

# 1 Finite element implementation of the coupled model

## 1.1 Weak coupling under periodic boundary conditions

### 1.1.1 Swif-Hohenberg equation

We recall that *Swift-Hohenberg equation* is a non-linear fourth order partial differential equation, defined as :

$$\frac{\partial \psi}{\partial t} = -\Gamma \frac{\delta \mathcal{F}}{\delta \psi} = -\Gamma [\psi + f'(\psi) + \Delta^2 \psi + 2\Delta \psi] \quad \text{with} \quad f(\psi) = -\frac{\epsilon}{2}\psi^2 - \frac{g}{3}\psi^3 + \frac{1}{4}\psi^4 \quad (1)$$

Several numerical methods have been proposed in the literature, trying to build a thermodynamically consistent and energy stable schemes while optimizing the computational costs. It is well known that a forward explicit euler scheme is unstable if the CFL-like conditions are not met ( $\Delta t \sim < \Delta x^4$ ). For this reason, a first semi-implicit method was proposed in Cheng and Warren, 2008, then this method was enhanced in Elsey and Wirth, 2013 where the authors added a stabilizing term to enforce energy stability. Following this, a second order Crank-Nicolson scheme was suggested in Gomez and Nogueira, 2012 in combination with a Newton-Raphson method to adress the non linear scheme. Moreover, to deal with the non-linear term, different operator splitting methods were proposed, such as first and second order convex splitting Hu et al., 2009. Finally, we refer to spectral method used in conjunction with these splitting methods (e.g Lee, 2017) and pseudo-spectral studied in Zhai et al., 2021. In what comes next, we follow the finite elements scheme suggested in Qi, 2024, based on the classically used mixed formulation of fourth order partial differential equations.

We consider a domain  $\Omega$  with a given triangulation  $\mathcal{T}_h$  such that  $\Omega = \bigcup_{U \in \mathcal{T}_h} U$  with  $h$  being the maximal length of the triangles. We consider the scalar finite element element functional space  $V_h^q$  defined as:

$$V_h^q = \{f_h \in H_{prt}^1(\Omega) \mid f_h|_U \in \mathcal{P}_q, \forall U \in \mathcal{T}_h\} \quad (2)$$

Where,  $H_{per}^1(\Omega)$  is the standard  $H_1 = W^{s,p}$  Sobolev space with enforced periodic boundary conditions all around  $\partial\Omega$ . We recall that  $H_{per}^1(\Omega)$  is equipped with the standard  $L^2$  inner product which with denote by  $\langle \cdot, \cdot \rangle$ . Finally, the space  $\mathcal{P}_q$  denotes the space of degrees up to  $q$ .

The continuous mixed formulation of the Swif-Hohenberg equation eq. (1), is based on introducing a new function  $\omega \in H_{per}^1(\Omega)$ , such that  $\omega = \Delta\psi$ . The coupled system is thus:

$$\begin{cases} \frac{\partial \psi}{\partial t} = -\Gamma [\psi + f'(\psi) + \Delta\omega + 2\omega] \\ \omega = \Delta\psi \end{cases} \quad (3)$$

To obtain the weak formulation of the previous coupled problem, we multiply the first equation with a test function  $u_h \in V_h^q$ , and the second one with  $v_h \in V_h^q$ .

$$\begin{cases} \langle \partial_t \psi, u_h \rangle = -\Gamma [\langle \psi + f'(\psi), u_h \rangle + \langle \Delta\omega, u_h \rangle + 2\langle \omega, u_h \rangle] \\ \langle \omega, v_h \rangle = \langle \Delta\psi, v_h \rangle \end{cases} \quad (4)$$

Using the divergence theorem we can get rid of the second order space derivatives as follows:

$$\forall f, u_h \in H_{per}^1(\Omega) \quad \langle \Delta f, u_h \rangle = -\langle \nabla f, \nabla u_h \rangle + \int_{\partial\Omega} u_h \nabla f \cdot dS \quad (5)$$

The boundary term vanishes because of periodicity and we can formulate eq. (4) as a semi-discretized weak problem:

Find  $\chi_h = (\psi_h, \omega_h) \in (V_h^q)^2$ , such that :

$$\forall u_h, v_h \in V_h^q \quad \begin{cases} \langle \partial_t \psi_h, u_h \rangle = -\Gamma [\langle \psi_h + f'(\psi_h), u_h \rangle - \langle \nabla \omega_h, \nabla u_h \rangle + 2\langle \omega_h, u_h \rangle] \\ \langle \omega_h, v_h \rangle = -\langle \nabla \psi_h, \nabla v_h \rangle \end{cases} \quad (6)$$

With known initial conditions  $\psi_h^{t=0}$  and  $\omega_h^{t=0}$ .

