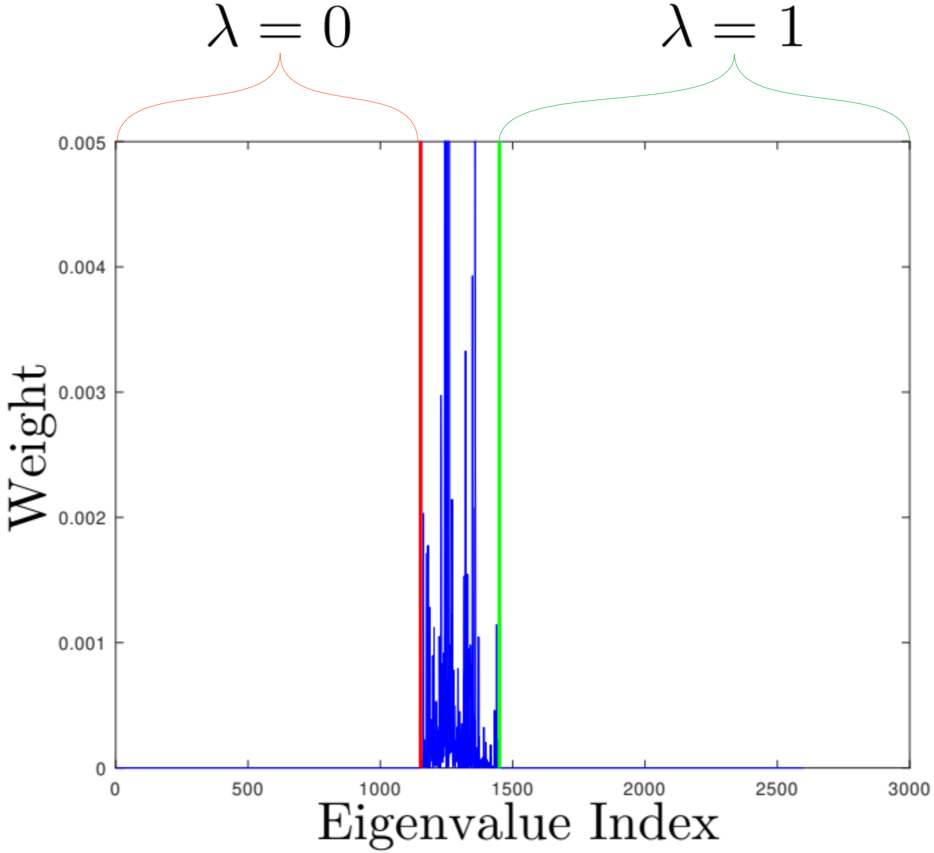


The absence of an abrupt change
in the spectral measure
would defy common intuition.

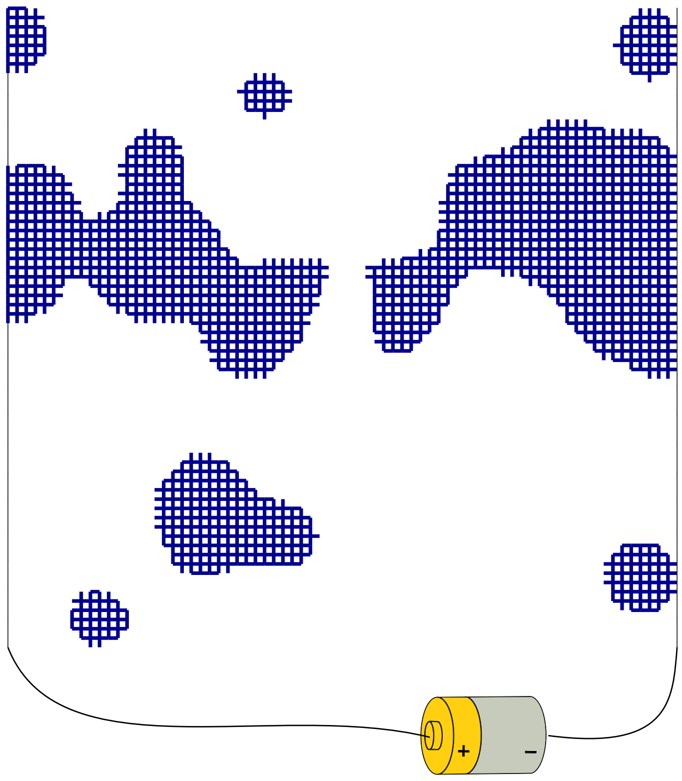
The direct calculation of spectral measures presents us with this geometric equivalent of a spark.

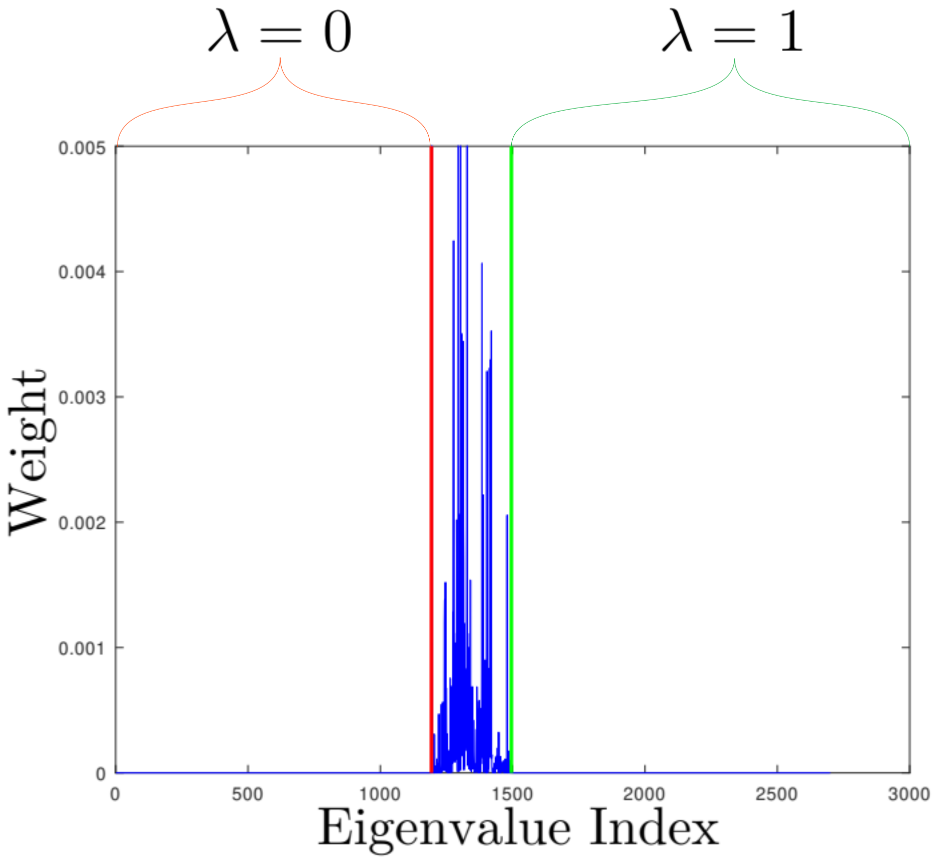
An Unmistakable Signal





An Unmistakable Signal





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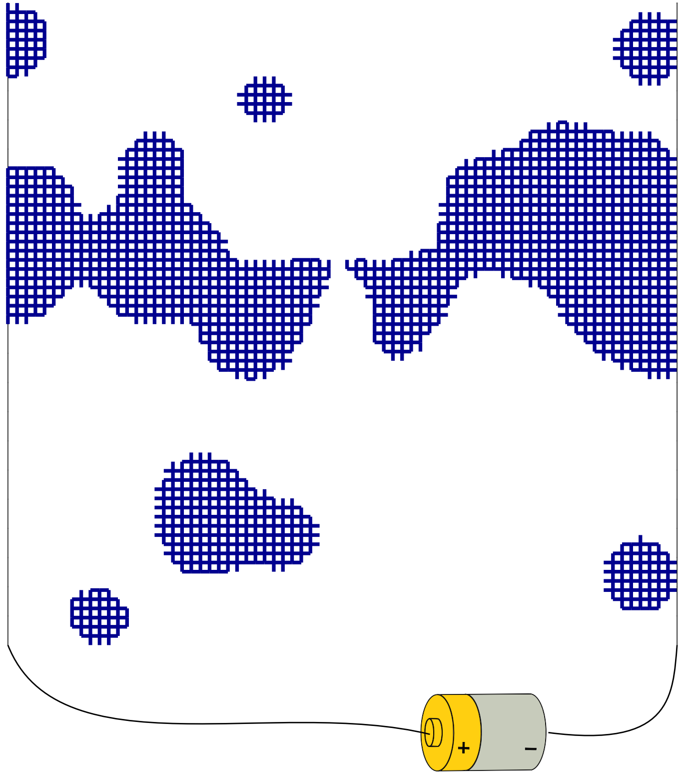

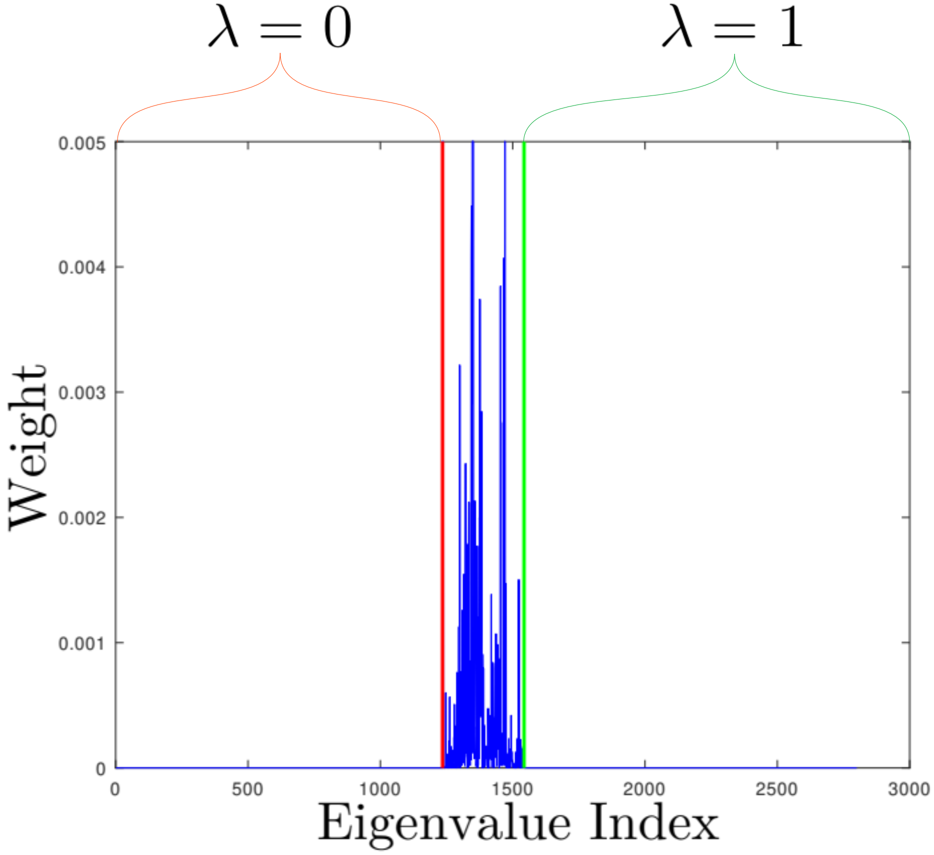

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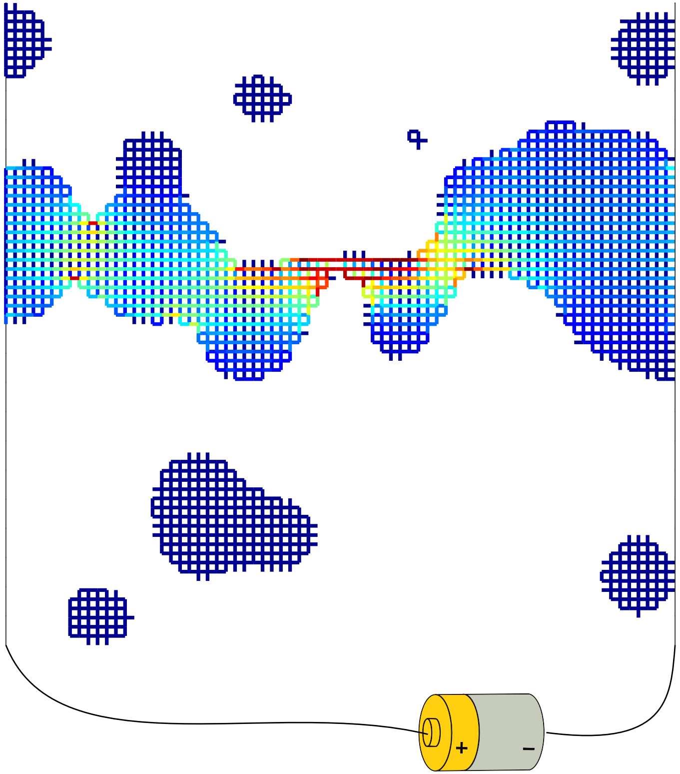

