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

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Plan

- Introduction of the model
- Local existence result
- Global existence result

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, e.g. [6, 3, 12, 2, 1, 5, 14, 16, 13, 4, 15]. These materials consist of many small monocrystalline grains which are separated by interfaces or grain boundaries.

Grain Growth Simulation

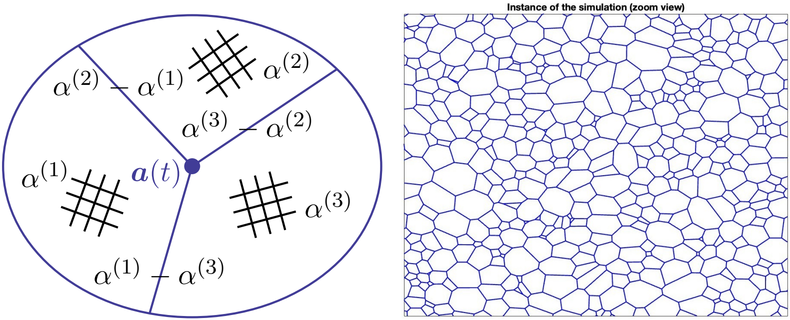

Figure 1: Left figure: A schematic plot of three grain boundaries that meet at a triple junction point $\boldsymbol{a}(t)$. For each $i, j \in \{1, 2, 3\}$, $\alpha^{(j)} = \alpha^{(j)}(t)$ represents the lattice orientation that corresponds to grid lines on the figure and the differences $\alpha^{(i)} - \alpha^{(j)}$ represent the lattice misorientations. Right figure: An instance of the simulation of the $2D$ grain network that is a collection of grain boundaries and triple junction points [8, 5].

Vertex Model

We have a coupled ODE model for lattice orientaions $\alpha^{(j)}(t)$ and triple junctions points $\boldsymbol{a}(t)$ which we call *vertex model*.
$N \to \infty$ limit of the vertex model resulting in the following free energy with inhomogeneous absolute temperature $D(x)$:

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

together with the dissipation relation

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

Nonlinear PDE Model

(nFP-D)

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

- $f(x,t)$ 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.

Known Results

- Local existence of solutions known under natural (no flux) boundary conditions [9]. This result comes after an application of three different change of variables. The authors also assume $f_0 \in C_x^{2+\beta}$ but as a solution they just get $f \in C_{x,t}^{2+\beta,1+\beta/2}$.
- Asymptotic behaviour of the solutions under the assumption that classical global solutions on $\mathbb{T}^d$ exist [10, 7].

More Explicit form of the PDE

By applying the product rule, it is possible to separate the linear and nonlinear part:
(nFP)

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

Here L_{FP} is a divergence form linear operator as defined below:

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

We assume there is a $\theta > 0$ indepedent from $(x,t) \in \mathbb{T}^d \times [0,\infty)$ such that $\frac{D(x)}{\pi(x,t)} \geq \theta$.

Definition (Fundamental solution [11, p. 3])

Let $\partial_t - L$ be a second order uniformly parabolic differential operator. We call $K(x, t; y, s)$ to be the *fundamental solution* of $\partial_t - L$ in $\mathbb{T}^d \times [0, T]$ if the following two properties hold:

(P1) $K(x, t; y, s)$ is solution of $\partial_t h = Lh$ as a function of $(x, t) \in \mathbb{T}^d \times [0, T]$ for every fixed (y, s) with $y \in \mathbb{T}^d$ and $s < t \leq T$,

(P2) for every continuous function f_0 on $\mathbb{T}^d$, K satisfies the limit relation given below

$$\lim_{t \to s} \int_{\mathbb{T}^d} K(x, t; y, s) f_0(y) dy = f_0(x).$$

Comparison Principle

Let $\partial_t - L$ be a second-order uniformly parabolic divergence form operator with

$$Lf \coloneqq \nabla \cdot \nabla(a(x,t)f) + b(x,t) \cdot \nabla f + c(x,t)f.$$

Then, the fundamental solution K of $\partial_t - L$ satisfies the following comparison principle:

$$\exp\left(c_{\inf}(t-s)\right) \leq \int_{\mathbb{T}^d} K(x,t;y,s)dy \leq \exp\left(c_{\sup}(t-s)\right)$$

where $c_{\inf}$ and $c_{\sup}$ denotes the infimum and supremum of the coefficient $c(x,t)$.