The existence and uniqueness of a solution for this semi-discretized scheme was proven in Qi, 2024 using galerkin spectral method. In addition, the author studied and demonstrated the convergence of the scheme for  $\mathcal{P}_1$  and  $\mathcal{P}_2$  polynomial spaces.

In order to introduce the fully discrete scheme, we use *Crank-Nicolson* method to treat the time derivatives. An explicit Eulers scheme would require a time step roughly  $dt < dx^4$ , whereas a CN scheme is known for it's second order stability and allows for larger timesteps.

Find  $\chi_h^{n+1} = (\psi_h^{n+1}, \omega_h^{n+1}) \in (V_h^q)^2$ , given  $\chi_h^n = (\psi_h^n, \omega_h^n)$ , such that  $\forall u_h, v_h \in V_h^q$  :

$$\begin{cases} \langle \psi_h^{n+1}, u_h \rangle = \langle \psi_h^n, u_h \rangle - dt \Gamma \left[ \langle \frac{\psi_h^{n+1} + f'(\psi_h^{n+1}) + \psi_h^n + f'(\psi_h^n)}{2}, u_h \rangle - \langle \frac{\nabla \omega_h^{n+1} + \nabla \omega_h^n}{2}, \nabla u_h \rangle \right. \\ \left. + 2 \langle \frac{\omega_h^{n+1} + \omega_h^n}{2}, u_h \rangle \right] \\ \langle \omega_h^{n+1}, v_h \rangle = - \langle \nabla \psi_h^{n+1}, \nabla v_h \rangle \end{cases} \quad (7)$$

Where  $dt$  is the timestep. The problem requires an initialization  $\psi_h^{t=0}$  and  $\omega_h^{t=0}$ .

This fully discretized scheme introduces a nonlinear term, due to the non linear nature of the function  $f$ . At each time iteration, this problem is tackled using a Newton-Raphson iterative solver in conjunction with a Krylov solver for all the linear equation, as well as the Newton internal subiteration with a convergence critereon based on residuals. To go into details, the previous system in eq. (7) can compactly written as (we drop the  $h$  subscript for convenience):

$$\text{Given } \chi_h^n, \text{ Find } \chi_h^{n+1}, \text{ such that : } F(\chi_h^{n+1}, \chi_h^n, u_h, v_h) = 0 \quad \forall u_h, v_h \in V_h^q \quad (8)$$

Within a finite-element approximation, we can assemble from the previous system eq. (7) a jacobian matrix  $\mathcal{J}[(\chi_h^{n+1})_k]$  as well as residual vector  $F((\chi_h^{n+1})_k)$  which easily set up our Newton iterative scheme. The subscript  $k$  is linked to Newton's method internal iterations:

$$(\chi_h^{n+1})_{k+1} = (\chi_h^{n+1})_k - \mathcal{J}[(\chi_h^{n+1})_k]^{-1} F((\chi_h^{n+1})_k) \quad (9)$$

Which ultimately defines a reccurent sequence to be iterated until convergence critereon is reached as determined by a given tolerance.

### 1.1.2 Mechanical problem

We recall that in this section we solve a uncoupled FDM-PFC model in which the evolution the evolution of the scalar field  $\psi$  is independent of Mechanical state and is solely prescribed by the SH equation eq. (1). As introduced in Upadhyay and Viñals, 2024, the scalar field  $\psi$  can be used to extract a dislocation density tensor  $\alpha$  which will be used to solve the Mechanical problem. In fact, within the weakly non linear region with  $|\varepsilon| \ll 1$ , the order parameter  $\psi$  can be expanded in terms of the slow varying amplitudes of the resonant modes  $q_n$  (Skaugen et al., 2018). We can write:

$$\psi(\mathbf{r}, t) = \psi_0 + \sum_{n=1}^N A_n(\mathbf{r}, t) e^{i q_n \cdot \mathbf{r}} + c.c \quad (10)$$