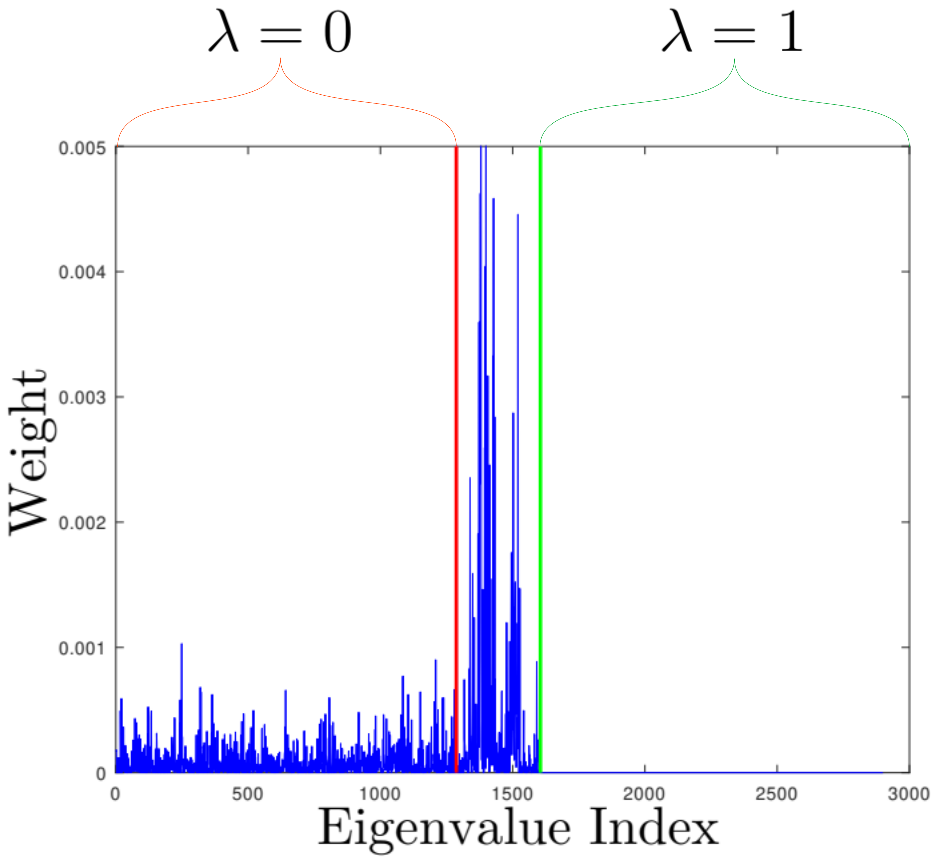

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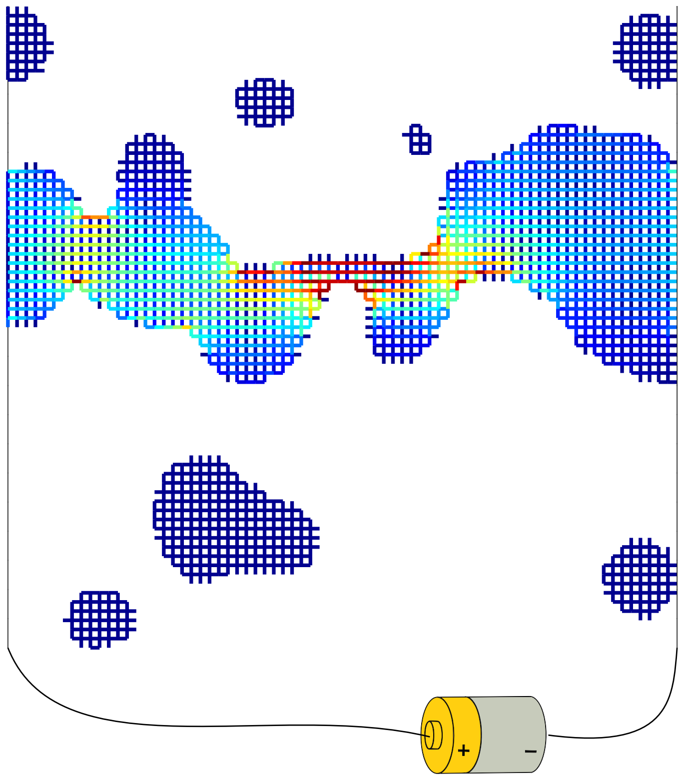
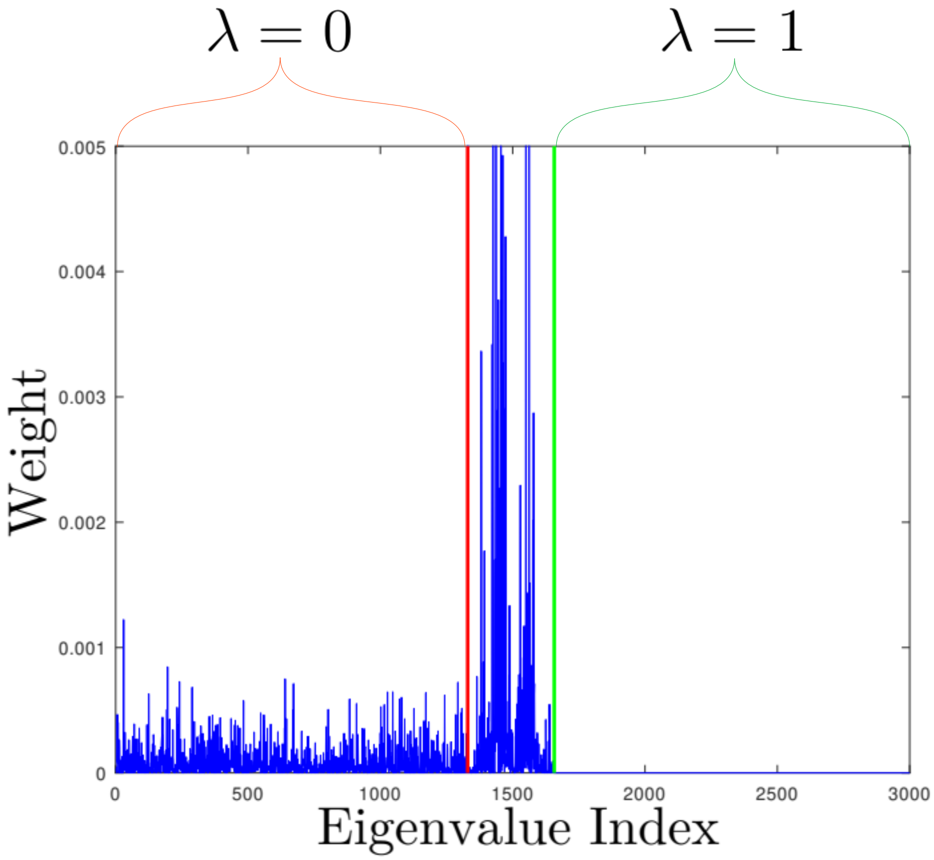
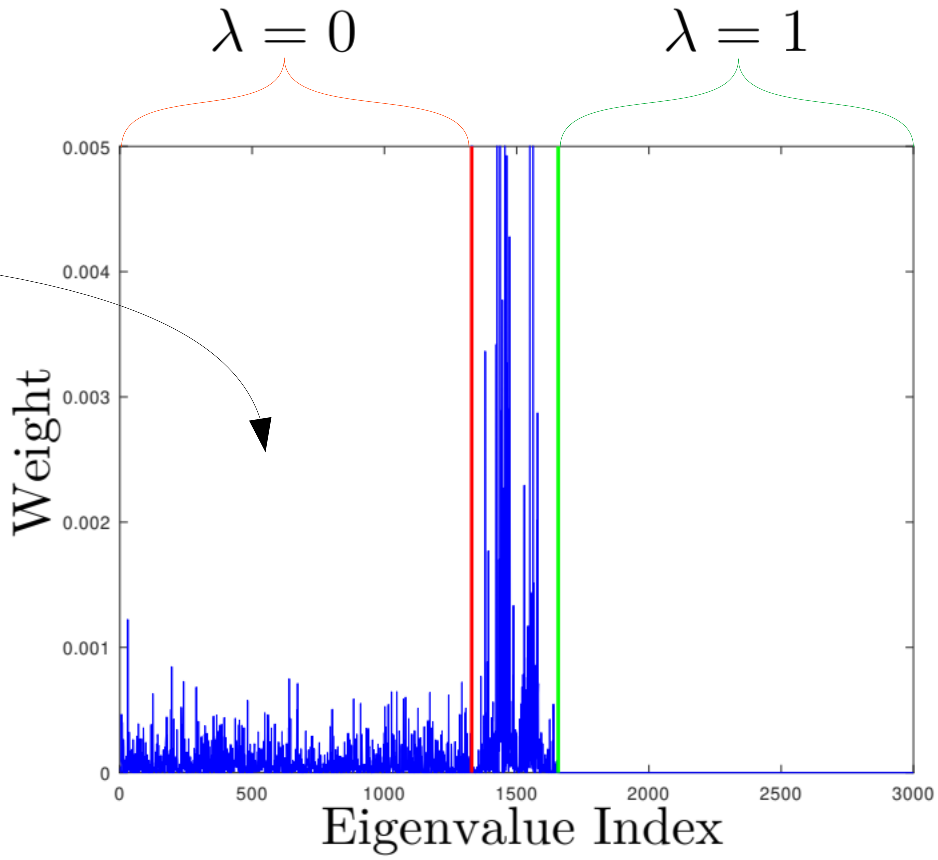




An Unmistakable Signal

α

defined in terms of
max eigenvalue weight
within the null



$\alpha \neq 0$ Percolated

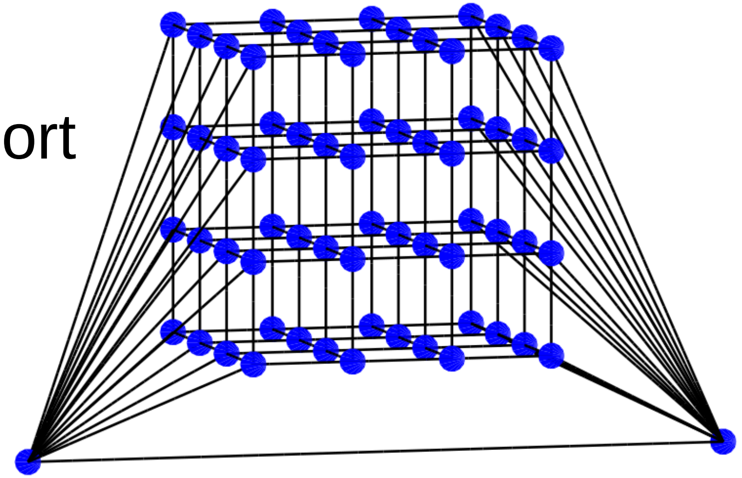
$\alpha = 0$ Not Percolated

Striking Yet Anticipated

N. Benjamin Murphy and I discussed this striking signal for years.
However, prior work noted the significance of this resonant mode.

We had nothing to prove...

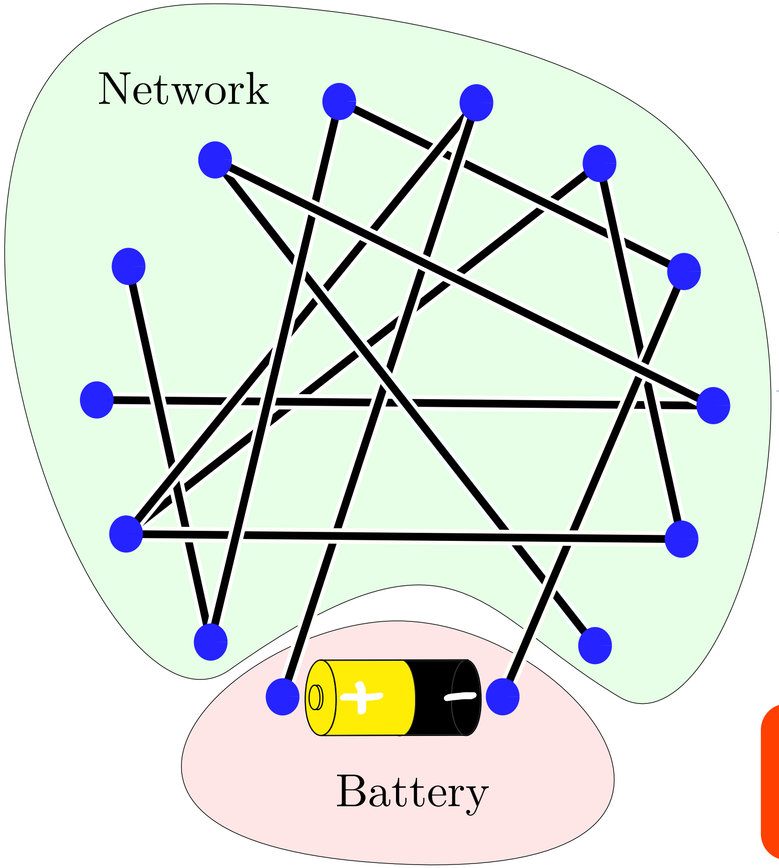
...until, we discussed applying the bulk transport framework to spanning trees and other graphs with Tom Alberts.

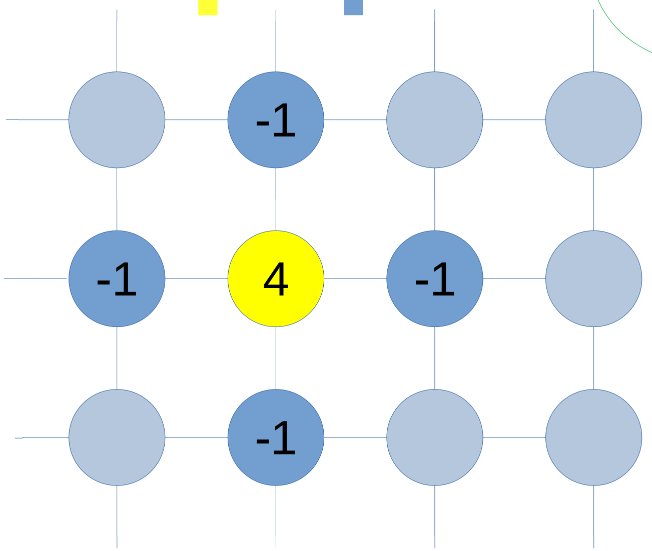


The Graph Laplacian Perspective

$$L = D - A = M^t M \quad = \text{“}\,\nabla \cdot \nabla = \nabla^2\,\text{”}$$

Incidence Matrix





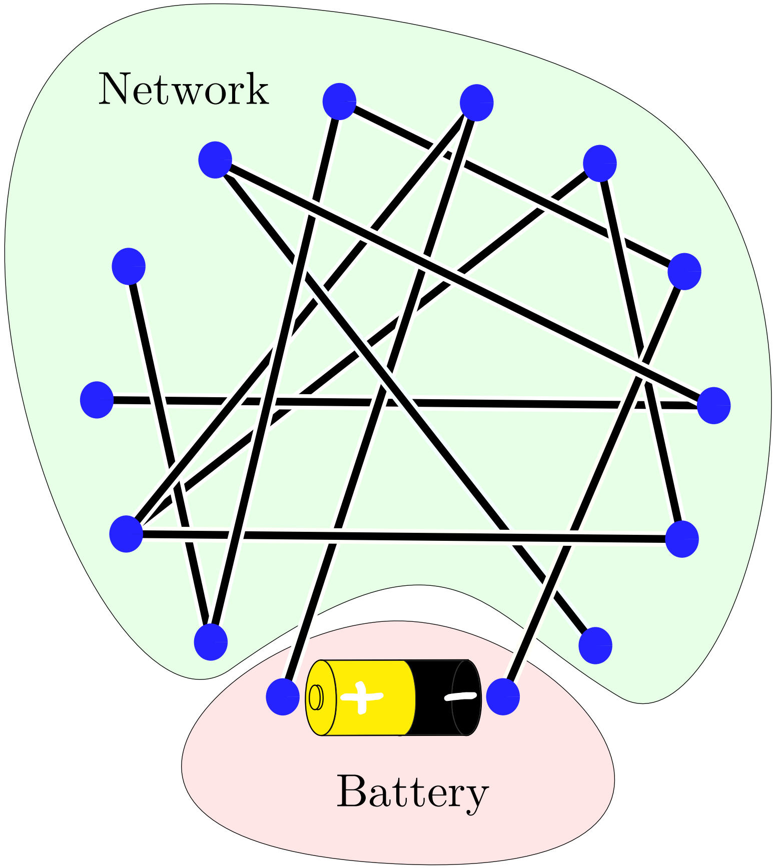
edges define connectivity
NOT spatial geometry

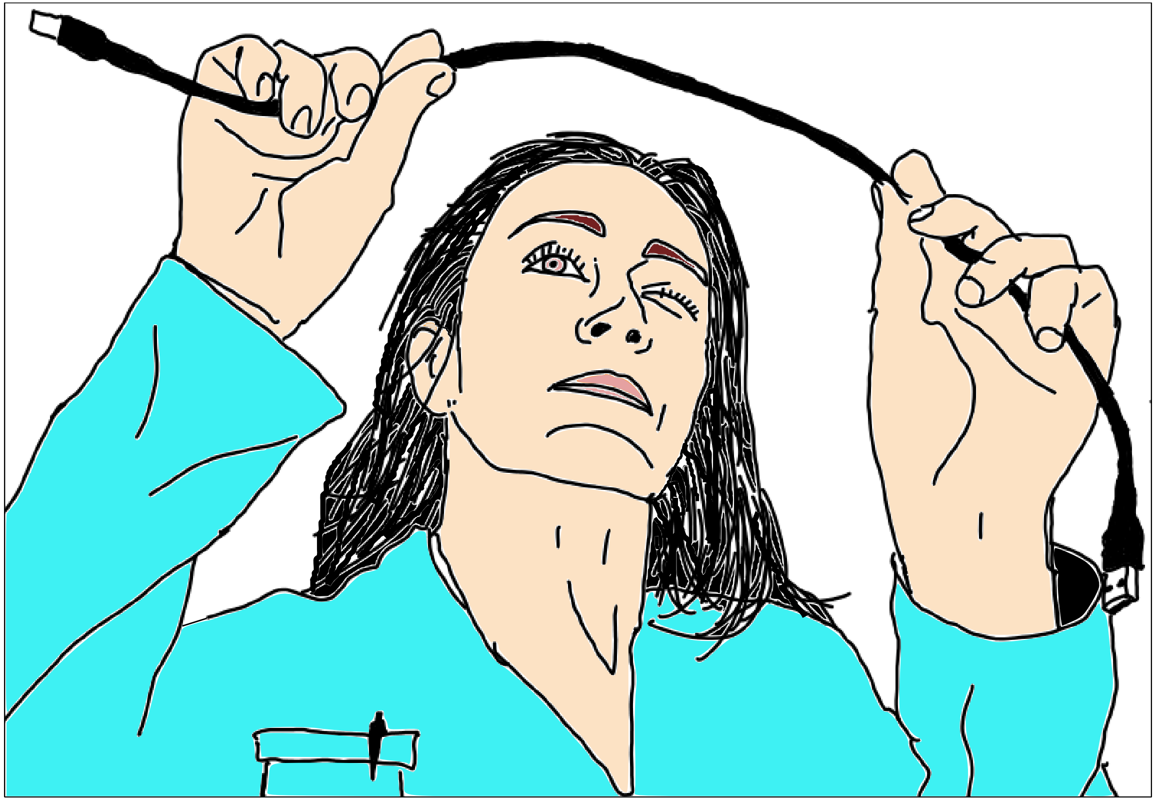
L
node functions

vs.

