Towards a gradient flow for microstructure:

microstructure meets Boltzmann

David Kinderlehrer

Department of Mathematical Sciences and
Center for Nonlinear Analysis
Carnegie Mellon University

Entropies, the Geometry of Nonlinear Flows, and their Applications

Banff International Research Station
for Mathematical Innovation and Discovery

Research supported by NSF DMR 0520425, DMS 0405343, DMS 0305794, DMS 0806703, DMS 0635983, DMS 0915013, DMS 1112984 OISE-0967140 and Simons Foundation Grant 415673.

Collaborators

Patrick Bardsley (Texas) Katayun Barmak (Columbia)
Eva Eggeling (Graz) Maria Emelianenko (George Mason)
Yekaterina Epshteyn (Utah) Xin Yang Lu (Lakehead)
Richard Sharp (Microsoft) Shlomo Ta'asan (CMU)

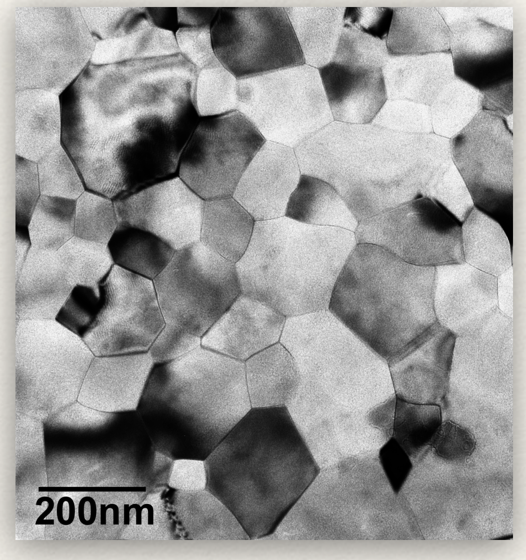
[1] Patrick Bardsley, Katayun Barmak, Eva Eggeling, Yekaterina Epshteyn, David Kinderlehrer, and Shlomo Ta'asan. Towards a gradient flow for microstructure. Atti Accad. Naz. Lincei Rend. Lincei Mat. Appl., 28(4):777–805, 2017.

[2] K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R. Sharp, and S. Ta'asan. Critical events, entropy, and the grain boundary character distribution. Phys. Rev. B, 83(13):134117, Apr 2011.

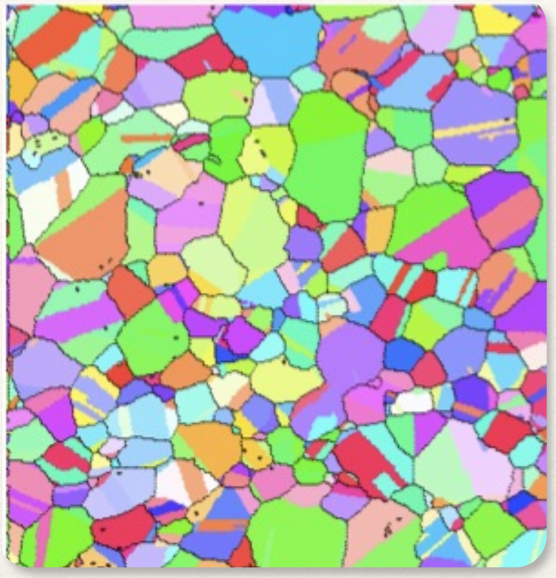
[3] Katayun Barmak, Eva Eggeling, Maria Emelianenko, Yekaterina Epshteyn, David Kinderlehrer, Richard Sharp, and Shlomo Ta'asan. An entropy based theory of the grain boundary character distribution. Discrete Contin. Dyn. Syst., 30(2):427–454, 2011.

thanks to Gregory Rohrer, Anthony Rollett,
Russell Schwab. Xiang Xu,
Center for Nonlinear Analysis &
Carnegie Mellon Materials Research Science and
Engineering Center

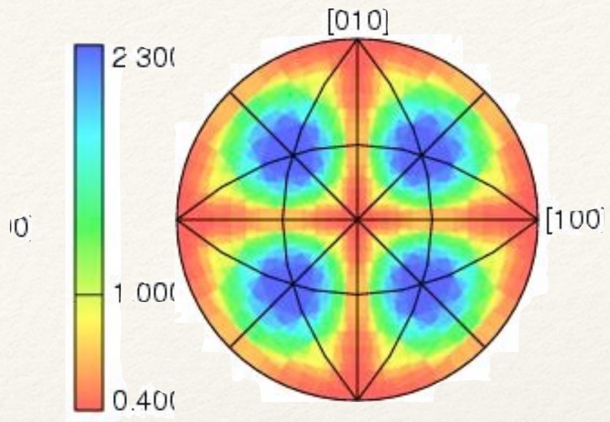
material microstructure texture



Al thin film (Barmak)
resistivity of thin films:
Mayadas-Schatzke theory



Ni cells showing orientations



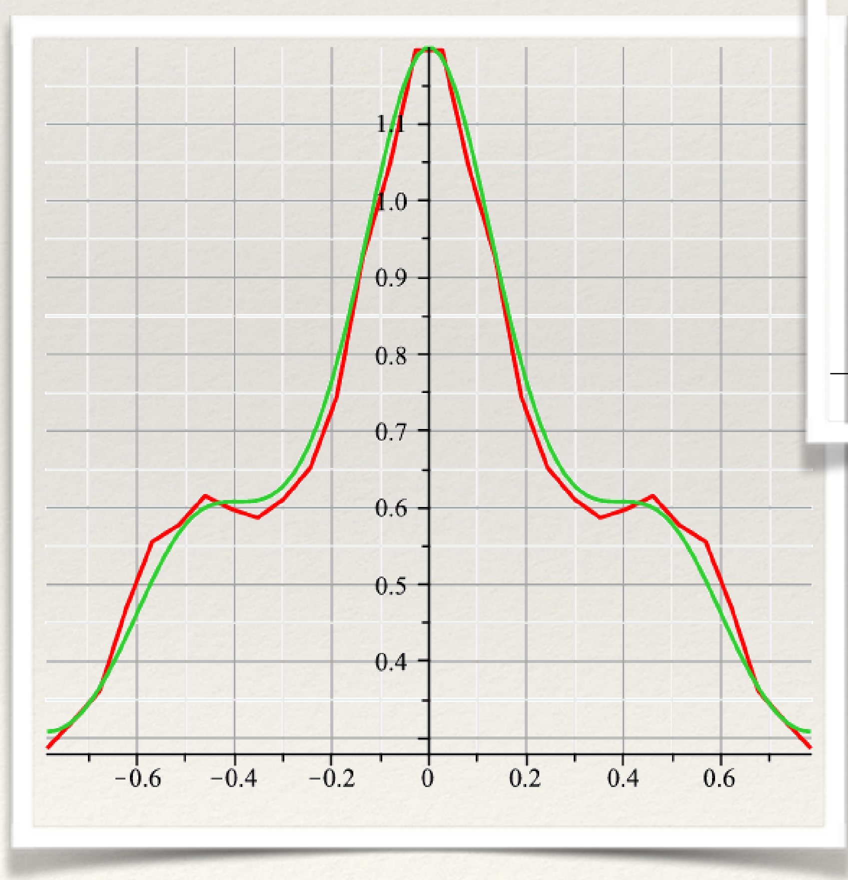
Al: conventional pole figure
showing distribution of
cell boundaries: **not uniform**

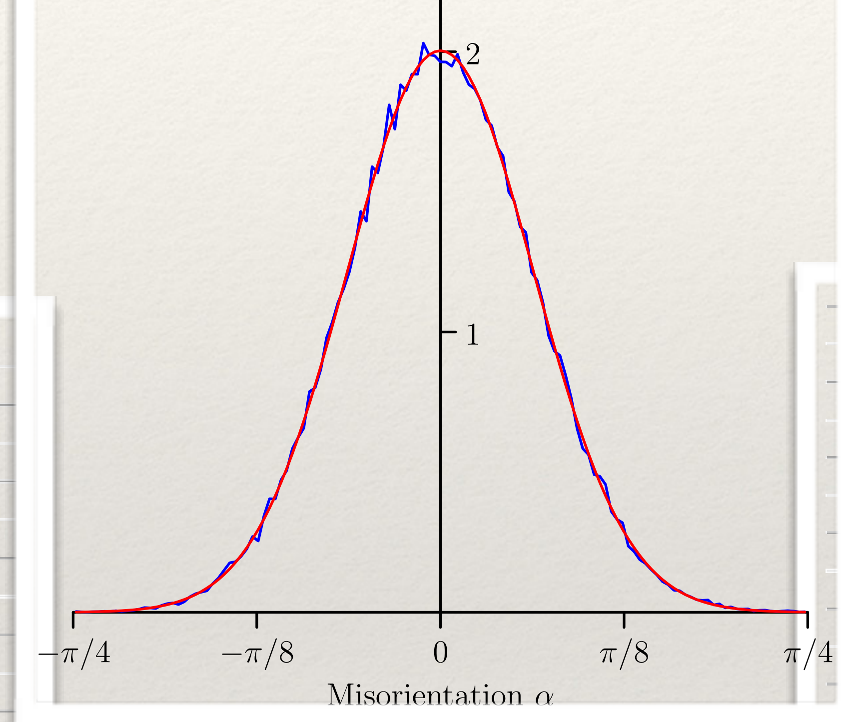
- Cellular structures are ubiquitous: most materials, natural and engineered, are polycrystalline, consisting of a myriad of small grains separated by interfaces, the grain boundaries. Our interest is texture.

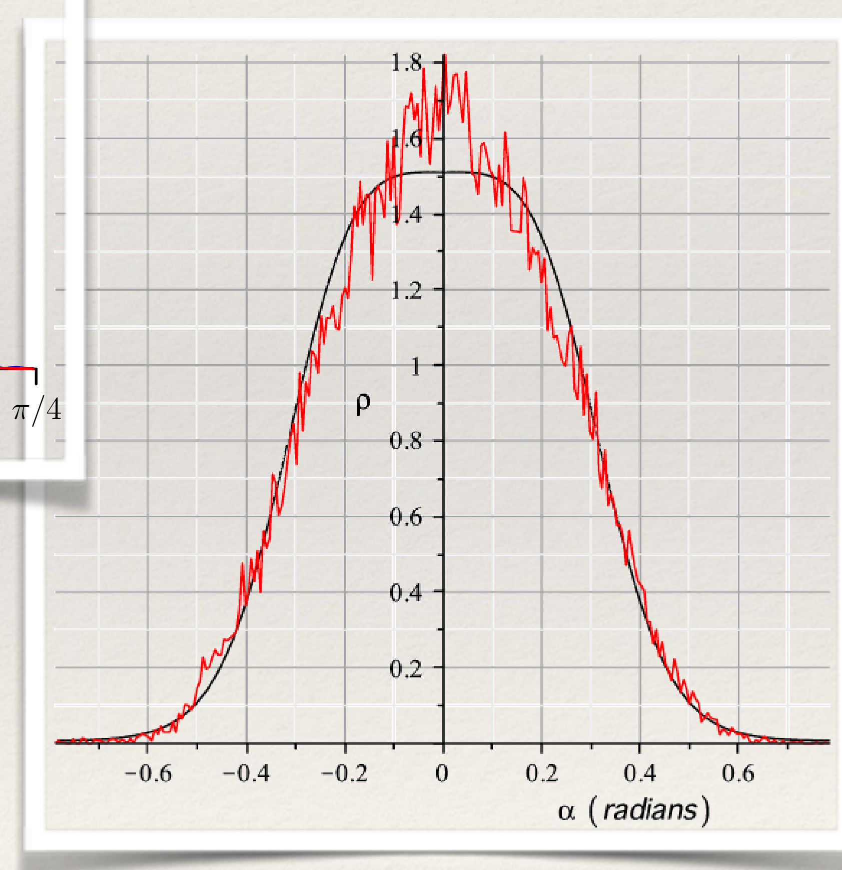
- Microstructures coarsen, according to thermodynamics with topological constraints, dissipating energy as some cells, or grains, expand, while others disappear.