Gaussian Bounds

Theorem ([11, Thm. 7, Ch. 9], [11, Thm. 8, Ch. 9], [11, p. 255] (adapted))

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 $t - s \leq 1$, the following Gaussian bounds hold on K and its derivatives:

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

and

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

Gaussian Bounds (continued)

Here $\beta \in (0, 1)$ and $c, C > 0$ are constants which depend on the dimension, uniform parabolicity constant λ of L, uniform upper bound of the coefficients of L, Hölder regularity of the coefficients of L, and order of the derivatives $a, b \in \mathbb{Z}_{\geq 0}$. Note that, $2a + b \leq 2 + l$.

Integral Bounds

Corollary (Integral bounds on the fundamental solution)

Let $\partial_t - L$ be a second-order uniformly parabolic operator in non-divergence form which satisfies the assumptions of Theorem 2 for $l = 1$. Then we have the following integral bounds on the fundamental solution K of $\partial_t - L$ and its derivatives:

(1)
$$\int_{t'}^{t} \int_{\mathbb{T}^d} \left| \nabla_y K(x, t; y, s) \right| dy ds \leq C \left| t - t' \right|^{1/2},$$

(2)
$$\int_{0}^{t'} \int_{\mathbb{T}^d} \int_{t'}^{t} \left| \partial_\tau \nabla_y K(x', \tau; y, s) \right| d\tau dy ds \leq C \left| t - t' \right|^{1/2},$$

and

(3)
$$\int_{0}^{t} \int_{\mathbb{T}^d} \left| \nabla_y K(x, t; y, s) - \nabla_y K(x', t; y, s) \right| dy ds \leq C t^{(1-\beta)/2} \left| x - x' \right|^{\beta}.$$

Assumptions

(A1) $\frac{D(x)}{\pi(x,t)} \geq \theta$ for all $(x,t) \in \mathbb{T}^d \times [0,\infty)$ for some arbitrary $\theta > 0$ which is independent from x and t. With this assumption, the linear part of (nFP), $\partial_t - L_{\mathrm{FP}}$, defines a linear second-order uniformly parabolic differential operator.

(A2) The coefficients of L_{FP} when they are considered in non-divergence form: $\frac{D(x)}{\pi(x,t)}$, $\frac{\nabla\phi(x)}{\pi(x,t)} + \nabla\left(\frac{D(x)}{\pi(x,t)}\right)$, and $\nabla\cdot\left(\frac{\nabla\phi(x)}{\pi(x,t)}\right)$ are bounded and belongs to $C^{1+\beta,\beta/2}_{x,t}(\mathbb{T}^d \times [0,\infty))$. In addition, the coefficient of the nonlinear part, $\frac{\nabla D(x)}{\pi(x,t)}$ satisfies the same assumptions. Here, $\beta \in (0,1)$ is Hölder exponent of the coefficients.

Assumptions (continued)

(A3) $\Lambda \geq f_0(x) \geq 4\mu$ for some arbitrary but fixed $\Lambda, \mu > 0$ which are independent from $x \in \mathbb{T}^d$.

(A4) There is $C_D \geq 1$ which is independent from $x \in \mathbb{T}^d$ such that $D(x) \geq C_D$. There are also $C_\pi^{\text{low}}, C_\pi^{\text{up}} > 0$ which are independent from $(x,t) \in \mathbb{T}^d \times [0,\infty)$ such that $C_\pi^{\text{low}} \leq \pi(x,t) \leq C_\pi^{\text{up}}$ [7].