$\chi\Gamma\chi$
edge functions

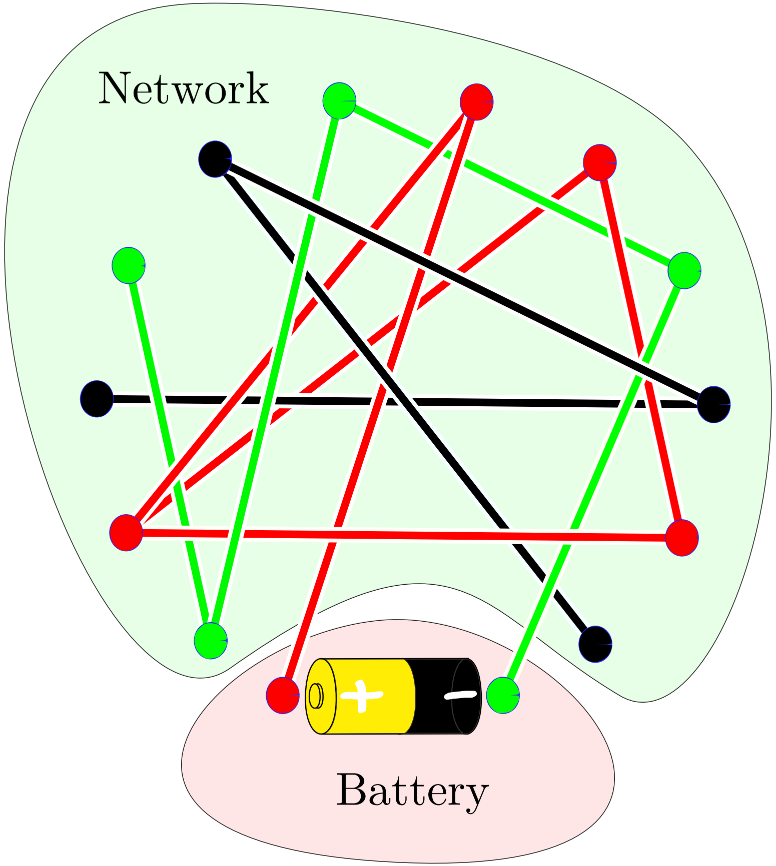
“Connect the USB cable?”
”But, it’s already connected.”

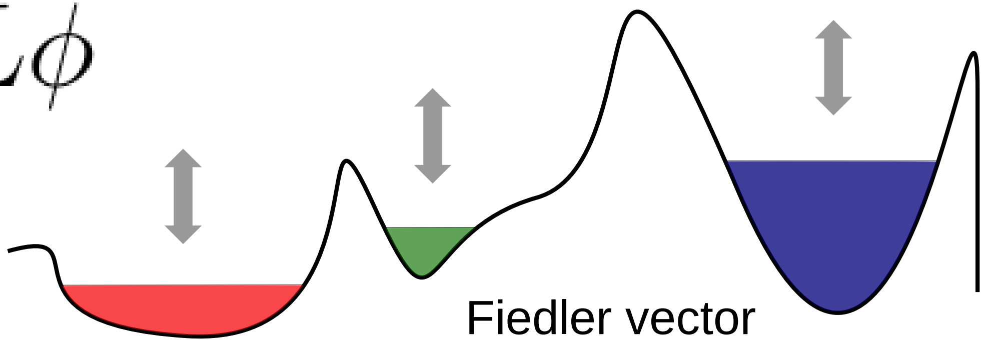




Algebraic Connectivity

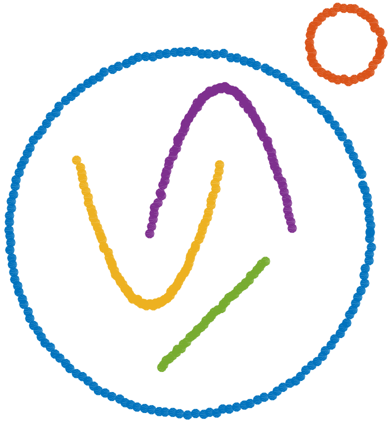
$$0 = L\phi$$





Fiedler vector

spectral clustering



β indicates a voltage difference on the battery terminals within the null of L, for the network.

$\beta \neq 0$ Network Insulates

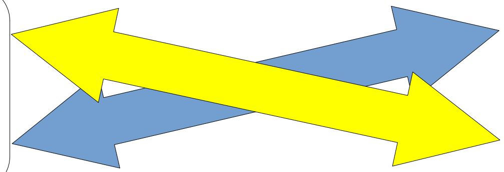
$\beta = 0$ Network Conducts

$\chi\Gamma\chi$ and L in Shared Terms

$$\alpha\beta = 0$$

$\alpha \neq 0$ Percolated

$\alpha = 0$ Not Percolated

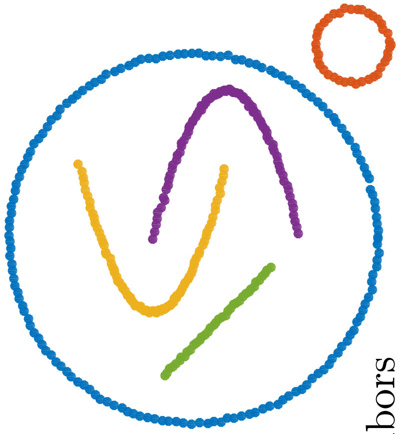


$\beta \neq 0$ Network Insulates

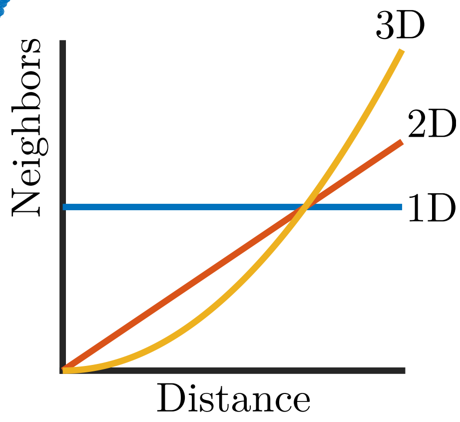
$\beta = 0$ Network Conducts

Cross Pollination Between Homogenization and Graph Theory

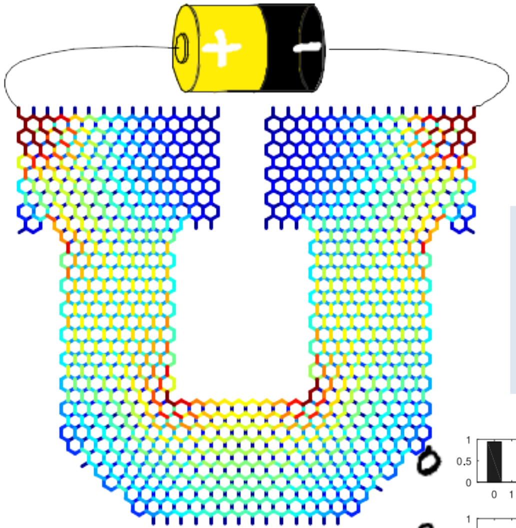
L and $\chi^{\Gamma}\chi$ Encode Different Information



“discovers the true dimension”



Spectral Clustering

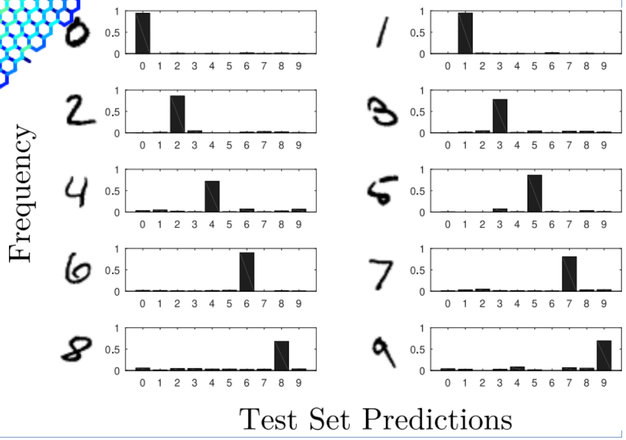


?

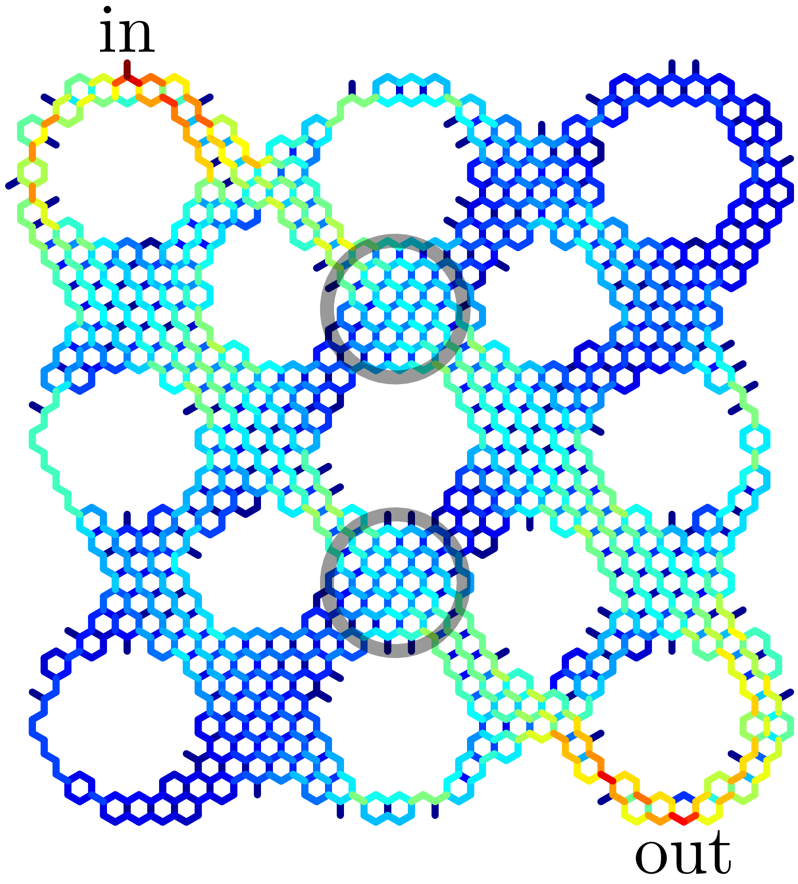
neural net with composite inspired architecture

Graph Sparsification

?



(Mis)Information Diffusion

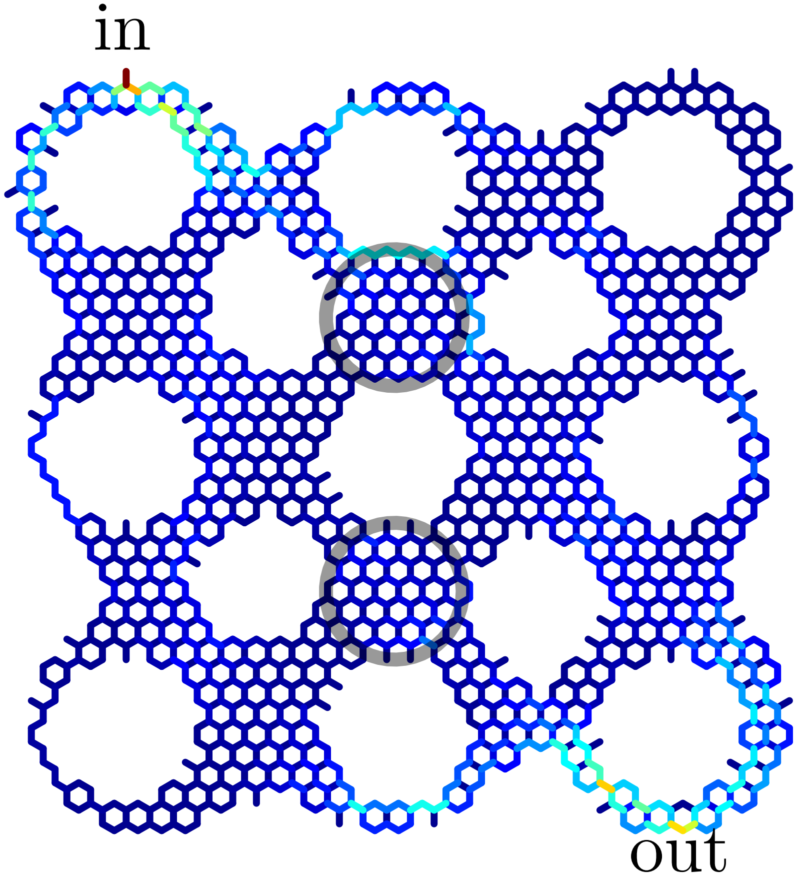


- Nodes = people in a network
- Edges = message passing

Edges within the circles behave identically to all other edges.

Messages pass from “in” to “out”.

(Mis)Information Diffusion

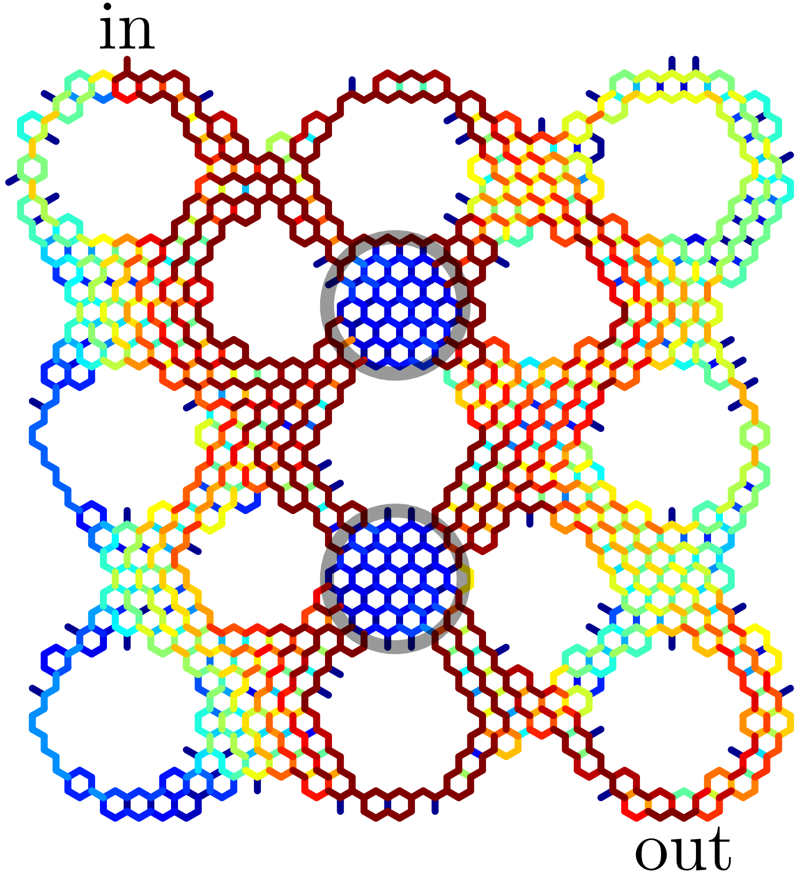


- Nodes = people in a network
- Edges = message passing

Edges within the circles transmit no information.

Messages not transmitted.

(Mis)Information Diffusion



- Nodes = people in a network
- Edges = message passing

Edges within the circles “lie.”

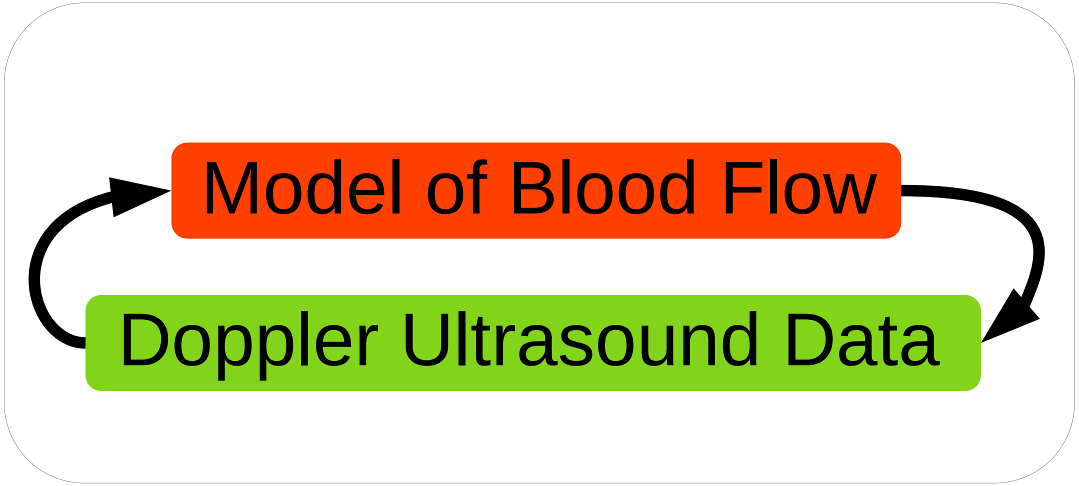
Network resonances are prominent.

