

# PAC Report

Simon Bignold

(Advisor: Christoph Ortner ; 2nd Advisor: Charles Elliott)

## 1. Introduction

In this project we consider the relatively new area of Phase Field Crystal (PFC) theory initially proposed in [3]. We provide a brief motivation for considering this theory and then outline a derivation from the more widely studied Density Functional Theory (DFT). We then proceed to outline some numerical approaches to simulating PFC and the results of some simulations. Finally we outline some avenues for further possible work. This project is still in an exploratory phase where we hope to gain insight into profitable research avenues in PFC.

### 1.1 Motivation

The idea of PFC was first introduced in [3] as a method of producing crystalline structures. It is shown in this paper that this model has the virtue of having an energy functional that is minimised by three different states (or phases): a constant phase, a hexagonal lattice and a striped phase, where different phases can be obtained by altering a parameter of the functional and the total mass of the system (see figure 1(a) of [3]). We can consider PFC as a model for a physical situation where the constant phase represents a liquid and the hexagonal lattice represents a crystalline solid. In a later paper [4] PFC is derived from the older theory of density functional theory which adds to the interest of PFC as it may be able to give insight into DFT. PFC has the advantage that the energy functional has a relatively simple explicit form, this is not in general true of DFT which is extremely difficult to work with directly. A review paper which also gives an insight into possible applications of PFC is found in [2].

### 1.2 Mathematical Model

PFC is defined such that the energy of the system is given by the energy functional

$$(1) \quad \mathcal{F}[u] = \int_{\Omega} \frac{u}{2} (\Delta + 1)^2 u - \delta \frac{u^2}{2} + \frac{u^4}{4} dx$$

where  $u : \mathbb{R}^n \rightarrow \mathbb{R}$  is a density perturbation (the exact relation to the density is considered in the next section) so that its integral is constant,

$$u_{av} = \int_{\Omega} u dx.$$

We are interested in the equilibrium state of our system which is obtained by minimising our functional, whilst keeping the integral of  $u$  constant. The standard approach to this (i.e. the approach considered in [3]) is to consider the  $H^{-1}$  gradient flow of the energy functional, i.e.

$$(2) \quad u_t = \Delta \frac{\delta \mathcal{F}[u]}{\delta u}$$

which automatically enforces the conservation of  $u$ . This leads to the partial differential equation (known as the PFC equation)

$$(3) \quad \frac{\partial u}{\partial t} = \Delta ((\Delta + 1)^2 u - \delta u + u^3).$$

As stated above and shown in figure 1(a) of [3] we can change the  $u$  that minimises the functional from striped to hexagonal to constant by altering the values of  $u_{av}$  and  $\delta$ .

## 2. Derivation of PFC from DFT

My MSc thesis [6] focused on DFT (see [7] for an introduction) specifically considering the hard-core gas potential in a classical context. We develop a link between DFT and PFC this was first shown in [4] and is also covered extensively in Section 2 of [2]. DFT can be considered as a simplification of the grand canonical model of statistical mechanics (see Section 4.1 of [9])- this link is explored in [8]. To see this we consider a system of  $N \in \mathbb{N}$  particles with positions  $x_i$  confined to a  $d$ -dimensional box  $\Lambda \subset \mathbb{R}^d$ . The Hamiltonian of the system is then

$$H_{\Lambda}^{U_1}(X_N) = \sum_{i=1}^N U_1(x_i) + \sum_{1 \leq i < j \leq N} U_2(|x_i - x_j|)$$

where  $X_N = (x_1, \dots, x_N) \in \Lambda^N$  and  $U_1 : \mathbb{R}^d \rightarrow \mathbb{R}$  is the external potential.  $U_2 : \mathbb{R}^d \rightarrow \mathbb{R}$  is the interaction potential taken to be a pairwise potential that depends only on the distance between particles.

The canonical Gibbs ensemble is characterised in the following way (compare page 20 of [9] where an  $N!$  accounts for indistinguishability of particles). Let  $\Gamma_{\Lambda} = (\Lambda \times \mathbb{R}^d)^N$  and equip it with the Borel  $\sigma$ -algebra  $\mathcal{B}_{\Lambda}$  on  $\Gamma_{\Lambda}$ . Then the probability measure  $\gamma_{\Lambda}^{\beta, \mu} \in \mathcal{P}(\Gamma_{\Lambda}, \mathcal{B}_{\Lambda})$  with density

$$(4) \quad \hat{\rho}_{\beta}^{\Lambda, N}(X_N) = \frac{\exp[-\beta H_{\Lambda}^{U_1}(X_N)]}{N! Z_{\Lambda}(N, \beta)}$$

is called the canonical ensemble.

The normalisation constant  $Z_{\Lambda}(N, \beta)$  is called the partition function.

$$(5) \quad Z_{\Lambda}(N, \beta) = \frac{1}{N!} \int_{\Lambda^N} \exp[-\beta H_{\Lambda}^{U_1}(X_N)] \mathrm{d}X_N$$

and

$$\beta = \frac{1}{k_B T},$$

is the inverse temperature, scaled by  $k_B$ . Following page 23 of [9] we know that the (Helmholtz) free energy can be written as

$$(6) \quad \mathcal{F}_{\beta}^{\Lambda, N}[U_1] = -\beta^{-1} \ln[Z_{\Lambda}(\beta, N)].$$

We now introduce the fundamental quantity of DFT, the density, giving three equivalent definitions

$$\begin{aligned} \rho_{\beta, N}^{\Lambda}(x) &= \int_{\Lambda^N} \sum_{i=1}^N \delta(x - x_i) \hat{\rho}_{\beta}^{\Lambda, N}(X_N) \mathrm{d}X_N \\ &= N \int_{\Lambda} \dots \int_{\Lambda} \hat{\rho}_{\beta}^{\Lambda, N}(X_N) \mathrm{d}x_2 \dots \mathrm{d}x_N \\ &= \frac{\delta \mathcal{F}_{\beta}^{\Lambda, N}[U_1]}{\delta U_1(x)} \end{aligned}$$

where importantly

$$N = \int_{\Lambda} \rho_{\beta, N}^{\Lambda}(x) \mathrm{d}x.$$

A process completely analogous to the one detailed for the grand canonical ensemble in Section 2 of [10], detailed for the canonical ensemble in Section 4 of [11], shows the existence of a functional  $\mathcal{F}_{HK}$  (the Hohenberg-Kohn functional) minimised at the equilibrium