Proof of Local Existence

We apply a fixed point argument by treating the nonlinearity of the PDE as a source term:
(LPNE)

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

As a Banach space, we set $X \coloneqq C^0(\mathbb{T}^d \times [0,T])$ which is equipped with a sup-norm:

$$\|f\|_X \coloneqq \sup_{(x,t) \in \mathbb{T}^d \times [0,T]} |f(x,t)| .$$

Then, we work on the closed subspace $Y \subset X$:

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

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

Map

As we can see, (LPNE) is linear in the variable u and by Duhamel's principle its solution can be written as:

$$u = \int_{\mathbb{T}^d} K(x,t;y,0) f_0(y) dy$$
$$+ \int_0^t \int_{\mathbb{T}^d} K(x,t;y,s) \nabla_y \cdot \left(\frac{\nabla D(y)}{\pi(y,s)} f(y,s) \log f(y,s) \right) dyds$$

where K is the fundamental solution of the second-order uniformly parabolic operator $\partial_t - L_{\mathrm{FP}}$ where L_{FP} defined as in (LO) and its coefficients satisfy Assumption (A1).

Map

Definition (Map)

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

(M)

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

where $V(y,s) := \frac{\nabla D(y)}{\pi(y,s)}$.

Lipschitz Estimates

Our nonlinear Fokker-Planck type equation (nFP) contains logarithmic nonlinearity so, we should be able to control this term. To this end, for any f and g in $Y \subset X$, we have the following norm estimates:

$$\|\log f - \log g\|_X \leq \frac{1}{\mu}\|f - g\|_X \tag{4}$$

and

$$\|\log f\|_X \leq \frac{R}{\mu} + |\log \mu| + 1. \tag{5}$$

They are just a consequence of the fact that log is $\frac{1}{\mu}$-Lipschitz on $[\mu, \infty)$ and the triangle inequality.

Time Bound

We choose the following time bound:

$$T^{1/2} \le \min\left\{ \frac{\min\{\mu, 1\}}{2\left(CR\left(\frac{2R}{\mu} + |\log \mu| + 1\right)\|V\|_{\sup} + 1\right)}, \left(\frac{\log 2}{|W_{\inf}| + |W_{\sup}| + 1}\right)^{1/2} \right\}.$$

- $R = 1 + \mu + 2\|f_0\|_{C^0(\mathbb{T}^d)}$ with $\mu > 0$,
- $V = \frac{\nabla D}{\pi}$,
- C is a constant as in Gaussian bounds,
- $W_{\inf}$ and $W_{\sup}$ denotes the infimum and supremum of the coefficient $W(x,t) := \nabla \cdot \left(\frac{\nabla \phi(x)}{\pi(x,t)}\right)$ of the zeroth order term in $\partial_t - L_{\mathrm{FP}}$.

First Lemma

Lemma (Well-definiteness of the map)

The map (M) *is well-defined i.e. maps Y to itself.*

Sketch of Proof.

Step 1: From the definition of map (M), we have the decomposition

$$(\Psi f)(x,t) = (\Psi_{f_0,\text{linear}})(x,t) + (\Psi_{f,\text{nonlinear}})(x,t).$$

Step 2: $\Psi f \geq \mu$ whenever $f \geq \mu$.

Step 3: $\|\Psi f\|_X \leq R$ whenever $\|f\|_X \leq R$. $\square$

$\Psi f \geq \mu$ whenever $f \geq \mu$

$$
\begin{aligned}
\Psi f &= \int_{\mathbb{T}^d} K(x,t;y,0) f_0(y) dy \\
&\quad - \int_0^t \int_{\mathbb{T}^d} \nabla_y K(x,t;y,s) \cdot V(y,s) f(y,s) \log f(y,s) dy ds \\
&\geq 4\mu \exp(W_{\inf} t) - \|f\|_X \|\log f\|_X \|V\|_{\sup} \int_0^t \int_{\mathbb{T}^d} |\nabla_y K(x,t;y,s)| \\
&\geq 4\mu \exp(-|W_{\inf}|\, T) - CRT^{1/2} \|V\|_{\sup} \left(\frac{R}{\mu} + |\log \mu| + 1 \right) \\
&\geq 2\mu - \min\{\mu, 1\} \\
&\geq \mu.
\end{aligned}
$$

Contraction Property

Lemma

The map (M) *is* $\frac{1}{2}$*-contraction mapping on* Y *i.e.*

$$\|\Psi f - \Psi g\|_X \leq \frac{1}{2}\|f - g\|_X$$

holds for any $f, g \in Y$.

Existence of a Fixed Point

Corollary

There exists a unique fixed point f of the map (M) *i.e.*

$$f = \Psi f.$$

Proof.