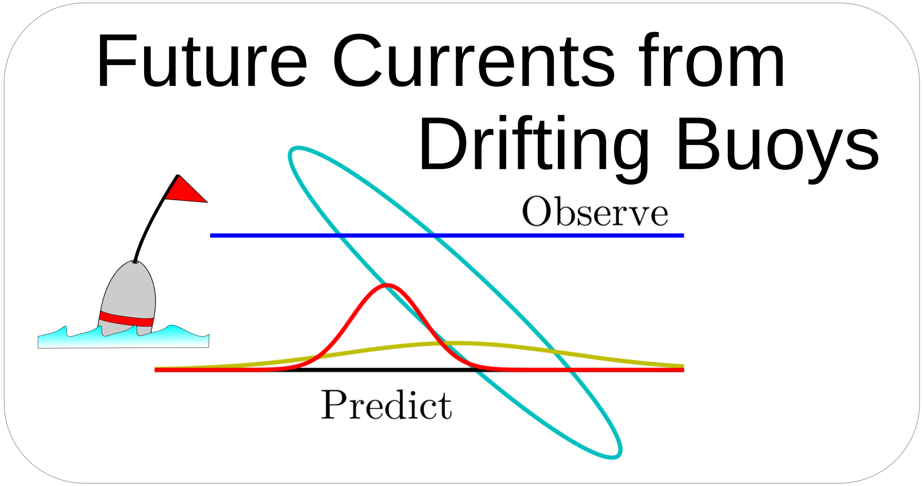
Tools of Homogenization Theory

Applied Statistics

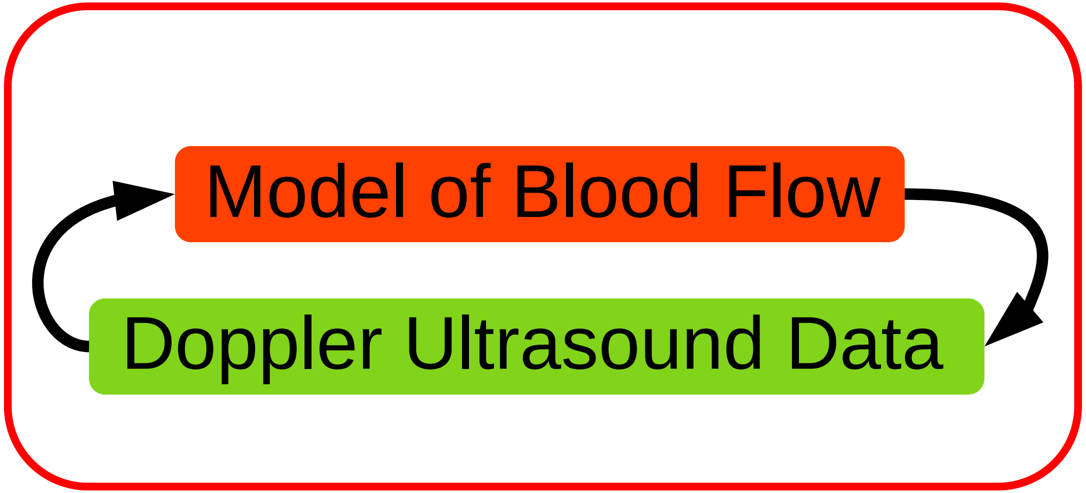
Two Perspectives on Percolation Transitions
Morison, Murphy, Cherkaev,
Golden, Alberts, Wang
(in preparation)

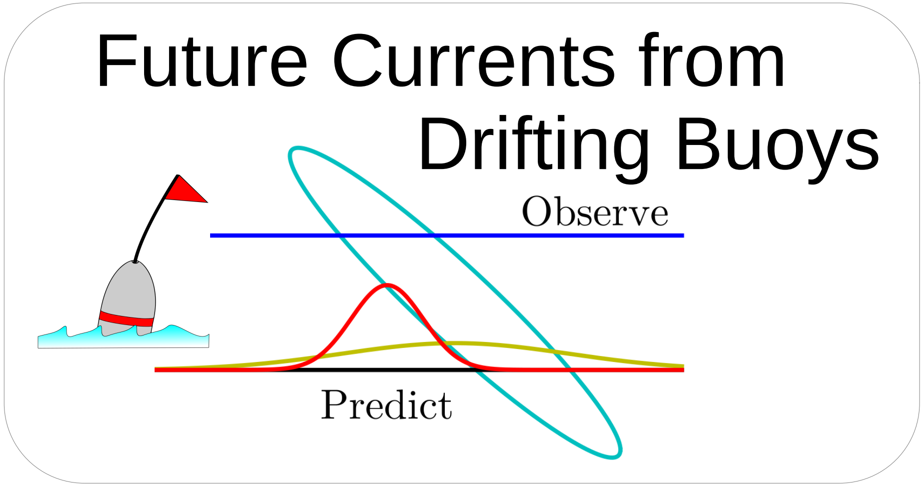
Flipped Priorities in Applied Statistics



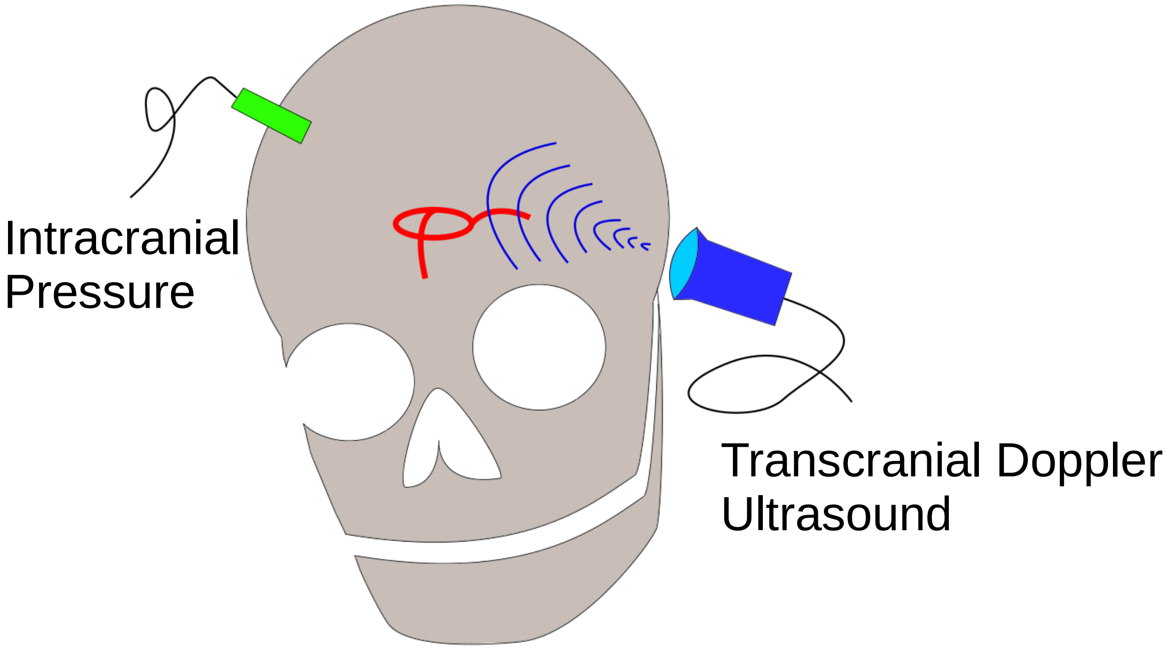


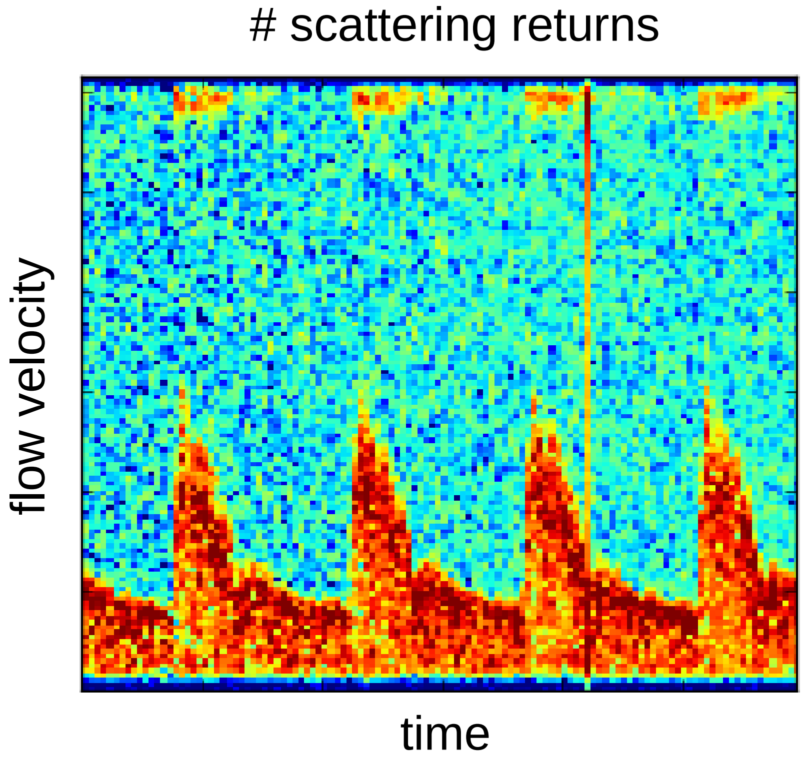
Flipped Priorities in Applied Statistics





Head Trauma & Cerebral Blood Flow

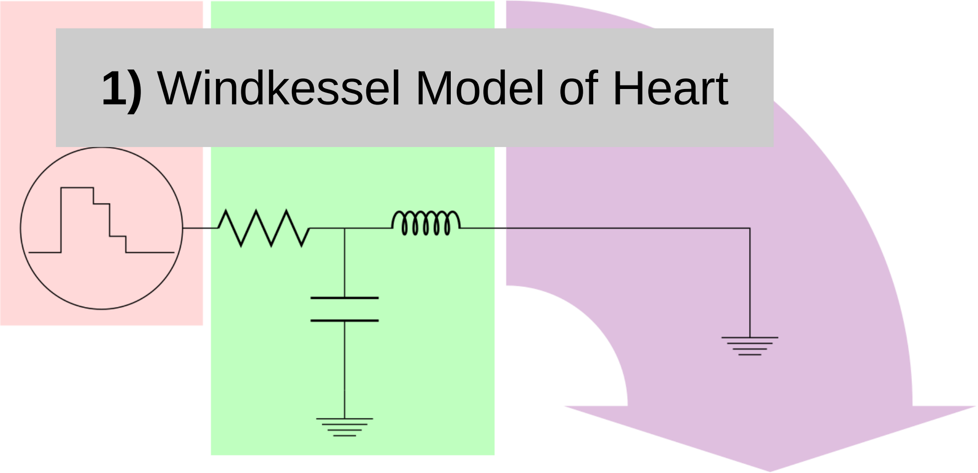




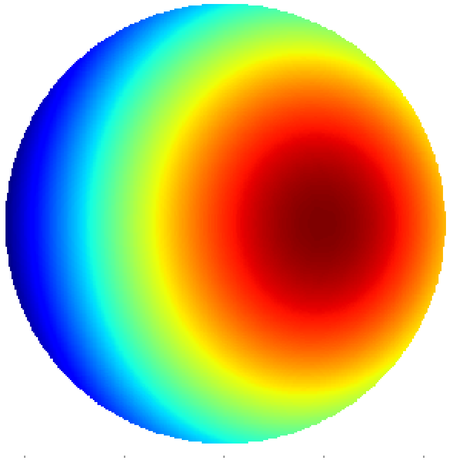
Can we avoid invasive measurements?

A “Forward” Model

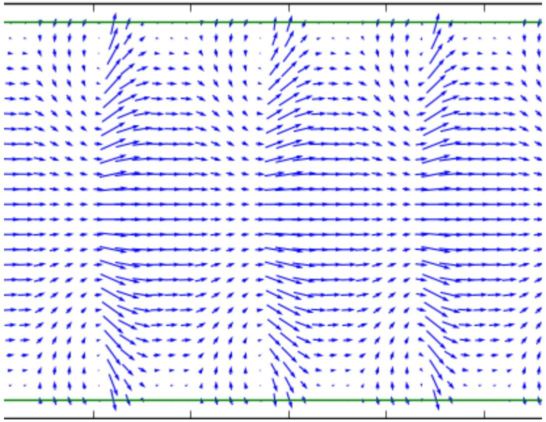
1) Windkessel Model of Heart

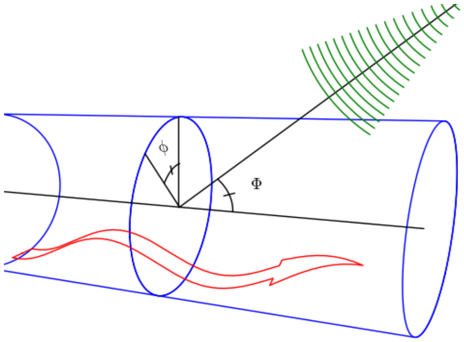


3) Relative Geometry
Of Ultrasound Focus



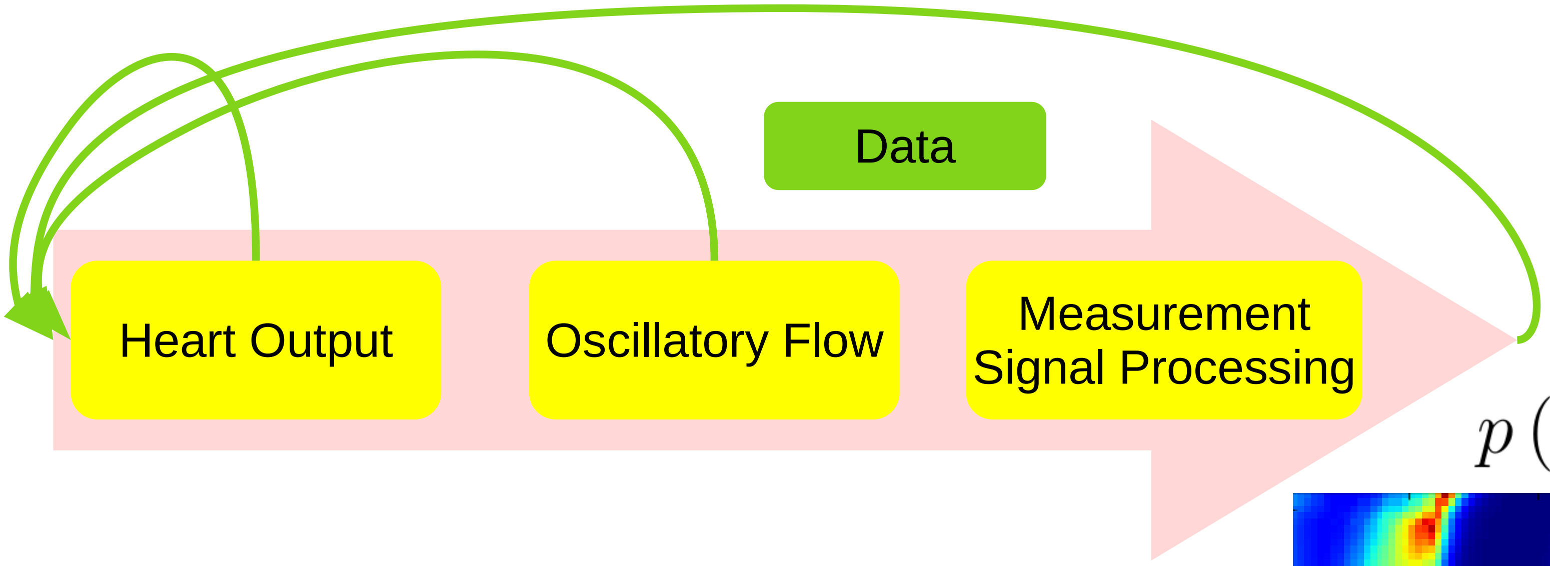
2) Womersley's solution
for pulsatile flow
in an elastic tube





