Finite volume methods for gradient-flow crystal growth problems

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1 Introduction

The growth of cubical crystalline surfaces, formed by chemicals such as CuO_2, is often modelled by an energy minimisation process. A two dimensional surface $h(x, y)$, modelling the crystal height, is said to have the free energy

$$E[h] = \iint W(\nabla h) + \frac{1}{2}\varepsilon^2(\Delta h)^2 \, \mathrm{d}x \, \mathrm{d}y \tag{1}$$

where W is a trigonally symmetric potential

$$W(p, q) = -\frac{1}{6}\left(q^2 + p^2\right) + \frac{1}{9}\left(q^3 - 3qp^2\right) + \frac{1}{6}\left(q^2 + p^2\right)^2 \tag{2}$$

and $0 < \varepsilon \ll 1$ is a given small constant. The minimisation of the energy E, with the given potential, leads to the kind of faceted surfaces shown in the figure.

The process of energy minimisation is modelled by the partial differential equation

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left[D_p W(\nabla h)\right] + \frac{\partial}{\partial y}\left[D_q W(\nabla h)\right] - \varepsilon^2 \Delta^2 h \tag{3}$$

where $D_p W$ and $D_q W$ are the derivatives of W with respect to the first and second arguments, respectively. This equation is the gradient flow of the energy E in the space L^2, since it can be written as

$$\frac{\partial h}{\partial t} = -\frac{\delta E}{\delta h}, \tag{4}$$

where $\frac{\delta E}{\delta h}$ is the variational derivative of E with respect to h (a sort of "gradient" in L^2). As such, the value of E can only decrease in time; this is a fundamental property of the dynamics of Eq. (3), and it strongly determines its evolution.

While the physics and the asymptotics of this process are well-understood [5, 4], the numerical simulation of Eq. (3) is highly non-trivial. The two-scale nature of the energy, given by the small parameter ε, leads to stiff dynamics. Furthermore, a numerical approximation to the solution of this equation might not guarantee the dissipation of the energy: the value of E could increase, leading to an erroneous state.

2 Numerical scheme for 1D reduced equation

2.1 1D reduced equation

Note that the 2D potential W is minimised by the three symmetric gradients $\mathbf{m} = p\mathbf{i}+q\mathbf{j} \in G$ of lengths 1,

$$G := \left\{ \frac{\sqrt{3}}{2}\mathbf{i} + \frac{1}{2}\mathbf{j}, -\frac{\sqrt{3}}{2}\mathbf{i} + \frac{1}{2}\mathbf{j}, -\mathbf{j} \right\} \tag{5}$$

with a minimum of $-\frac{1}{9}$. Then a natural choice for the 1D potential W is

$$W(p) = \frac{4}{9}(\frac{p^4}{4} - \frac{p^2}{2}) \tag{6}$$

as it is minimised at ± 1 with a minimum of $-\frac{1}{9}$.

Then the reduced 1D equation is given by

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left[\frac{\partial W}{\partial p}(\nabla h)\right] - \varepsilon^2 \Delta^2 h \tag{7}$$

$$DW(p) = \frac{\partial W}{\partial p} = \frac{4}{9}(p^3 - p) \tag{8}$$

2.2 Numerical scheme

Assume we want to solve the equation on the computational domain $[0, L]$. It is divided into N cells $C_i = \left[x_{i-1/2}, x_{i+1/2}\right]$, all with uniform size $\Delta x = L/N$, so that the centres of the cells satisfy $x_i = (i-1)\Delta x + \Delta x/2, i \in \{1, \ldots, N\}$. In each of the cells C_i we define the cell average h_i as

$$h_i(t) = \frac{1}{\Delta x}\int_{C_i} h(x,t)dx. \tag{9}$$

For the time discretisation, we define $t_n = n\Delta t$ where $n \in \mathbb{Z}$ so that h_i^n is the solution to the discretised PDE at cell C_i and time t_n.

Convex splitting of the potential $W(p)$ is

$$W(p) = W_c(p) - W_e(p) = \frac{p^4}{9} - \frac{2p^2}{9} \tag{10}$$

so

$$DW(p) = DW_c(p) - DW_e(p) = \frac{4}{9}p^3 - \frac{4}{9}p \tag{11}$$

We impose the following BCs:

$$DW^n_{\frac{1}{2}} = 0 = DW^n_{N+\frac{1}{2}}, (\nabla\Delta h)^n_{\frac{1}{2}} = 0 = (\nabla\Delta h)^n_{N+\frac{1}{2}}, (\Delta h)^n_0 = 0 = (\Delta h)^n_{N+1} \tag{12}$$