density, such that at equilibrium

$$\mathcal{F}_\beta^{\Lambda N}[U_1] = \inf_{\tilde{\rho}(x)} \left[ \mathcal{F}_{HK}[\tilde{\rho}] + \int_{\Lambda} U_1(x) \tilde{\rho}(x) dx \right]$$

where the infimum is over the space of absolute continuously probability measures having Lebesgue density. From equation 56 of [11]

$$\tilde{\rho}(x) = \frac{1}{N!} \int_{\Lambda} \dots \int_{\Lambda} f_N \sum_{i=1}^N \delta(x - x_i) dX_N$$

where  $f_N$  is an arbitrary  $N$ -body distribution satisfying

$$\frac{1}{N!} \int_{\Lambda} \dots \int_{\Lambda} f_N dX_N = 1.$$

Since we know that the free energy is minimised at equilibrium at constant temperature (see Section 1.3 of [12]) at equilibrium

$$\mathcal{F}_\beta^{\Lambda N}[U_1] = \mathcal{F}_{HK}[\rho_{\beta,eq,N}^\Lambda] + \int_{\Lambda} U_1(x) \rho_{\beta,eq,N}^\Lambda(x) dx$$

where  $\rho_{\beta,eq,N}^\Lambda(x)$  is the one-particle density at equilibrium.

We obtain the free energy at equilibrium by minimising the Hohenberg-Kohn functional and adding the integral product of the minimising density and the external potential. We will therefore concentrate on calculating the Hohenberg-Kohn functional. For ease of calculation, we define a functional  $\mathcal{F}_{\beta,exc}[\rho_{\beta,N}^\Lambda]$  so that we can split this functional into two

$$\mathcal{F}_{HK}[\rho_{\beta,N}^\Lambda] = \mathcal{F}_{\beta,id}[\rho_{\beta,N}^\Lambda] + \mathcal{F}_{\beta,exc}[\rho_{\beta,N}^\Lambda],$$

where  $\mathcal{F}_{\beta,id}$  is the Hohenberg-Kohn functional associated with the ideal gas.

Following Section 2 of [2] we assume the existence of a constant reference density, this is quite a restrictive assumption which is not strictly necessary for the expansion but is normally assumed we also consider this later, and perform a formal expansion of the excess free energy around it

$$\mathcal{F}_{\beta,exc}[\rho_{\beta,N}^\Lambda] \approx \mathcal{F}_{\beta,exc}^{(0)}(\rho_{ref}) + \beta^{-1} \sum_{n=1}^{\infty} \frac{1}{n!} \mathcal{F}_{exc}^{(n)}[\rho_{\beta,N}^\Lambda]$$

where

$$(7) \quad \mathcal{F}_{exc}^{(n)}[\rho_{\beta,N}^\Lambda] = - \int \dots \int c^{(n)}(x_1, \dots, x_n) \prod_{i=1}^n \Delta \rho_\beta(x_i) dx_1 \dots dx_n$$

with

$$c^{(n)}(x_1, \dots, x_n) = -\beta \left. \frac{\delta^n \mathcal{F}_{\beta,exc}[\rho_{\beta,N}^\Lambda]}{\delta \rho_{\beta,N}^\Lambda(x_1) \dots \delta \rho_{\beta,N}^\Lambda(x_n)} \right|_{\rho_{ref}} \quad \text{and} \quad \Delta \rho_\beta(x) = \rho_{\beta,N}^\Lambda(x) - \rho_{ref}.$$

The first term is a constant independent of  $\rho_{\beta,N}^\Lambda(x)$  so can be safely ignored, this form was also used in Section 6.2 of [10]. Consideration of translational and rotational symmetry gives  $c^{(1)}(x_1) = 0$ .

The simplest approximation of our functional (first seen in [13]) which has any contribution from the density is therefore

$$(8) \quad \mathcal{F}_{\beta,exc}[\rho_{\beta,\mu}] \approx \mathcal{F}_{\beta,exc}^{(0)}(\rho_{ref}) - \frac{1}{2}\beta^{-1} \int \int c^{(2)}(x_1 - x_2) \Delta\rho_{\beta,\mu}(x_1) \Delta\rho_{\beta,\mu}(x_2) dx_1 dx_2.$$

We now consider the ideal gas contribution, here there is no internal interaction between particles i.e.  $U_2(x_1, x_2) = 0$ . Thus using the formula (6) for free energy and the partition function (5) we have

$$(9) \quad \mathcal{F}_{\beta}^{\Lambda N}[U_1] = \beta^{-1} \left( \ln[N!] - N \ln \left[ \underbrace{\int_{\Lambda} \exp[-\beta U_1(x)] dx}_{z(\Lambda)} \right] \right).$$

Using the definition of the one-particle density as the functional derivative of the free energy we have

$$(10) \quad \rho_{\beta,N}^{\Lambda}(x) = \frac{N \exp[-\beta U_1(x)]}{z(\Lambda)}.$$

We want to re-arrange the free energy given by (9) to isolate the  $U_1$  dependent part. Re-arranging (10) we have

$$\ln[z(\Lambda)] = -\ln \left[ \frac{\rho_{\beta,N}^{\Lambda}(x)}{N} \right] - \beta U_1(x)$$

using that the integral of  $\rho_{\beta,N}^{\Lambda}(x)$  is  $N$  we have from (9)

$$(11) \quad \mathcal{F}_{\beta}^{\Lambda N}[U_1] = \beta^{-1} (\ln[N!] - N \ln N) + \beta^{-1} \int_{\Lambda} \rho_{\beta,N}^{\Lambda}(x) \ln[\rho^{(1)}(x)] dx + \int_{\Lambda} \rho_{\beta,N}^{\Lambda}(x) U_1(x) dx.$$

We have Stirling's approximation (see [14])

$$\ln[N!] = N \ln N - N + O(\ln N).$$

Using this in (11) we have

$$\mathcal{F}_{\beta}^{\Lambda N}[U_1] = \beta^{-1} \int_{\Lambda} \rho_{\beta,N}^{\Lambda}(x) (\ln[\rho^{(1)}(x)] - 1) dx + \int_{\Lambda} \rho_{\beta,N}^{\Lambda}(x) U_1(x) dx + O(\ln N).$$

It is postulated that all ensembles are equivalent in the thermodynamic limit  $|\Lambda|, N \rightarrow \infty$  see Section 5 of [9]. To do this we want to find the free energy per particle and give it in terms of the one-particle density per particle and then in any system we re-scale by the number of particles.