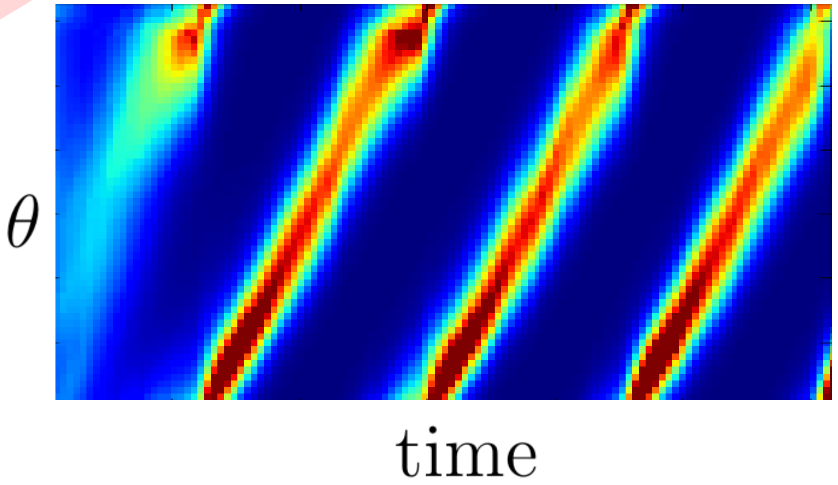
4) Velocity Field to
Scattering Volume
Calculation and
Signal Processing

A Recursive Bayesian Estimator



$$p\left(s|\theta,r\right)$$

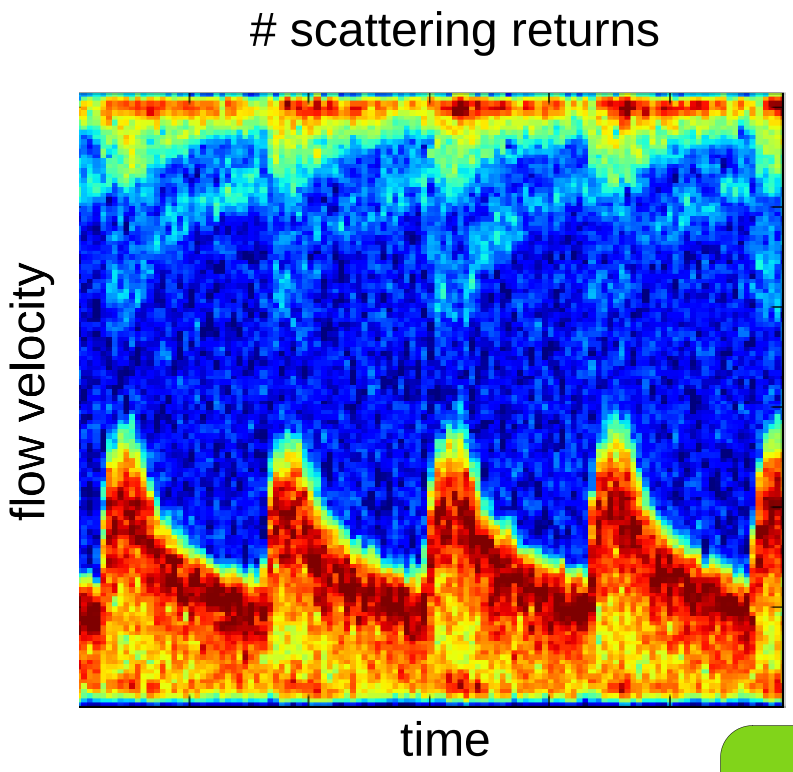
$$p\left(\theta_i|s_1,s_2,\ldots,s_i\right)$$

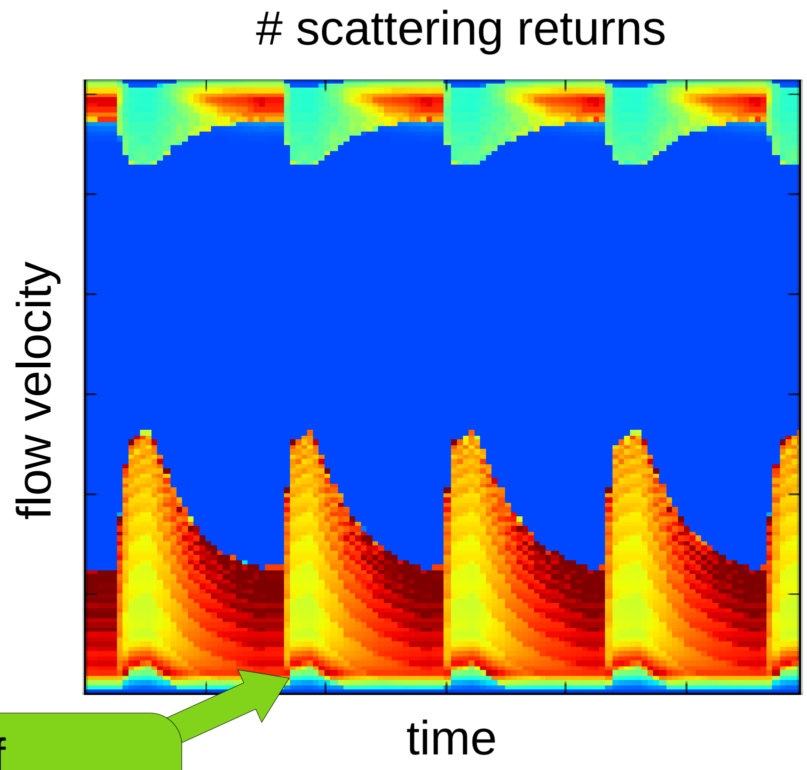


$$p\left(\theta_i,r_i\right)=F\left(p\left(\theta_{i-1},r_{i-1}\right)\right)$$

$$p\left(\theta_i,r_i|s_i\right)=p\left(s_i|\theta_i,r_i\right)p\left(\theta_i,r_i\right)$$