- Grain Boundary Character Distribution (GBCD) is a portrayal of texture and shows that the boundary network has order.

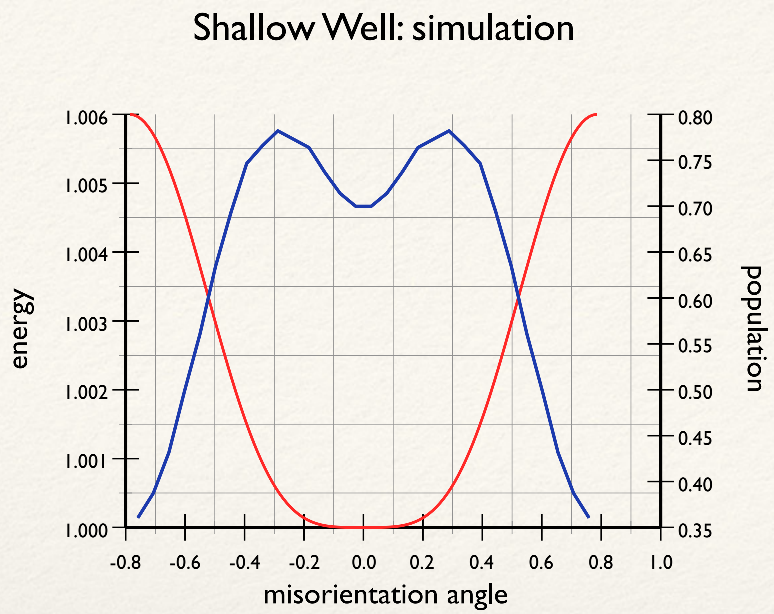
- Simulate the evolution of this network using conventional univerally accepted theory. This by itself is an enterprise.
- Harvest GBCD statistics
- interfacial energy depends on crystallography alone $\Rightarrow$ GBCD is a Boltzmann distribution.
- Among the simplest distributions, corresponding to independent trials with respect to the interfacial energy density. Why does such simplicity emerge from such complexity?

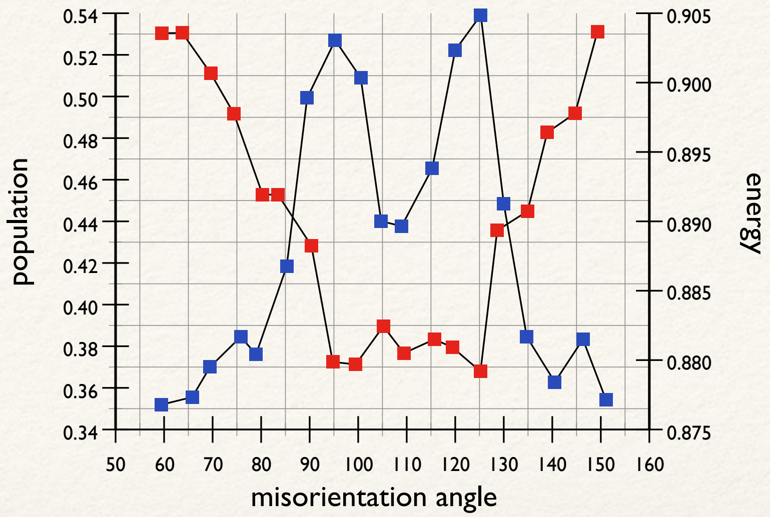




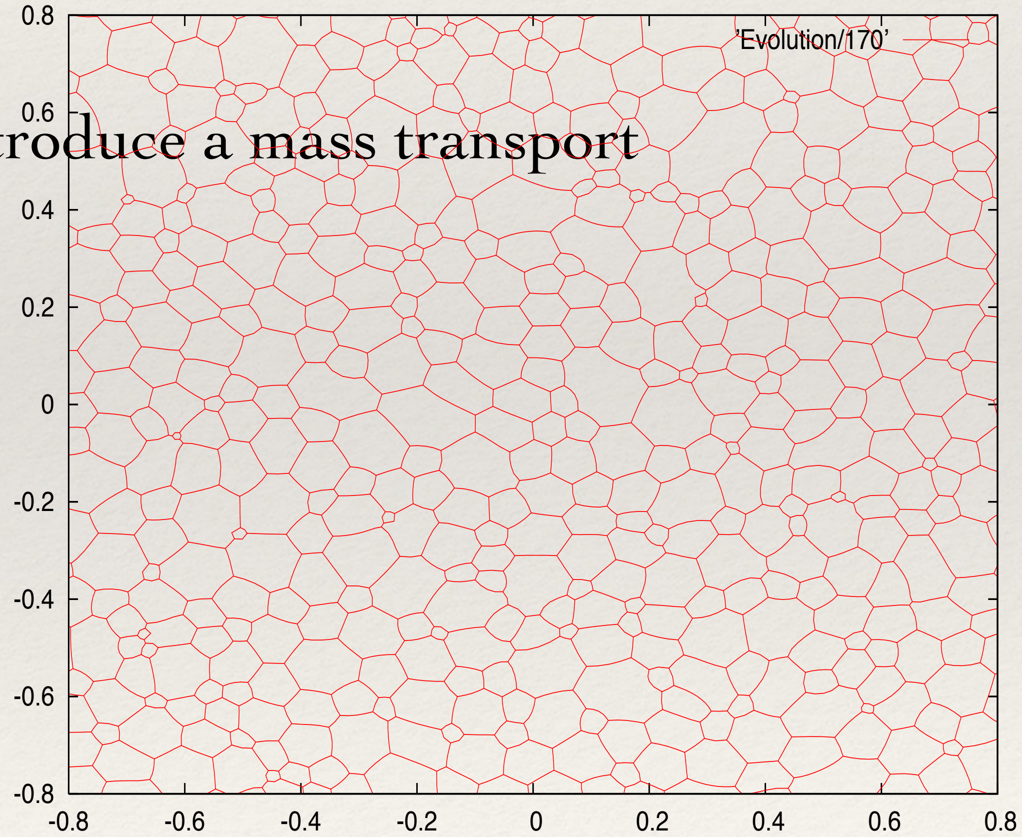


scrapbook of Boltzmanns





consistent with experiment



- GBCD is the solution of an equation: will introduce a mass transport based theory

gradient flow

gradient flow for Fokker-Planck (De Giorgi minimizing movements)
Ambrosio, Gigli, Savaré
Santambrogio

$$F(\rho) = \int_\Omega (\psi\rho + \sigma\rho\log\rho)dx \quad \text{free energy}$$

$$\frac{\partial\rho}{\partial t} = \frac{\partial}{\partial x}(\sigma\frac{\partial\rho}{\partial x} + \psi'\rho) \text{ in } \Omega \qquad \rho \geqq 0, \quad \int_\Omega \rho dx = 1$$

$$\sigma\frac{\partial\rho}{\partial x} + \psi'\rho = 0 \text{ on } \partial\Omega$$

conventional gradient flow: $\dfrac{d\xi}{dt} = -\nabla\varphi(\xi)$ De Giorgi

$$\varphi(\xi(t)) - \varphi(\xi(t+\tau)) - \left(\frac{1}{2}\int_t^{t+\tau} |\nabla\varphi|^2 dt' + \frac{1}{2}\int_t^{t+\tau} |\frac{d\xi}{dt}|^2 dt'\right)$$

$$\leqq 0$$

$$= 0 \;\Leftrightarrow\; \text{only for gradient flow}$$

ρ gradient flow for

$$F(\rho) = \int_\Omega \Big(\psi\rho + \sigma\rho\log\rho)dx$$

$$\Leftrightarrow$$

$$\rho_t = (\sigma\rho_x + \psi'\rho)_x \text{ in } \Omega$$

characterized by

$$F(\rho)\Big|_{t_0} - \Big\{F(\rho)\Big|_{t_0+\tau} + \frac{1}{2}\int_{t_0}^{t_0+\tau}\int_\Omega (\sigma\frac{\rho_x}{\rho} + \psi')^2\rho dx dt + \frac{1}{2}\int_{t_0}^{t_0+\tau}\int_\Omega v^2\rho dx dt\Big\}$$
$$= 0,\ t_0, \tau \geqq 0,$$
$$\rho_t + (v\rho)_x = 0,$$

which comes from

$$\frac{d}{dt}F(\rho) = \int_\Omega (\sigma\frac{\rho_x}{\rho} + \psi')v\rho dx$$
$$\geqq -\frac{1}{2}\int_\Omega (\sigma\frac{\rho_x}{\rho} + \psi')^2\rho dx - \frac{1}{2}\int_\Omega v^2\rho dx$$

entropy by itself does not characterize a gradient flow

realize solution of equation (and gradient flow)
as implicit scheme for the (Kantorovich-Rubinstein-)Wasserstein metric

given $\rho^* = \rho^{(k-1)}$ determine $\rho^{(k)} = \rho$ as the solution of

$$\frac{1}{2\tau} d(\rho, \rho^*)^2 + F_\sigma(\rho) = \inf$$

Jordan, K, Otto
(SIAM Math Anal 1998)

Set

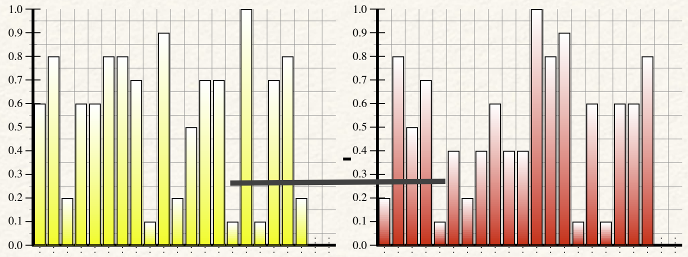
$$\rho^{(\tau)}(x,t) = \rho^{(\tau,k)}(x) \text{ for } (k-1)\tau < t \leqq k\tau$$

$$\rho = \lim_{\tau \to 0} \rho^{(\tau)} \qquad \text{is solution of FP}$$

discrete Euler equation is

$$\frac{1}{\tau}(x-\phi)+(\sigma\frac{\rho_x}{\rho}+\psi')=0 \text{ in } \Omega$$

$$\phi = \text{transfer function from } \rho \text{ to } \rho^*$$



idea of mass transport

GF condition satisfied with = with W metric at level of the implicit scheme:

$$\frac{1}{\tau}d(\rho,\rho^*)^2=\frac{1}{\tau}\int_\Omega (x-\phi(x))^2\rho dx=\tau\int_\Omega(\sigma\frac{\rho_x}{\rho}+\psi')^2\rho dx$$

