Stochastic particle systems related to grain boundary coarsening

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Joint work with Govind Menon (Brown University) and Robert Pego (Carnegie Mellon University)

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Coarsening in Networks

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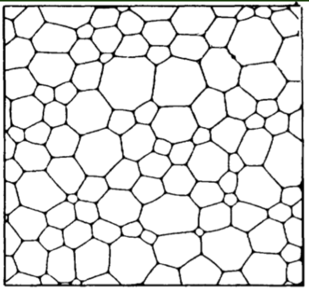
Grain boundary coarsening is observed in polycrystalline ceramics and metals and gas diffusion between cells of a foam. Under two-dimensions with isotropic surface tension, grain boundaries evolve by curve shortening flow- for an evolving curve $\gamma(x,t) \subset \mathbb{R}^2$, edges $\gamma(x,t)$ move with respect to their curvatures:

$$\gamma_t(x,t) = \kappa \vec{n}(x,t).$$

Grains are faces of a trivalent network G. At junctions, by force balance we have Herring's condition: edges at vertices must meet at 120 degrees.



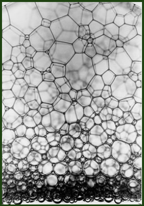
A two dimensional foam. (Glazier, Gross, and Stavans '87)

Previous work

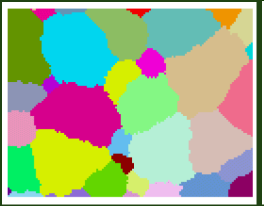
Physical experiments
Bubble sorting: Hutzler ’00
Empirical laws: Aboav ’70, Lewis ’28
Foam packing: Newhall et al. ’12

Numerical simulation
Potts models: Anderson et al. ’84, Zöllner/Streitenberger ’04
Level set methods: Esedoglu/Elsey/Smereka ’11, Zhao et al ’96, Merriman/Bence/Osher ’94
Others: Kinderlehrer/Livshits/Ta’asan ’06, Lazar et al ’11

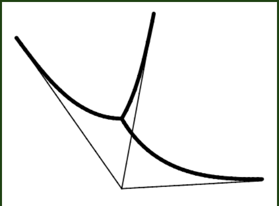
Geometry and analysis
Single junction: Schnurer/Schulze ’07, Mazzeo/Saez ’07
Flow of lens: Schnurer et al. ’11, Bellettini/Novaga ’09



Wet foam (NASA)



Potts model (Zöllner)



Flow through triple junction (Schnurer, Schulze)

Evolution of individual grains

Assuming that a grain does not change its topology (number of sides), we have the following simple rule relating the topology and geometry of single grains:

Theorem
(von Neumann's "$n-6$" rule) A grain with area $A(t)$ and n sides satisfies

$$\frac{dA}{dt} = \frac{\pi M}{3}(n-6).$$

Here M is a constant based on material properties. In particular, grains with less than six sides shrink, grains with more than six sides grow, and grains with six sides keep the same area.

The first proof of this fact is due to Von Neumann in 1952, and appeared in the discussion section of a metallurgical journal. The reasoning assumes all edges evolve as arcs of constant curvature. Mullins provided a generalization for smooth boundaries in 1956.

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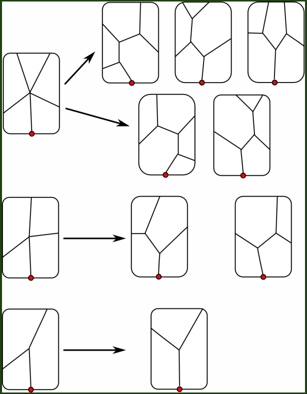
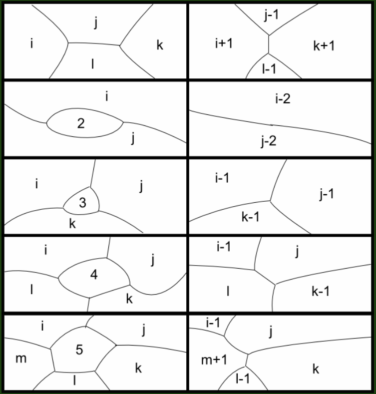
Flowing through singularities





The $N-6$ rule implies that grains can vanish in a network. Also, edges can undergo side switching, in which one side vanishes, and another is created.