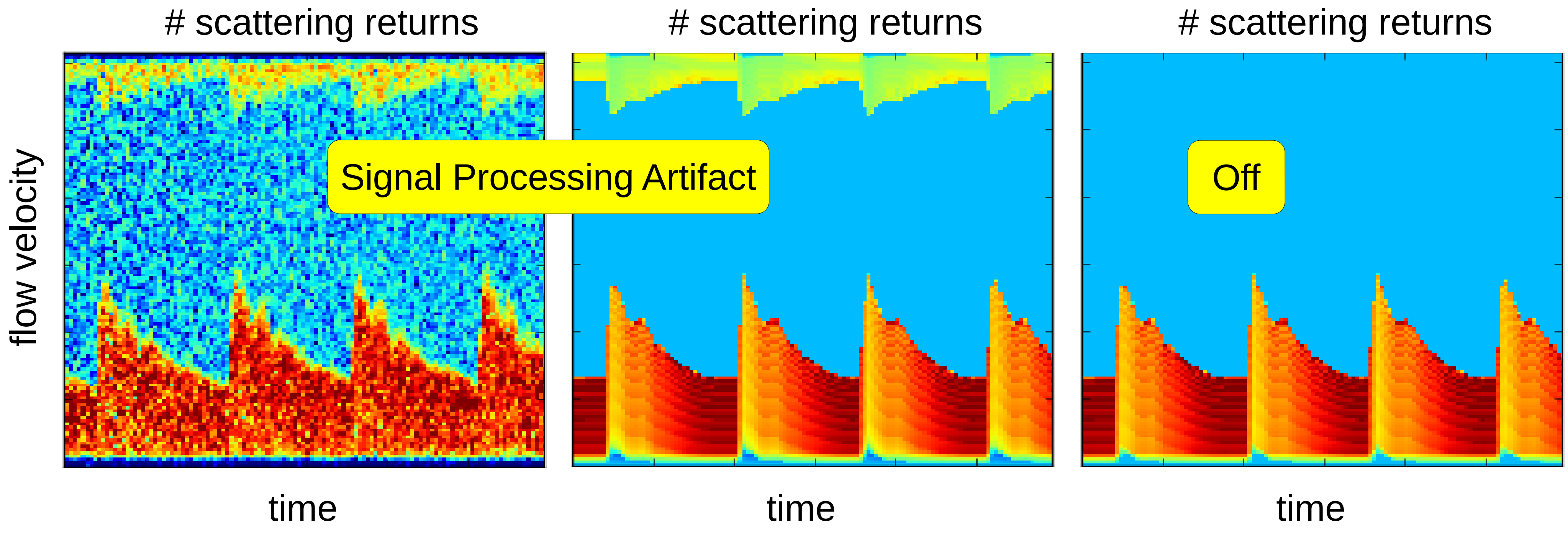
Data vs Model



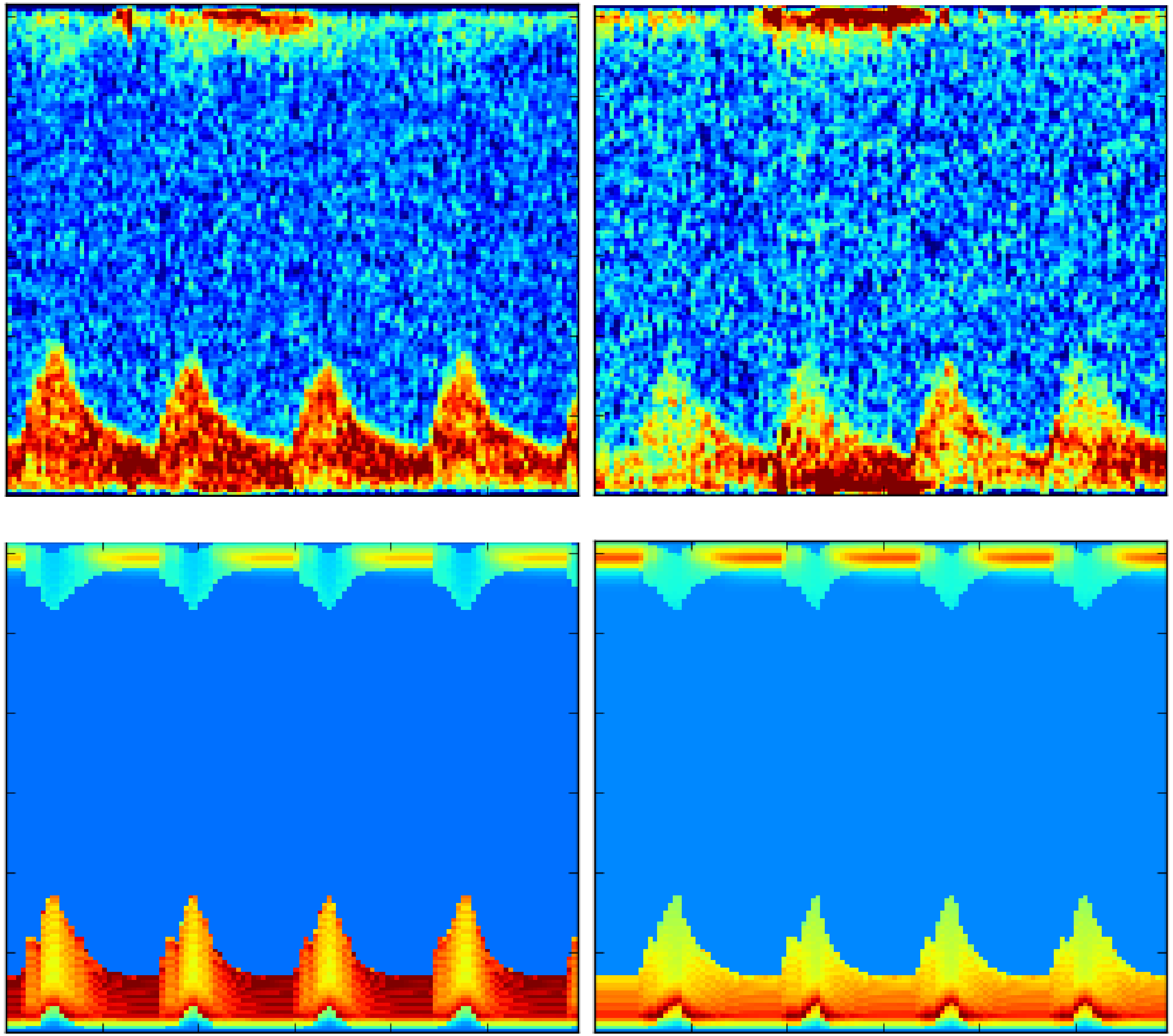


Signal of
Interaction Between
Flow and Vessel Wall

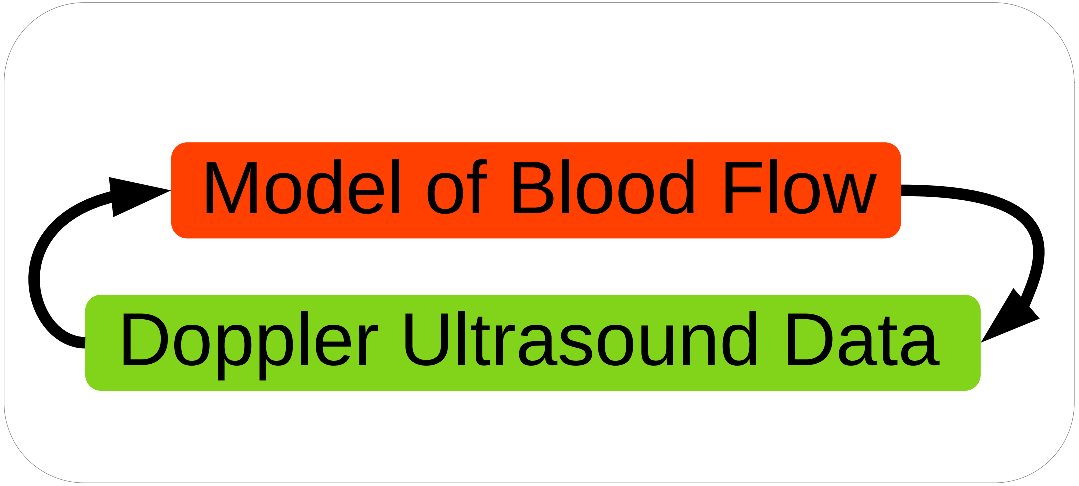
Advantage of a Closed Form Model

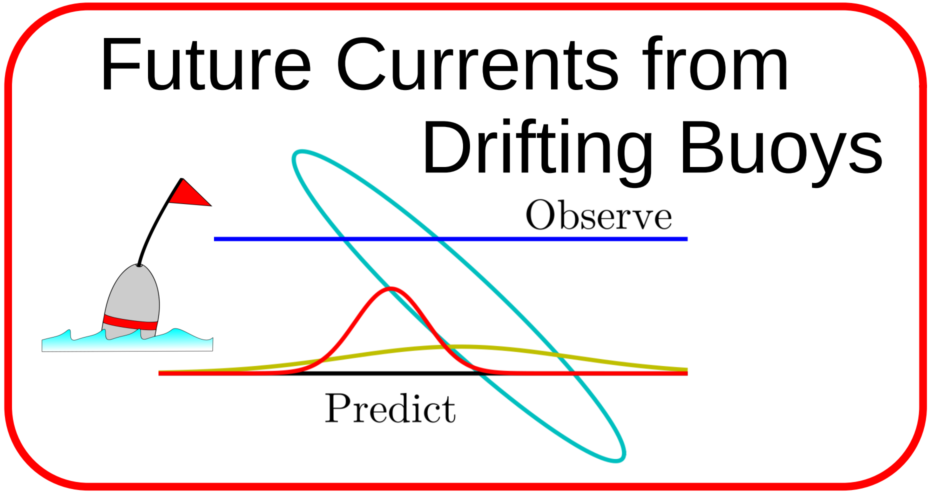


Same Patient Different Focal Point

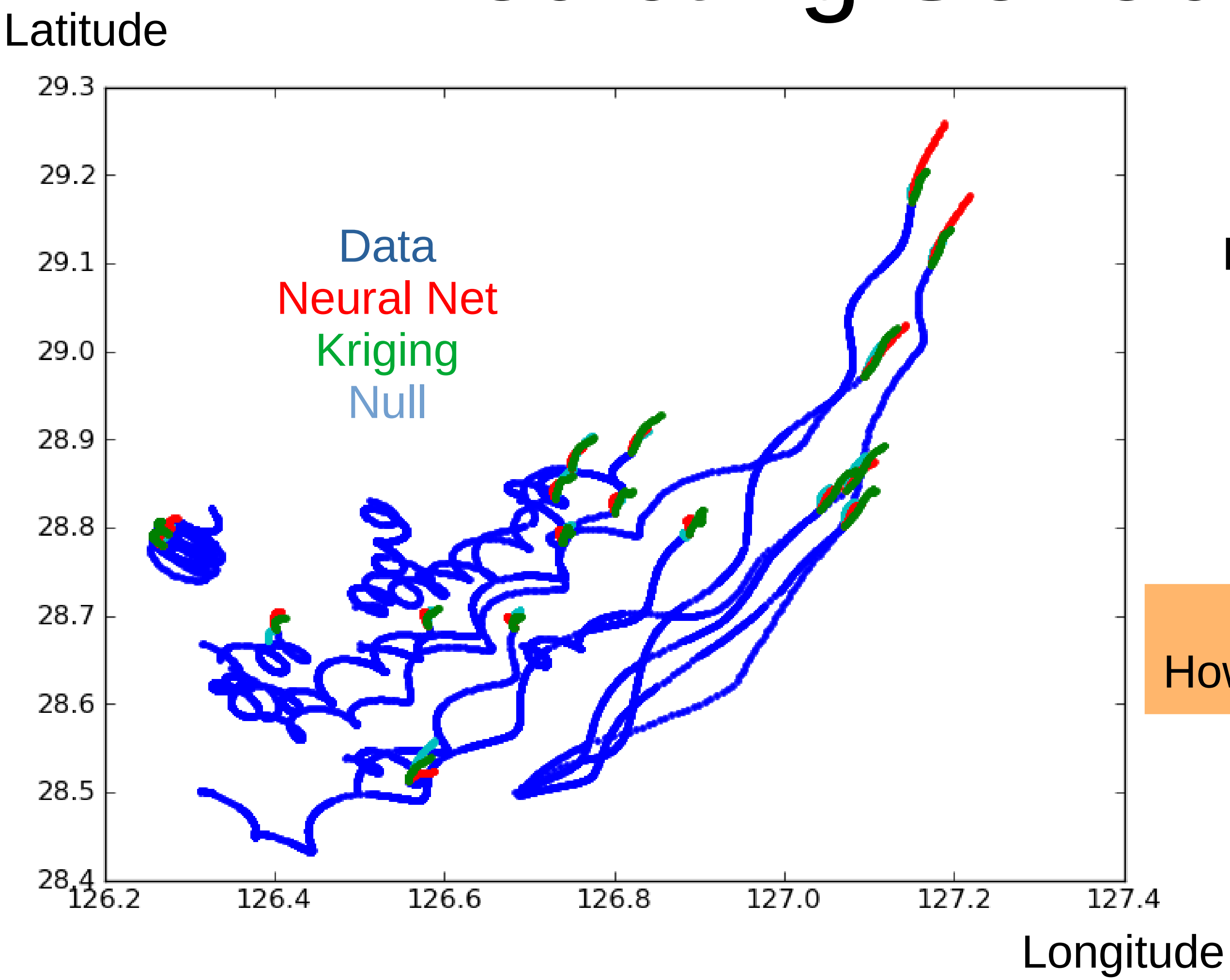


Flipped Priorities in Applied Statistics

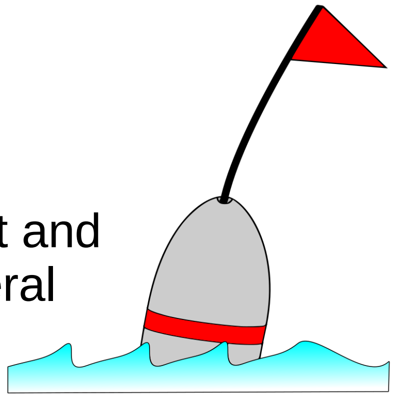




Predicting Sonobuoy Drift

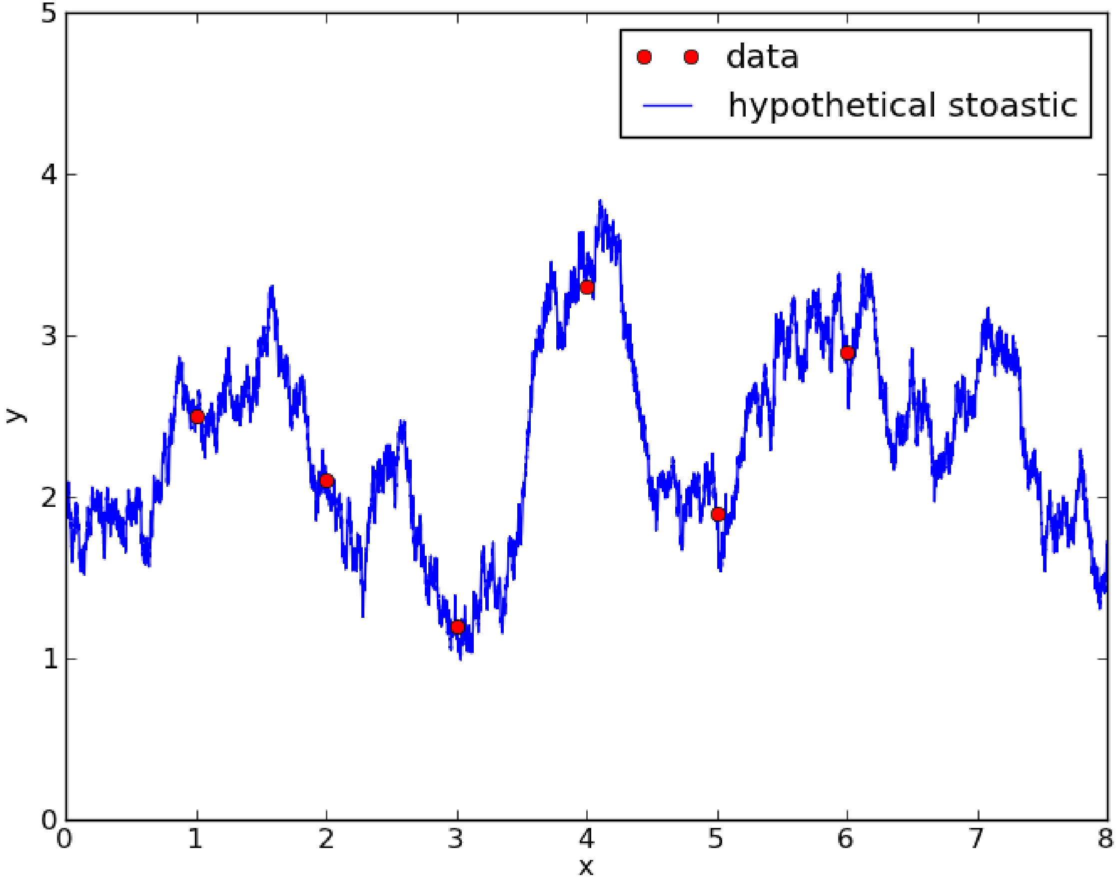


Predict Future Drift and Currents in General



After the sea trial, we asked:
How could we use ensemble forecasts?

Optimal Interpolation



Domain Experts

$$y = Xc + \varepsilon$$

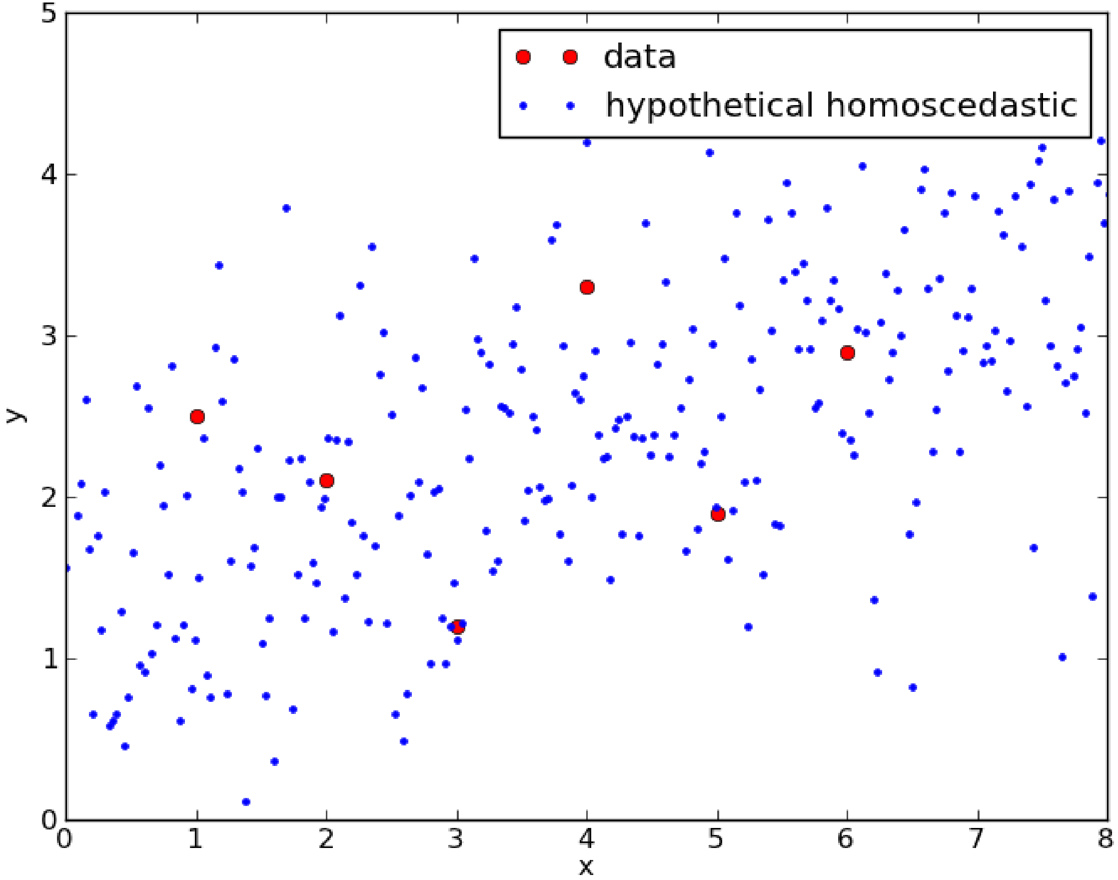
$$\begin{pmatrix} E[cc^t] & 0 \\ 0 & E[\varepsilon\varepsilon^t] \end{pmatrix}$$

Linear Statistics

$$a^* = \mu_a + C_{ab}C_{bb}^{-1}\left(b - \mu_b\right)$$

$$C_{aa|b} = C_{aa} - C_{ab}C_{bb}^{-1}C_{ab}^t$$

Optimal Interpolation



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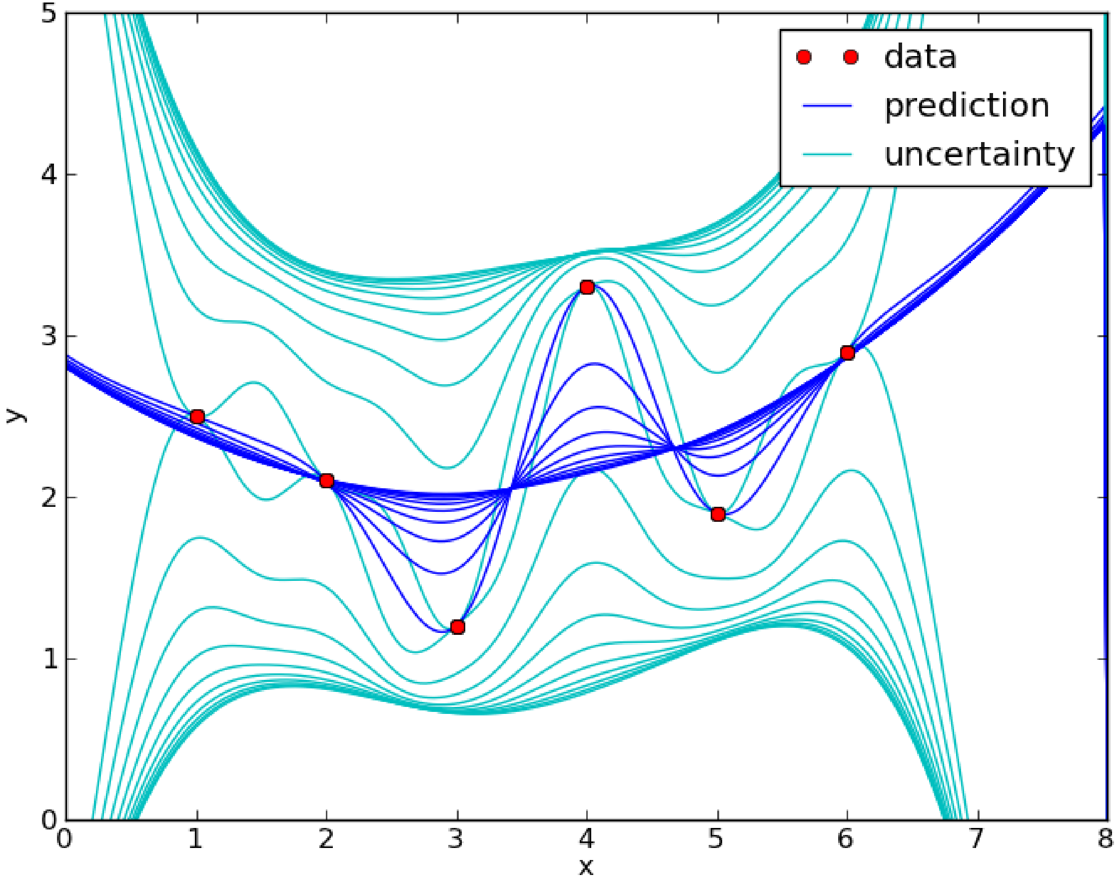
Optimal Interpolation