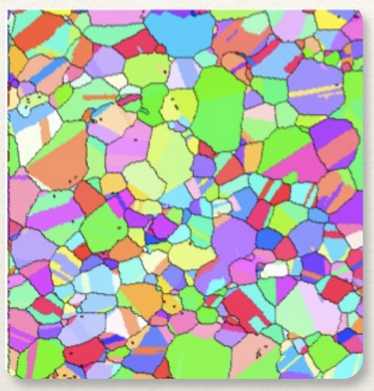
leads to
discrete GF conditions

$$F(\rho^{(k-1)})-\left\{F(\rho^{(k)})+\frac{1}{\tau}d(\rho^{(k-1)},\rho^{(k)})^2\right\}=0,$$

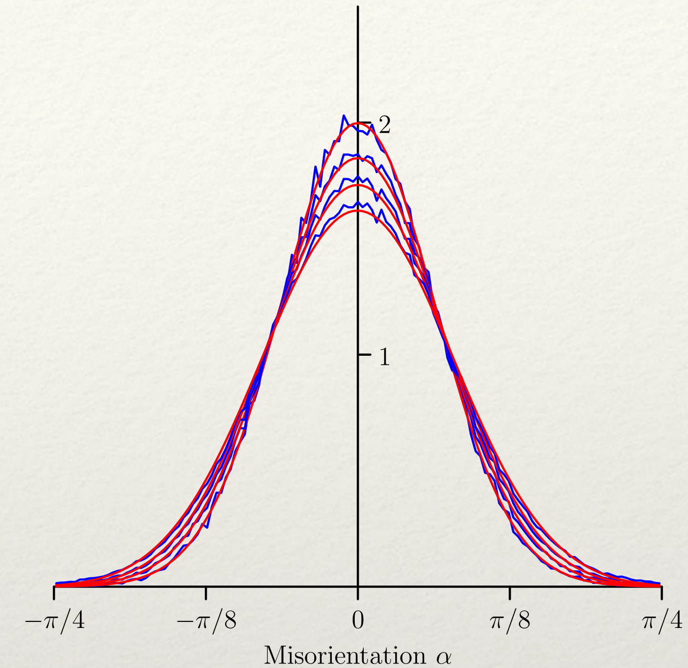
$$F(\rho^{(k-1)})-\left\{F(\rho^{(k)})+\tau\int_\Omega(\sigma\frac{\rho_x^{(k)}}{\rho^{(k)}}+\psi')^2\rho^{(k)}dx\right\}=0$$

our theme:

- the collection of harvested statistics satisfies the discrete GF conditions and thus GBCD statistics arise as the iterates of the W-implicit scheme



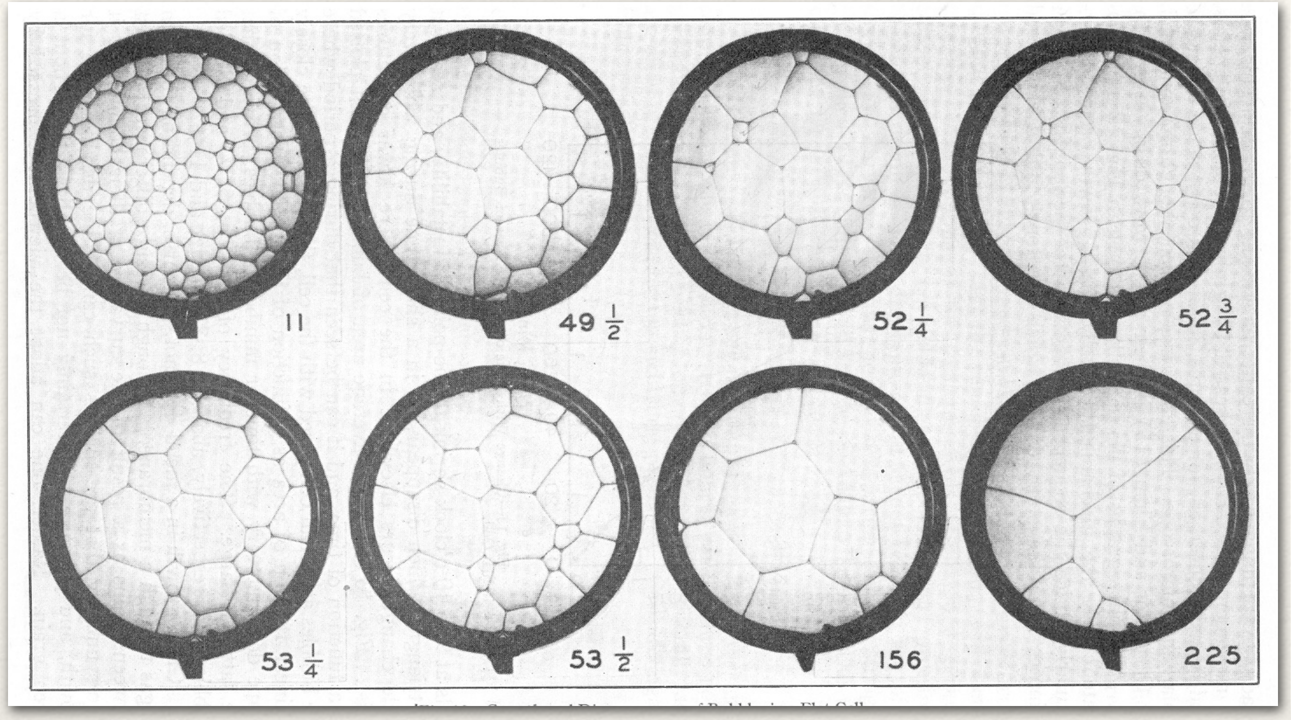
gradient flow

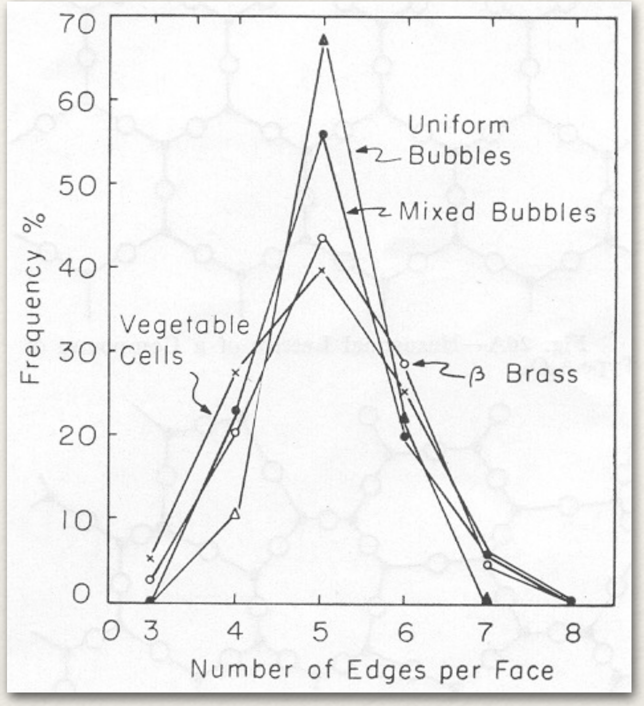


- GBCD is a gradient flow $\Rightarrow$ solution of Fokker-Planck PDE

- verification is astonishingly accurate
- can we explore other systems?

C.S. Smith (1951) on microstructural coarsening





(Le Caer's Law)

Soap froth

The average number of facets per cell = 6 (constraint on Euler characteristic of simplicial decomposition of the plane when only triple junctions are permitted)*

coarsening is governed by two global features

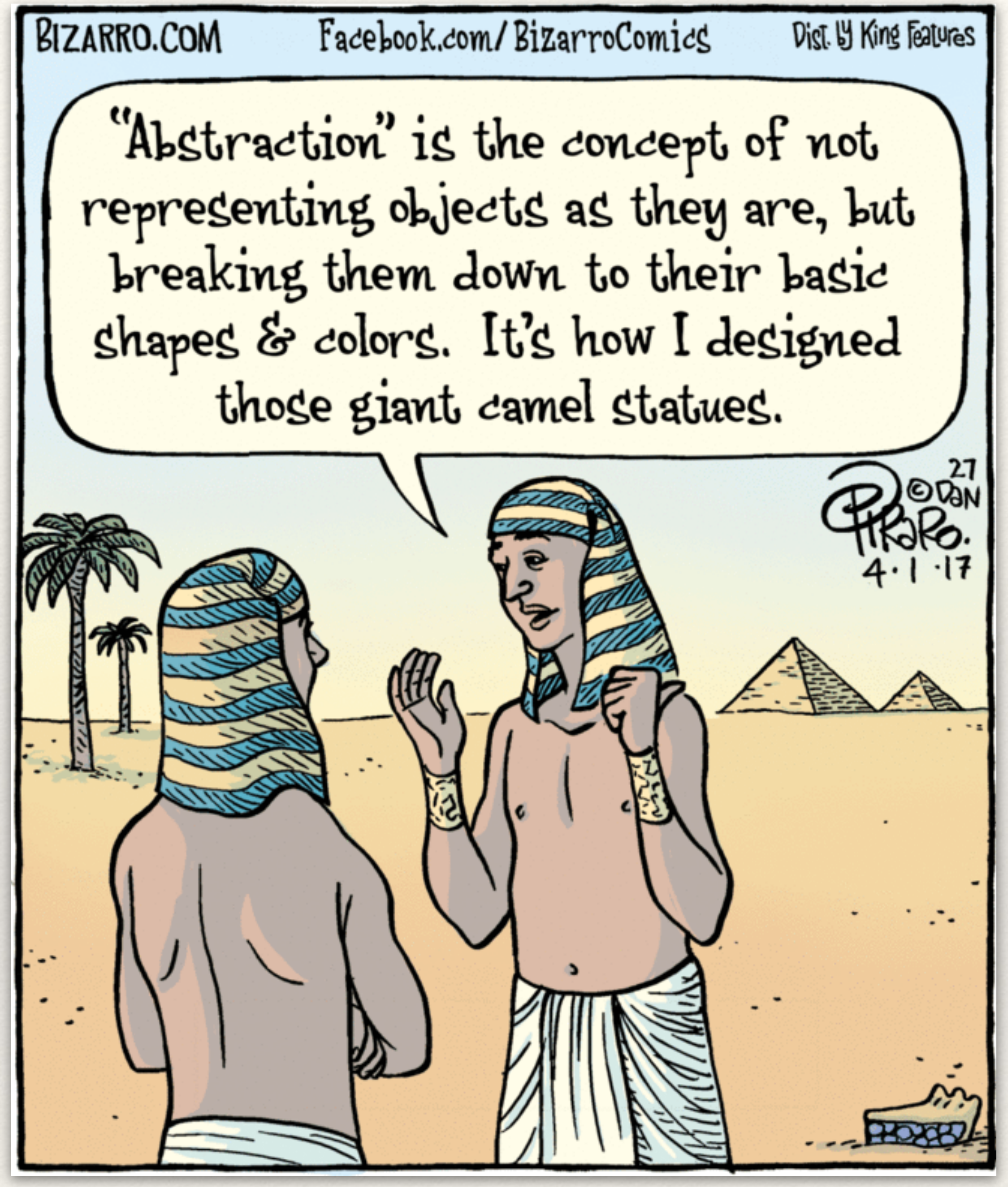
- cell growth according to a local evolution law

in competition with

- space filling constraint

simulation is the testbed to examine these two features

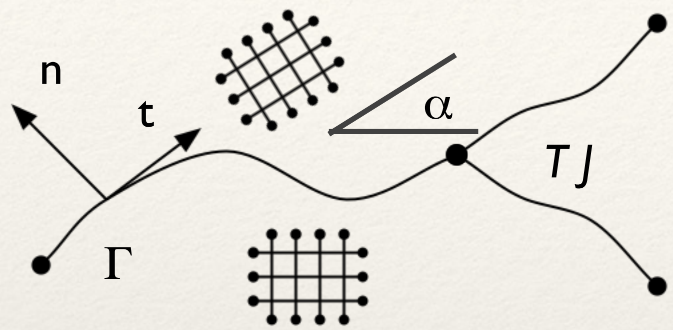
* W.G. Graustein, Ann. of Math., 1932; applied to plant cells