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Mean field models

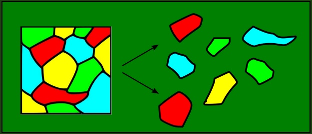
Several kinetic models from physicists (Fradkov '94, Flyvbjerg '88, Marder '88) were created for area densities $f_n(x,t)$ of grains with n sides. The general form is transport equation with an intrinsic source term:

$$\boxed{\partial_t f_n(x,t) + (n-6)\partial_x f_n(x,t) = F(f)}.$$

- Transport corresponds to advection of grains by the $n-6$ rule.
- $F(f)$ is the topological flux, which arises from grain annihilation, with form

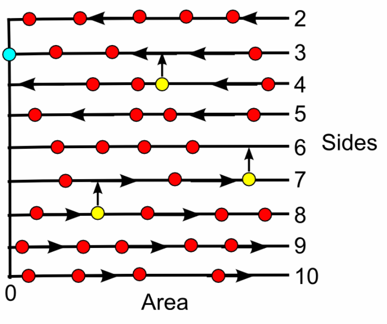
$$F(f) = \sum_{l=2}^{5}(l-6)f_l(0,t)\left(\sum_{m=2}^{\infty} A_{lm}(t) f_m(x,t)\right)$$

- The terms $(l-6)f_l(0,t)$ for $l = 2,3,4,5$ are rates of loss for l sided grains.
- To determine $F(f)$, mean field rules are created for how grains are selected to gain/lose sides (these rules eliminate correlations between grains)



The M-species model

Prelimit behavior for kinetic equations can be understood by the following diagram



Interpretation: Each particle represents a grain, with area given by horizontal position, and lines represent possible topologies. By $n - 6$ rule, grains move sideways at constant rate. When a particle hits the origin, it is removed, and other particles are randomly selected move vertically, indicating a mutation. This is an example of a piecewise deterministic Markov process.

Kinetic equations

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Kinetic equations for number densities $f_\sigma(x,t)$ for species σ are

$$
\begin{aligned}
\partial_t f_\sigma(x,t) + v_\sigma \partial_x f_\sigma(x,t) &= j_\sigma := j_\sigma^+(x,t) - j_\sigma^-(x,t), \\
j_\sigma^+(x,t) &= \sum_{k=1}^{M} \left(\sum_{l=1}^{M_-} \dot{L}_l J_{\sigma k} W_k^{(l)}(t) + \beta\gamma(t) J_{\sigma k} w_k \right) f_k(x,t), \\
j_\sigma^-(x,t) &= \left(\sum_{l=1}^{M_-} \dot{L}_l K W_\sigma^{(l)}(t) + \beta\gamma(t) K w_\sigma \right) f_\sigma(x,t), \\
\dot{L}_l &= -f_l(0,t) v_l, \quad l = 1, \dots, M_-.
\end{aligned}
$$

The M-species model contains several parameters:

v_σ - velocity of species

K - how many particles mutate at singular event

$W_\sigma, \gamma(t) w_\sigma$-tier weights at singular event

$J_{\sigma k}$-rules for how particles mutate

β- rate of interior events

Well-posedness

Let X denote the space of continuous and integrable functions $f = (f_1, \dots, f_M) : [0, \infty) \to \mathbb{R}^M$ equipped with the norm

$$\|f\| := \|f\|_{L^1} + \|f\|_{L^\infty}, \quad \|f\|_{L^1} := \sum_{\sigma=1}^{M} \|f_\sigma\|_{L^1}, \quad \|f\|_{L^\infty} := \sum_{\sigma=1}^{M} \|f_\sigma\|_{L^\infty}.$$

Theorem

Assume given positive $f_0 \in X$. There exists a (possibly infinite) time $T_* > 0$ and a unique map $f \in C([0, T_*); X)$ with $f(0) = f_0$ such that f is a positive, mild solution to the kinetic equations on each interval $[0, T]$ with $0 < T < T_*$. Further, $\lim_{t \to T_*} f(t) = 0$ if $T_* < \infty$.

Proof sketch: Express integral form of kinetic equations as

$$f(x,t) = f(x - v_\sigma t, 0) + \int_0^t j_\sigma(x - v_\sigma(t-\tau), \tau) d\tau.$$

Find Lipschitz estimate on total flux j_σ and apply contraction mapping principle.

Hydrodynamic limit

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For a limit of the stochastic particle system to the kinetic equations, we have a tightness result - a subsequence of measures $\mu^{n_k} \to \mu$ in the Skorokhod topology $\mathbb{D}([0, T], \mathcal{M}(\mathbb{R}^+)^M)$ which solves a weak form of the kinetic equations.