$$\rho^1(x) = \frac{\rho_{\beta,N}^{\Lambda}(x)}{N}.$$

Then in a system of size  $N_1$  we want

$$\rho_{N_1}(x) = N_1 \rho^1(x)$$

thus

$$\int_{\Lambda} \rho_{N_1}(x) dx = N_1.$$

Since  $\mathcal{F}_{\beta,exc}$  is such that re-scaling the density and the functional by the same constant has no effect we need only consider the ideal gas part. The free energy per particle is given as

$$\frac{\mathcal{F}_{\beta}^{\Lambda N}[U_1]}{N} = \beta^{-1} \int_{\Lambda} \rho^{(1)}(x) (\ln[N_1 \rho^{(1)}(x)] - 1) dx + \int_{\Lambda} \rho^{(1)}(x) U_1(x) dx + \beta^{-1} \ln \left[ \frac{N}{N_1} \right] + \frac{O(\ln N)}{N}.$$

Then we can take the thermodynamic limit (i.e.  $|\Lambda|, N \rightarrow \infty$ ) then the free energy for a system of  $N_1$  particles is

$$\mathcal{F}[\rho_{N_1}] = \beta^{-1} \int_{\Lambda} \rho_{N_1}(x) (\ln [\rho_{N_1}(x)] - 1) dx + \int_{\Lambda} \rho_{N_1}(x) U_1(x) dx + \beta^{-1} N_1 \ln \left[ \frac{N}{N_1} \right].$$

the final term, the  $N$  dependent term, is independent of  $\rho$ , all  $\rho$  that have integral  $N_1$  will have this term, and since we are only interested in the difference between free energies we can ignore the terms.

Thus the ideal gas part of our Hohenberg-Kohn functional is

$$(12) \quad \mathcal{F}_{\beta, id}[\rho_{N_1}] = \beta^{-1} \int_{\Lambda} \rho_{N_1}(x) (\ln (\rho_{N_1}(x)) - 1)$$

which agrees with the same quantity in the grand canonical ensemble derived on page 4 of [7] (up to a constant in the logarithmic term that arises from consideration of particles with momentum and quantum considerations).

If we know the reference density is constant and the deviation from the density is small we can re-write the density as

$$(13) \quad \rho_{N_1} = \rho_{ref}(1 + \psi(x))$$

As mentioned above the assumption that there is a constant reference density is a restrictive requirement, physically this amounts to assuming that all the structures we are considering are just deviations from a uniform body. Whilst unusual the Taylor expansion could still be carried out with non-constant density however the logarithmic expansion for the ideal gas below and the gradient expansion will both be problematic. This equation also implicitly gives that

$$\int_{\Omega} \psi dx = 0$$

which again restricts the structures, however the derivation of  $u$  below suggests that this condition just enforces that the integral of  $u$  is constant which we already have, although the constant is now constrained to some extent.

Inserting (13) into our ideal gas equation (12) we have

$$\mathcal{F}_{\beta, id}[\rho_{N_1}] = \beta^{-1} \int_{\Omega} \rho_{ref}(1 + \psi(x)) (\ln[\rho_{ref}(1 + \psi(x))] - 1) dx.$$

Using the Taylor expansion of the logarithm we have

$$(14) \quad \mathcal{F}_{\beta, id}[\rho_{N_1}] = \mathcal{F}_{\beta, id}[\rho_{ref}] + \beta^{-1} \rho_{ref} \int_{\Omega} a_0 \psi(x) + \frac{\psi(x)^2}{2} - \frac{\psi(x)^3}{6} + \frac{\psi(x)^4}{12} + O(\psi(x)^5) dx$$

where

$$a_0 = \ln [\rho_{ref}].$$

If we use the same approximation for the density in our expression for the excess energy (c.f. (8))

$$\mathcal{F}_{\beta, exc}[\rho_{N_1}] = \mathcal{F}_{\beta, exc}[\rho_{ref}] - \frac{\rho_{ref}^2 \beta^{-1}}{2} \int_{\Omega} \int_{\Omega} c^{(2)}(x_1, x_2) \psi(x_1) \psi(x_2) dx_1 dx_2$$

where we have used that

$$\Delta \rho(x_i) = \rho_{ref} \psi(x).$$

where  $\psi(x)$  is translational invariant, this follows from the translation invariance of  $U_2$ .

Using the definition of a convolution and that the Fourier transform of a convolution is the product of the Fourier transforms of the functions in the convolution

$$\mathcal{F}_{\beta,exc}[\rho_{N_1}] = \mathcal{F}_{\beta,exc}[\rho_{ref}] - \frac{\rho_{ref}^2 \beta^{-1}}{2} \int_{\Omega} \mathfrak{F}^{-1} \left[ \hat{c}^{(2)}(k) \hat{\psi}(k) \right] \psi(x_1) dx_1.$$

We expand  $\hat{c}^{(2)}$  as a Taylor series around  $k = 0$  and use that odd terms vanish by symmetry of  $\hat{c}^{(2)}$

$$\mathcal{F}_{\beta,exc}[\rho_{N_1}] = \mathcal{F}_{\beta,exc}[\rho_{ref}] - \frac{\rho_{ref}^2 \beta^{-1}}{2} \int_{\Omega} \mathfrak{F}^{-1} \left[ \sum_{m=0}^{\infty} c_{2m} k^{2m} \hat{\psi}(k) \right] \psi(x_1) dx_1.$$

Using that

$$\mathfrak{F}^{-1} \left[ k^{2m} \hat{\psi}(k) \right] = (-1)^m \nabla^{2m} \psi(x)$$

we have

$$(15) \quad \mathcal{F}_{\beta,exc}[\rho_{N_1}] = \mathcal{F}_{\beta,exc}[\rho_{ref}] - \frac{\rho_{ref}^2 \beta^{-1}}{2} \int_{\Omega} \psi(x_1) \sum_{m=0}^{\infty} c_{2m} (-1)^m \nabla^{2m} \psi(x_1) dx_1.$$

We can re-combine our ideal gas functional (14) and our excess energy functional (15) to give

$$\begin{aligned} \mathcal{F}_{HK}[\rho_{N_1}] &= \mathcal{F}_{HK}[\rho_{ref}] - \frac{\rho_{ref}^2 \beta^{-1}}{2} \int_{\Omega} \psi(x_1) \sum_{m=0}^{\infty} c_{2m} (-1)^m \nabla^{2m} \psi(x_1) dx_1 \\ &\quad + \beta^{-1} \rho_{ref} \int_{\Omega} a_0 \psi(x) + \frac{\psi(x)^2}{2} - \frac{\psi(x)^3}{6} + \frac{\psi(x)^4}{12} + O(\psi(x)^5) dx. \end{aligned}$$

