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Step Evolution for Crystals of Finite Size: The ADL Case

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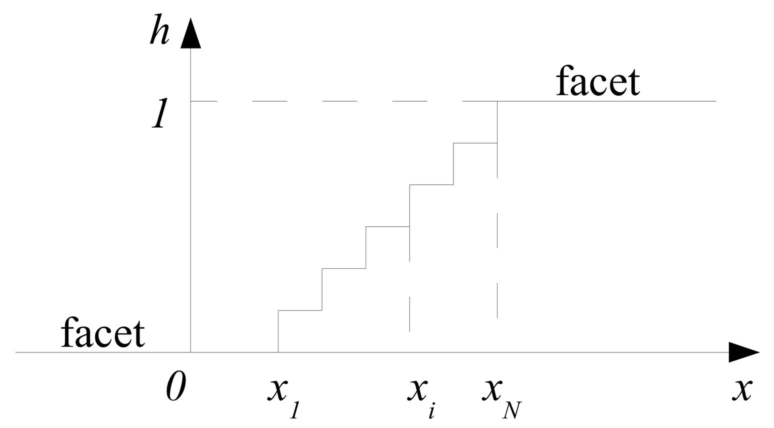
Step Equations of motion

The figure below shows a one-dimensional stepped surface separated by two flat surfaces called facets.



The step equations of motion are:

$$\dot{x}_1 = (x_3 - x_2)^{-3} - 2\,(x_2 - x_1)^{-3}$$

$$\dot{x}_2 = (x_4 - x_3)^{-3} - 3\,(x_3 - x_2)^{-3} + 3\,(x_2 - x_1)^{-3}$$

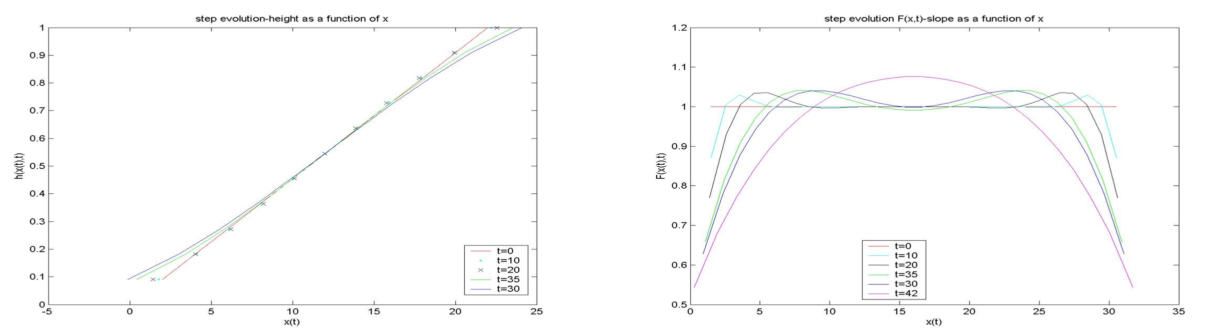
$$\begin{aligned}\dot{x}_i = {} & [(x_{i+2} - x_{i+1})^{-3} - 2\,(x_{i+1} - x_i)^{-3} + (x_i - x_{i-1})^{-3}] \\ & -[(x_{i+1} - x_i)^{-3} - 2\,(x_i - x_{i-1})^{-3} + (x_{i-1} - x_{i-2})^{-3}]\end{aligned}$$

for $i = 3, 4, \ldots, N-2$, and

$$\begin{aligned}\dot{x}_{N-1} = {} & -3\,(x_N - x_{N-1})^{-3} + 3\,(x_{N-1} - x_{N-2})^{-3} \\ & -(x_{N-2} - x_{N-3})^{-3}\end{aligned}$$

$$\dot{x}_N = 2\,(x_N - x_{N-1})^{-3} - (x_{N-1} - x_{N-2})^{-3}$$

Energy estimates show that the solution exists, and simulations show the behavior



of the height and the slope. Prior work on the continuum limit of step dynamics has mainly focused on the slope $F(x,t)$ as a function of spatial position and time [2][3]. The edge of each facet is then a free boundary.

We focus instead on the slope $u(h,t)$ as a function of height and time – a choice also used by Fok, Margetis, and Rosales in the radial case [1][2]. This approach has two key advantages: (a) there are no free boundaries, and (b) the step equations (written in terms of the reciprocals of the step differences $z_i = x_{i+1} - x_i$) become the natural finite-difference discretization of a PDE for u.