There's evidence that more is true: we conjecture a concentration inequality of the form

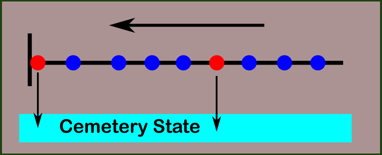
$$\mathbb{P}\left(\sup_{s\in[0,T]} d(\mu^n(s), \mu(s)) > \varepsilon\right) \leq C_1(\varepsilon)\exp(-nC_2(\varepsilon)).$$

Where d is the BL distance which metrizes the weak topology of measures. This conjecture is based on a minimal model for the M-species model which produces a similar estimate.

A minimal model: 'Removal-Driven Thinning'

For understanding the main machinery in calculating the total loss $L_\sigma^n(t)$, consider a minimal, one species model:

1. Particles travel toward the origin at unit speed.
2. When a particle hits the origin, remove the particle and also another randomly chosen particle.
   For initial empirical measures $\mu_0^n \to \mu_0$, can we describe convergence rates of $\mu_t^n \to \mu_t$ and $L^n(t) \to L(t)$?



Removal driven thinning

Explicit solution

The limiting equation for total number, assuming densities $f(x,t)$, is

$$\partial_t f(x,t) - \partial_x f(x,t) = -\frac{f(0,t)}{\int_0^\infty f(x,t)dx} f(x,t), \quad x,t \in (0,\infty).$$

$$f(x,0) = f_0(x), \quad x \in (0,\infty).$$

While nonlinear, it is straightforward to obtain an explicit solution

$$f(x,t) = \beta(t) f_0(x+t),$$

$$\beta(t) = \int_t^\infty f_0(x)dx.$$

Thus, $f(x,t)$ is a translated and scaled copy of its initial conditions. Less intuitive is a formula for the total loss at the origin

$$L(t) = \frac{1}{2}\left(1 - \left(\int_t^\infty f_0(x)\right)^2\right).$$

With uniform initial data $f_0 = \mathbf{1}_{[0,1]}$, for example, this gives

$$L(t) = t - \frac{t^2}{2}, \quad t \in [0,1].$$

The quadratic term accounts for particles removed before arrival at the origin.

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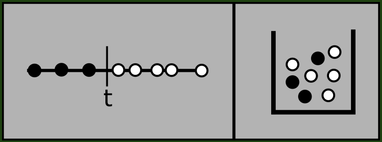
An urn model

How to compare $L^n(t)$ with $L(t)$? For the finite model, color balls at position less than t black, and those at position at least t white. Perform the following draw for a "diminishing urn" with n balls, w of which are white, and b are black.

1. Remove a black ball.
2. Randomly remove another ball.

Repeat until all black balls are removed. What is $X_{w,b}$, the number of white balls remaining?



One-d loss model

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Urn models

The model described is one example of a large class of sampling methods called diminishing urns. The main object of interest is the replacement matrix

$$M = \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix}.$$

For an urn with white and black balls, randomly select a ball:

- If a white ball is selected, add α white balls and β black balls.
- If a black ball is selected, add γ white balls and δ black balls.

Repeat until no black balls remain. Let $X_{w,b}$ be the number of remaining white balls.

For an urn with w white and b black balls, we can condition on a single draw to obtain a recurrence relation for the mgf $h_{w,b}(z) = \mathbb{E}[\exp(z \cdot X_{w,b})]$, given by

$$h_{w,b}(z) = \frac{w}{w+b} h_{w+\alpha,b+\beta} + \frac{b}{w+b} h_{w+\gamma,b+\delta}.$$

For large w, b, what are limiting quantities for $X_{w,b}$ (e.g. LLN, central limit theorems)? Depending on the type of urn, limiting distributions can take several forms (Kumaraswamy, Weibull, Normal).

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Examples

Some increasingly interesting scenarios:

Classical Sampling. Select a ball. If the ball is replaced $M = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$. If not, $M = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$.

The Ehrenfest Urn (1907). A simple model of diffusion for particles moving between two regions. $M = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$.

The OK Corral (Williams/McIlroy-'98). Two groups of outlaws shoot at each other. Randomly select which outlaw shoots. Then $M = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$.