Following [4] we curtail at fourth order in both  $\psi$  and the gradient, it is claimed in [3] that this order is the lowest order that enables the formation of stable crystalline phases. The functional minus the part evaluated at the reference density is

$$\begin{aligned} \Delta \mathcal{F}_{HK}[\rho_{N_1}] &\approx - \frac{\rho_{ref}^2 \beta^{-1}}{2} \int_{\Omega} \psi(x_1) \sum_{m=0}^2 c_{2m} (-1)^m \nabla^{2m} \psi(x_1) dx_1 \\ &\quad + \beta^{-1} \rho_{ref} \int_{\Omega} a_0 \psi(x) + \frac{\psi(x)^2}{2} - \frac{\psi(x)^3}{6} + \frac{\psi(x)^4}{12} dx. \end{aligned}$$

Since we Taylor expand  $\hat{c}^{(2)}$

$$\begin{aligned} \hat{c}_n &= \frac{1}{n!} \frac{\partial^n \hat{c}}{\partial k^n}(0) \\ &= \int \frac{(ix)^n c^{(2)}(x)}{n!} dx \end{aligned}$$

so the relevant coefficients in the gradient expansion alternate in sign.

Discarding the linear terms we have

$$(16) \quad \Delta \mathcal{F}_{HK}[\rho_{N_1}] \approx \beta^{-1} \rho_{ref} \int_{\Omega} A \psi(x)^2 + B \psi(x) \nabla^2 \psi(x) + C \psi(x) \nabla^4 \psi(x) - \frac{\psi(x)^3}{6} + \frac{\psi(x)^4}{12} dx$$

where

$$A = \frac{1}{2} (1 + |c_0| \rho_{ref}) \quad B = \frac{1}{2} |c_2| \rho_{ref} \quad C = \frac{1}{2} |c_4| \rho_{ref}.$$

We would like to reformulate our functional difference to be of the form

$$(17) \quad \tilde{\mathcal{F}} = \int \left( \frac{\tilde{\psi}}{2} \left( -\ell + (k_0^2 + \nabla^2)^2 \right) \tilde{\psi} + \frac{\tilde{\psi}^4}{4} \right) d\tilde{x}.$$

This is the form initially given for PFC theory in [3]. Substitution of  $\tilde{\psi} = \alpha(1 - 2\psi(x))$  in (17), neglecting constant contributions and terms linear in  $\psi$  and terms that vanish on the boundary shows this is equivalent to (16) divided by  $12\rho_{ref}\beta^{-1}C^2$  (compare equations 42-44 [2]). Where

$$\alpha = \frac{1}{\sqrt{24C}} \quad k_0^2 = \frac{B}{2C} \quad \ell = \frac{1}{8C} - \frac{A}{C} + \frac{B^2}{4C^2}.$$

Using the transform  $k_0^2 x_i = \tilde{x}_i$ , (17) can be re-written as

$$\tilde{\mathcal{F}}[\tilde{\psi}] = k_0^{-2d} \int_{\Omega} \frac{k_0^4}{2} \tilde{\psi} (\Delta + 1)^2 \tilde{\psi} - \frac{\ell}{2} \tilde{\psi}^2 + \frac{1}{4} \tilde{\psi}^4 d\tilde{x}$$

using  $\tilde{\psi} = k_0^2 u$  we have

$$\tilde{\mathcal{F}}[u] = k_0^{8-2d} \int_{\Omega} \frac{u}{2} (\Delta + 1)^2 u - \frac{\ell}{2k_0^4} u^2 + \frac{1}{4} u^4 d\tilde{x}$$

which by relabelling the coefficient of the square gives a constant multiplying our original functional (1).

### 3. Initial Numerical Approach

We now consider several methods of minimising the PFC functional (1). Initially we consider a numerical approach to simulating the equation (3) following the techniques of [1]. Following [1] we consider our  $\Omega$  to be a rectangle with periodic boundary conditions. The principle behind [1] is to add and subtract a constant multiplying a stabilising term and split the functional into a convex and a concave functional i.e.

$$\mathcal{F}[u] = \mathcal{F}_c[u] - \mathcal{F}_e[u]$$

where

$$\begin{aligned} \mathcal{F}_c[u] &= \int_{\Omega} \frac{u}{2} (\Delta + 1)^2 u - \frac{\delta}{2} u^2 + \frac{C}{2} |Lu|^2 dx \\ \mathcal{F}_e[u] &= \int_{\Omega} \frac{C}{2} |Lu|^2 - \frac{1}{4} u^4 dx \end{aligned}$$

where  $L = 1, L = \nabla$ . For  $C > \max(2, \delta)$  the first functional is convex. However the second functional is only convex if  $\|u\|_{L^\infty}^2 \leq \frac{C}{3} \min(1, \nu)$  (see page 5 [1]), where we need a bounded domain for Poincaré's inequality (which has constant  $\nu$ ) in the case  $L = \nabla$ .

We then enforce time discretisation with  $\mathcal{F}_c$  evaluated at  $u^{n+1}$  and  $\mathcal{F}_e$  evaluated at  $u^n$ . Then using (2) we have

$$\frac{u^{n+1} - u^n}{\tau} = \Delta \left( (\Delta + 1)^2 u^{n+1} - \delta u^{n+1} + CLL^* u^{n+1} - CLL^* u^n + (u^n)^3 \right)$$

where  $L^*L = 1$  or  $L^*L = -\Delta$  for  $L = 1, L = \nabla$  respectively.

The periodic boundary conditions allow us to solve in Fourier space and use the fast Fourier transform. This follows the method of [1] with minor adaptations to allow for rectangular rather than square domains.

