

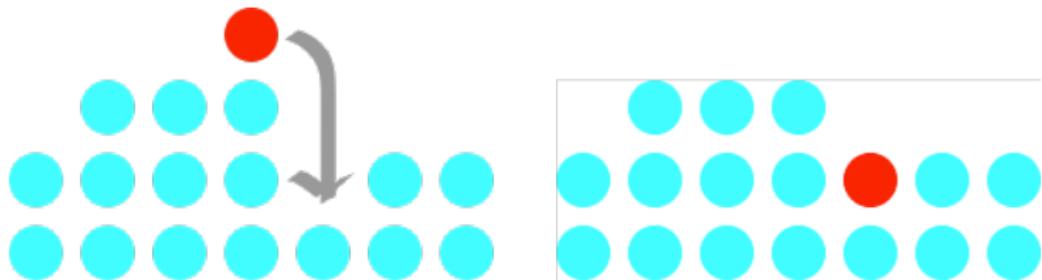
On 4th order nonlinear thin-film like PDEs describing crystal surface evolution

Joint work with Jon Weare (NYU), Anya Katsevich (MIT),
Dio Margetis (Maryland), Katy Craig (UCSB), Li Wang
(Minnesota), Yuan Gao (Purdue), Jianfeng Lu (Duke),
Jian-Guo Liu (Duke)

Jeremy L. Marzuola

Mathematics Department University of North Carolina, Chapel Hill

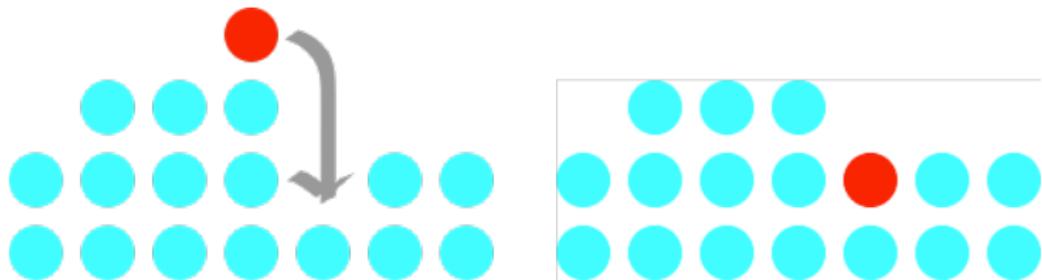
81st Fujihara Seminar - June 3, 2024



Each surface atom breaks the bonds with its nearest (horizontal) neighbors at a random (exponentially distributed) time and then jumps (uniformly) to one of its neighboring sites.

The rate at which those bonds are broken depends on the energy barrier that must be overcome in breaking them.... but atoms with lots of horizontal neighbors will move infrequently and neighbors with no (adatoms) or few horizontal neighbors will move more frequently.

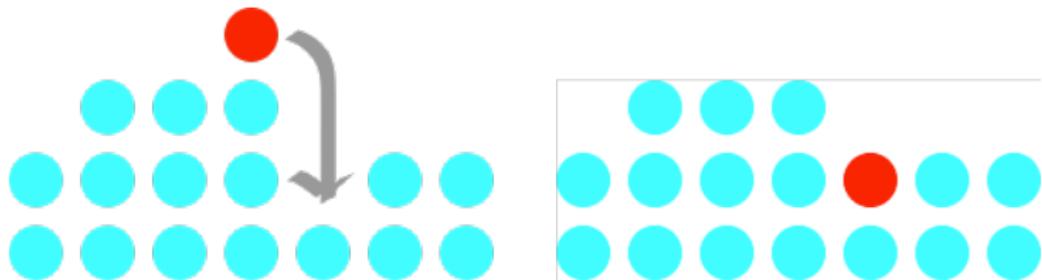
Macroscopically you might expect convex regions to move more slowly than concave regions.



Each surface atom breaks the bonds with its nearest (horizontal) neighbors at a random (exponentially distributed) time and then jumps (uniformly) to one of its neighboring sites.

The rate at which those bonds are broken depends on the energy barrier that must be overcome in breaking them.... but atoms with lots of horizontal neighbors will move infrequently and neighbors with no (adatoms) or few horizontal neighbors will move more frequently.

Macroscopically you might expect convex regions to move more slowly than concave regions.



Each surface atom breaks the bonds with its nearest (horizontal) neighbors at a random (exponentially distributed) time and then jumps (uniformly) to one of its neighboring sites.

The rate at which those bonds are broken depends on the energy barrier that must be overcome in breaking them.... but atoms with lots of horizontal neighbors will move infrequently and neighbors with no (adatoms) or few horizontal neighbors will move more frequently.

Macroscopically you might expect convex regions to move more slowly than concave regions.

We model the crystal surface as an indexed set of integer valued random variables $h_N(t, \alpha) \in \mathbb{Z}$ where $\alpha \in \mathbb{T}_N^d$ (the d -dimensional torus).

The jumps:

$h_N \rightarrow J_\alpha J^\beta h_N$ add an atom at β and subtract one from α

where

$$J_\alpha h_N(\gamma) = \begin{cases} h_N(\alpha) - 1, & \gamma = \alpha \\ h_N(\gamma), & \gamma \neq \alpha \end{cases} \quad \text{and} \quad J^\alpha h_N(\gamma) = \begin{cases} h_N(\alpha) + 1, & \gamma = \alpha \\ h_N(\gamma), & \gamma \neq \alpha \end{cases}$$

Now we need the **rates**...

We need an estimate of the energy barrier that must be overcome in breaking an atom's neighbor bonds.

If we define the total energy of the surface to be:

$$H(h_N) = \sum_{\alpha \in \mathbb{T}_N} \sum_{i \leq d} V(\nabla_i^+ h_N(\alpha))$$

where

$$\nabla_i^+ g(\alpha) = g(\alpha + \mathbf{e}_i) - g(\alpha) \quad \text{and} \quad \nabla_i^- g(\alpha) = g(\alpha) - g(\alpha - \mathbf{e}_i)$$

then the (symmetrized) change in energy that results from removing the atom at site α :

$$n_\alpha(h_N) = \frac{1}{2} \sum_{i \leq d} (V(\nabla_i^+ J_\alpha h_N(\alpha)) - V(\nabla_i^+ h_N(\alpha)) \\ + V(\nabla_i^- J_\alpha h_N(\alpha)) - V(\nabla_i^- h_N(\alpha))).$$

The rate at which the atom at site α breaks its bonds and becomes free to move is

$$e^{-2Kn_\alpha(h_N)}$$

The rate at which an atom breaks its bonds and moves to any particular neighbor is

$$r_N(\alpha) = \frac{1}{2d} e^{-2Kn_\alpha(h_N)}$$

The generator is

$$\mathcal{A}_N f(h_N) = \sum_{\substack{\alpha, \beta \in \mathbb{T}_N^d \\ |\alpha - \beta| = 1}} r_N(\alpha) \left(f(\mathbf{J}_\alpha^\beta h_N) - f(h_N) \right).$$

$h(t, \cdot)$ is reversible with respect to the distribution

$$\rho_N^m \propto \begin{cases} e^{-K \sum_{\alpha \in \mathbb{T}_N} \sum_{i \leq d} V(\nabla_i^+ h_N(\alpha))}, & \text{if } \sum_{\alpha \in \mathbb{T}_N} h_N(\alpha) = m \\ 0, & \text{otherwise} \end{cases}$$

with $m = \sum_{\alpha \in \mathbb{T}_N} h_N(0, \alpha)$

Our objective is to characterize the non-equilibrium continuum (large N) behavior of the surface.