The Cannibal Urn (Pittel '82). Cannibals and noncannibals inhabit a shared space. A randomly chosen person eats a noncannibal. A noncannibal becomes a cannibal by eating another noncannibal. Thus $M = \begin{bmatrix} -2 & -1 \\ 1 & 0 \end{bmatrix}$.

Asymptotic normality

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Suppose the fraction of noncannibals to cannibals approaches $\rho \in [0,1]$. For the cannibal urn, Pittel shows that for some functions $\phi(\rho)$ and $\psi(\rho)$, for $X_{w,b}$ denoting the total number of draws until exhaustion, and $w + b = n$,

$$\frac{X_{w,b} - n\phi(\rho)}{\sqrt{n\psi(\rho)}} \Rightarrow Z, \quad Z \sim N(0,1)$$

Proof sketch: compare the mgf $h_{w,b}(z)$ for $X_{w,b}$ to $g_{w,b}(z)$, the mgf of a normal $Z \sim N(\phi(w/b), \psi(w/b))$. Then an asymptotic analysis shows that $g_{w,b}(z)$ approximately satisfies the recurrence relation for $h_{w,b}(z)$ when

$$\phi' - \phi = 0, \quad \phi(1) = 1,$$

$$\psi' - \psi + \phi^2\rho(1-\rho) = 0, \quad \psi(1) = 0.$$

These are simple to solve:

$$\phi(\rho) = \exp(\rho - 1), \quad \psi(\rho) = \exp[2(\rho-1)](\rho^2 - 3\rho + \rho - \exp(1-\rho)).$$

Concentration inequality for loss measure

For the one species model, the replacement matrix is $M = \begin{bmatrix} -2 & -1 \\ 0 & -1 \end{bmatrix}$. Using methods similar to Pittel,

$$\frac{X_{w,b} - n\phi(\rho)}{\sqrt{n\psi(\rho)}} \Rightarrow Z, \quad Z \sim N(0,1)$$

hold when

$$\rho\phi'(\rho) - 2\phi(\rho) = 0, \quad \phi(1) = 1,$$

$$\rho\psi' - 2\psi(\rho) + 4\rho^3(1-\rho) = 0, \quad \psi(1) = 0.$$

Thus

$$\phi(\rho) = \rho^2, \quad \psi(\rho) = 2\rho^2(1-\rho)^2.$$

The upshot: the random quantity $X_{w,b}$ is intimately related to the total number of particles which hit the origin: $L^n(t) = \frac{n - X_{w,b}}{2}$. From exponential tails of the normal, the CLT can be converted into a concentration inequality:

$$\mathbb{P}(|L^n(t) - L(t)| > \frac{\varepsilon}{2}) \leq \frac{2}{\varepsilon} e^{-8n\varepsilon^2}.$$

The main concentration inequality

Let F be the limiting CDF of the minimal model, and d be the BL metric on measures in $[0, \infty)$ which metrizes the weak topology:

$$d(F,G) = \sup_{\|\varphi\|_{BL} \leq 1} \int_0^\infty \varphi(x) d(F(x) - G(x)),$$

$$\|\varphi\|_{BL} = \sup_x |\varphi(x)| + \sup_{x,y} \frac{|\varphi(x) - \varphi(y)|}{|x - y|}.$$

Let $\mu^n(t)$ be an empirical measure of n particles, and $\mu(t)$ be the limiting measure satisfying the limiting kinetic equations. With the two previous results, we may state our final theorem:

Theorem

There exists a universal constant $\kappa > 0$ *and* $M_\varepsilon(F_0) > 0$ *such that for every* $\varepsilon > 0$ *and* $T > 0$ *there exists* M_ε *satisfying*

$$\mathbb{P}\left(\sup_{t \in [0,T]} d(\mu^n(t), \mu(t)) > \varepsilon \right) \leq M_\varepsilon e^{-\kappa n \varepsilon^2}.$$

Summary:

Some directions to look at:

Theoretical:

- A full concentration estimate of hydrodynamic convergence.
- A rigorous explanation of stabilization of network statistics.

Numerical:

- Convergence to stable statistics from specialized initial conditions.
- Generalization to nonhomogeneous media.
- Improved understanding of fitting parameters.

References:

Concentration inequalities for a removal-driven thinning process. With Govind Menon. Quarterly of Applied Mathematics.

The Fokker-Planck equation for residual times under an intrinsic scaling. Preprint.

Analysis and simulations of kinetic models for two-dimensional grain boundary coarsening. With Govind Menon and Robert Pego. Preprint.