We re-arrange and discretise in space

$$(18) \quad (1 - \tau\Delta_h [(\Delta_h + 1)^2 - \delta + CL^*L]) U_j^{n+1} = U_j^n - \tau\Delta_h [CL^*LU_j^n - (U_j^n)^3]$$

where the discrete Laplacian is using the second difference

$$(19) \quad \Delta_h U_j^n = \sum_{i=1}^d \frac{U^n_{j+e_i} - 2U^n_j + U^n_{j-e_i}}{h_i^2}.$$

We use the discrete Fourier transform, for simplicity we will work in two dimensions in an  $m_1 \times m_2$  grid . The discrete Fourier transform is then, see equation 2.5 of [5],

$$\widehat{U}^n[k] = \sum_{j_1=1}^{m_1} \sum_{j_2=1}^{m_2} U^n_{j_1, j_2} \exp \left[ -2\pi i \left( \frac{k_1 j_1}{m_1} + \frac{k_2 j_2}{m_2} \right) \right].$$

We need the Fourier transform of the discrete Laplacian (19). Using the linearity of the Fourier transform, after some changes of variables, our discrete Laplacian becomes

$$\begin{aligned} \widehat{\Delta_h U_j^n} &= \sum_{i=1}^d \frac{1}{h_i^2} \left( \exp \left[ \frac{2\pi i k_i}{m_i} \right] - 2 + \exp \left[ -\frac{2\pi i k_i}{m_i} \right] \right) \widehat{U}^n[k] \\ &= \sum_{i=1}^d \frac{2}{h_i^2} \left( \cos \left[ \frac{2\pi k_i}{m_i} \right] - 1 \right) \widehat{U}^n[k] \end{aligned}$$

where in the second line we have used the formulation of  $\cos$  in terms of exponentials (this should be easy to extend to higher dimensional domains of the form of cuboids or hyper-rectangles). Writing

$$F[k] = \sum_{i=1}^d \frac{2}{h_i^2} \left( \cos \left[ \frac{2\pi k_i}{m_i} \right] - 1 \right)$$

we have

$$(20) \quad \widehat{\Delta_h U_j^n} = F[k] \widehat{U}^n[k]$$

and we see that in  $k$ -space the action of the operator  $\Delta_h$  becomes multiplication by  $F[k]$ . Now we can transform (18) into Fourier space to obtain

$$(1 - \tau F[k] [(F[k] + 1)^2 - \delta + C (-F[k])^\omega]) \widehat{U}^{n+1}[k] = \widehat{U}^n[k] + \tau F[k] \left[ (\widehat{U}^n[k])^3 - C (-F[k])^\omega \widehat{U}^n[k] \right]$$

where

$$\omega = \begin{cases} 0 & \text{if } L = 1 \\ 1 & \text{if } L = \nabla \end{cases}$$

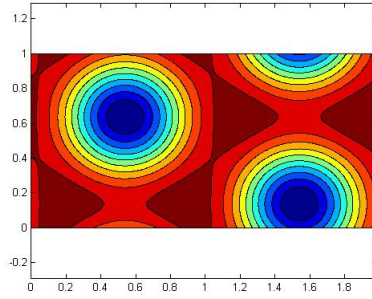
re-arranging for an iterative process we have

$$\widehat{U}^{n+1}[k] = \frac{\widehat{U}^n[k] + \tau F[k] \left[ (\widehat{U}^n[k])^3 - C (-F[k])^\omega \widehat{U}^n[k] \right]}{(1 - \tau F[k] [(F[k] + 1)^2 - \delta + C (-F[k])^\omega])}.$$

We now implement this in Matlab using a similar code to page 12 of [1]. With  $\omega = 0$  and parameters  $\tau = 1$ ,  $\delta = 0.9$ ,  $C = 100$ ,  $m_1 = m_2 = 512$  and  $\bar{u} = 0.5$  on a 2D domain  $4\pi \times 2\pi$  starting with random initial conditions we can generate a unit cell for the hexagonal phase after approximately 8000 time steps (shown below).  $\bar{u}$  is the average value of  $u$

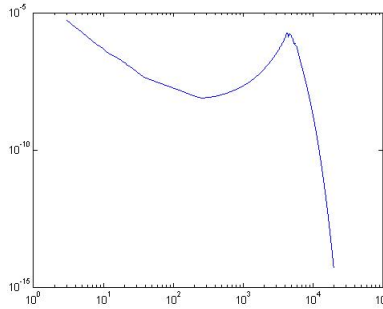
$$\bar{u} = \frac{1}{|\Omega|} \int_{\Omega} u dx$$





The lack of six fold symmetry is an unresolved numerical issue. We show below the graph of the error against the time step on a log-log scale, where the error is given as the maximum difference between successive time steps, normalised by the norm of the current time step (we set the first two errors to 0 so the graph is well-scaled )

$$(21) \quad e^{n+1} = \frac{\|u^{n+1} - u^n\|_{L^\infty}}{\|u^{n+1}\|_{L^\infty}}$$



#### 4. Further Numerical Approaches

As noted above there appears to be slight numerical issues with the unit cell produced using the PFC equation. Different approaches to simulating the PFC equation have been considered in [15] and [16]. However we note that the PFC equation is high order in its derivatives and therefore is stiff. In general we are only interested in the equilibrium of the system, as stated above this is obtained by minimising the functional (1). Although this is done by equation (3), which also conserves the integral of  $u$ , it may not be the most efficient method of minimising the functional (1). We are interested in the most efficient descent method, however formulating this is a long term aim which may prove difficult. Here we will concentrate on constructing a steepest descent method where we can prove the convergence of the method. Once we obtain such a method we hope to be able to analyse the size of domains on which such a method would converge and the constraints on the discretisation imposed by such a method. We note that in the method above the value of  $C$  is highly dependent on domain see [1].

Initially we consider a problem such that if we choose the correct search direction our energy functional is reduced.

First we define a quadratic functional

$$(22) \quad \Phi(v, u) = \frac{1}{2} \|\Delta v + v\|_{L^2}^2 - \langle l(u), v \rangle + \frac{\gamma}{2} \|v\|_{L^2}^2.$$

where

$$(23) \quad \langle l(u), v \rangle = -\delta \mathcal{F}(u, v).$$

We also define the inner product

$$(24) \quad \langle M_\gamma v, v \rangle = \|\Delta v + v\|_{L^2}^2 + \gamma \|v\|_{L^2}^2$$

where we have a norm

$$\|v\|^2 = \langle M_1 v, v \rangle$$

and the dual norm

$$(25) \quad \|\delta \mathcal{F}(u)\|_* = \sup_{\|\varphi\|=1} \langle l(u), \varphi \rangle.$$