But first...

This is oversimplified but physically reasonable:

The atoms mostly jiggle around on their sites but eventually climb out of the potential well (from bonds with neighbors) confining them. The escape event is rare and it's reasonable to assume that

- 1 the rate is dominated by the change in energy and
- 2 the projection of the system onto the site occupation number remains Markovian.

A couple of examples

- 1 Suppose $V(z) = |z|$. Then

$$n_\alpha(h_N) + 2^{d-1} = \sum_{\substack{\beta \in \mathbb{T}_N^d \\ |\alpha - \beta| = 1}} \mathbf{1}_{(h_N(\alpha) \leq h_N(\beta))},$$

i.e. up to an additive constant (a time rescaling), the generalized coordination number is the number of bonds that need to be broken to free the atom at lattice site α .

- 2 Suppose $V(z) = z^2$. Then

$$n_\alpha(h_N) - 2d = \sum_{i \leq d} \nabla_i^+ h_N(\alpha) - \nabla_i^- h_N(\alpha),$$

i.e. up to an additive constant, the generalized coordination number is the discrete Laplacian of the surface at lattice site α .

Why this model?

This model is far from perfect:

- 1 no substrate interactions (e.g. elasticity),
- 2 no defects (e.g. vacancies),
- 3 many systems require modeling the electronic structure (probably via DFT) to get correct barrier heights for estimating jump rates,
- 4 ...

But it is close to models used in very large scale simulations.

These models have not been considered by mathematicians but close relatives have been studied:

Funaki and Spohn (1997) studied the hydrodynamic limit of

$$dh_N(t, \alpha) = -\frac{\partial H(h_N)}{\partial h_N(\alpha)} dt + \sqrt{2K^{-1}} dW(t)$$

where here $h_N(t, \alpha) \in \mathbb{R}$

They show that if

$$\bar{h}_N(t, x) = N^{-1} h_N(N^4 t, \alpha) \text{ where } Nx \in \cap_{i=1}^d \left[\alpha_i - \frac{1}{2}, \alpha_i + \frac{1}{2} \right)$$

then \bar{h}_N converges to the solution of the PDE

$$\partial_t h = K \operatorname{div} [\sigma_C(\nabla h)]$$

The surface tension is defined by $\sigma_C(u) = \nabla \mathcal{F}_C(u)$ where

$$\mathcal{F}_C(u) = \frac{1}{K} \sup_{\sigma \in \mathbb{R}^d} \left\{ \sigma^\top u - \log \int_{w \in \mathbb{R}^d} e^{-K \sum_{i \leq d} V(w_i) + K \sigma^\top w} dw \right\}$$

$$u = \frac{\int w e^{-K \sum_{i \leq d} V(w_i) + K \sigma(u)^\top w} dw}{\int e^{-K \sum_{i \leq d} V(w_i) + K \sigma(u)^\top w} dw}$$

They show that if

$$\bar{h}_N(t, x) = N^{-1} h_N(N^4 t, \alpha) \text{ where } Nx \in \cap_{i=1}^d \left[\alpha_i - \frac{1}{2}, \alpha_i + \frac{1}{2} \right)$$

then \bar{h}_N converges to the solution of the PDE

$$\partial_t h = K \operatorname{div} [\sigma_C(\nabla h)]$$

The surface tension is defined by $\sigma_C(u) = \nabla \mathcal{F}_C(u)$ where

$$\mathcal{F}_C(u) = \frac{1}{K} \sup_{\sigma \in \mathbb{R}^d} \left\{ \sigma^\top u - \log \int_{w \in \mathbb{R}^d} e^{-K \sum_{i \leq d} V(w_i) + K \sigma^\top w} dw \right\}$$

$$u = \frac{\int w e^{-K \sum_{i \leq d} V(w_i) + K \sigma(u)^\top w} dw}{\int e^{-K \sum_{i \leq d} V(w_i) + K \sigma(u)^\top w} dw}$$

Nishikawa (2002) extended Funaki and Spohn's approach to

$$dh(t, \alpha) = \Delta \frac{\partial H(h)}{\partial h(\alpha)} dt + \sqrt{-2K^{-1} \Delta} dW(t)$$

where

$$\Delta g(\alpha) = \sum_{i \leq d} \nabla_i^+ g(\alpha) - \nabla_i^- g(\alpha).$$

He proved that \bar{h}_N converges to the solution of the PDE

$$\partial_t h = -K \Delta [\operatorname{div} [\sigma_C(\nabla h)]]$$

Recent work of Armstrong-Wu (2019) shows that $\sigma_C \in C^{2,\beta}$ for some $\beta > 0$. What can we say about σ_D ??

This last overdamped Langevin equation for continuous height variables can be derived from the KMC model by introducing a vanishing lattice constant.

Replace $V(z)$ by $V(az)$, rescaling time appropriately, and taking $a \rightarrow 0$.

One can then apply Nishikawa's result to make an approximate statement about the scaling limit of the KMC equations.

This was pointed out by Haselwandter and Vvedensky.

The small lattice constant limit sacrifices interesting features.

For example, if V is symmetric and if h_N is a solution of the SDE then $-h_N$ is also a solution.

Remember that in the KMC model convex regions are much stickier than concave regions.

Krug, Dobbs, and Majaniemi studied the evolution of a model very similar to our KMC models in 1D when $V(z) = |z|$

They first argue for

$$\partial_t h = -K \Delta [\operatorname{div} [\sigma_D(\nabla h)]]$$

with $\sigma_D(u) = \nabla \mathcal{F}_D(u)$ where

$$\mathcal{F}_D(u) = \frac{1}{K} \sup_{\sigma \in \mathbb{R}^d} \left\{ \sigma^T u - \log \sum_{z \in \mathbb{Z}^d} e^{-K \sum_{i \leq d} V(z_i) + K \sigma^T z} \right\}$$

Then at the end of the paper they give arguments supporting

$$\partial_t h = \Delta \left[e^{-K \operatorname{div}[\sigma_D(\nabla h)]} \right]$$

As they point out... this PDE gives the first PDE when curvature of the surface is small.

M-Weare (2013): The correct limit depends on the scaling regime.

And the standard scaling regime may tell us less about the physics.