BIZARRO.COM
Facebook.com/BizarroComics
Dist. by King Features
"Abstraction" is the concept of not representing objects as they are, but breaking them down to their basic shapes & colors. It's how I designed those giant camel statues.
27 ©DAN PIRARO. 4·1·17

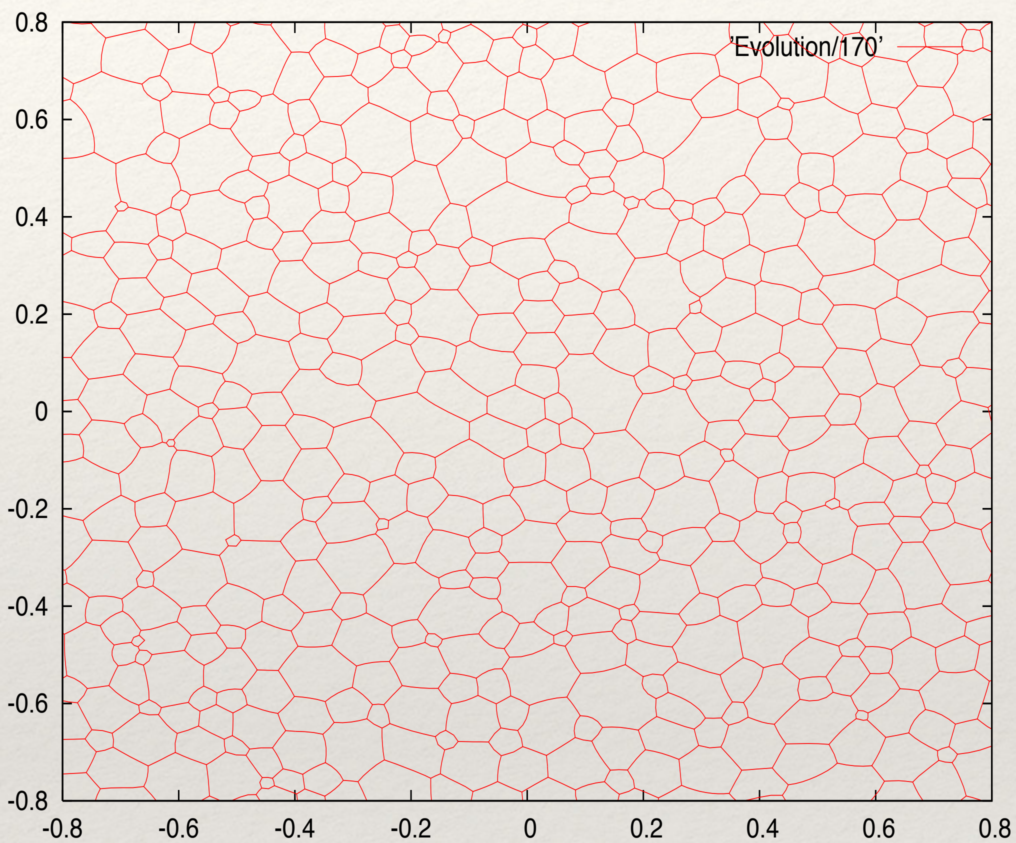
Evolving networks (reprise)

- local evolution

curvature driven growth: Burkart and Read $\rightarrow$ .... $\rightarrow$ Mullins and Herring



$$n = (\cos\theta, \sin\theta)$$
$$v_n = \text{normal velocity}$$
$$\kappa = \text{curvature}$$
$$\psi(n,\alpha) = \text{GB energy}$$



$$v_n = \mu(\psi_{\theta\theta} + \psi)\kappa \text{ on } \Gamma$$ Mullins Equation

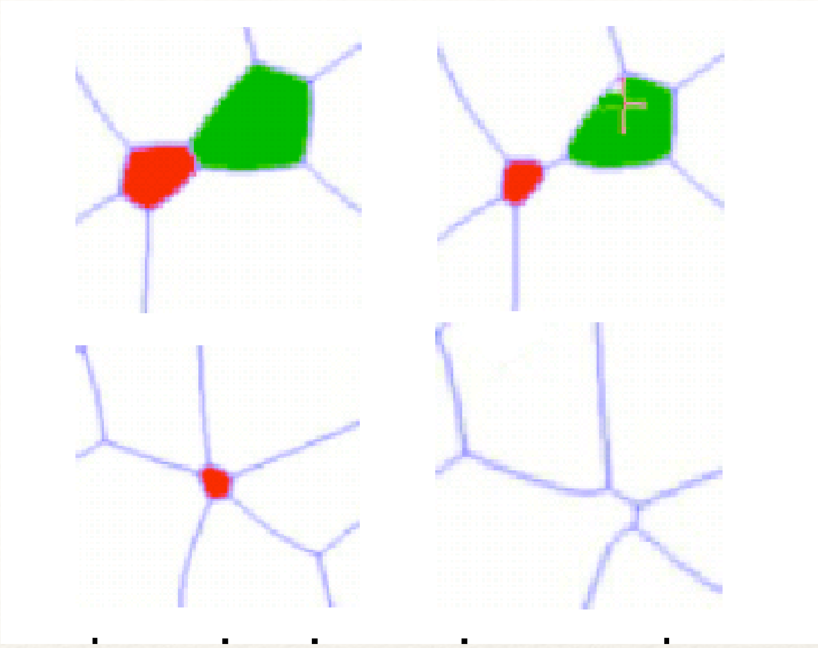
$$\sum_{TJ}(\psi_\theta n + \psi t) = 0 \quad \text{at} \quad \text{TJ's}$$ Herring Condition

- space filling constraint

critical events or rearrangement events:

facet interchange

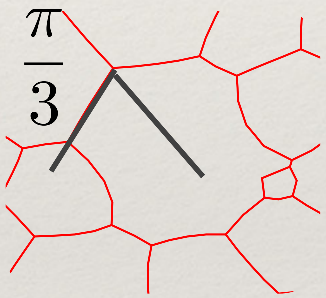
grain deletion

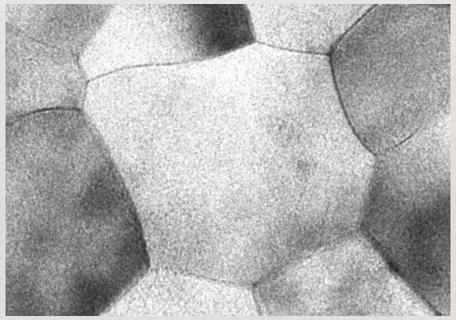


von Neumann-Mullins n - 6 rule:

if a cell has n facets then

$$\frac{dA}{dt} = c(n-6) \text{ when } \psi = \text{const.}$$





recent result of MacPherson & Srolovitz (2007)
for high dimension (Hadwiger measure)

Bronsard & Reitich
K & Liu

Dissipation

$$E(t) = \sum_{\{\Gamma\}} \int_\Gamma \psi(n,\alpha)|t|ds$$

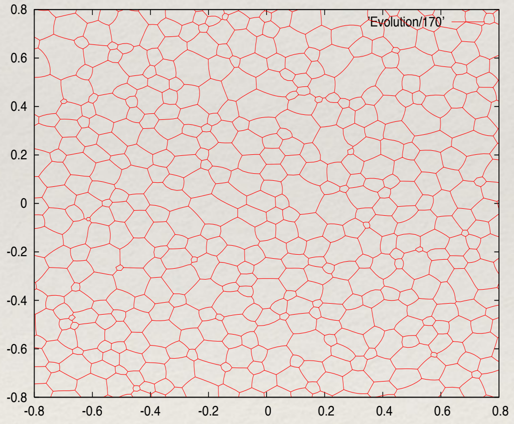
energy

$$\frac{dE}{dt} = -\sum_{\Gamma} \int_\Gamma v_n^2 ds + \sum_{\{TJ\}} v \cdot \sum_{TJ} (\psi_\theta n + \psi t)$$

$$\leqq \quad 0$$

Herring Condition

local dissipation equation
(no critical events)
ensemble of inertia free springs



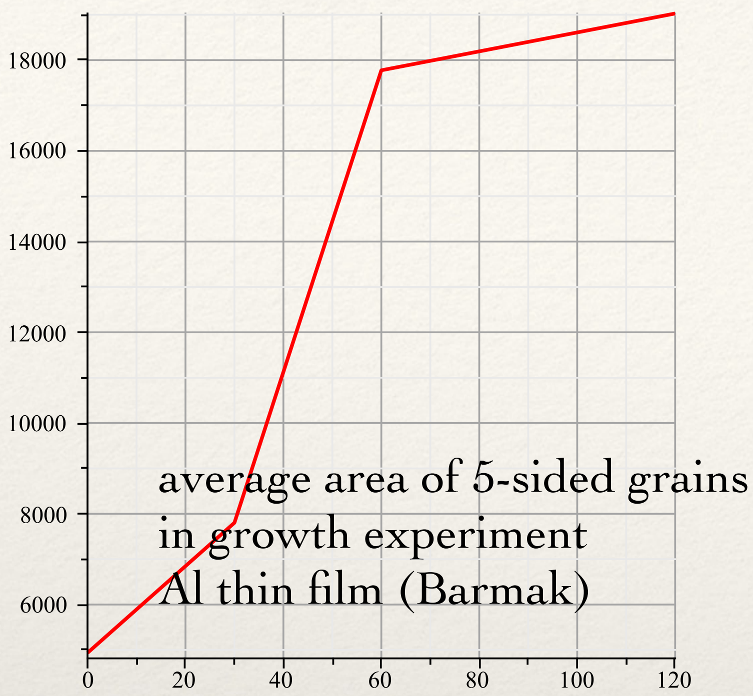
$$\sum_{\{\Gamma\}} \int_0^\tau \int_\Gamma v_n^2 ds dt + E(\tau) = E(0)$$