### **Lemma 1 (Stability)**

We know

$$\exists! v = \operatorname{argmin} \Phi(v, u).$$

Then in 2 dimensions, for sufficiently large  $\gamma(\|u\|_{L^\infty}, \|\delta \mathcal{F}(u)\|_*)$ . If  $\|u\|_{L^\infty}, \|\delta \mathcal{F}(u)\|_* < \infty$

$$\mathcal{F}(u + v) \leq \mathcal{F}(u) - \beta \langle M_\gamma v, v \rangle$$

### **Proof**

First consider the difference in the functional

$$\mathcal{F}(u + v) - \mathcal{F}(u) = \int \frac{1}{2} (\Delta v + v)^2 - \delta uv - \frac{\delta v^2}{2} + (\Delta v + v)(\Delta u + u) + u^3 v + \frac{3}{2} u^2 v^2 + uv^3 + \frac{v^4}{4}.$$

Then we can re-write using (23)

$$\mathcal{F}(u + v) - \mathcal{F}(u) = \frac{1}{2} \|\Delta v + v\|_{L^2}^2 - \langle l(u), v \rangle + \frac{3}{2} \int u^2 v^2 + \int uv^3 + \frac{1}{4} \|v\|_{L^4}^4 - \frac{\delta}{2} \|v\|_{L^2}^2.$$

Using (22) we have

$$(26) \quad \begin{aligned} \mathcal{F}(u + v) - \mathcal{F}(u) &= \Phi(u, v) - \frac{\gamma}{2} \|v\|_{L^2}^2 - \frac{\delta}{2} \|v\|_{L^2}^2 + \frac{3}{2} \int u^2 v^2 + \int uv^3 + \frac{1}{4} \|v\|_{L^4}^4 \\ &\leq \Phi(u, v) - \left( \frac{\gamma}{2} + \frac{\delta}{2} - \frac{3}{2} \|u\|_{L^\infty}^2 \right) \|v\|_{L^2}^2 + \|u\|_{L^\infty} \|v\|_{L^3}^3 + \frac{1}{4} \|v\|_{L^4}^4. \end{aligned}$$

By an interpolation of Hölder's inequality we have

$$(27) \quad \|v\|_{L^3}^3 \leq \|v\|_{L^2} \|v\|_{L^4}^2.$$

As we are in 2 dimensions, we also have a version of Ladyzhenskaya's inequality (see equation 5.7 of [20] for  $v : \mathbb{T}^2 \rightarrow \mathbb{R}$ , and Theorem 9.3 of [19] for  $v : \mathbb{R}^2 \rightarrow \mathbb{R}$ )

$$(28) \quad \|v\|_{L^4} \leq \|v\|_{L^2}^{\frac{1}{2}} \|v\|_{H^1}^{\frac{1}{2}}.$$

We can show

$$(29) \quad \|v\|_{H^1}^2 \leq K(\|v\|_{L^2}^2 + \|\Delta v + v\|_{L^2}^2).$$

$$\begin{aligned} \|\nabla v\|_{L^2}^2 &\leq \int |v(\Delta v + v) - v^2| \\ &\leq \int |v(\Delta v + v)| + \int v^2 \\ &\leq \|v\|_{L^2} \|\Delta v + v\|_{L^2} + \|v\|_{L^2}^2 \quad \text{by Cauchy-Schwarz} \\ &\leq \|v\|_{L^2}^2 \left( \frac{1}{2\epsilon} + 1 \right) + \frac{\epsilon}{2} \|\Delta v + v\|_{L^2}^2 \end{aligned}$$

where we use Young's inequality with  $\epsilon$ . If

$$\frac{\epsilon}{2} = \frac{1}{2\epsilon} + 1$$

then

$$\|\nabla v\|_{L^2}^2 \leq \frac{\epsilon}{2} (\|v\|_{L^2}^2 + \|\nabla v + v\|_{L^2}^2)$$

where  $\epsilon$  is just a constant number independent of  $\Omega$  etc. In fact  $\epsilon = 1 + \sqrt{2}$ . Adding the  $L^2$  norm of  $v$  to both sides and taking  $K$  as  $1 + \frac{\epsilon}{2}$  gives (29).

From (22) using (24) we have

$$\Phi = \frac{1}{2} \langle M_\gamma v, v \rangle - \langle l(u), v \rangle.$$

We can show that minimising this functional is equivalent to solving the problem

$$(30) \quad \langle l(u), w \rangle = \langle M_\gamma v, w \rangle \quad \forall w \in H$$

where  $H$  is the Hilbert space  $H^2$  with  $\int v = 0$ . (30) has a unique solution since the left-hand side is bounded and the right-hand side is bounded and coercive.

Thus we have using (24) and the associated norm

$$\Phi(v, u) = -\frac{1}{2} \|v\|^2 - \frac{(\gamma - 1)}{2} \|v\|_{L^2}^2.$$

Using this and (27) in (26) we have

$$\begin{aligned} \mathcal{F}(u + v) - \mathcal{F}(u) &\leq - \left( \frac{(2\gamma - 1)}{2} + \frac{\delta}{2} - \frac{3}{2} \|u\|_{L^\infty} \right) \|v\|_{L^2}^2 - \frac{1}{2} \|v\|^2 + (\|u\|_{L^\infty} \|v\|_{L^2} + \|v\|_{L^4}^2) \|v\|_{L^4}^2 \\ &\leq - \left( \frac{(2\gamma - 1)}{2} + \frac{\delta}{2} - \frac{3}{2} \|u\|_{L^\infty} \right) \|v\|_{L^2}^2 - \frac{1}{2} \|v\|^2 \\ &\quad + (\|u\|_{L^\infty} \|v\|_{L^2} + \|v\|_{L^2} \|v\|_{H^1}) \|v\|_{L^2} \|v\|_{H^1} \quad \text{using (28)}. \end{aligned}$$

Using (29) we have

$$\begin{aligned} \mathcal{F}(u + v) - \mathcal{F}(u) &\leq - \left( \frac{(2\gamma - 1)}{2} + \frac{\delta}{2} - \frac{3}{2} \|u\|_{L^\infty} \right) \|v\|_{L^2}^2 - \frac{1}{2} \|v\|^2 \\ &\quad + (\|u\|_{L^\infty} \|v\|_{L^2} + \|v\|_{L^2} K \|v\|) \|v\|_{L^2} K \|v\|. \end{aligned}$$

Young's inequality on the first term in the second bracket gives

$$\|u\|_{L^\infty} \|v\|_{L^2}^2 \|v\| \leq \frac{(\|u\|_{L^\infty} \|v\|_{L^2})^2}{2} + \frac{\|v\|^2 \|v\|_{L^2}^2}{2}.$$