The phase information included in the complex amplitudes  $A_n$  is used to define a distorted configuration with respect to a perfect lattice. As a matter of fact, the slow varying amplitudes transforms the phase as  $\theta_n \rightarrow \theta_n^0 - q_n \cdot \mathbf{u}$ , where  $\mathbf{u}$  is the displacement field (Skogvoll et al., 2022):

$$\mathbf{u}(\mathbf{r}) = -\frac{3}{N q_0^2} \sum_{n=1}^N q_n \theta(\mathbf{r}) \quad (11)$$

Accessing the complex amplitudes  $A_n$  can be formulated as a demodulation problem that can be tackled through many techniques as we will list in the strongly coupled case. For now, we follow the method proposed in Skogvoll et al., 2022 based on coarse graining. We introduce a coarse graining operator  $X \mapsto \langle X \rangle$  defined as a convolution with a gaussian filter  $\mathcal{G}$  having a length scale  $a_0$ . Let  $X$  be a generic scalar field defined over the domain  $\Omega$ . It's corresponding coarse-grained value is

$$\langle X \rangle(\mathbf{r}) = \frac{1}{(2\pi a_0^2)^{d/2}} \int_{\Omega} d\mathbf{r}' X(\mathbf{r}') e^{-\frac{\|\mathbf{r} - \mathbf{r}'\|^2}{2a_0^2}} = (X * \mathcal{G})(\mathbf{r}) \quad (12)$$

Due to the fact that the complex amplitudes  $A_n$  vary on a length scale much larger than  $a_0$ , one can easily write:

$$A_n(\mathbf{r}) \approx \langle \psi(\mathbf{r}) e^{-i\mathbf{q}_n \cdot \mathbf{r}} \rangle \quad (13)$$

proof?

The typical value of the gaussian kernel length scalar is  $a_0 = 2\pi/q_0$  with  $q_0$  being the characteristic wave vector length of a perfect reference lattice. The major advantage of this method is that it can be efficiently computed using fourier transform. In fact, since the Fourier transform of a gaussian kernel is still a gaussian kernel but with an inverse scale, we can define the kernel once in the fourier space:

$$G(\mathbf{r}) = \frac{1}{(2\pi a_0^2)^{d/2}} e^{-\frac{\|\mathbf{r}\|^2}{2a_0^2}} \Rightarrow \tilde{G}(\boldsymbol{\xi}) = \mathcal{F}[G] = e^{-2a_0^2\pi^2\|\boldsymbol{\xi}\|^2} \quad (14)$$

Using this displacement field or equivalently the slow varying amplitudes, one can define a configurational distortion:

$$\mathbf{Q}(\mathbf{r}) = -\frac{d}{N} \sum_{n=1}^N \mathbf{q}_n \otimes \Im \left( \frac{\nabla A_n}{A_n} \right) \quad (15)$$

An in analogy with linear elasticity, we define a configurational stress simply as :

$$\boldsymbol{\sigma}^Q = \mathbb{C} : \mathbf{Q} \quad (16)$$

add  $\sigma^\psi$  and compare

As discussed in the first part, the phase field crystal support stable and isolated defects which can be accessed using phase singularities. With being said, the configurational distortion can be used to defined the phase field dislocation density tensor  $\bar{\alpha}$ :

$$\bar{\alpha} = \nabla \times \mathbf{Q} \quad (17)$$

Within the uncoupled model, this dislocation density can serve to formulate a static FDM problem. Find an elastic distortion field  $\mathbf{U}$  given a dislocation density tensor  $\alpha$ . This static FDM is solved using *Stokes-Helmholtz* decomposition  $\mathbf{U} = \mathbf{U}^\perp + \mathbf{U}^\parallel$ , with  $\mathbf{U}^\parallel$  being the compatible part satisfying  $\nabla \times \mathbf{U}^\parallel = 0$  and  $\mathbf{U}^\perp$  the incompatible one, verifying  $\nabla \cdot \mathbf{U}^\perp = 0$ .

