Global Well-Posedness of a Nonlinear Fokker-Planck Type Model of Grain Growth

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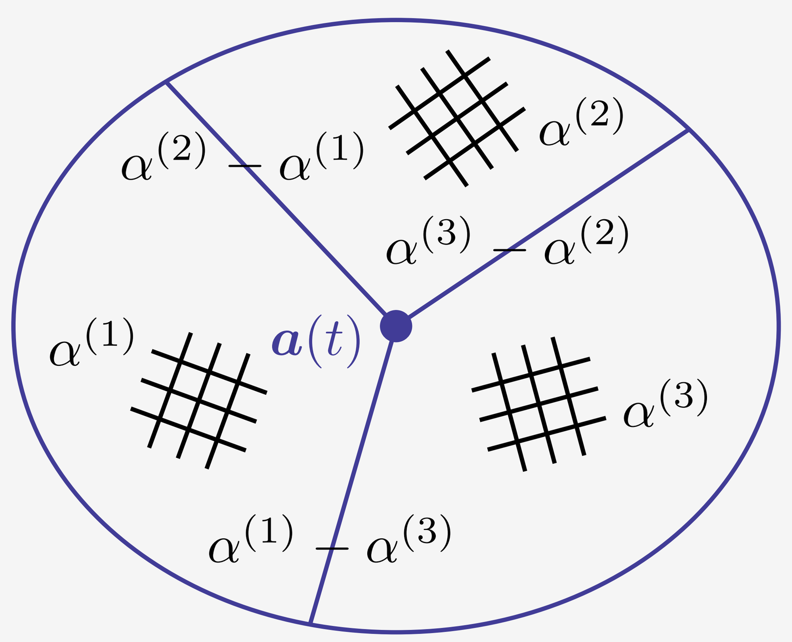
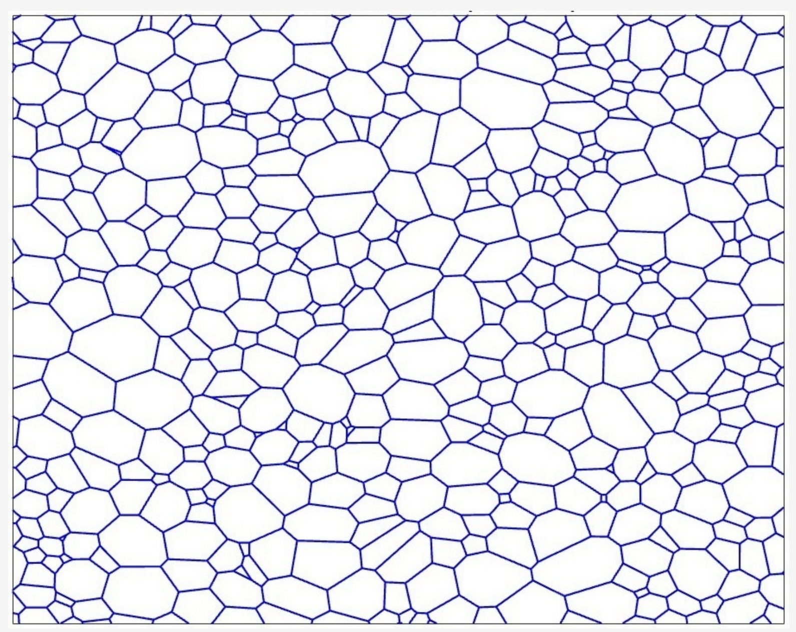
What is Grain Growth?

- Grain growth is a highly complex multiscale-multiphysics process appearing in materials science which describes the evolution of the microstructure of polycrystalline materials [1, 2].
- These materials consist of many small monocrystalline grains which are separated by grain boundaries.
- The changes in grain size affect the material's electrical, thermal, etc. properties, which are important in the engineering of new materials.

Simulation & Free Energy





- $a(t)$ is the triple junction point, $\alpha^{(j)} = \alpha^{(j)}(t)$'s are lattice orientations, and $\alpha^{(i)} - \alpha^{(j)}$'s are lattice misorientations.
- There is a coupled ODE system in terms of $a(t)$ and $\alpha^{(j)}(t)$, which we call the *vertex model* [3]. Since $N \gtrsim 10^4$ in applications, it is convenient to study $N \to \infty$ limit of the vertex model resulting in the following free energy with inhomogeneous absolute temperature $D(x)$:

$$F[f] = \int_{\mathbb{T}^d} (D(x)f(x,t)(\log f(x,t) - 1) + \phi(x)f(x,t))\, dx$$

together with the dissipation relation

$$\frac{d}{dt}F[f] = -\int_{\mathbb{T}^d} \frac{f}{\pi(x,t)} |\nabla(D(x)\log f + \phi(x))|^2\, dx.$$

Nonlinear PDE Model

$$\text{(nFP)} \quad \begin{cases} \dfrac{\partial f}{\partial t} = \nabla \cdot \left(\dfrac{f}{\pi(x,t)} \nabla\left(D(x)\log f + \phi(x)\right)\right), & x \in \mathbb{T}^d,\ t > 0, \\ f(x,0) = f_0(x), & x \in \mathbb{T}^d. \end{cases}$$

- $f(x,t)$ will be a probability density function,
- $\pi(x,t) > 0$ is mobility function,
- $D(x) > 0$ is absolute temperature function,
- $\phi(x)$ is energy density of a grain boundary.