In the $h \sim N^{-1}h_N$, $s \sim N^4t$, $x \sim N^{-1}\alpha$ regime we argue for

$$\partial_t h = -\frac{K}{2d} \Delta [\text{div} [\sigma_D(\nabla h)]]$$

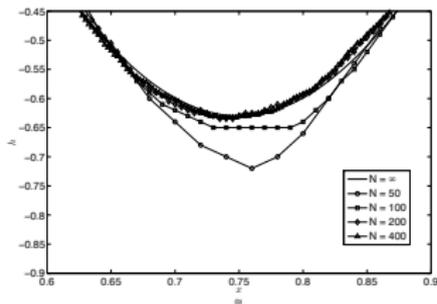
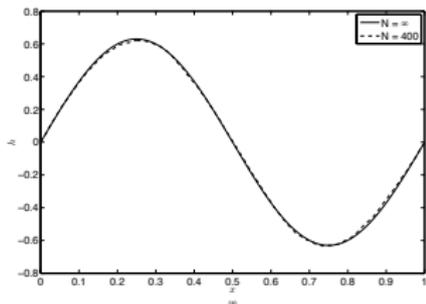


Figure: $V = z^2$ for $T = 1e - 1$ at $K = 1.5$

In the $h \sim N^{-1}h_N$, $s \sim N^4t$, $x \sim N^{-1}\alpha$ regime we argue for

$$\partial_t h = -\frac{K}{2d} \Delta [\text{div} [\sigma_D(\nabla h)]]$$

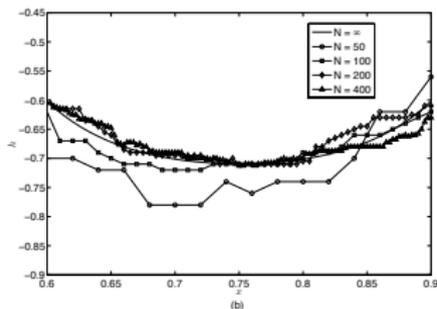
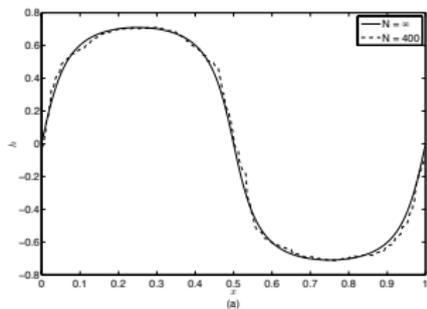


Figure: $V = |z|$ for $T = 1e-3$ at $K = 1.5$

Now suppose that for some $p > 1$

$$V(\kappa u) = \kappa^p V(u) \quad \text{for all } \kappa > 0$$

Letting $q = \frac{p}{p-1}$ and scaling like

$$h \sim N^{-q} h_N \quad s \sim N^{q+2} t \quad x \sim N^{-1} \alpha$$

we argue that \bar{h}_N converges to the solution of

$$\partial_t h = \frac{1}{2d} \Delta \left[e^{-K \sum_{i \leq d} V'(\partial_{x_i} h)} \partial_{x_i}^2 h \right]$$

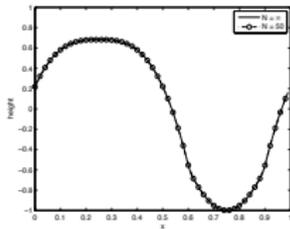


Figure: $V = |z|^{3/2}$ for $T = 1e - 12$ at $K = 1.5$

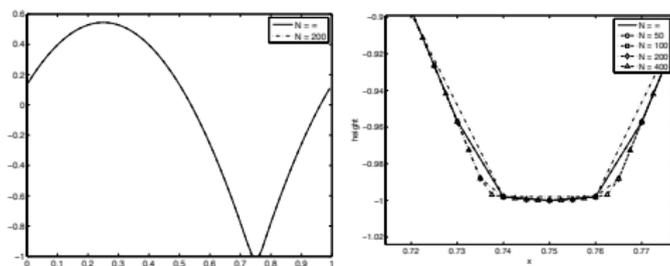


Figure: $V = z^2$ for $T = 1e - 20$ at $K = 1.5$

- For the rough pde with $p = 1$ and the continuous surface tension, jointly with Jian-Guo Liu, Jianfeng Lu and Dio Margetis (2019) we derived the exponential PDE in the $p = 1$ case and studied facet dynamics for that model. This is related to the work of Giga-Kohn (2011), Giga-Giga (2010) on Total Variation flows.
- The PDE takes the form

$$\partial_t h = \partial_{xx} e^{-\partial_x \left(\frac{\partial_x h}{|\partial_x h|} \right)}, \quad h(x, 0) = h_0(x),$$

- For the rough pde with $p = 1$ and the continuous surface tension, jointly with Jian-Guo Liu, Jianfeng Lu and Dio Margetis (2019) we derived the exponential PDE in the $p = 1$ case and studied facet dynamics for that model. This is related to the work of Giga-Kohn (2011), Giga-Giga (2010) on Total Variation flows.
- The PDE takes the form

$$\partial_t h = \partial_{xx} e^{-\partial_x \left(\frac{\partial_x h}{|\partial_x h|} \right)}, \quad h(x, 0) = h_0(x),$$

- For a non-exponential version of this model,

$$\partial_t h = -\partial_{xx} \partial_x \left(\frac{\partial_x h}{|\partial_x h|} \right), \quad h(x, 0) = h_0(x),$$

Giga-Giga (2010) proved the existence of shock-like solutions satisfying

$$\begin{cases} \dot{h}_f = -\frac{3}{x_f^3(t)}, \\ \dot{x}_f(h_0(x_f) - h_f) = -3x_f^{-2}. \end{cases}$$

- There are implicit facet dynamics that can be derived and relate to a jump forming at the point of minima and maxima.
- Numerical methods also need to be carefully developed to capture jumps.

- There are implicit facet dynamics that can be derived and relate to a jump forming at the point of minima and maxima.
- Numerical methods also need to be carefully developed to capture jumps.

- In this case, the energy supports the formation of jump discontinuities. The front of a facet (x_f, h_f) can be shown to obey the Differential-Algebraic system of equations

$$\left\{ \begin{array}{l} \dot{X}_f = \frac{\dot{x}_f F(X_f)}{1 - x_f F'(X_f)} , \\ \dot{h}_f = -2F(X_f)^2 , \\ \dot{x}_f (h_0(x_f) - h_f) = -2x_f F(X_f)^2 , \end{array} \right.$$

where the variable X_f is an extra variable included to enforce an algebraic condition.

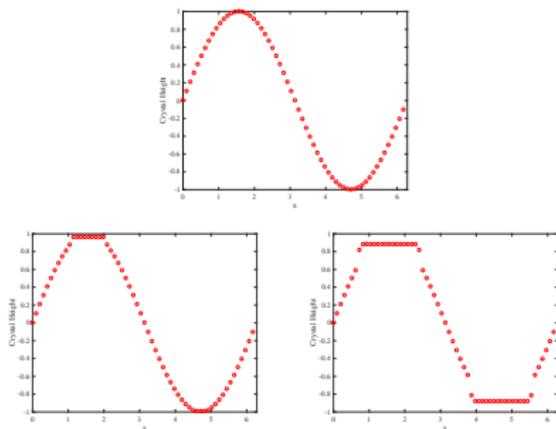


Figure: Snapshots of evolving surface height profile, $h(x, t)$, under initial data $h(0, x) = \sin(x)$ (top panel) by fourth-order total variation flows given by: exponential PDE with regularization parameter $\nu = 10^{-3}$ on a time scale $T = 10^{-4}$ (bottom left panel); and by PDE with regularization parameter $\nu = 10^{-3}$ on a time scale $T = 10^{-2}$ (bottom right panel).