The PDE is an L^2 steepest descent for a suitable energy, and its solution is asymptotically self-similar. We prove this in the discrete setting – establishing the existence, uniqueness, and global stability of the similarity solution.

Notation: $x_i(t)$ for step positions; $z_i = x_{i+1} - x_i$ for step differences; $y_i = 1/z_i$ for the discrete slope; $u = u(h,t)$ is the continuum slope as a function of height and time; $\phi(h)$ is the self similar solution; $w(h,s)$ is the slope in "similarity variables" ($w = t^{1/4}u$, $s = \log t$).

Story

1. The step equations suggest a **PDE for the slope** as a function of height:

$$\begin{aligned} u_t &= -u^2 (u^3)_{hhhh} \\ u(0,t) &= u(1,t) = 0 \\ u^3_{hh}(0,t) &= u^3_{hh}(1,t) = 0 \end{aligned} \tag{1}$$

   The discretization of this PDE is $\dot{y}_i = -y_i^2\,\Delta^2 y_i^3$, $i = 3, \ldots, N-3$, where Δ is the discrete Laplacian. Then with $y_i = 1/z_i$, we get the ODE's for $z_i = x_{i+1} - x_i$, namely, $\dot{z}_i(t) = \Delta^2 z_i^{-3}$. These are equivalent to the step equations.

2. **Simulations** of the above equations show self similar behavior.

3. Solutions are indeed **asymptotically self-similar**. The following sketch uses continuum language (u, ϕ, and w), but our analysis is presently complete only for the **discrete setting** (y_i, ϕ_i, w_i). (The main reason: we can show y_i never vanishes, but we do not know whether u can vanish.)

   - The PDE (1) is the L^2-steepest descent of the energy functional

$$E(u) = \int_0^1 \frac{1}{6}(u^3_{hh})^2 dh \tag{2}$$

   - The self-similar solution $\phi(h)$: $u(h,t) = t^{-\frac{1}{4}}\phi(h)$. ϕ satisfies:

$$\frac{1}{4}\phi = \phi^2(\phi^3)_{hhhh} \tag{3}$$

     with $\phi(0) = \phi(1) = 0$ and $\phi^3_{hh}(0) = \phi^3_{hh}(1) = 0$.

   - This similarity solution is the unique positive critical point of the energy functional

$$E(w) = \int_0^1 -\frac{1}{8}w^2 + \frac{1}{6}(w^3_{hh})^2 dh \tag{4}$$

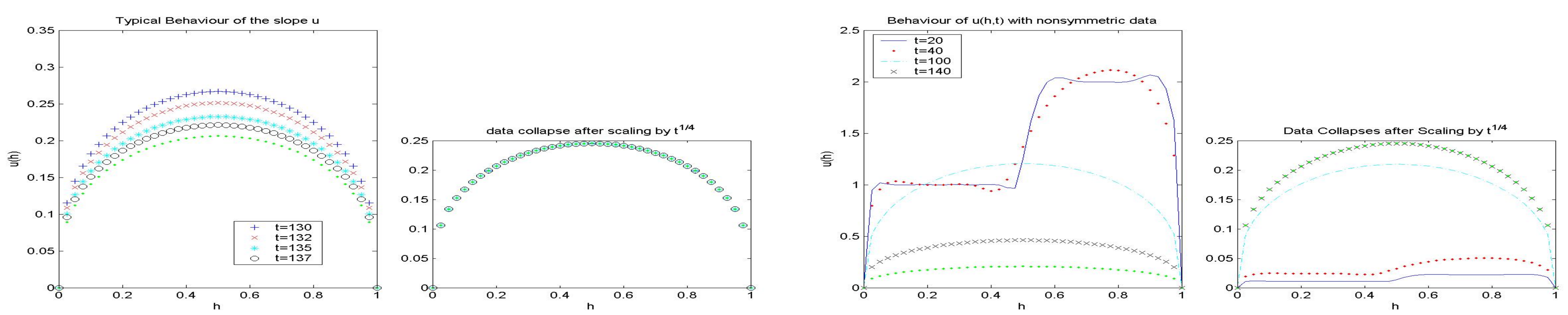
   - To see the asymptotic self-similarity, let $s = \log\, t$ and $w(h,s) = t^{\frac{1}{4}}u(h,t)$. The PDE becomes

$$w_s = \frac{1}{4}w - w^2(w^3)_{hhhh} \tag{5}$$

     with $w(0,s) = w(1,s) = 0$ and $w^3_{hh}(0,s) = w^3_{hh}(1,s) = 0$. This is the L^2-steepest descent of $E(w)$. So we expect (and prove) $w \to \phi$ as $s \to \infty$. Thus u is asymptotically self-similar.