Thus we have

$$(31) \quad \begin{aligned} \mathcal{F}(u + v) - \mathcal{F}(u) &\leq - \left( \frac{(2\gamma - 1)}{2} + \frac{\delta}{2} - \frac{3}{2} \|u\|_{L^\infty} - \frac{K \|u\|_{L^\infty}^2}{2} \right) \|v\|_{L^2}^2 - \frac{1}{2} \|v\|^2 \\ &\quad + \frac{3}{2} K \|v\|_{L^2}^2 \|v\|^2. \end{aligned}$$

(30) gives

$$\|v\|^2 + (\gamma - 1) \|v\|_{L^2}^2 = \langle l(u), v \rangle.$$

Using (25)

$$\|v\|^2 + (\gamma - 1) \|v\|_{L^2}^2 \leq \|v\| \| \delta \mathcal{F}(u) \|_*$$

using Young's inequality with  $\epsilon = 2$  we have

$$4(\gamma - 1) \|v\|_{L^2}^2 \leq \| \delta \mathcal{F}(u) \|_*^2.$$

using this in (31) we have

$$\mathcal{F}(u + v) - \mathcal{F}(u) \leq - \left( \frac{(2\gamma - 1)}{2} + \frac{\delta}{2} - \frac{3}{2} \|u\|_{L^\infty} - \frac{K \|u\|_{L^\infty}^2}{2} \right) \|v\|_{L^2}^2 - \left( \frac{1}{2} - \frac{3K \| \delta \mathcal{F}(u) \|_*^2}{8(\gamma - 1)} \right) \|v\|^2.$$

□

**Remark**

The previous Lemma should be easily applicable in 3D where the Ladyzhenskaya's inequality becomes

$$\|u\|_{L^4} \leq \|u\|_{L^2}^{\frac{1}{4}} \|u\|_{H^1}^{\frac{3}{4}}$$

this means that the proof will have to be adapted which we hope to achieve later.

Following Lemma 1 we can minimise the functional (1) by solving

$$\langle M_\gamma v, v \rangle = -\delta \mathcal{F}(u, v).$$

This is equivalent to

$$(\Delta^2 + 2\Delta + (1 + \gamma)) v = -(\Delta + 1)^2 u + \delta u - u^3.$$

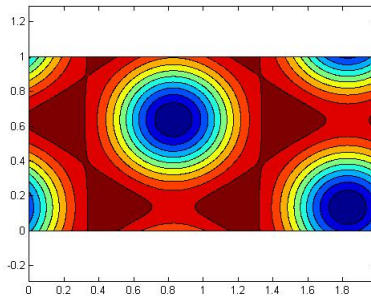
We know that Fourier transform of  $\Delta_h$  is  $F$  (20) thus the Fourier transformed equation after re-arrangement and discretising in space is

$$\hat{V}_j = -\frac{(F + 1)^2 \hat{U}_j - \delta \hat{U}_j + \widehat{U}_j^3}{(F^2 + 2F + (1 + \gamma))}.$$

We know  $u^{n+1} = u^n + v$ . Thus

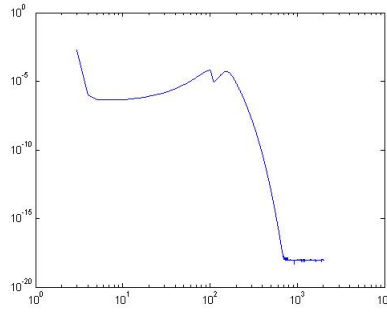
$$\hat{U}_j^{n+1} = \hat{U}_j^n - \frac{(F + 1)^2 \hat{U}_j^n - \delta \hat{U}_j^n + \widehat{U}_j^{n3}}{(F^2 + 2F + (1 + \gamma))}.$$

Again using Matlab with the parameters  $\delta = 0.9$ ,  $\gamma = 2$ ,  $m_1 = m_2 = 512$  and  $\bar{u} = 0.5$  on a 2D domain  $4\pi \times 2\pi$  starting with random initial conditions we can generate a unit cell for the hexagonal phase after approximately 200 time steps



Again there is a slight discrepancy from six-fold symmetry, this may be related to numerical accuracy and not the optimisation since it does not appear to depend on the method, however the much shorter simulation time for this method seems optimistic. We have not yet proved convergence, obviously we need  $\|u\|_{L^\infty}$  (and  $\|\delta \mathcal{E}(u)\|_{*}$ ) bounded which we have not yet shown, if we proved this we have stability of the scheme. The bound on  $\|u\|_{L^\infty}$  is critical as in general it may fail to be bounded. To prove convergence of this method we would also need the method to be first order consistent.

We show below the graph of the error against the time step on a log-log scale where the error is given as (21) (we set the first two errors to 0 so the graph is well-scaled).



In the scheme above we enforce conservation of  $u$  by setting the change between successive time-steps of the first Fourier mode to zero.

$$\widehat{u}^{n+1}[0] - \widehat{u}^n[0] = 0$$

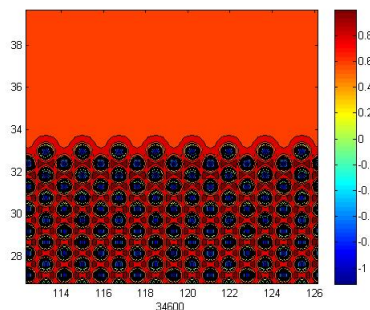
without this we are implementing a generalisation of the  $L^2$  flow of our functional (1). The classic  $L^2$  flow of our functional is just the Swift-Hohenberg equation for which there is also some mathematical literature e.g. [17]. There is a suggestion for implementing a  $L^2$  gradient flow in [1].

## 5. Lattice Deformations

We now consider the simulation of lattices and in particular lattices with defects. Once we have generated a unit cell we can build a lattice of arbitrary size (subject to memory constraints) by placing unit cells next to each other. We can then consider various types of deformations to the lattice.