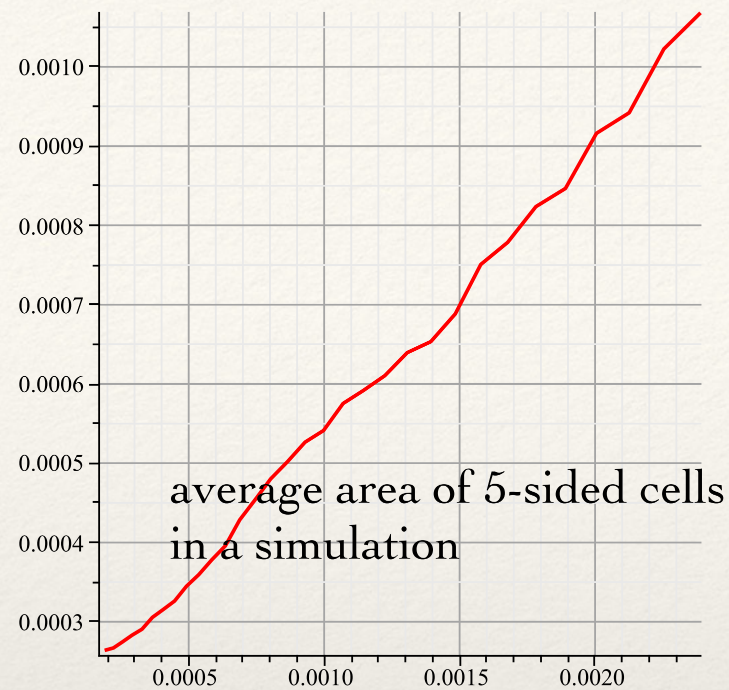
dissipation

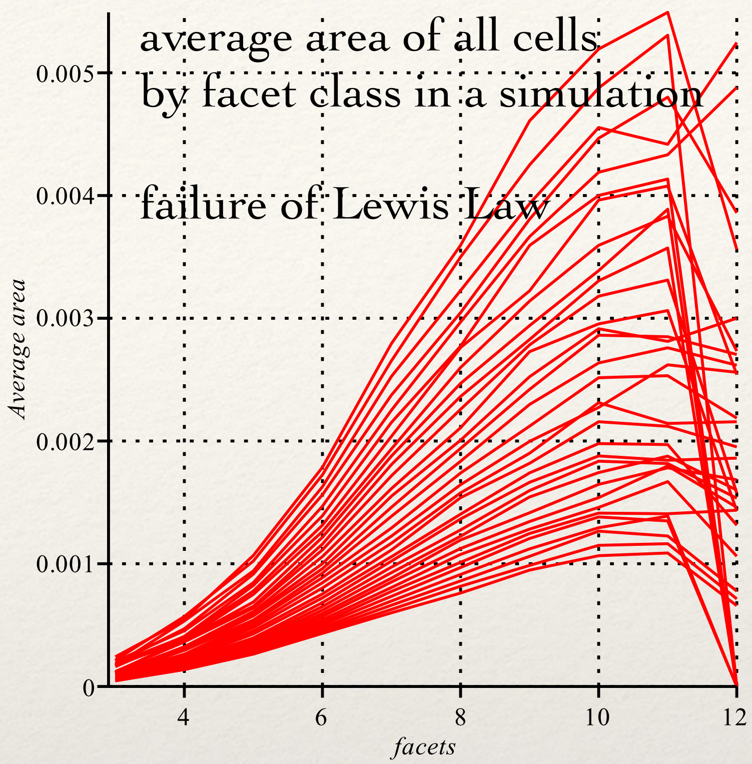
objective: upscale to a dissipation relation for GBCD
success leads to explanation of the Boltzmann

stochasticity in network coarsening

entropy role for rearrangement events







- coarsening does not follow von Neumann-Mullins *n - 6* rule:

➥

- suggests importance of the effect of network rearrangement events

leads to simplifed coarsening model:
rearrangement without curvature

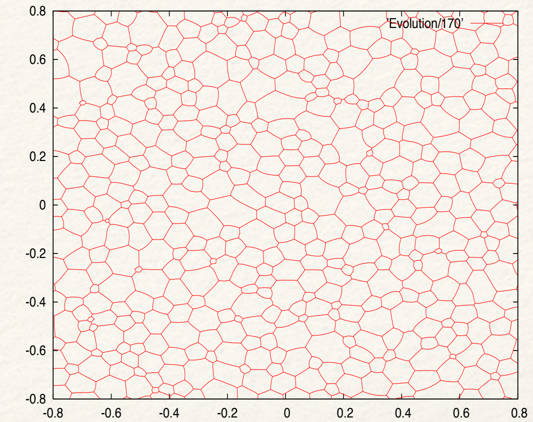
another system we seek to establish as a gradient flow
will defer discussion

outline of theory

$\psi = \psi(\alpha)$ α lattice misorientation

$$E(t) = \sum_{\{\Gamma\}} \int_\Gamma \psi \, d\alpha$$

$$\sum_{\{\Gamma\}} \int_0^\tau \int_\Gamma v_n^2 \, ds\, dt + E(\tau) = E(0)$$



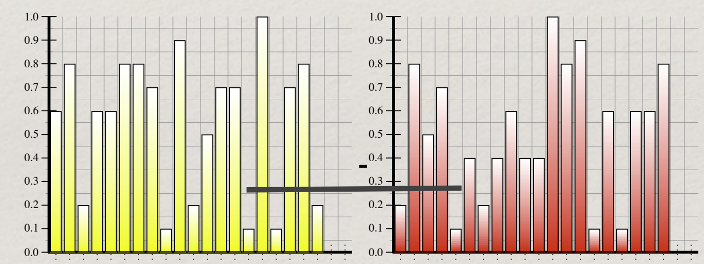
$\rho(\alpha, t)$ GBCD upscale of ensemble

$$F_\sigma(\rho) = \int_\Omega (\psi\rho + \sigma\rho\log\rho)\, d\alpha$$

$$\mu \int_0^\tau \int_\Omega v^2 \rho \, d\alpha\, dt + \qquad F_\sigma(\rho)\Big|_\tau \le F_\sigma(\rho)\Big|_0$$

competitor for the Wasserstein metric

$$\frac{\mu}{2\tau} d(\rho|_\tau, \rho|_0)^2 +$$

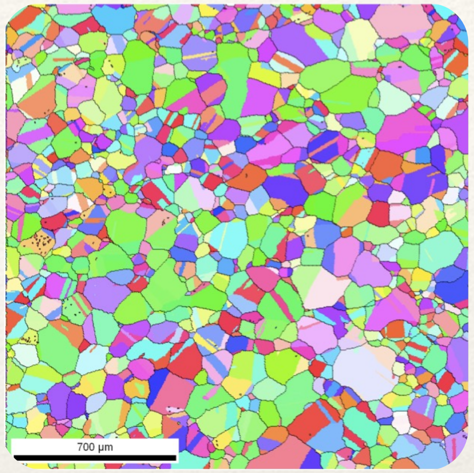


idea of mass transport

gives rise to dissipation relation for GBCD:

$$\frac{\mu}{2\tau} d(\rho|_\tau, \rho|_0)^2 + F_\sigma(\rho)\Big|_\tau \le F_\sigma(\rho)\Big|_0$$

Success $\Rightarrow$ $\rho(\alpha,t)$ = GBCD, empirical first order texture statistic, resembles solution of a F-P Equation



determine parameter σ

employ (Kullback-Leibler) relative entropy

$$\Phi_\lambda(\rho) = \Phi(\rho \| \rho_\lambda) = \int_\Omega \rho \log \frac{\rho}{\rho_\lambda} d\alpha \geqq 0$$

$$\text{with } \rho_\lambda(\alpha) = \frac{1}{Z_\lambda} e^{-\frac{\psi(\alpha)}{\lambda}}, \ Z_\lambda = \int_\Omega e^{-\frac{\psi(\alpha)}{\lambda}} d\alpha$$

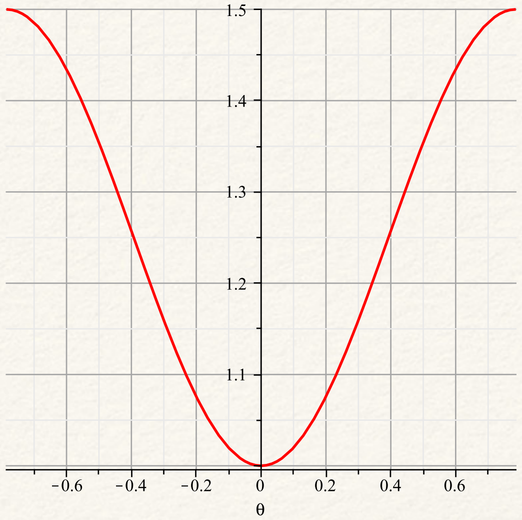
$$= \int_\Omega (\psi_\lambda \rho + \rho \log \rho) d\alpha, \quad \psi_\lambda = \frac{\psi}{\lambda} + \log Z_\lambda, \ \int_\omega \psi_\lambda d\alpha = 1$$

maximimum liklihood
calculate dual function

$\Phi_\sigma(\rho) \to 0$ as $t \to \infty$ for solution of FP equation

2D coarsening

GBCD statistic (averaged over 10 trials)