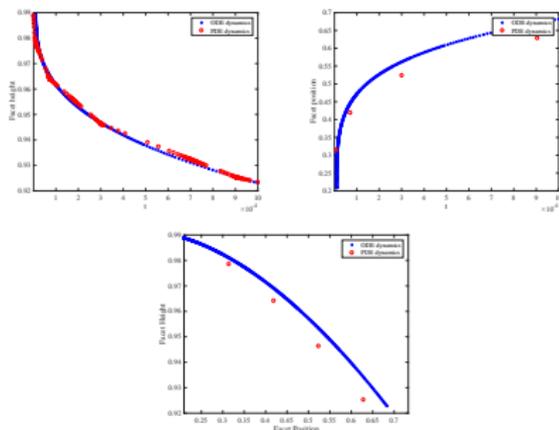


Figure: (Color Online) Plots of facet height $h_f(t)$ versus time, t (top left panel), facet position $x_f(t)$ versus t (top right panel) and facet height versus facet position ($x_f(t)$, $h_f(t)$) (bottom panel). The initial data is taken from the PDE evolution as $x_f(t_0) = \frac{\pi}{15}$, $h_f(t_0) = .98879899$ with $t_0 = 5 \times 10^{-7}$. The numerical experiments for the ODEs and PDE are then compared up to time $T = 10^{-3}$.

- These PDEs can be related to the total variation flow in H^{-1} for the given energy.

$$E[h] = \gamma \int_{\Omega} \left(|\nabla h| + \frac{g}{3} |\nabla h|^3 \right) dx \quad (\Omega \subset \mathbb{R}^2),$$

- For $g > 0$, due to presence of the (less singular) term $|\partial_x h|^3$ in the surface energy, the solution to this PDE no longer develops jumps in the height profile. This is expected from other studies in the non-weighted H^{-1} total variation flow.

- These PDEs can be related to the total variation flow in H^{-1} for the given energy.

$$E[h] = \gamma \int_{\Omega} \left(|\nabla h| + \frac{g}{3} |\nabla h|^3 \right) dx \quad (\Omega \subset \mathbb{R}^2),$$

- For $g > 0$, due to presence of the (less singular) term $|\partial_x h|^3$ in the surface energy, the solution to this PDE no longer develops jumps in the height profile. This is expected from other studies in the non-weighted H^{-1} total variation flow.

- Recent progress on Exponential PDE with $p = 2$ by J.G. Liu, Y. Gao, J. Lu, X. Xu, R. Granero-Belinchon, M. Magliocca, R. Strain, D. Ambrose, JLM,
- There are three main approaches:
 1. A small data theory in the Weiner Algebra space (Granero-Belinchon, Magliocca; Liu-Strain; Ambrose, GLLM).
 2. A large data weak solution theory similar to the entropy solutions of Bernis-Friedman (Liu-Xu, GLLM).
 3. A small data, quasilinear approach for the u equation, see certain recent results of Quoc Hung Nguyen on quasilinear parabolic models.

- Recent progress on Exponential PDE with $p = 2$ by J.G. Liu, Y. Gao, J. Lu, X. Xu, R. Granero-Belinchon, M. Magliocca, R. Strain, D. Ambrose, JLM,
- There are three main approaches:
 1. A small data theory in the Weiner Algebra space (Granero-Belinchon, Magliocca; Liu-Strain; Ambrose, GLLM).
 2. A large data weak solution theory similar to the entropy solutions of Bernis-Friedman (Liu-Xu, GLLM).
 3. A small data, quasilinear approach for the u equation, see certain recent results of Quoc Hung Nguyen on quasilinear parabolic models.

- One can even include 2nd order effects of evaporation and deposition to arrive at at PDE of the form:

$$\partial_t h = \Delta e^{-\Delta h} + (1 - e^{-\Delta h}).$$

See Gao-Liu-Lu-M (2020).

- Define

$$u := e^{-\Delta h}.$$

The equation can be formally recast as

$$\partial_t u = -u\Delta[\Delta u + (1 - u)].$$

- One can even include 2nd order effects of evaporation and deposition to arrive at at PDE of the form:

$$\partial_t h = \Delta e^{-\Delta h} + (1 - e^{-\Delta h}).$$

See Gao-Liu-Lu-M (2020).

- Define

$$u := e^{-\Delta h}.$$

The equation can be formally recast as

$$\partial_t u = -u\Delta[\Delta u + (1 - u)].$$

- For weak solutions, use a regularized method to first prove the existence and strict positivity for regularized solution u_ε to a properly modified equation below, then take limit $\varepsilon \rightarrow 0$. For $0 < \alpha < 1$, the regularization of the u equation we consider is

$$\begin{cases} \partial_t u_\varepsilon = -\frac{u_\varepsilon^{1+\alpha}}{u_\varepsilon^\alpha + \varepsilon^\alpha} (\partial_x^4 u_\varepsilon - \partial_x^2 u_\varepsilon), & \text{for } t \in [0, T], x \in \mathbb{T}; \\ u_\varepsilon(0, x) = u_0(x) + \varepsilon, & \text{for } x \in \mathbb{T}. \end{cases}$$

Singularity Formation for $p=2$

- Using the change of variables $u = e^{-\Delta h}$, the 4th equations of motion become

$$u_t = -u\Delta^2 u.$$

- There is a related 2nd order model of the form

$$u_t = u\Delta u.$$

- Note, one of these looks a bit like the thin-film equation and one looks a bit like the porous medium equation, but without gradient structure!

Singularity Formation for $p=2$

- Using the change of variables $u = e^{-\Delta h}$, the 4th equations of motion become

$$u_t = -u\Delta^2 u.$$

- There is a related 2nd order model of the form

$$u_t = u\Delta u.$$

- Note, one of these looks a bit like the thin-film equation and one looks a bit like the porous medium equation, but without gradient structure!

Singularity Formation for $p=2$

- Using the change of variables $u = e^{-\Delta h}$, the 4th equations of motion become

$$u_t = -u\Delta^2 u.$$

- There is a related 2nd order model of the form

$$u_t = u\Delta u.$$

- Note, one of these looks a bit like the thin-film equation and one looks a bit like the porous medium equation, but without gradient structure!

- Self-similar solutions that are quartic in the 4th order case and quadratic in the 2nd order case can be found, but they do not behave well with respect to boundary conditions.

4th Order Singularity Formation

4th Order Singularity Formation Zoom In

2nd Order Avoided Singularity

- Note, setting $v = u_x$, we get

$$\partial_t v = vv_x + uv_{xx},$$

which resembles an Euler equation with variable coefficient viscosity. It was observed by Tarek Elgindi that using the maximum principle this solution cannot form a true singularity. With David Ambrose and Doug Wright, we are now pursuing this as a means of capturing both the transition layer between self-similar profiles and trying to build solutions that almost form singularities in the 2nd order case and do indeed form singularities in the 4th order problem.