4. **Energy Estimates** include: $\int_0^1 (\triangle^{-1}\frac{1}{u})^2 \leq (C\,t + d)^2$, and $\frac{1}{2}\|u\|^2_{L^2[0,1]}(T) + \int_0^T \int_0^1 (u^3_{hh})^2 dh\, dt = \frac{1}{2}\|u_0\|^2_{L^2[0,1]}$.

Numerical Simulations



Numerical simulations show that starting with "any" positive initial data, and scaling by $t^{1/4}$,the data collapses into one graph, that of $\phi(h)$. This confirms that the evolution in similarity variables approaches the self-similar solution $\phi(h)$ as $t \to \infty$.

Self Similar Solution

Uniqueness: For positive ϕ, equation (3) can be written as

$$\frac{1}{4\,\phi} = (\phi^3)_{hhhh}$$

Suppose there are two positive critical points ϕ_1 and ϕ_2 satisfying the above ODE. Then

$$\frac{\phi_2 - \phi_1}{4\,\phi_1\,\phi_2} = (\phi_1^3 - \phi_2^3)_{hhhh}$$

Multiplying by $\phi_1^3 - \phi_2^3$ and integrating from 0 to 1

$$\int_0^1 \frac{(\phi_1^3 - \phi_2^3)\,(\phi_2 - \phi_1)}{4\,\phi_1\,\phi_2} = \int_0^1 (\phi_1^3 - \phi_2^3)(\phi_1^3 - \phi_2^3)_{hhhh}$$

Factorizing the left hand side and integrating by parts twice the right hand side:

$$-\int_0^1 \frac{(\phi_1 - \phi_2)^2\,(\phi_1^2 + \phi_1\,\phi_2 + \phi_2^2)}{4\,\phi_1\,\phi_2} = \int_0^1 (\phi_1^3 - \phi_2^3)^2_{hh}$$

Boundary terms vanish due to the given boundary conditions. Hence

$$\int_0^1 \frac{(\phi_1 - \phi_2)^2\,(\phi_1^2 + \phi_1\,\phi_2 + \phi_2^2)}{4\,\phi_1\,\phi_2} + \int_0^1 (\phi_1^3 - \phi_2^3)^2_{hh} = 0$$

Each of the above terms is nonnegative, thus $\phi_1 = \phi_2$.

Current Work

- **Is there a facet?** Numerical simulations suggest that as $N \to \infty$, the facet width, $x_N - x_1$ remains finite.

N	10	100	1000	2000	3000
$x_N - x_1$	4.2752	5.1787	5.3737	5.3937	5.4018

  In the continuum setting, this is equivalent to

$$x_N - x_1 = \int_{x_1}^{x_N} dx = \int_0^1 \frac{dx}{dh}dh = \int_0^1 \frac{1}{u}dh < \infty\,.$$

- **Convergence** of the numerical scheme.
- **Positivity** of u: If $u_0 > 0$, then is it true that $u > 0$ for all t? This is true in the discrete setting (y_i).
- **The DL case** is the other rate limiting process in crystal growth. In this case, the proposed PDE is: $u_t = -u^2\,(u(u^3)_{hh})_{hh}$ with $u(0,t) = u(1,t) = 0$.

References

[1] P.W. Fok, R.R. Rosales, D. Margetis. Unification of Step bunching phenomena on vicinal surfaces. *Physical Review B*, 76: 033408, 2007.

[2] Pak-Wing Fok, Rodolfo R. Rosales, and Dionisios Margetis. Facet evolution on supported nanostructures: the effect of finite height. *Physical Review B*, 78: 235401, 2008.

[3] Navot Israeli and Daniel Kandel. Decay of one-dimensional surface modulations. *Physical review B*, 62(20):13 707, 2000.