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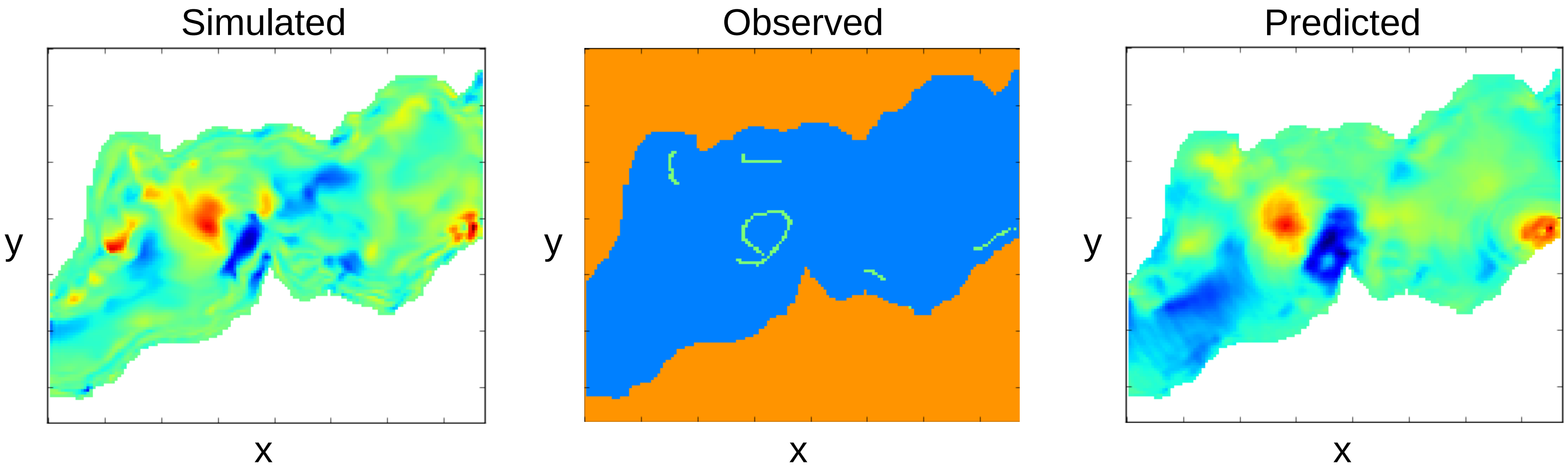
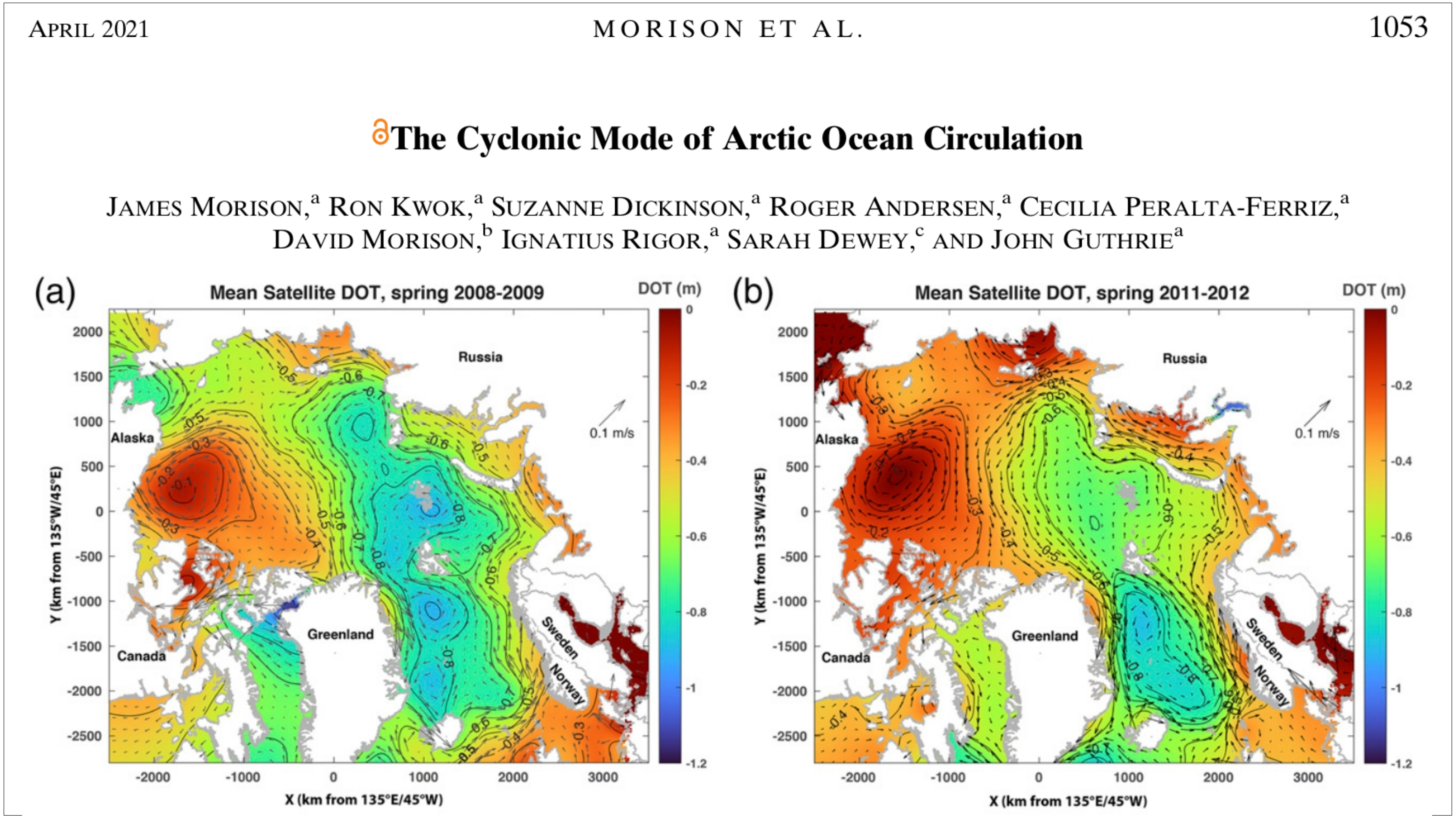
Proof of Concept



Velocity in x-Direction

Simulation of Tidal Flow at Three Tree Point Puget Sound by Sally Warner

Interdisciplinary Exchange of Predictions and Uncertainty



The Cyclonic Mode of Arctic Ocean Circulation

JAMES MORISON,[a] RON KWOK,[a] SUZANNE DICKINSON,[a] ROGER ANDERSEN,[a] CECILIA PERALTA-FERRIZ,[a] DAVID MORISON,[b] IGNATIUS RIGOR,[a] SARAH DEWEY,[c] AND JOHN GUTHRIE[a]

ICESat vs CryoSat-2

Leads vs Open Ocean

Along Track Data

Geoid Model Errors

Let the scientists do the science.

Thank You For Your Consideration!

Directorate: National Security

Division: Computing and Analytics

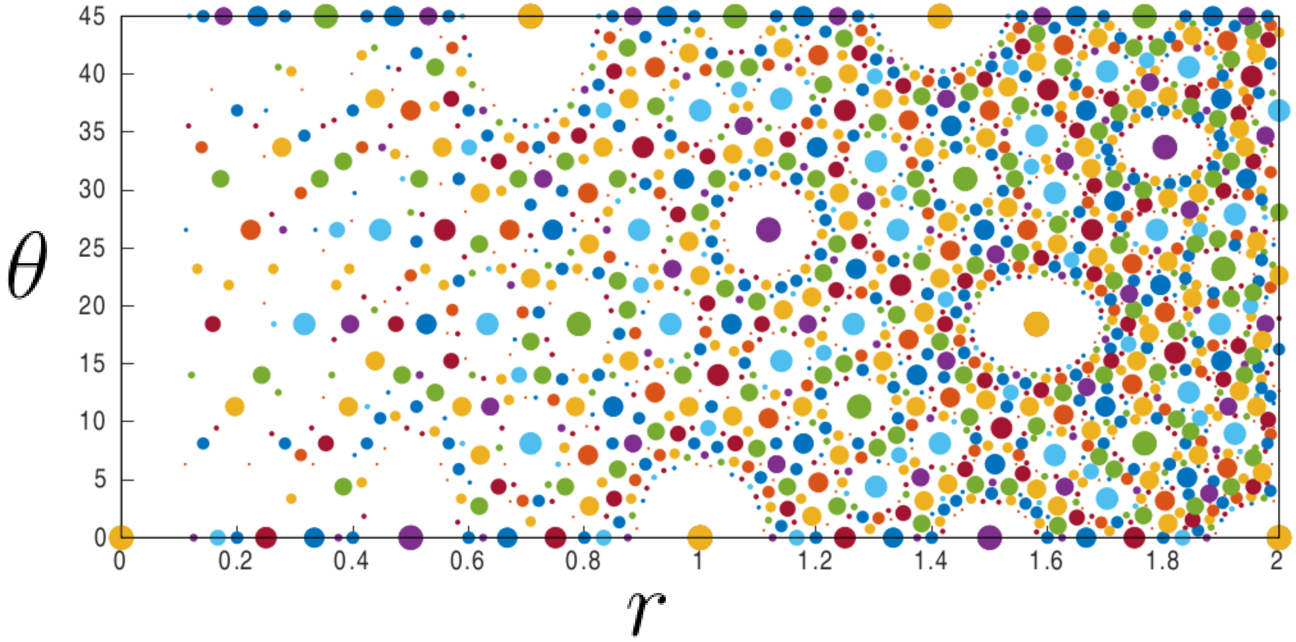
Group: Applied Statistics and Computational Modeling

Oct 20, 2021

Pacific Northwest
NATIONAL LABORATORY

Fractal Constellation of Periodic Systems

Beyond simple curiosity, calculating the distribution of (r,θ) pairs with finite L allows us to identify regions of (r,θ) where periodic systems are absent.



The identity transform and other “pathological” systems stand out.

Fractal Constellation of Periodic Systems

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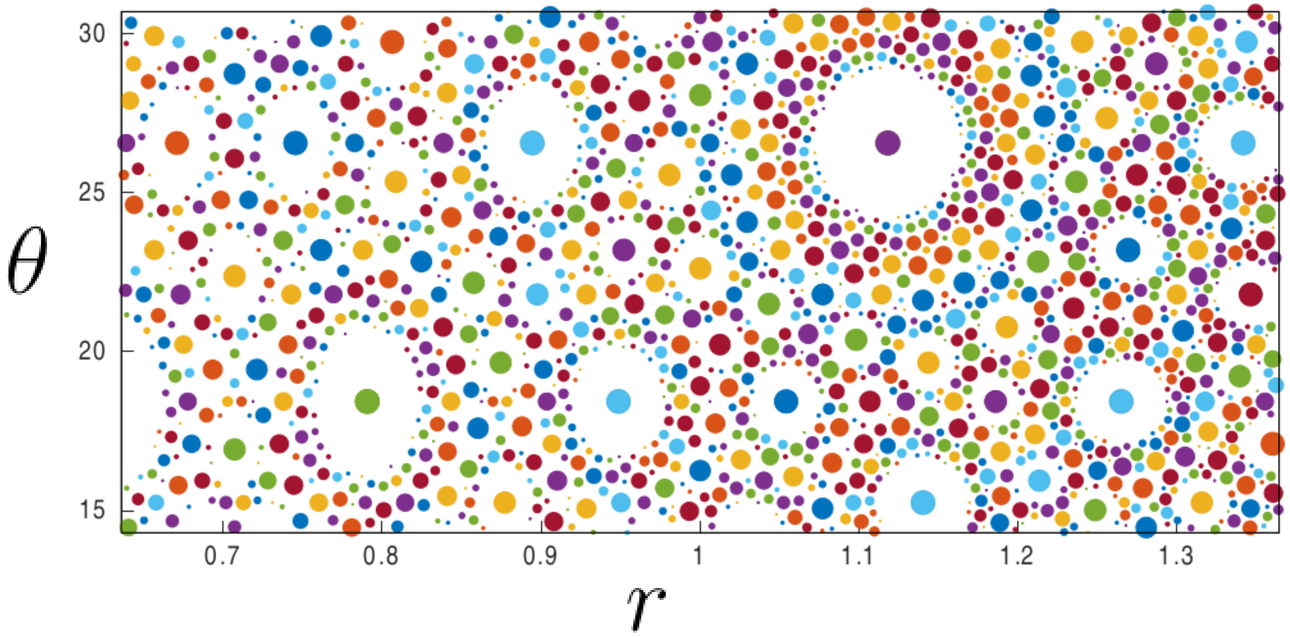

We zoom in a little.

Fractal Constellation of Periodic Systems

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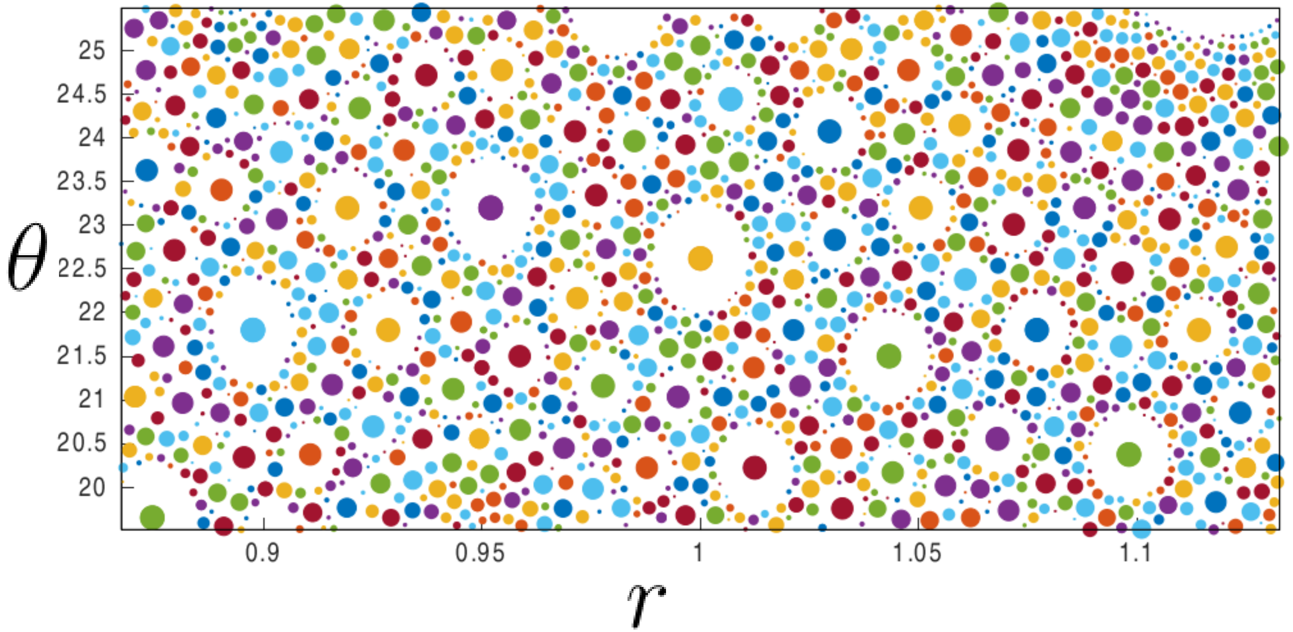

Short period systems seem to have “halos” of long period neighbors.

Fractal Constellation of Periodic Systems

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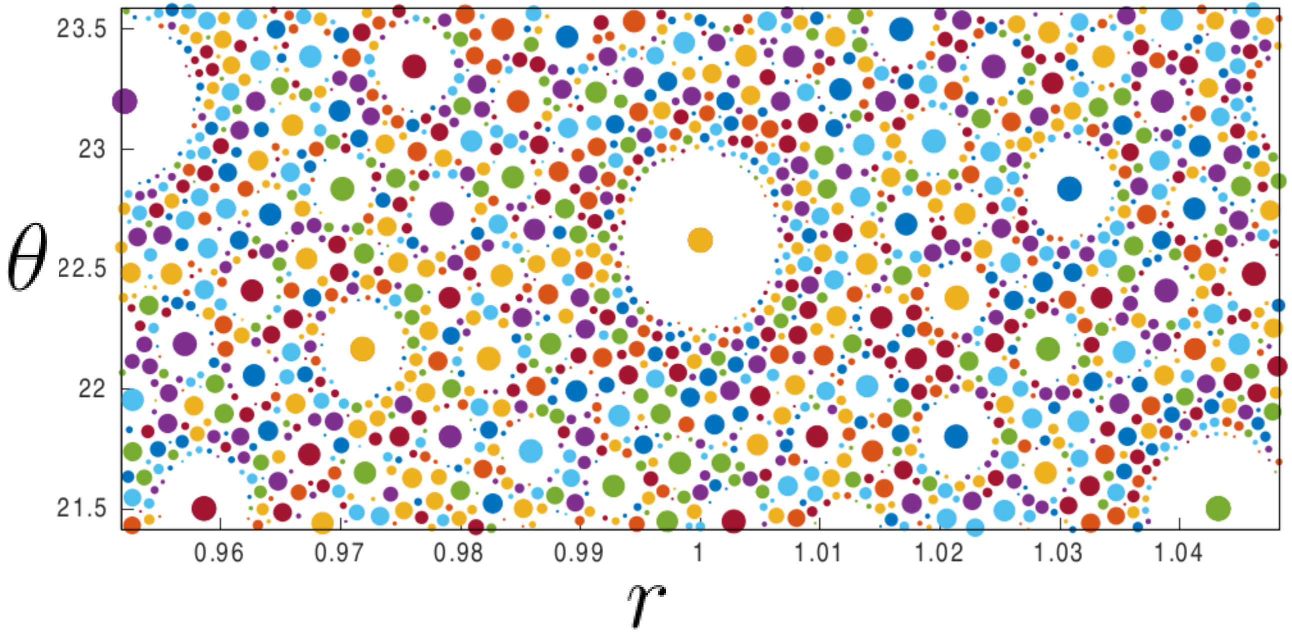
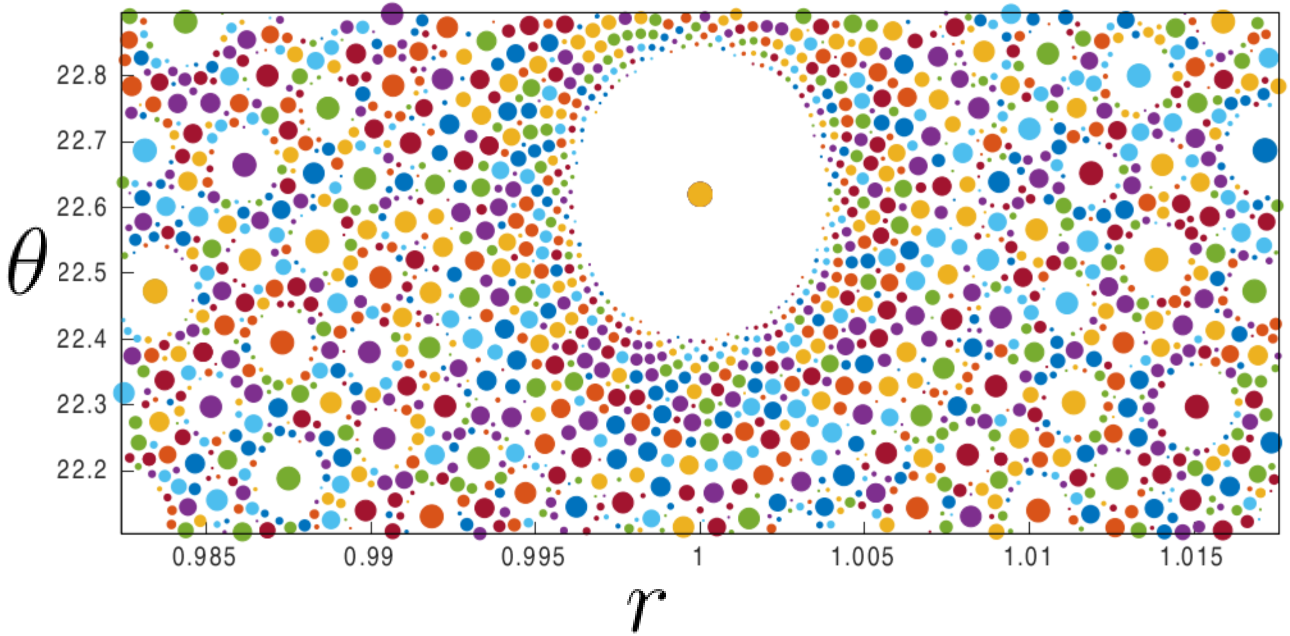


We zoom in towards one short period system.