- With Yuan Gao, Jian-Guo Liu, Jianfeng Lu and Anya Katsevich (2021), we considered Metropolis-style rates and analyzing dynamics in comparison to the Adatom KMC models. These rates have some distinct differences and a temperature dependence in the form of the limiting PDEs can be seen. We focus here on the case $p = 2$ as many calculations become more explicit. The PDE limit proposed here is of the form

$$\partial_t h(t, x) = \partial_x \left(e^{[-\partial_x^3 h(t, x)]} - e^{[\partial_x^3 h(t, x)]} \right).$$

- This is NOT quite the exact limit you get from the KMC system, but it is close as the temperature gets large. See the works by Katsevich exploring this (2022,2023).

- With Yuan Gao, Jian-Guo Liu, Jianfeng Lu and Anya Katsevich (2021), we considered Metropolis-style rates and analyzing dynamics in comparison to the Adatom KMC models. These rates have some distinct differences and a temperature dependence in the form of the limiting PDEs can be seen. We focus here on the case $p = 2$ as many calculations become more explicit. The PDE limit proposed here is of the form

$$\partial_t h(t, x) = \partial_x \left(e^{[-\partial_x^3 h(t, x)]} - e^{[\partial_x^3 h(t, x)]} \right).$$

- This is NOT quite the exact limit you get from the KMC system, but it is close as the temperature gets large. See the works by Katsevich exploring this (2022,2023).

- Recall, we are generally interested in the models we consider of the form:

$$h_t = \Delta e^{-\Delta_p h}$$

for Δ_p the p -Laplacian for $p \geq 1$ given by the Euler-Lagrange equation for the surface energy

$$E(h) = \frac{1}{p} \int |\nabla h|^p dx.$$

- Recently, with Craig, Liu, Lu and Wang, we have introduced a gradient flow structure numerical flow that allows one to numerically solve

$$h_t = \Delta e^{-\Delta_1 h}$$

using the FORMAL gradient flow structure

$$h_t + \nabla \cdot \left(M(h) \nabla \frac{\partial \mathcal{E}}{\partial h} \right) = 0,$$
$$M(h) = e^{-\Delta_1 h}, \quad \mathcal{E}(h) = \|\nabla h\|_{L^1}.$$

- Examples:

- ① $M(h) = 1 \rightarrow H^{-1}$ gradient flow,

- ② $M(h) = h \rightarrow W_2$ gradient flow,

- ③ $M(h)$ non-negative, concave \rightarrow weighted W_2 gradient flow
(See Carrillo-Lisini-Savaré-Slepcev (2009),
Dolbeault-Nazaret-Savaré (2009), Lisini-Matthew-Savaré
(2019), ...)

- ④ $M(h) \in \text{Lin}(\mathbb{R}^{\ell \times d}, \mathbb{R}^{\ell \times d}) \rightarrow$ gradient system (Liero-Mielke
(2013))

- Our mobility is a nonlinear function of the 1-Laplacian and hence falls well outside existing theories, but....

- Examples:
 - 1 $M(h) = 1 \rightarrow H^{-1}$ gradient flow,
 - 2 $M(h) = h \rightarrow W_2$ gradient flow,
 - 3 $M(h)$ non-negative, concave \rightarrow weighted W_2 gradient flow (See Carrillo-Lisini-Savaré-Slepcev (2009), Dolbeault-Nazaret-Savaré (2009), Lisini-Matthew-Savaré (2019), ...)
 - 4 $M(h) \in \text{Lin}(\mathbb{R}^{\ell \times d}, \mathbb{R}^{\ell \times d}) \rightarrow$ gradient system (Liero-Mielke (2013))
- Our mobility is a nonlinear function of the 1-Laplacian and hence falls well outside existing theories, but....

Recent Advances with formal H^{-1} gradient flow for $p = 1$ using ideas of Otto (2001), Giga-Giga (2010), ...

- Suppose $0 \leq M(h) \in L^1(\mathbb{T}^d)$. Define

$$\Delta_h v = \nabla \cdot (M(h) \nabla v).$$

- We define the weighted Hilbert space

$$\|v\|_{H_h^1}^2 = \int_{\mathbb{T}^d} M(h) |\nabla v|^2 dx = - \int_{\mathbb{T}^d} v \Delta_h v dx.$$

- We have the dual space:

$$\|\psi\|_{H_h^{-1}}^2 = - \int_{\mathbb{T}^d} \psi \Delta_h^{-1} \psi dx.$$

- And the sub-differential

$$\partial_{H_h^{-1}} \mathcal{E}$$

and gradient

$$\nabla_{H_h^{-1}} \mathcal{E}(\psi).$$

Recent Advances with formal H^{-1} gradient flow for $p = 1$ using ideas of Otto (2001), Giga-Giga (2010), ...

- Suppose $0 \leq M(h) \in L^1(\mathbb{T}^d)$. Define

$$\Delta_h v = \nabla \cdot (M(h) \nabla v).$$

- We define the weighted Hilbert space

$$\|v\|_{H_h^1}^2 = \int_{\mathbb{T}^d} M(h) |\nabla v|^2 dx = - \int_{\mathbb{T}^d} v \Delta_h v dx.$$

- We have the dual space:

$$\|\psi\|_{H_h^{-1}}^2 = - \int_{\mathbb{T}^d} \psi \Delta_h^{-1} \psi dx.$$

- And the sub-differential

$$\partial_{H_h^{-1}} \mathcal{E}$$

and gradient

$$\nabla_{H_h^{-1}} \mathcal{E}(\psi).$$

Recent Advances with formal H^{-1} gradient flow for $p = 1$ using ideas of Otto (2001), Giga-Giga (2010), ...

- Suppose $0 \leq M(h) \in L^1(\mathbb{T}^d)$. Define

$$\Delta_h v = \nabla \cdot (M(h) \nabla v).$$

- We define the weighted Hilbert space

$$\|v\|_{H_h^1}^2 = \int_{\mathbb{T}^d} M(h) |\nabla v|^2 dx = - \int_{\mathbb{T}^d} v \Delta_h v dx.$$

- We have the dual space:

$$\|\psi\|_{H_h^{-1}}^2 = - \int_{\mathbb{T}^d} \psi \Delta_h^{-1} \psi dx.$$

- And the sub-differential

$$\partial_{H_h^{-1}} \mathcal{E}$$

and gradient

$$\nabla_{H_h^{-1}} \mathcal{E}(\psi).$$

Recent Advances with formal H^{-1} gradient flow for $p = 1$ using ideas of Otto (2001), Giga-Giga (2010), ...

- Suppose $0 \leq M(h) \in L^1(\mathbb{T}^d)$. Define

$$\Delta_h v = \nabla \cdot (M(h) \nabla v).$$

- We define the weighted Hilbert space

$$\|v\|_{H_h^1}^2 = \int_{\mathbb{T}^d} M(h) |\nabla v|^2 dx = - \int_{\mathbb{T}^d} v \Delta_h v dx.$$

- We have the dual space:

$$\|\psi\|_{H_h^{-1}}^2 = - \int_{\mathbb{T}^d} \psi \Delta_h^{-1} \psi dx.$$

- And the sub-differential

$$\partial_{H_h^{-1}} \mathcal{E}$$

and gradient

$$\nabla_{H_h^{-1}} \mathcal{E}(\psi).$$

Recent Advances with formal H^{-1} gradient flow for $p = 1$ using ideas of Otto (2001), Giga-Giga (2010), ...