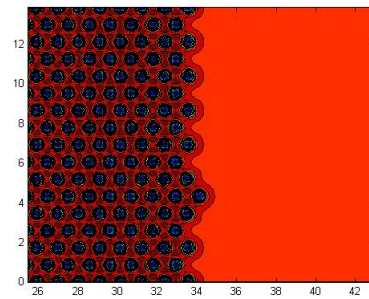
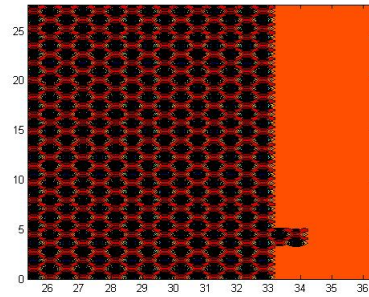
### 5.1 Surface

If we consider a large domain then by reference to the physical intuition of [3] we hope to be able to create a simulation of a surface by implanting a lattice created from a series of unit cells into a domain with constant density (representing a liquid). The constant background is initialised by setting  $\bar{u}$  to a constant, the constant must be chosen with care, if it is too small (close to the lattice  $\bar{u}$ ) the lattice will grow to cover the whole domain and if it is too large the lattice structure dissolves, for convenience we suggest this value represents the vacuum. The results below show a surface where the unit cell is generated using the  $H^{-1}$  gradient flow numerical scheme on a domain  $2.4\pi \times 2\sqrt{3}\pi$  with  $\bar{u} = 0.5$ , the background  $\bar{u} = 0.7$ , the size of the lattice is 32 unit cells by 128 unit cells in total domain  $\frac{4\sqrt{3}}{3}32(1.2) \times 128\sqrt{3}$  and  $C = 100$ ,  $\tau = 1$  are used throughout, the  $x$ -axis of the total domain is given  $m = 512$  and the other axes are scaled appropriately. This image is zoomed in on the surface and taken 2000 time steps after the lattice has been initialised in the vacuum.



Now we have created a surface we can deform the surface in a small way by placing a single unit cell on top of the surface. Below, using the same parameters as for the surface above,

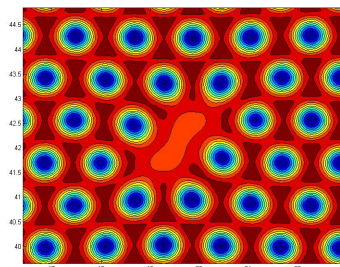
we show the initial condition of the lattice in the vacuum and the system after 10000 time steps

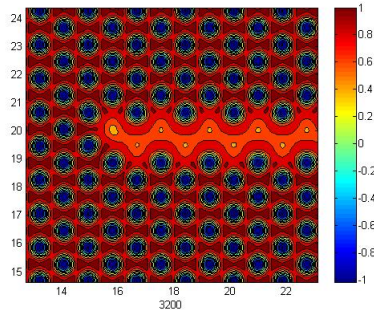


For all the simulations above the  $H^{-1}$  gradient flow of Section 3 is used for the evolution of the surface.

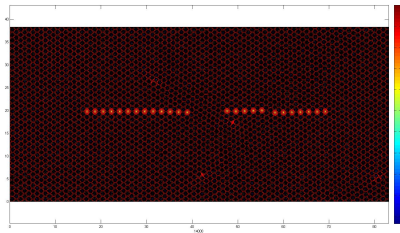
## 5.2 Lattice Dislocation

We now hope to be able to create a lattice dislocation. To do this we create a lattice made of unit cells and remove some unit cells and set the value of  $\bar{u}$  to the vacuum value in the hole created. Below we show a lattice where the unit cell is generated using the  $H^{-1}$  gradient flow numerical scheme on a domain  $2.4\pi \times 2\sqrt{3}\pi$  with  $\bar{u} = 0.5$ , the background  $\bar{u} = 0.7$ , the size of the lattice is 32 unit cells by 48 unit cells in total domain  $C = 100$ ,  $\tau = 1$  are used throughout, the  $x$ -axis of the total domain is given  $m = 512$  and the other axis is scaled appropriately. The first image shows the results of removing a unit cell (this gives a site vacancy) after 5000 time steps and the second image shows the result of removing a strip 32 unit cells and 1 unit cells wide running parallel to the  $y$  axis from the centre after approximately 300 time steps.





For all the simulations above the  $H^{-1}$  gradient flow of Section 3 is used for the evolution of the lattice. One would expect that the fracture in the lattice would disappear as it is energetically unfavourable, this may be a long term phenomenon that is not seen due to the slow evolution of the system. It is hoped that using more efficient methods including perhaps the method of Section 4 will allow us to perform faster simulations which may give results that agree with our intuition. A simulation using the method of Section 4 using the same parameters with  $\gamma = 2$  appears to show the gap closing, see the image below after 14000 time steps.



## 6. Further Work

As mentioned above this project is in the exploratory phase and thus there is a considerable amount of further work to be done. At the moment our long-term ambition is to coarse-grain the PFC model to obtain a continuum elasticity model. We will also consider a multi-scale approach to be able to consider defects. To do this we will look at obtaining a refined optimisation method. We also wish to consider elastic deformations by applying a "macroscopic" external field.

### 6.1 Refinement of the optimisation method

As mentioned above we have implemented our minimisation procedure in two ways. However we have not yet assessed which is the best for our purposes. The method of [1] requires a domain dependent stabilisation constant which we hope to avoid. The method of Section 4 looks more optimistic but needs greater consideration.

There are several internal refinement required for each method before it is optimal. Following [3] we know there are several values of  $\delta$  and  $\bar{u}$  such that the function  $u$  that minimises the functional (1) is the hexagonal lattice, currently we have chosen these arbitrarily however it may prove that choosing these carefully will speed up our method. The stabilisation constants  $C$  (for the method of [1]) and  $\gamma$  (for the method of Section 4) have also been chosen without great care and it is likely that the correct choice of these constants would vastly improve the speed of our method, in particular it may be possible to make  $\gamma$  iteration dependent so that it is optimised at each time-step which should vastly increase calculation speed.

The method of Section 4 also need some specific refinements. In order to prove stability of this method we will need to check  $\|u\|_{L^\infty}$  (and  $\|\delta\mathcal{F}(u)\|_*$ ) is bounded, as mentioned above this may not be generally true. Also we would like  $\gamma$  and the rate of convergence to

be independent of the domain size and the discretisation parameter.

In the long term once we have refined the method of Section 4 we would like to be able to explore whether analysis of this scheme allows us to say anything generally about the PFC evolution equations. It would also be useful to compare our method to other methods for simulating the PFC equation and possibly link to work simulating the Swift-Hohenberg equation.

## 6.2 Elastic Deformation

A class of deformations that we have not yet considered but is important is the class of elastic deformations. In this case we would create a lattice and apply a force-field, which varies on a scale larger than the atom size, if the system returns to equilibrium after the force-field has been removed we will have generated an elastic deformation. We will first attempt this numerically and then see if we can obtain analytical results, we believe that we may be able to consider this situation analytically by considering the outer variation of crystalline and near-crystalline equilibrium states. In the case where we have a lattice with a surface we would possibly obtain results that would be useful in the analysis of surface Cauchy-Born methods which is an active area of research e.g. [18].

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