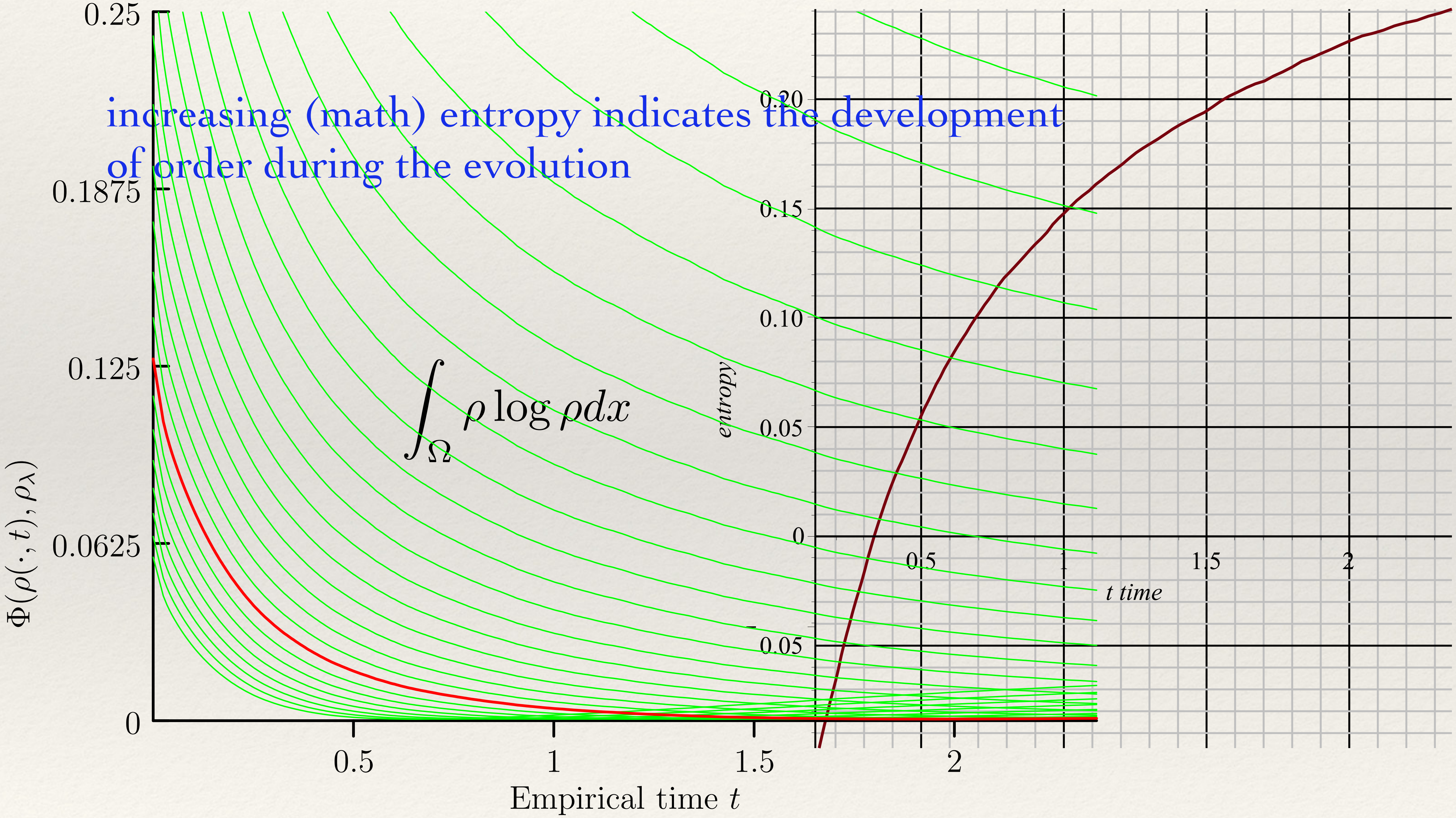


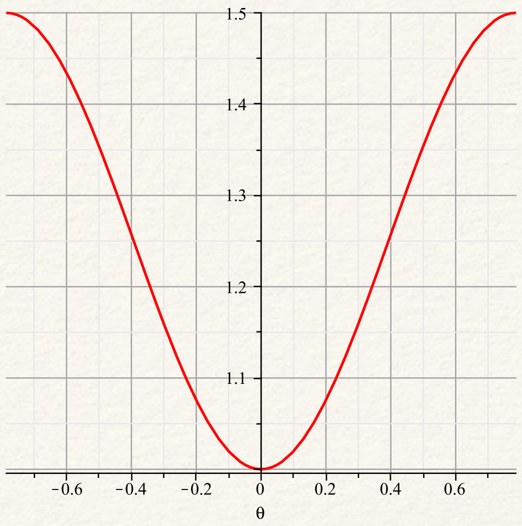
$$\psi(\alpha) = 1 + \epsilon \sin^2 2\alpha, \epsilon = \frac{1}{2}$$

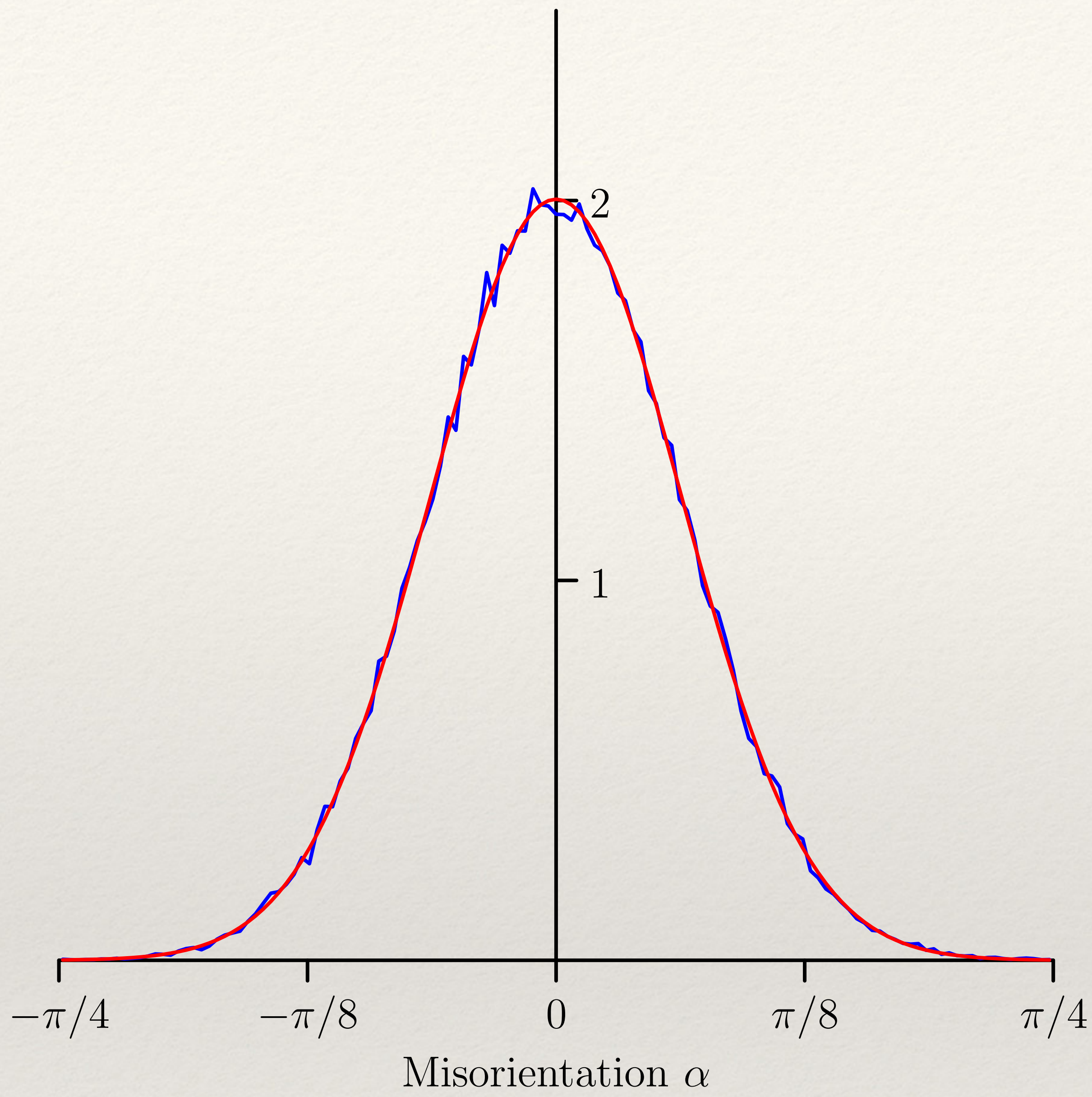
$$\rho_\lambda(\alpha) = \frac{1}{Z_\lambda} e^{-\frac{\psi(\alpha)}{\lambda}}$$

$$\Phi_\lambda(\rho \| \rho_\lambda) = \int_\Omega \rho \log \frac{\rho}{\rho_\lambda} d\alpha \geqq 0; \quad \Phi_\sigma \to 0 \text{ as } t \to \infty$$

increasing (math) entropy indicates the development of order during the evolution







blue: empirical distribution (10 trials)
20,000 initial cells
red: Boltzmann for σ determined by relative entropy condition

gradient flow (validation: de Giorgi minimizing movements)

our context: discrete sampling of a process
exploit the implicit scheme

$$\frac{1}{2\tau}d(\rho,\rho^*)^2 + F(\rho) = \inf$$

Euler equation is

$$\frac{1}{\tau}(x-\phi(x)) + (\sigma\frac{\rho_x}{\rho} + \psi') = 0 \text{ in } \Omega \qquad \phi = \text{transfer function from } \rho \text{ to } \rho^*$$

GF condition satisfied with = with W metric at level of the implicit scheme

$$\frac{1}{\tau}d(\rho,\rho^*)^2 = \frac{1}{\tau}\int_\Omega (x-\phi(x))^2\rho dx = \tau\int_\Omega (\sigma\frac{\rho_x}{\rho} + \psi')^2\rho dx$$

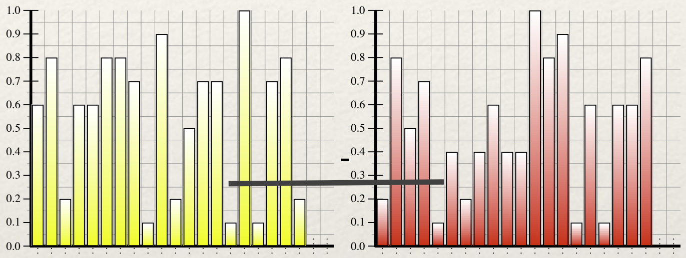
Label the frames $\{\rho_j\}$

$$F(\rho_{j-1}) - \left\{F(\rho_j) + \frac{1}{\tau} d(\rho_{j-1}, \rho_j)^2\right\} \approx 0$$

$$F(\rho_{j-1}) - \left\{F(\rho_j) + \tau \int_\Omega (\sigma \frac{\rho_{jx}}{\rho_j} + \psi')^2 \rho_j dx\right\} \approx 0$$

verify these conditions

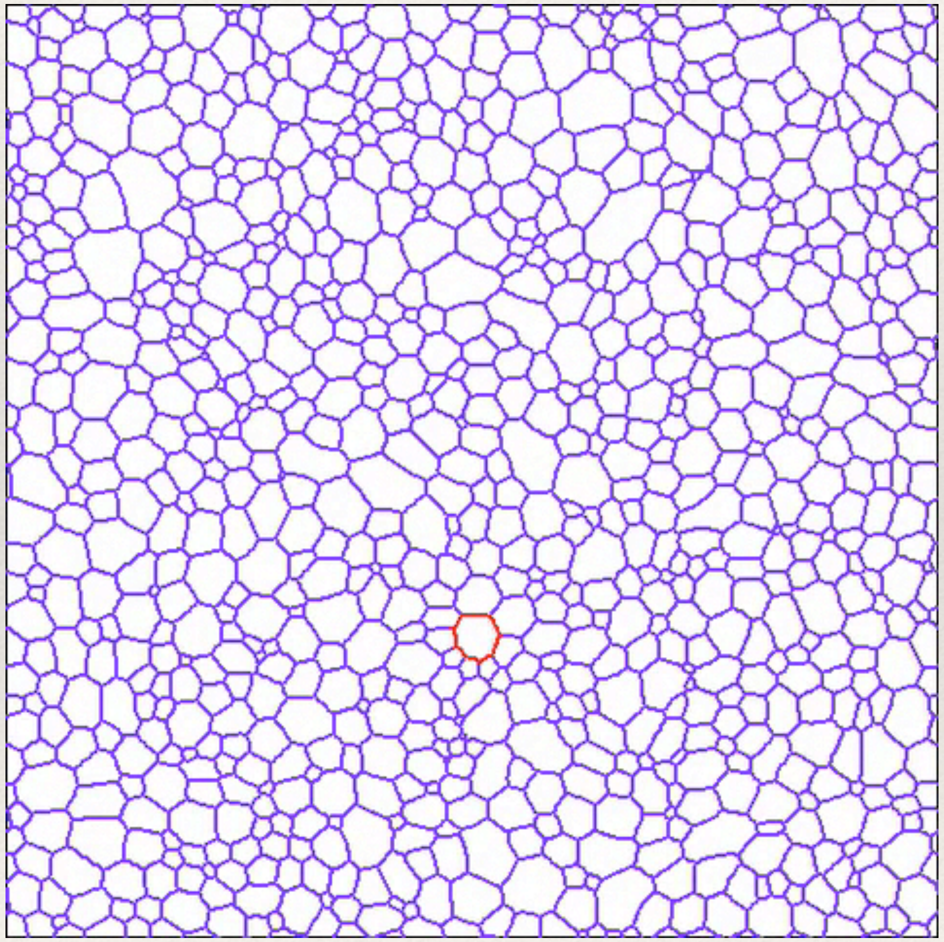
$\Rightarrow$



the frames $\{\rho_j\}$ arise as the iterates in an implicit scheme

sampling
calibration and rescaling

essential to establish time scale
regard the simulation steps, 'frames,' as samples of an evolving process