- To get to a well-defined gradient flow, we require that the time derivative of $h(t)$ makes sense wrt $\|\cdot\|_{H_{h(t)}^{-1}}$ and that $M(h(t))$ remains in L^1 and ≥ 0 for all t .

$$\partial_t h = -\nabla_{H_h^{-1}} \mathcal{E}(h) \Leftrightarrow \partial_t h + \Delta_h \frac{\partial E}{\partial h} = 0 \Leftrightarrow \partial_t h + \nabla \cdot M(h) \nabla \frac{\partial E}{\partial h} = 0$$

Recent Advances with formal H^{-1} gradient flow for $p = 1$ using ideas of Otto (2001), Giga-Giga (2010), ...

- To get to a well-defined gradient flow, we require that the time derivative of $h(t)$ makes sense wrt $\|\cdot\|_{H_h^{-1}}$ and that $M(h(t))$ remains in L^1 and ≥ 0 for all t .



$$\partial_t h = -\nabla_{H_h^{-1}} \mathcal{E}(h) \Leftrightarrow \partial_t h + \Delta_h \frac{\partial \mathcal{E}}{\partial h} = 0 \Leftrightarrow \partial_t h + \nabla \cdot M(h) \nabla \frac{\partial \mathcal{E}}{\partial h} = 0$$

Our proposed numerical method - Mobility

- Even with a smooth profile, $e^{-\Delta_1 h}$ is not really well-defined since $\Delta_1(\sin(x)) \sim -2\delta_{\pi/2}(x) + 2\delta_{3\pi/2}(x)$.
- Prior works have considered the mobility formulation of the Total Variation flow, see (Giga-Giga (2010)) in which they consider a Mobility that is of the form given by the Taylor expansion $e^x \approx 1 + x$.
- Given that the exponential breaks convex/concave symmetry, we consider of mollified mobility. Given

$$\phi \in C_c^\infty(\mathbb{T}^d), \quad \phi \geq 0, \quad \int \phi dx = 1, \quad \phi_\epsilon(x) = \epsilon^{-d} \phi(x/\epsilon),$$

we define

$$M_\epsilon(h) := e^{-\phi_\epsilon * \Delta_1 h}.$$

Our proposed numerical method - Mobility

- Even with a smooth profile, $e^{-\Delta_1 h}$ is not really well-defined since $\Delta_1(\sin(x)) \sim -2\delta_{\pi/2}(x) + 2\delta_{3\pi/2}(x)$.
- Prior works have considered the mobility formulation of the Total Variation flow, see (Giga-Giga (2010)) in which they consider a Mobility that is of the form given by the Taylor expansion $e^x \approx 1 + x$.
- Given that the exponential breaks convex/concave symmetry, we consider of mollified mobility. Given

$$\phi \in C_c^\infty(\mathbb{T}^d), \quad \phi \geq 0, \quad \int \phi dx = 1, \quad \phi_\epsilon(x) = \epsilon^{-d} \phi(x/\epsilon),$$

we define

$$M_\epsilon(h) := e^{-\phi_\epsilon * \Delta_1 h}.$$

Our proposed numerical method - Mobility

- Even with a smooth profile, $e^{-\Delta_1 h}$ is not really well-defined since $\Delta_1(\sin(x)) \sim -2\delta_{\pi/2}(x) + 2\delta_{3\pi/2}(x)$.
- Prior works have considered the mobility formulation of the Total Variation flow, see (Giga-Giga (2010)) in which they consider a Mobility that is of the form given by the Taylor expansion $e^x \approx 1 + x$.
- Given that the exponential breaks convex/concave symmetry, we consider of mollified mobility. Given

$$\phi \in C_c^\infty(\mathbb{T}^d), \quad \phi \geq 0, \quad \int \phi dx = 1, \quad \phi_\epsilon(x) = \epsilon^{-d} \phi(x/\epsilon),$$

we define

$$M_\epsilon(h) := e^{-\phi_\epsilon * \Delta_1 h}.$$

Our proposed numerical method - time discretization

- We consider a semi-implicit time stepping scheme similar to for instance the JKO framework, see also Murphy-Walkington (2019) in the Porous Medium Equation.

$$h^{n+1} \in \arg \min_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|_{H_{h^n}^{-1}}^2$$

- Or...

$$\frac{h^{n+1} - h^n}{\tau} = -\nabla \cdot \left(M(h^n) \nabla \frac{\partial \mathcal{E}}{\partial h^{n+1}} \right).$$

- For the Total Variation Energy (L^1), if $h^n \in D(E)$ and $0 \leq M(h^n) \in L^1$, there exists a unique solution to h^{n+1} !!

Our proposed numerical method - time discretization

- We consider a semi-implicit time stepping scheme similar to for instance the JKO framework, see also Murphy-Walkington (2019) in the Porous Medium Equation.



$$h^{n+1} \in \arg \min_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|_{H_{h^n}^{-1}}^2$$

- Or...

$$\frac{h^{n+1} - h^n}{\tau} = -\nabla \cdot \left(M(h^n) \nabla \frac{\partial \mathcal{E}}{\partial h^{n+1}} \right).$$

- For the Total Variation Energy (L^1), if $h^n \in D(E)$ and $0 \leq M(h^n) \in L^1$, there exists a unique solution to h^{n+1} !!

Our proposed numerical method - time discretization

- We consider a semi-implicit time stepping scheme similar to for instance the JKO framework, see also Murphy-Walkington (2019) in the Porous Medium Equation.



$$h^{n+1} \in \arg \min_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|_{H_{h^n}^{-1}}^2$$

- Or...

$$\frac{h^{n+1} - h^n}{\tau} = -\nabla \cdot \left(M(h^n) \nabla \frac{\partial \mathcal{E}}{\partial h^{n+1}} \right).$$

- For the Total Variation Energy (L^1), if $h^n \in D(E)$ and $0 \leq M(h^n) \in L^1$, there exists a unique solution to h^{n+1} !!

Our proposed numerical method - time discretization

- We consider a semi-implicit time stepping scheme similar to for instance the JKO framework, see also Murphy-Walkington (2019) in the Porous Medium Equation.



$$h^{n+1} \in \arg \min_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|_{H_{h^n}^{-1}}^2$$

- Or...

$$\frac{h^{n+1} - h^n}{\tau} = -\nabla \cdot \left(M(h^n) \nabla \frac{\partial \mathcal{E}}{\partial h^{n+1}} \right).$$

- For the Total Variation Energy (L^1), if $h^n \in D(E)$ and $0 \leq M(h^n) \in L^1$, there exists a unique solution to h^{n+1} !!

- We have the optimization

$$\begin{aligned} h^{n+1} &\in \arg \min_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|_{H_{h^n}^{-1}}^2 \\ &= \arg \min_h (f(Kh) + g(h)) \end{aligned}$$

for Z, H Hilbert spaces to be explained, $f : Z \rightarrow \mathbb{R}$,
 $g : H \rightarrow \mathbb{R}$ convex, $K : H \rightarrow Z$ a bounded linear operator.