Then the semi-implicit numerical scheme is given by

$$\frac{h_i^{n+1}-h_i^n}{\Delta t} = -\xi_i^{n+1} = \frac{1}{\Delta x}(DW_{i+\frac{1}{2}}^{n+1} - DW_{i-\frac{1}{2}}^{n+1}) - \frac{\varepsilon^2}{2}((\Delta^2 h)_i^n + (\Delta^2 h)_i^{n+1}) \tag{13}$$

$$DW_{i+\frac{1}{2}}^{n+1} = DW_c\left((\nabla h)_{i+\frac{1}{2}}^{n+1}\right) - DW_e\left((\nabla h)_{i+\frac{1}{2}}^{n}\right) \tag{14}$$

$$(\nabla h)_{i+\frac{1}{2}}^n = \left(\frac{\partial h}{\partial x}\right)_{i+\frac{1}{2}}^n = \frac{h_{i+1}^n - h_i^n}{\Delta x} \quad \text{for} \quad i = 0, \ldots, N \tag{15}$$

$$(\Delta^2 h)_i^n = \left(\frac{\partial^4 h}{\partial x^4}\right)_i^n = \frac{h_{i+2}^n - 4h_{i+1}^n + 6h_i^n - 4h_{i-1}^n + h_{i-2}^n}{(\Delta x)^4} \quad \text{for} \quad i = 1, \ldots, N \tag{16}$$

3 Findings

3.1 Simulations

Below are the simulations of the evolution of the solution to the 1D equation with sinusoidal initial data.

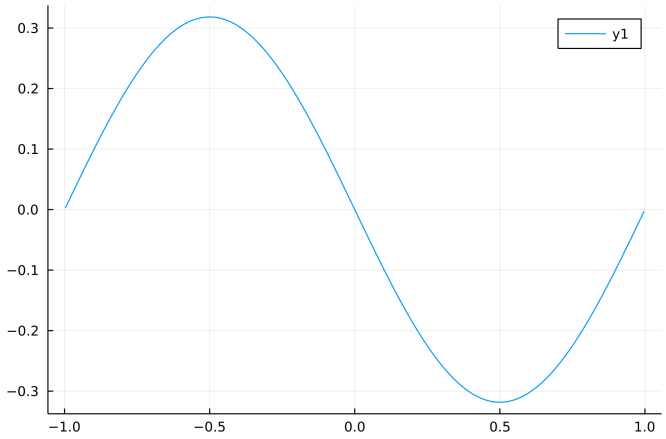

Figure 1: Initial condition

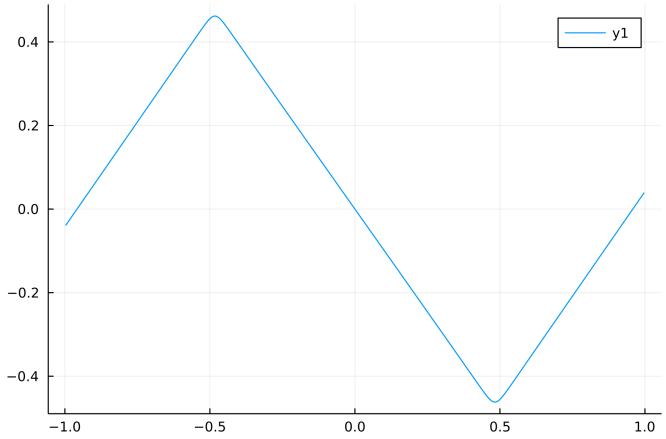

Figure 2: Final solution

From an arbitrary initial condition, we observe the coarsening of the solution, i.e. the curve become largely piecewise linear with a few sharp turning points as time goes by, mimicking the growth characteristics of CuO_2.

3.2 Properties of the scheme

The numerical scheme exhibits the following two important analytic properties that are observed at the continuous level:

(i) Conservation of mass $\sum_{i=1}^{N} h_i^n = \sum_{i=1}^{N} h_i^{n+1}$, meaning the crystal can neither be produced nor disappear from the system.

(ii) Dissipation of the discrete free energy, defined as

$$E_\Delta^n = \Delta x \sum_{i=1}^{N} W_{i+\frac{1}{2}}^n + \Delta x \sum_{i=1}^{N} \frac{\varepsilon^2}{2} ((\Delta h)_i^n)^2 \tag{17}$$

where $W_{i+\frac{1}{2}}^n = W_{c,i+\frac{1}{2}}^n - W_{e,i+\frac{1}{2}}^n = W_c\left((\nabla h)_{i+\frac{1}{2}}^n\right) - W_e\left((\nabla h)_{i+\frac{1}{2}}^n\right)$. Then we have $E_\Delta^{n+1} \leq E_\Delta^n$. This shows that the 'energy' can only decrease over time, reaching a more stable state.

4 Implications

The crystal equation is one example of a broader class of equations exhibiting a gradient-flow structure. These equations have the universal property of energy dissipation.

Since it is very challenging to solve such equations analytically (giving a exact expression of the solution) we resort to numerical methods, solving the equation at a discrete level. It is crucial that we preserve the energy dissipation property at the discrete level to get a correct evolution of the solution. We found that by using the classical technique, convex splitting of the potential function, helped dissipate the energy. This shows that the technique could potentially work for a broader class of equations.

In addition, these type of stiff problems mean that any conditionally energy stable scheme requires a very fine time discretisation and thus very high computational costs. A semi-implicit scheme gave unconditional energy stability and thus produced very fast simulations. This suggests that implicit schemes could potentially be the first choice for stiff problems.

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