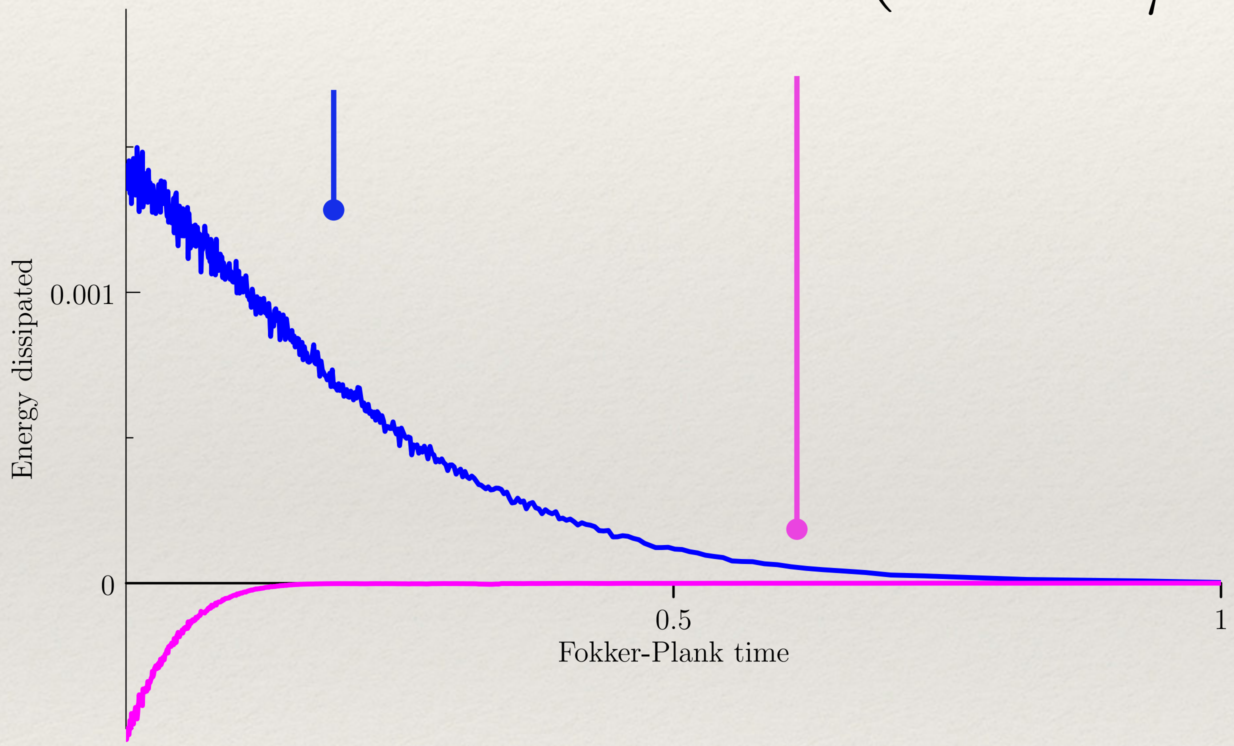
establish the sequence of time intervals
of the frames by comparison
with a computed solution of
the PDE

an inverse problem:
'machine time' ≠ 'fokker planck time'

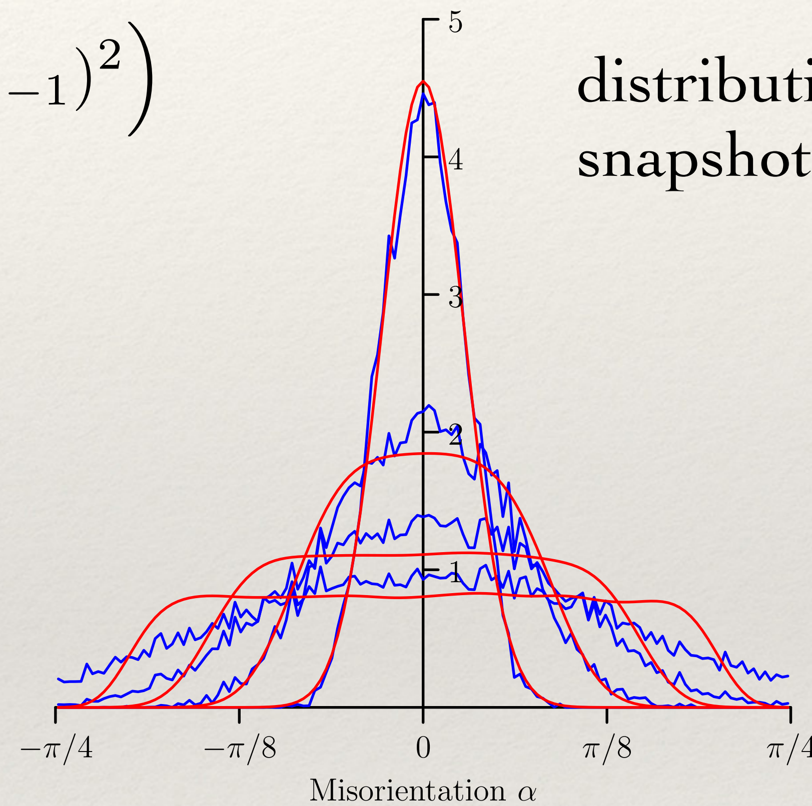
holds even for simple systems like
Ehrenfest Urn

simplified problem
coarsening: energy decay and dissipation

$$F(\rho_{j-1}) - F(\rho_j) \qquad F(\rho_{j-1}) - \left(F(\rho_j) + \frac{1}{\tau} d(\rho_j, \rho_{j-1})^2\right)$$



initial population
19 K intervals



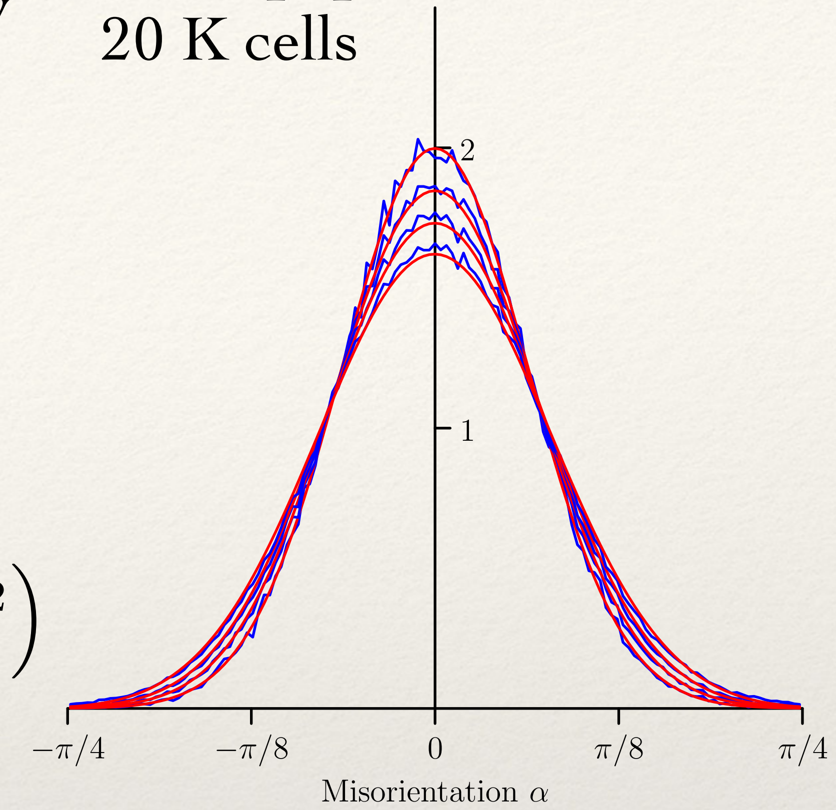
distribution
snapshots

2D coarsening: energy decay and dissipation

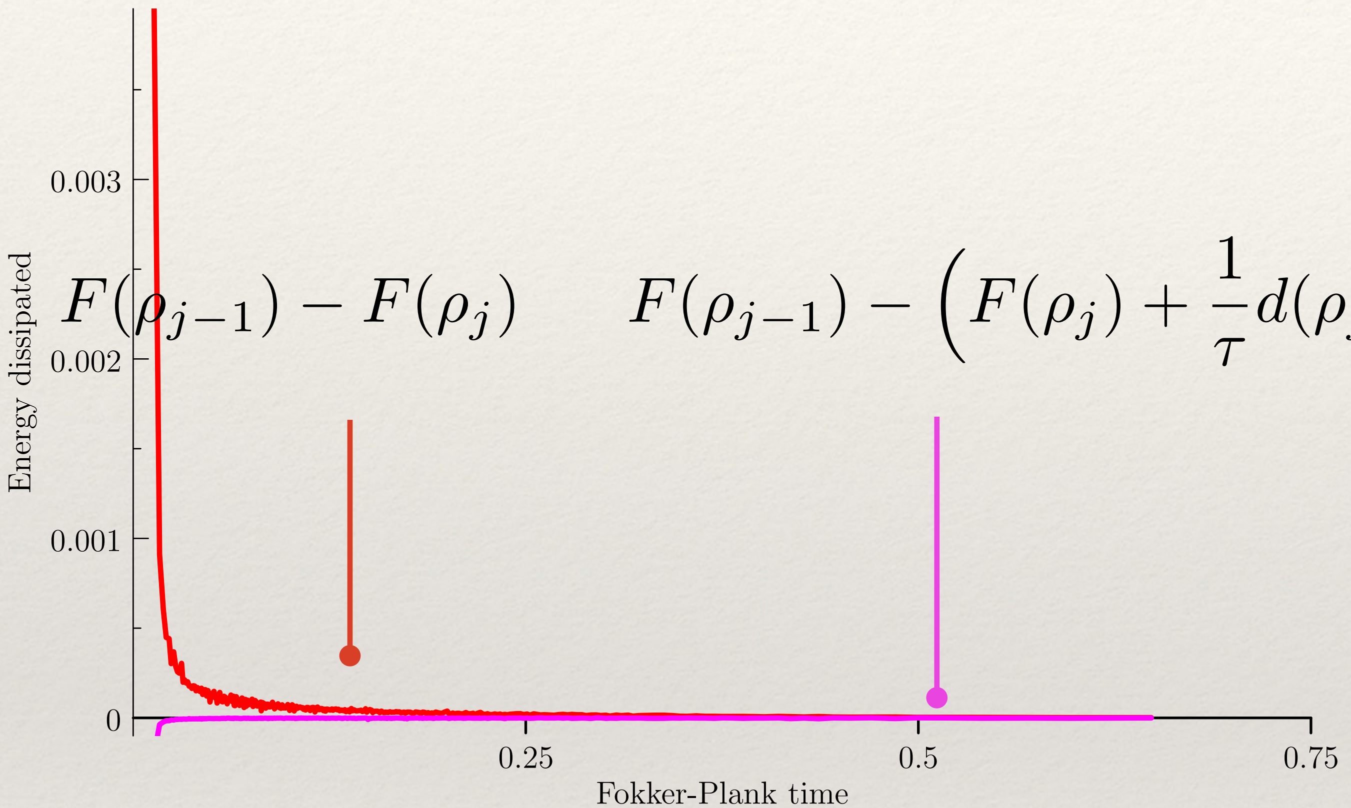
GBCD evolution consistent with gradient flow