- Such schemes can be regularized and solved using a primal-dual algorithm to solve inner and outer optimization problems!! See (Laborde-Benamou-Carlier (2016), Carrillo-Craig-Wang-Wei (2019)).

- We have the optimization

$$\begin{aligned}h^{n+1} &\in \arg \min_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|_{H_{h^n}^{-1}}^2 \\ &= \arg \min_h (f(Kh) + g(h))\end{aligned}$$

for Z, H Hilbert spaces to be explained, $f : Z \rightarrow \mathbb{R}$,
 $g : H \rightarrow \mathbb{R}$ convex, $K : H \rightarrow Z$ a bounded linear operator.

- Such schemes can be regularized and solved using a primal-dual algorithm to solve inner and outer optimization problems!! See (Laborde-Benamou-Carlier (2016), Carrillo-Craig-Wang-Wei (2019)).

Our proposed numerical method - space discretization

- For our case, we are motivated by the work of Jacobs-Léger-Li-Osher (2019).
- Gradient descent of smooth, convex function $F(u) = f(Ku) + g(u)$ with a unique min at u^* .
- Convergence rate:

$$F(u_n) \leq F(u^*) + 2L_{\mathcal{H}} \frac{\|u^* - u_0\|_{\mathcal{H}}^2}{n + 4}.$$

Our proposed numerical method - space discretization

- For our case, we are motivated by the work of Jacobs-Léger-Li-Osher (2019).
- Gradient descent of smooth, convex function $F(u) = f(Ku) + g(u)$ with a unique min at u^* .
- Convergence rate:

$$F(u_n) \leq F(u^*) + 2L_{\mathcal{H}} \frac{\|u^* - u_0\|_{\mathcal{H}}^2}{n+4}.$$

Our proposed numerical method - space discretization

- For our case, we are motivated by the work of Jacobs-Léger-Li-Osher (2019).
- Gradient descent of smooth, convex function $F(u) = f(Ku) + g(u)$ with a unique min at u^* .
- Convergence rate:

$$F(u_n) \leq F(u^*) + 2L_{\mathcal{H}} \frac{\|u^* - u_0\|_{\mathcal{H}}^2}{n + 4}.$$

- Nesterov:

$$F(u_n) \leq F(u^*) + 4L_{\mathcal{H}} \frac{R^2}{(n+2)^2} + \min_{\|u-u_0\|_{\mathcal{H}} \leq R} (F(u) - F(u^*)).$$

Punchline: $\|u^* - u_0\|_{\mathcal{H}} = +\infty$ OK as long as

$$\min_{\|u-u_0\|_{\mathcal{H}} \leq R} (F(u) - F(u^*)) \rightarrow 0$$

as $R \rightarrow \infty$.

- The primal-dual algorithm is thus:

$$u_{n+1} = \arg \min_{u \in \mathcal{H}} g(u) + (u, K^T \bar{p}_n)_{\mathcal{H}} + \frac{1}{2\tau} \|u - u_n\|_{\mathcal{H}}^2,$$

$$p_{n+1} = \arg \max_{p \in \mathcal{Z}} -f^*(p) + (Ku_{n+1}, p)_{\mathcal{Z}} - \frac{1}{2\sigma} \|p - p_n\|_{\mathcal{Z}}^2,$$

$$\bar{p}_n = 2p_{n+1} - p_n.$$

- Cf. JLLO, Chambolle-Pock PDHG method, ...

- The primal-dual algorithm is thus:

$$u_{n+1} = \arg \min_{u \in \mathcal{H}} g(u) + (u, K^T \bar{p}_n)_{\mathcal{H}} + \frac{1}{2\tau} \|u - u_n\|_{\mathcal{H}}^2,$$

$$p_{n+1} = \arg \max_{p \in \mathcal{Z}} -f^*(p) + (Ku_{n+1}, p)_{\mathcal{Z}} - \frac{1}{2\sigma} \|p - p_n\|_{\mathcal{Z}}^2,$$

$$\bar{p}_n = 2p_{n+1} - p_n.$$

- Cf. JLLO, Chambolle-Pock PDHG method, ...

Our proposed numerical method - space discretization

- For us, we get the following:
- Outer time iteration:

$$h^{n+1} = \arg \min_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|_{H_{h^n}^{-1}}^2.$$

- Inner time iteration applied using a PDHG algorithm regularizing h with $(1/2\lambda)H^1$ and ϕ with an $(1/2\sigma)L^2$ regularizer ($(\sigma\lambda) \leq 1$):

$$h^{m+1} = \left(\frac{\tau}{\lambda} \Delta_{h^n} \Delta + I \right)^{-1} \left(\frac{\tau}{\lambda} \Delta_{h^n} \Delta h^{(m)} - \tau \Delta_{h^n} \nabla \cdot \phi^{(m)} + h^n \right),$$
$$\bar{h}^{(m+1)} = 2h^{(m+1)} - h^{(m)},$$
$$\phi^{(m+1)} = (I + \sigma \partial F^*)^{-1} (\phi^{(m)} + \sigma \nabla \bar{h}^{(m+1)})$$

where

$$(I + \sigma \partial F^*)^{-1}(u(x)) = \min\{u(x), 1\} \operatorname{sign}(u(x)).$$

Our proposed numerical method - space discretization

- For us, we get the following:
- Outer time iteration:

$$h^{n+1} = \arg \min_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|_{H_{h^n}^{-1}}^2.$$

- Inner time iteration applied using a PDHG algorithm regularizing h with $(1/2\lambda)H^1$ and ϕ with an $(1/2\sigma)L^2$ regularizer ($(\sigma\lambda) \leq 1$):

$$h^{m+1} = \left(\frac{\tau}{\lambda} \Delta_{h^n} \Delta + I \right)^{-1} \left(\frac{\tau}{\lambda} \Delta_{h^n} \Delta h^{(m)} - \tau \Delta_{h^n} \nabla \cdot \phi^{(m)} + h^n \right),$$

$$\bar{h}^{(m+1)} = 2h^{(m+1)} - h^{(m)},$$

$$\phi^{(m+1)} = (I + \sigma \partial F^*)^{-1} (\phi^{(m)} + \sigma \nabla \bar{h}^{(m+1)})$$

where

$$(I + \sigma \partial F^*)^{-1}(u(x)) = \min\{u(x), 1\} \operatorname{sign}(u(x)).$$

Our proposed numerical method - space discretization

- For us, we get the following:
- Outer time iteration:

$$h^{n+1} = \arg \min_h \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|_{H_{h^n}^{-1}}^2.$$

- Inner time iteration applied using a PDHG algorithm regularizing h with $(1/2\lambda)H^1$ and ϕ with an $(1/2\sigma)L^2$ regularizer ($(\sigma\lambda) \leq 1$):

$$h^{m+1} = \left(\frac{\tau}{\lambda} \Delta_{h^n} \Delta + I \right)^{-1} \left(\frac{\tau}{\lambda} \Delta_{h^n} \Delta h^{(m)} - \tau \Delta_{h^n} \nabla \cdot \phi^{(m)} + h^n \right),$$

$$\bar{h}^{(m+1)} = 2h^{(m+1)} - h^{(m)},$$

$$\phi^{(m+1)} = (I + \sigma \partial F^*)^{-1} (\phi^{(m)} + \sigma \nabla \bar{h}^{(m+1)})$$

where

$$(I + \sigma \partial F^*)^{-1}(u(x)) = \min\{u(x), 1\} \operatorname{sign}(u(x)).$$

What do we gain???