From previous two lemmas, we know that the map (M) is well-defined contraction mapping on Y so, by Banach's fixed point theorem, there exists a unique fixed point $f \in Y$ such that $f = \Psi f$ and this completes the proof. $\square$

Regularity

In our well-definitiess proof, due to behaviour of Gaussian bounds, we get something stronger which means that $\Psi_{f,\text{nonlinear}}(x,t)$ is β-Hölder in space.
We also know that $\Psi_{f_0,\text{linear}}(x,t)$ is β-Hölder in space as well.
As a conclusion, the map $\Psi f(x,t)$ is β-Hölder in space.

Regularity (continued)

Corollary

The unique fixed point f of (M) *belongs to*

$$f \in C^{2+\beta,1+\beta/2}_{\mathrm{loc}}(\mathbb{T}^d \times (0,T]).$$

So, this means f is two times differentiable in x and one time differentiable in t with Hölder continuous derivatives. Hence, f is the unique classical solution of (nFP).

Continuous Depence on Initial Data

Corollary

Let f *and* g *be solutions of* (nFP) *with initial data* f_0 *and* g_0 *respectively. Then the following continuity estimate holds*

$$\|f - g\|_X \leq 4\|f_0 - g_0\|_{C^0(\mathbb{T}^d)}.$$

Main Theorem

Theorem

Under the assumptions (A1), (A2), and (A3) the initial value problem (nFP) *is locally well posed on* Y*.*

Global Well-Posedness

Theorem

Under the assumptions (A1), (A2), (A3), and (A4) there exists a unique positive classical global solution of (nFP) *which belongs to*

$$f \in C_{\mathrm{loc}}^{2+\beta,1+\beta/2}(\mathbb{T}^d \times (0,\infty)).$$

Global Well-Posedness (continued)

The proof is based on repeating our local existence proof on nested time intervals $I_j := [0, jT']$ via induction and using a-priori estimate.

A priori estimates

Proposition ([10, Prop. 1.6], [7, Cor. 1.8])

Let $f(x,t)$ *be a classical solution of* (nFP). *Then for all* $(x,t) \in \mathbb{T}^d \times (0,\infty)$, *under Assumptions (A3) and (A4), the following two sided estimate holds on* $f(x,t)$*:*

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

Also, by using the upper and lower bounds of f^{eq} *from Lemma 1.6 of [7], it is possible to make it the above estimate uniform:*

$$m \leq f(x,t) \leq M$$

where $m, M > 0$ *are constants which are independent from* x *and* t*.*

Idea of the Proof

We will construct the solution via induction. Define

$$R' := 1 + \mu + 2\|f_0\|_{C^0(\mathbb{T}^d)} + 2M$$

and

$$T'^{1/2} := \min\left\{ \frac{\min\{\mu, 1, \frac{m}{4}\}}{2\left(CR'\left(\frac{2R'}{\gamma} + |\log\gamma| + 1\right)\|V\|_{\sup} + 1\right)}, \right.$$
$$\left. \left(\frac{\log 2}{|W_{\inf}| + |W_{\sup}| + 1}\right)^{1/2} \right\}$$

where $C > 0$ is a constant as in Gaussian bounds and $\gamma := \min\{\mu, \frac{m}{4}\}$. The claim is: for all $j \in \mathbb{Z}_{\geq 1}$, there is a classical solution of (nFP) on $[0, jT']$ satisfying $m \leq f \leq M$.

Updated Map

$$
\begin{aligned}
\Phi g(x,t) := &\int_{\mathbb{T}^d} K(x,t;y,kT')f_k(y,kT')dy \\
&- \int_{kT'}^{t}\int_{\mathbb{T}^d} \nabla_y K(x,t;y,s)\cdot \frac{\nabla D(y,s)}{\pi(y,s)} g(y,s)\log g(y,s)dyds
\end{aligned}
$$

on the following space

$$
\begin{aligned}
Y_k := \Big\{ g \in C^0(\mathbb{T}^d \times [kT',(k+1)T']) =: X_k \ \Big| \\
g \geq \min\left\{\mu, \frac{m}{4}\right\},\ \|g\|_{X_k} \leq R' \Big\}.
\end{aligned}
$$

Thank you!

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