Fractal Constellation of Periodic Systems

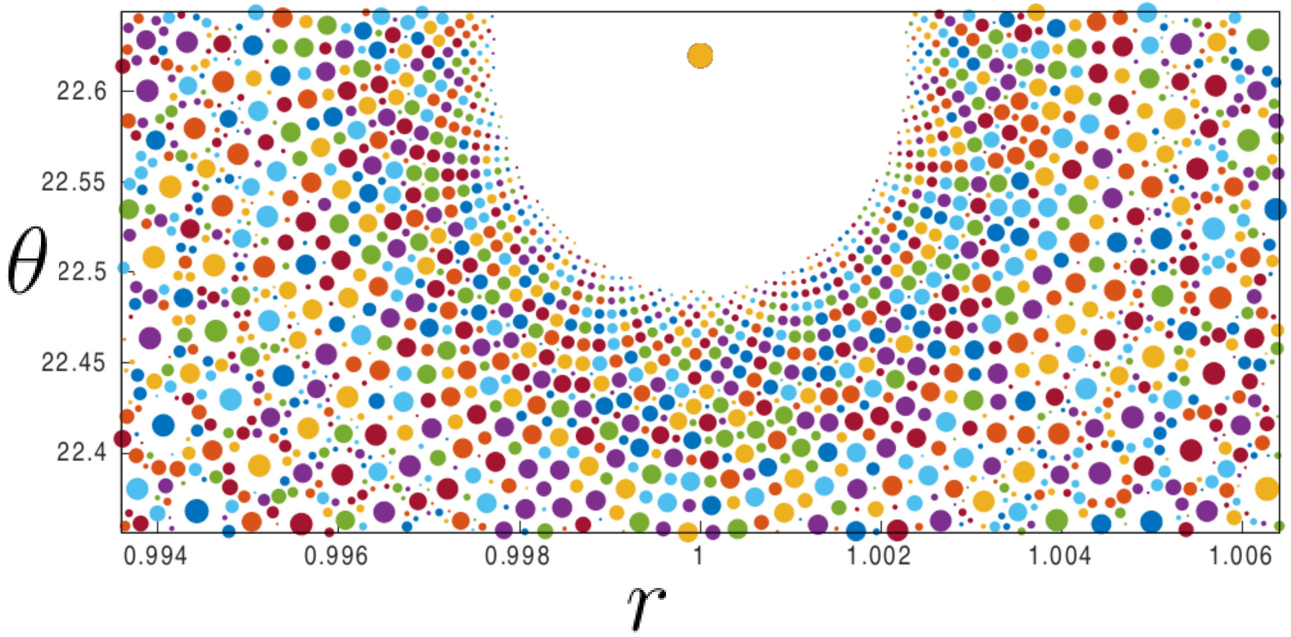
Beyond simple curiosity, calculating the distribution of (r,θ) pairs with finite L allows us to identify regions of (r,θ) where periodic systems are absent.



…a closer look into a “halo”...

Fractal Constellation of Periodic Systems

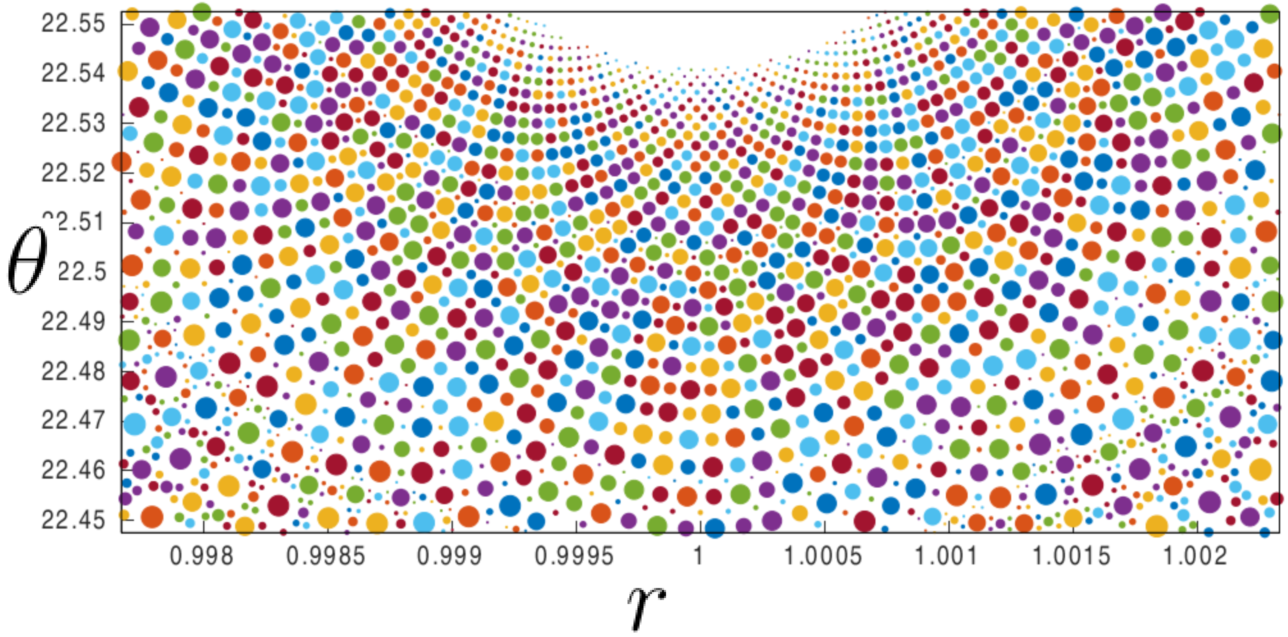
Beyond simple curiosity, calculating the distribution of (r,θ) pairs with finite L allows us to identify regions of (r,θ) where periodic systems are absent.



The distribution of short period systems seems orderly in some sense.

Fractal Constellation of Periodic Systems

Beyond simple curiosity, calculating the distribution of (r,θ) pairs with finite L allows us to identify regions of (r,θ) where periodic systems are absent.



...very ordered...

Fractal Constellation of Periodic Systems

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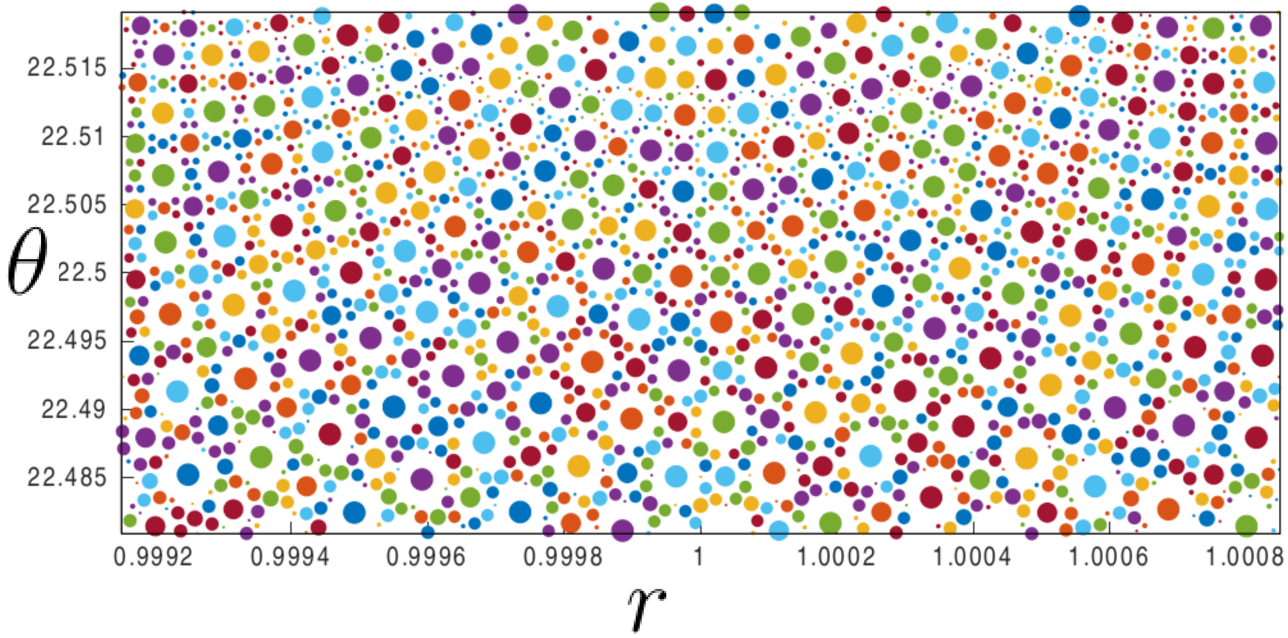
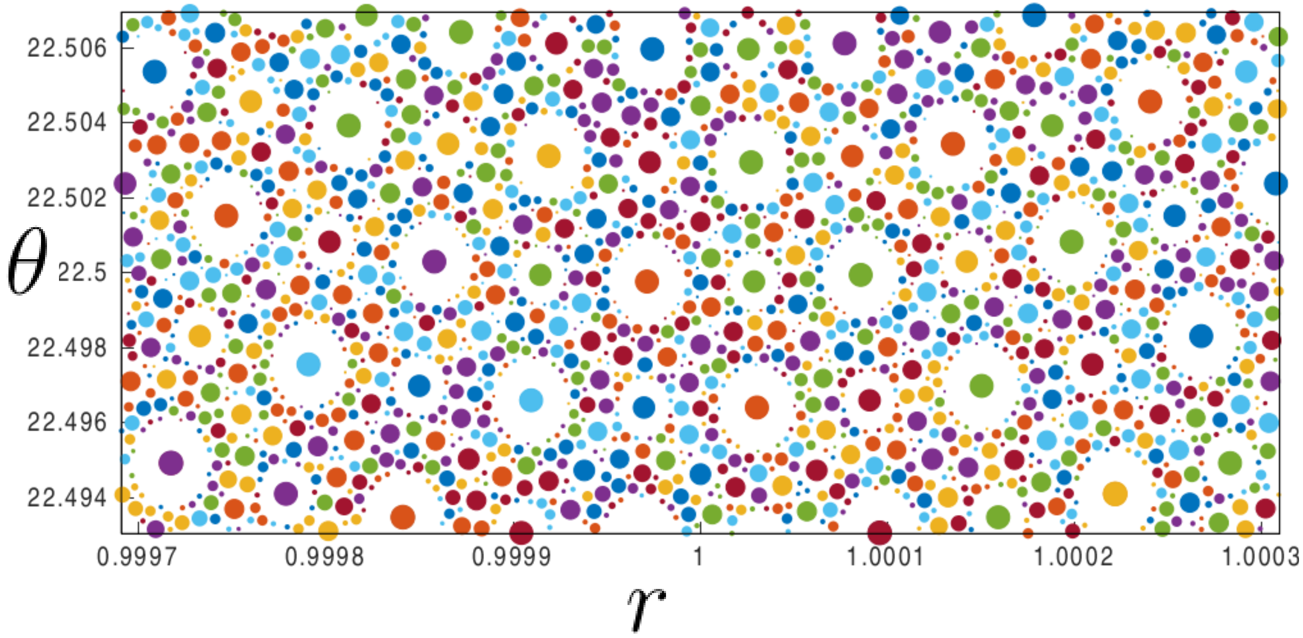


...closer in...

Fractal Constellation of Periodic Systems

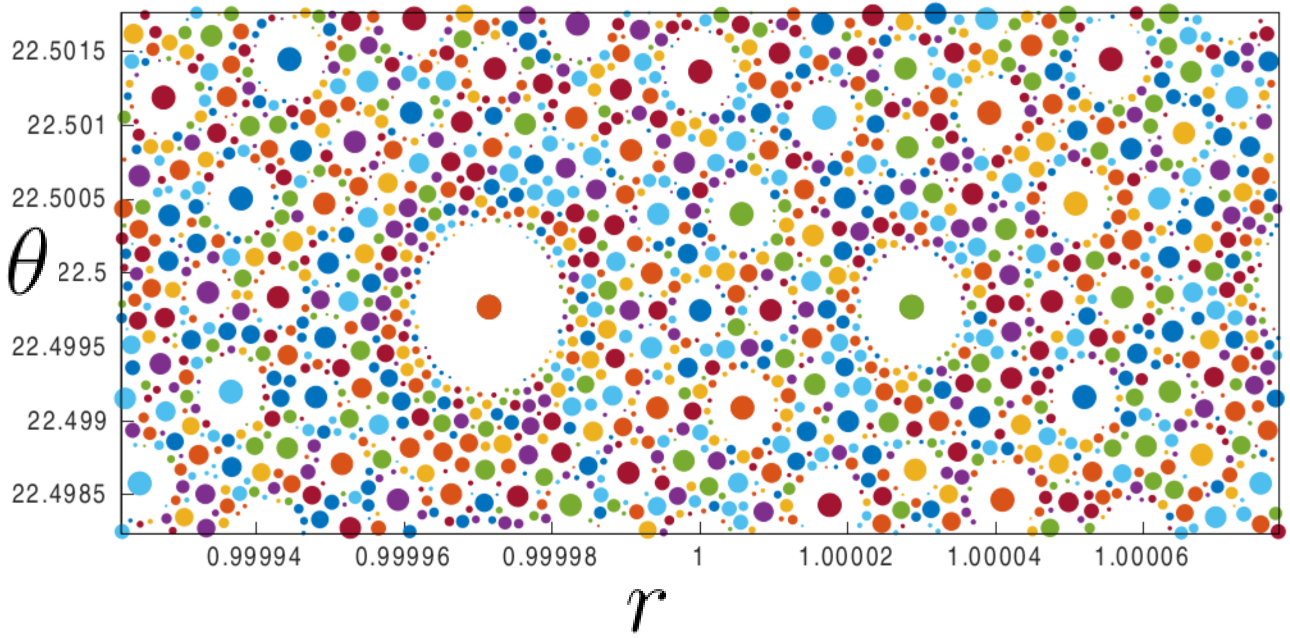
Beyond simple curiosity, calculating the distribution of (r,θ) pairs with finite L allows us to identify regions of (r,θ) where periodic systems are absent.



...more varied structure...

Fractal Constellation of Periodic Systems

Beyond simple curiosity, calculating the distribution of (r,θ) pairs with finite L allows us to identify regions of (r,θ) where periodic systems are absent.



We are back to a more "organic" appearing distribution of short period system parameters.

But, what about the inverse?

Desired Property

ϵ^*

Microgeometry

χ

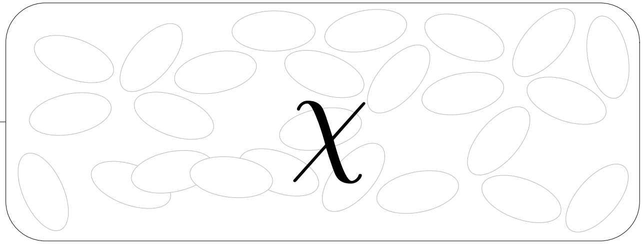
Constituent Materials

ϵ_1 ϵ_2

Stieltjes Integral Representation

Bergman (1980) Milton (1980) Golden and Papanicolaou (1983)

Microgeometry



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

Material Properties

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