$$\psi(\alpha) = 1 + \frac{1}{2}\sin^2(2\alpha)$$

initial population
20 K cells

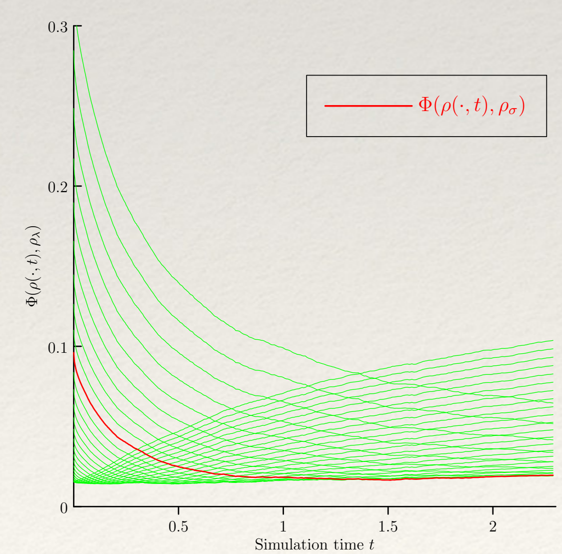


$$F(\rho_{j-1}) - F(\rho_j) \qquad F(\rho_{j-1}) - \left(F(\rho_j) + \frac{1}{\tau} d(\rho_j, \rho_{j-1})^2\right)$$



density plots at
20%, 40%, 60% 80% of cells deleted
compared with solution of FPE

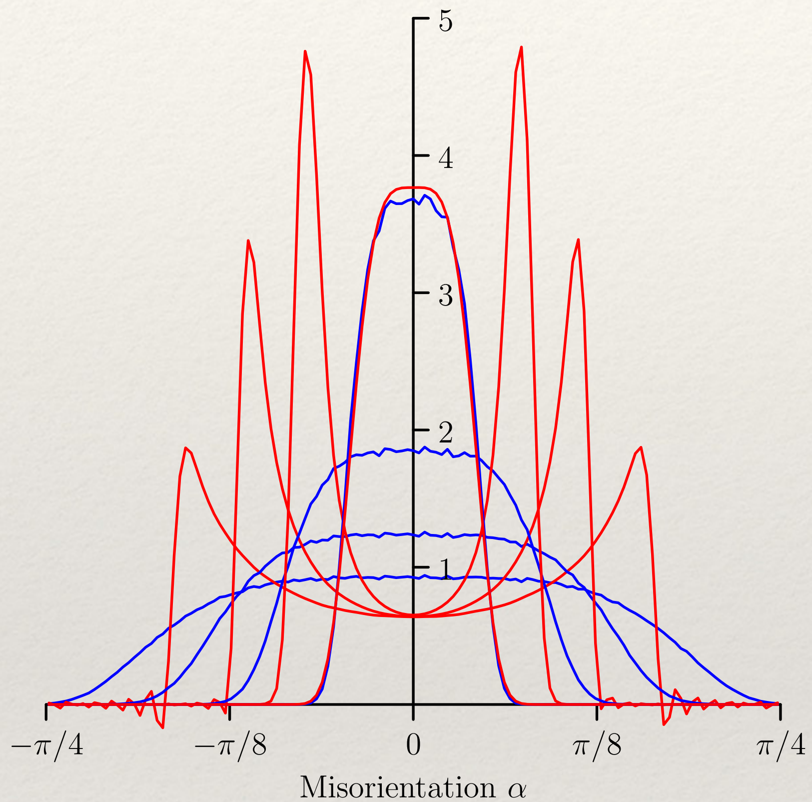
d^2 computed using K and Walkington



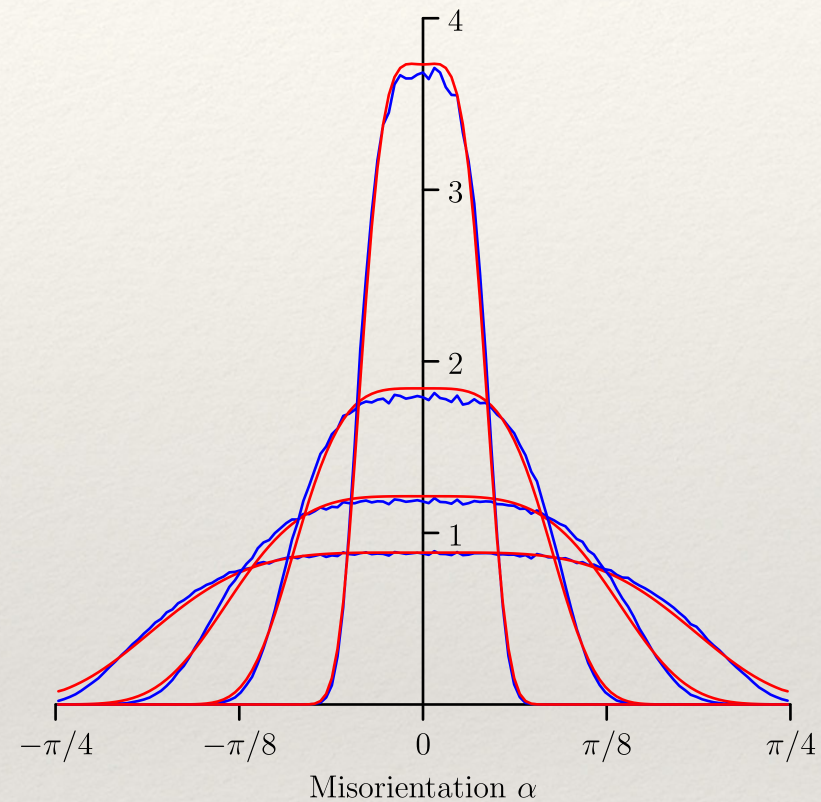
quartic potential

$$\psi(\alpha) = 1 + \epsilon \sin^4(2\alpha)$$

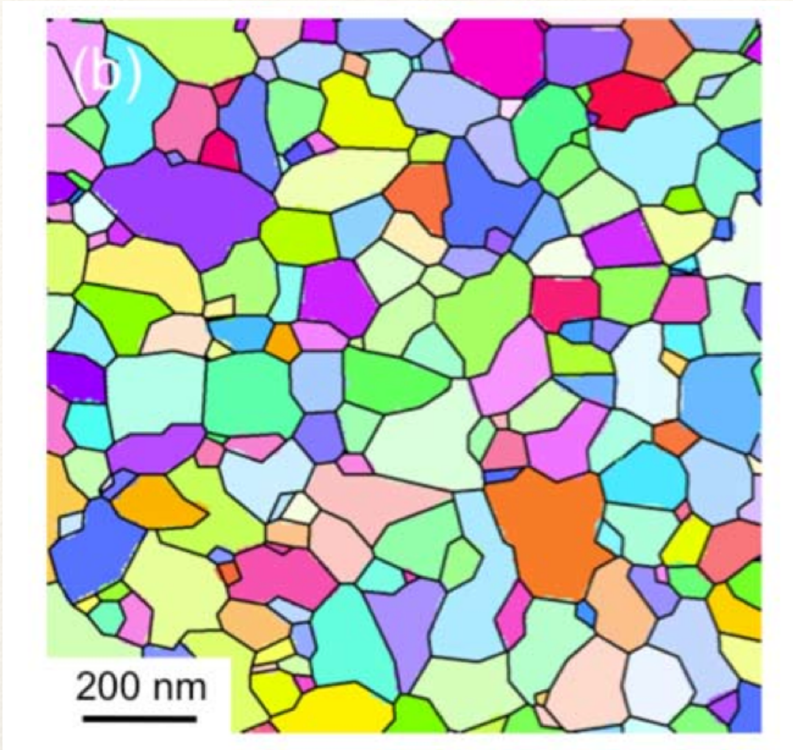
some challenges



comparison with
FPE



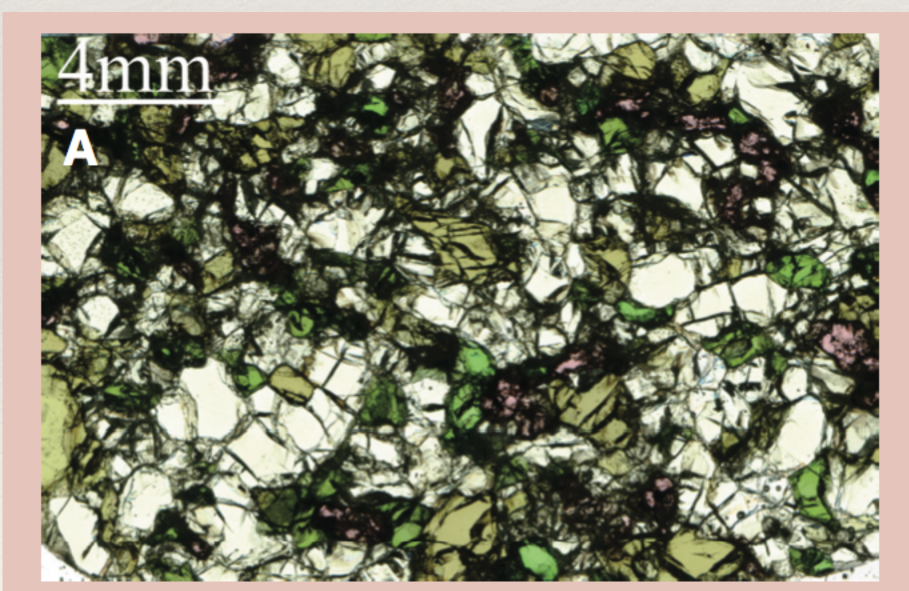
comparison with
FPE with time dependent
diffusion constant



Significant current interest

W/ferrite comparison

Xuan Liu, Dooho Choi, Hossein Beladi, Noel T. Nuhfer, Gregory S. Rohrer, and Katayun Barmak (2013)



GBCD for geological processes

K. Marquardt, Bayreuth

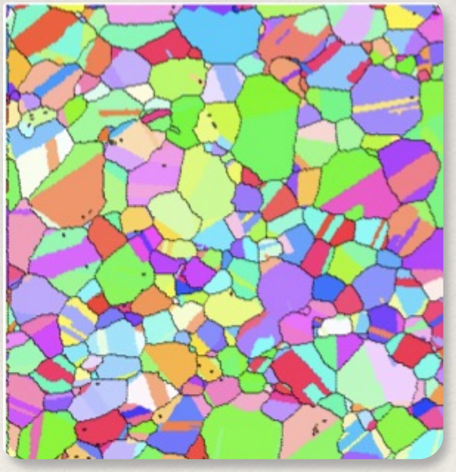
Summary

GBCD: relative character distribution

- consistency between experiment and simulation
- interfacial energy $\psi = \psi(\alpha) \Rightarrow$ GBCD is a Boltzmann distribution

mass transport based theory describes evolution of GBCD:
harvested statistics are iterates of implicit scheme
GBCD solution of a Fokker-Planck Equation

gradient flow identification is first use of mass transport in this context
other systems: eg., random walk



gradient flow