Proof Setup

$$\begin{cases} \dfrac{\partial u}{\partial t} = L_{\mathrm{FP}} u + \nabla \cdot \left(\dfrac{\nabla D(x)}{\pi(x,t)} f \log f\right), & x \in \mathbb{T}^d,\ t > 0, \\ u(x,0) = f_0(x), & x \in \mathbb{T}^d. \end{cases}$$

Here,

$$L_{\mathrm{FP}} u := \nabla \cdot \left(\frac{D(x)}{\pi(x,t)} \nabla u\right) + \frac{\nabla \phi(x)}{\pi(x,t)} \cdot \nabla u + \nabla \cdot \left(\frac{\nabla \phi(x)}{\pi(x,t)}\right) u.$$

- $\frac{D(x)}{\pi(x,t)} \geq \theta$ for some arbitrary $\theta > 0$.
- $\frac{D(x)}{\pi(x,t)}, \frac{\nabla \phi(x)}{\pi(x,t)} + \nabla\left(\frac{D(x)}{\pi(x,t)}\right)$, and $\nabla \cdot \left(\frac{\nabla\phi(x)}{\pi(x,t)}\right)$ are bounded and belongs to $C^{1+\beta,\beta/2}_{x,t}(\mathbb{T}^d \times [0,\infty))$. The coefficient of the nonlinear part, $\frac{\nabla D(x)}{\pi(x,t)}$ satisfies the same assumptions. Here, $\beta \in (0,1)$.
- $\Lambda \geq f_0(x) \geq 4\mu$ for some arbitrary $\Lambda, \mu > 0$.

As a Banach space, we set $X := C^0(\mathbb{T}^d \times [0,T])$ which is equipped with a sup-norm. Then, we work on the closed subspace $Y \subset X$:

$$Y := \{f \in X \mid f \geq \mu,\ \|f\|_X \leq R\}$$

where $R := 1 + \mu + 2\|f_0\|_{C^0(\mathbb{T}^d)}$.

Map

We define the map $\Psi : Y \to Y$, $f \mapsto u$ by the formula given below (M)

$$\begin{aligned} u = \Psi f(x,t) &= \int_{\mathbb{T}^d} K(x,t;y,0) f_0(y)\, dy \\ &\quad - \int_0^t \int_{\mathbb{T}^d} \nabla_y K(x,t;y,s) \cdot \frac{\nabla D(y)}{\pi(y,s)} f(y,s) \log f(y,s)\, dy ds \\ &=: \Psi_{f_0,\text{linear}}(x,t) + \Psi_{f,\text{nonlinear}}(x,t) \end{aligned}$$

where K is the fundamental solution of $\partial_t - L_{\mathrm{FP}}$.

Gaussian Bounds

Let K be the fundamental solution of the second-order uniformly parabolic operator $\partial_t - L$ in non-divergence form such that all of its coefficients are bounded and $C^{l+\beta,0}_{x,t}$-Hölder regular. Then, for all $x, y \in \mathbb{T}^d$ and $t - s \leq 1$ with $2a + b \leq 2l$, we have

$$\left|\partial_t^a \nabla_y^b K(x,t;y,s)\right| \leq C(t-s)^{-(d+2a+b)/2} \exp\left(\frac{-c\,|x-y|^2}{t-s}\right)$$

and

$$\begin{aligned} &|\nabla_y K(x,t;y,s) - \nabla_y K(x',t;y,s)| \\ &\quad \leq C\,|x-x'|^\beta (t-s)^{-(d+1+\beta)/2} \left(\exp\left(\frac{-c\,|x-y|^2}{t-s}\right) + \exp\left(\frac{-c\,|x'-y|^2}{t-s}\right)\right). \end{aligned}$$

Conclusions

- The map (M) is a well-defined $\frac{1}{2}$-contraction mapping on Y.
- There exists a unique fixed point f of the map (M).
- The continuity estimate $\|f - g\|_X \leq 4\|f_0 - g_0\|_{C^0(\mathbb{T}^d)}$ holds.

A priori Estimate

Let $f(x,t)$ be a classical solution of (nFP). Under the assumptions in Proof Setup with $D(x) \geq C_D \geq 1$ and $C^{\text{low}}_\pi \leq \pi(x,t) \leq C^{\text{up}}_\pi$, we have [4]:

$$\begin{aligned} &\exp\left(\frac{1}{D(x)} \min_{y \in \mathbb{T}^d}\left(D(y)\log\frac{f_0(y)}{f^{\text{eq}}(y)}\right)\right) f^{\text{eq}}(x) \\ &\quad \leq f(x,t) \leq \exp\left(\frac{1}{D(x)} \max_{y \in \mathbb{T}^d}\left(D(y)\log\frac{f_0(y)}{f^{\text{eq}}(y)}\right)\right) f^{\text{eq}}(x). \end{aligned}$$

Regularity

Gaussian bounds implies $\Psi_{f,\text{nonlinear}} \in C^\beta_x$ so, $f \in C^\beta_x$ and we conclude $F := \frac{\nabla D}{\pi} f \log f \in C^\beta_x$. Since the RHS of our PDE is in the gradient form ∇F, the standard form of the Schauder estimates don't apply. But a relatively recent reference [5] allows us to conclude $\nabla F \in C^{\beta,\beta/2}_{x,t}$. Then we have a right to apply the standard Schauder estimate to get $f \in C^{2+\beta,1+\beta/2}_{\text{loc}}$.

Main Result

There exists a unique positive classical global solution of (nFP) which belongs to $f \in C^{2+\beta,1+\beta/2}_{\text{loc}}(\mathbb{T}^d \times (0,\infty))$.

Future Directions

- JKO approach to the weak solutions of (nFP).
- Rigorous study of the $N \to \infty$, many particle, limit of the vertex model.

Acknowledgments & References

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