- We do not invert the 1-Laplacian!

$$(D^t D + \frac{\lambda}{\tau} A^{-1}(\cdot - h^n))^{-1} = (\frac{\tau}{\lambda} A D^t D u + h^n).$$

- Can choose λ quite large!

What do we gain???

- We do not invert the 1-Laplacian!

$$(D^t D + \frac{\lambda}{\tau} A^{-1}(\cdot - h^n))^{-1} = (\frac{\tau}{\lambda} A D^t D u + h^n).$$

- Can choose λ quite large!

- Let $d = 1$. Suppose the PDHG algorithm is initialized with

$$h^{(0)} = h^n, \phi^{(0)} = 0, \text{ where } \mathcal{E}(h^n) < \infty.$$

Then for all $\delta > 0$, there exist $\tilde{M}, \lambda, \sigma$ such that

$$F(h^{(M)}) - F(h^{n+1}) \leq \delta, \forall M \geq \tilde{M}, F(h) = \mathcal{E}(h) + \frac{1}{2\tau} \|h - h^n\|_{H_{h^n}^{-1}}^2.$$

- Extends to general $M(h)$ provided $M(h^n), 1/M(h^n) \in L^1$ (Cancés-Gallouët-Todeschi (2019)).
- The restriction $d = 1$ is to apply a Sobolev embedding. Different integrability on $1/M$ required to go to higher dimensions.
- If $\nabla h^n \in BV$, the estimates are quantitative:
 $\tilde{M} \sim \delta^{-2}, \lambda \sim \delta^{-1}, \sigma \sim \delta.$



$$\min_{\|h^n - h\|_{\mathcal{H}} \leq R} (F(h) - F(h^{n+1})) \rightarrow 0$$

as $R \rightarrow \infty$.

- Extends to general $M(h)$ provided $M(h^n), 1/M(h^n) \in L^1$ (Cancés-Gallouët-Todeschi (2019)).
- The restriction $d = 1$ is to apply a Sobolev embedding. Different integrability on $1/M$ required to go to higher dimensions.
- If $\nabla h^n \in BV$, the estimates are quantitative:
 $\tilde{M} \sim \delta^{-2}, \lambda \sim \delta^{-1}, \sigma \sim \delta.$

$$\min_{\|h^n - h\|_{\mathcal{H}} \leq R} (F(h) - F(h^{n+1})) \rightarrow 0$$

as $R \rightarrow \infty.$

- Extends to general $M(h)$ provided $M(h^n), 1/M(h^n) \in L^1$ (Cancés-Gallouët-Todeschi (2019)).
- The restriction $d = 1$ is to apply a Sobolev embedding. Different integrability on $1/M$ required to go to higher dimensions.
- If $\nabla h^n \in BV$, the estimates are quantitative:
 $\tilde{M} \sim \delta^{-2}, \lambda \sim \delta^{-1}, \sigma \sim \delta.$

$$\min_{\|h^n - h\|_{\mathcal{H}} \leq R} (F(h) - F(h^{n+1})) \rightarrow 0$$

as $R \rightarrow \infty.$

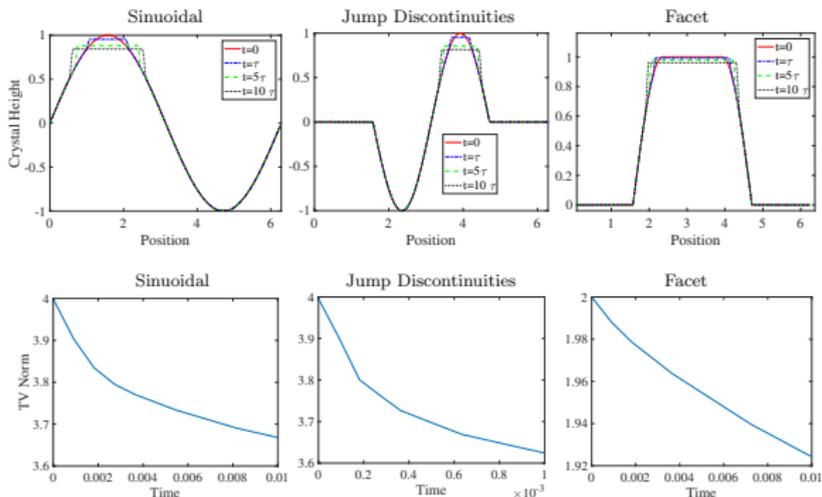
- Extends to general $M(h)$ provided $M(h^n), 1/M(h^n) \in L^1$ (Cancés-Gallouët-Todeschi (2019)).
- The restriction $d = 1$ is to apply a Sobolev embedding. Different integrability on $1/M$ required to go to higher dimensions.
- If $\nabla h^n \in BV$, the estimates are quantitative:
 $\tilde{M} \sim \delta^{-2}, \lambda \sim \delta^{-1}, \sigma \sim \delta.$



$$\min_{\|h^n - h\|_{\mathcal{H}} \leq R} (F(h) - F(h^{n+1})) \rightarrow 0$$

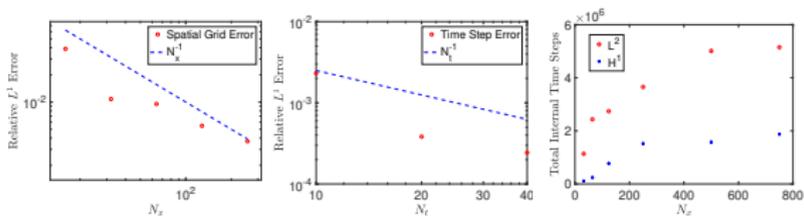
as $R \rightarrow \infty$.

Numerical Results: energy decrease



15

Numerical Results: convergence



Observations:

- Error vs N_x : slightly sublinear convergence (low spatial regularity)
- Error vs N_t : first order (semi-implicit Euler)
- Internal time steps vs N_t : importance of selecting correct Hilbert space

sinusoidal, ($N_x = 200$), ($N_t = 10$), $\sigma = 0.0005$, $\lambda = 500$, $\varepsilon = 0.05$, $T = 10^{-4}$

16

Basic questions remain unanswered:

- 1 Can we prove that the exponential PDE has a solution (in some space) for other p values, especially $p = 1$?
- 2 Can we prove convergence of the microscopic model to the PDE in our scaling regimes? See recent work of Katsevich!
- 3 Can we establish finite time singularity formation in the 2nd derivative in the case $p = 2$?
- 4 Full global strong solutions with $g > 0$? Convergence of dynamics as $g \rightarrow 0$?

There are also lots of great questions about the qualitative behavior that can be asked w.r.t. wetting and self-similarity.