The incompatible distortion  $\mathbf{U}^\perp$  is found by solving a *Poisson*-type of equation:

$$\nabla^2 \mathbf{U}^\perp = -\nabla \times \alpha \quad (18)$$

Under periodic assumptions, this can be simply solved by a spectral method (see Upadhyay and Viñals, 2024), with  $\tilde{\alpha} = \mathcal{F}(\alpha)$  the Fourier transform of the dislocation density tensor  $\alpha$ :

$$\mathbf{U}^\perp = \mathcal{F}^{-1} \left( \begin{cases} i \frac{(\tilde{\alpha} \cdot \boldsymbol{\mathcal{E}}) \cdot \mathbf{k}}{|\mathbf{k}|} & , |\mathbf{k}| \neq 0 \\ 0 & , |\mathbf{k}| = 0 \end{cases} \right) \quad (19)$$

Where  $\boldsymbol{\mathcal{E}}$  is the third order *Levi-Civita* tensor.

The compatible part, however, is obtained using linear elasticity and the equilibrium condition:

$$\nabla \cdot \boldsymbol{\sigma} = 0 \Rightarrow \nabla \cdot (\mathbb{C} : \mathbf{U}^\parallel) = -\nabla \cdot (\mathbb{C} : \mathbf{U}^\perp) \quad (20)$$

Which can be also solved by means of spectral methods:

$$\mathbf{U}^\parallel = \mathcal{F}^{-1} \left( \tilde{\mathbb{G}} : \mathbb{C} : \tilde{\mathbf{U}}^\perp \right) \quad (21)$$

$\tilde{\mathbb{G}}$  being the fourth order modified Green's tensor defined in the Fourier space:

$$\tilde{\mathbb{G}}_{ijkl} = \dots \text{check MURA1987} \quad (22)$$

Finally, the mechanical stress can be deduced using constitutive law:

$$\mathbf{U} = \mathbf{U}^\perp + \mathbf{U}^\parallel \Rightarrow \boldsymbol{\sigma} = \mathbb{C} : \mathbf{U} \quad (23)$$

The uncoupled model consist of solving the static FDM problem given the dislocation density as determined from configurational distortion  $\bar{\alpha}$  as determined by the order parameter  $\psi$ , i.e we set  $\alpha = \bar{\alpha}$ . Withot any intercation or impact from the mechanics on the scalar field evolution.

### 1.1.3 Uncoupled case, numerical algorithm

The previously introduced numerical scheme is implemented on the opensource FEM software FEniCS available as a frontend library under Python. All fourier transforms are performed using `numpy.fft` library. The following algorithm recapitulate the numerical procedure for solving the uncoupled PFC-FDM model.

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#### Algorithm 1: Uncoupled PFC-FDM model

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**Data:**  $\Omega, dx, dy, dt, \mathbb{C}, \psi(t=0), g, \varepsilon, tol$   
**Result:**  $Q, U, \sigma^Q, \sigma$   
 $t \leftarrow 0$ ;  
 $\psi_h^0 \leftarrow \psi(t=0)$ ;  
 $\omega_h^0 \leftarrow \Delta \psi^0$ ;  
**while**  $t < T$  **do**  
     $k = 0$ ;  
     $(\chi_h^{t+dt})_k \leftarrow (\psi_h^t, \omega_h^t)$ ;  
    FE assembly of  $F((\chi_h^{t+dt})_k)$  from eq. (7);  
     $res \leftarrow ||F((\chi_h^{t+dt})_k)||$ ;  
    **while**  $res > tol$  **do**  
        FE assembly of  $\mathcal{J}[(\chi_h^{n+1})_k]$  from eq. (7);  
         $(\chi_h^{t+dt})_{k+1} \leftarrow \text{RHS of eq. (9)}$ ;  
        FE assembly of  $F((\chi_h^{t+dt})_{k+1})$  from eq. (7);  
         $res \leftarrow ||F((\chi_h^{t+dt})_{k+1})||$ ;  
         $k \leftarrow k + 1$ ;  
    **end**  
     $(\psi_h^t, \omega_h^t) \leftarrow (\chi_h^{t+dt})_k$ ;  
     $A_n^{t+dt} \leftarrow ??$ ;  
     $Q^{t+dt} \leftarrow ??$ ;  
     $\sigma^Q \leftarrow ??$ ;  
     $\bar{\alpha}^{t+dt} \leftarrow \text{RHS of eq. (17)}$ ;  
     $\alpha^{t+dt} \leftarrow \bar{\alpha}^{t+dt}$ ;  
     $t \leftarrow t + dt$ ;  
**end**

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