

Hexagonal phase field lattice

Lucas Myers

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1 Hexagonal lattice phase-field and free energy

To begin, we create a scalar phase field ψ , which roughly corresponds to a time-average of the mass-density of atoms in the lattice. Hence, we would like to write down a form which has mass concentrated in a hexagonal lattice pattern. This looks like:

$$\psi(\mathbf{r}) = \psi_0 + \sum_n A_0 e^{i \mathbf{q}_n \cdot \mathbf{r}} \quad (1)$$

with ψ_0 some constant, A_0 an amplitude, and each \mathbf{q}_n a lattice vector, given by:

$$\mathbf{q}_1 = \hat{\mathbf{y}}, \quad \mathbf{q}_2 = \frac{\sqrt{3}}{2} \hat{\mathbf{x}} - \frac{1}{2} \hat{\mathbf{y}}, \quad \mathbf{q}_3 = -\frac{\sqrt{3}}{2} \hat{\mathbf{x}} - \frac{1}{2} \hat{\mathbf{y}} \quad (2)$$

We will use this as an initial configuration to make sure that we can create a stable configuration and iterate it in time.

The free energy corresponding to a hexagonal lattice is given by:

$$\mathcal{F}[\psi] = \int_{\Omega} \left[\frac{1}{2} [(\nabla^2 + 1) \psi]^2 + \frac{\epsilon}{2} \psi^2 + \frac{1}{4} \psi^4 \right] dV \quad (3)$$

where, if $\epsilon > 0$ the only stable solution is $\psi = \psi_0$, whereas $\epsilon < 0$ admits periodic solutions which we are interested in. Given this free energy, the corresponding time evolution is given by:

$$\frac{\partial \psi}{\partial t} = \nabla^2 \frac{\delta F}{\delta \psi} \quad (4)$$

Writing this out explicitly gives:

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= \nabla^2 \left[(\nabla^2 + 1)^2 \psi + \epsilon \psi + \psi^3 \right] \\ &= \nabla^2 (\nabla^2 + 1)^2 \psi + \epsilon \nabla^2 \psi + \nabla^2 \psi^3 \end{aligned} \quad (5)$$

2 Finite element method

To begin, we expand the equation as much as possible:

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= \nabla^6 \psi + 2 \nabla^4 \psi + (1 + \epsilon) \nabla^2 \psi + \nabla^2 \psi^3 \\ &= \nabla^6 \psi + 2 \nabla^4 \psi + (1 + \epsilon) \nabla^2 \psi + 3 \psi^2 \nabla^2 \psi + 6 \psi (\nabla \psi)^2 \end{aligned} \quad (6)$$

For technical reasons associated with the use of piecewise polynomials for the finite element method, we choose to define the following auxiliary variables:

$$\chi := \nabla^2 \psi, \quad \phi := \nabla^2 \chi = \nabla^4 \psi \quad (7)$$

Substituting these auxiliary variables into our original equations yields:

$$\frac{\partial \psi}{\partial t} = \nabla^2 \phi + 2\phi + (1 + \epsilon) \chi + 3\psi^2 \chi + 6\psi (\nabla \psi)^2 \quad (8)$$

Then we have three coupled second-order equations.

2.1 Time discretization

We may solve this equation numerically using the finite element method. To begin, we discretize in time. For this, we use a semi-implicit method parameterized by θ as in step 23 of the deal.II tutorials. This gives:

$$\begin{aligned} \frac{\psi_n - \psi_{n-1}}{\delta t} = & \theta \left[\nabla^2 \phi_n + 2\phi_n + (1 + \epsilon + 3\psi_n^2) \chi_n + 6\psi_n (\nabla \psi_n)^2 \right] \\ & + (1 - \theta) \left[\nabla^2 \phi_{n-1} + 2\phi_{n-1} + (1 + \epsilon + 3\psi_{n-1}^2) \chi_{n-1} + 6\psi_{n-1} (\nabla \psi_{n-1})^2 \right] \end{aligned} \quad (9)$$

Here δt is the discrete timestep and θ is the discretization parameter: $\theta = 1$ corresponds to a fully-implicit method, $\theta = 0$ is a fully explicit method, and $\theta = 1/2$ is a Crank-Nicolson method. Of course, the definitions of the auxiliary variables still hold for timestep n and $n - 1$.

2.2 Linearizing the equation

Given that the equation is nonlinear, we must use Newton-Rhapson method to solve for each timestep. Because we have a series of three coupled equations, the residual is a three-component function defined at every point. The components are then given by:

$$\begin{aligned} R_1(\psi_n, \chi_n, \phi_n) &= \psi_n - \delta t \theta \left[\nabla^2 \phi_n + 2\phi_n + (1 + \epsilon + 3\psi_n^2) \chi_n + 6\psi_n (\nabla \psi_n)^2 \right] \\ &\quad - \psi_{n-1} - \delta t (1 - \theta) \left[\nabla^2 \phi_{n-1} + 2\phi_{n-1} + (1 + \epsilon + 3\psi_{n-1}^2) \chi_{n-1} + 6\psi_{n-1} (\nabla \psi_{n-1})^2 \right] \\ R_2(\psi_n, \chi_n, \phi_n) &= \chi_n - \nabla^2 \psi_n \\ R_3(\psi_n, \chi_n, \phi_n) &= \phi_n - \nabla^2 \chi_n \end{aligned} \quad (10)$$

Since our residual is vector-valued, the Gateaux derivative will be a matrix which acts on a vector-valued deviation $[\delta\psi, \delta\chi, \delta\phi]^T$. Taking the Gateaux derivative one row at a time yields:

$$\begin{aligned} dR_1(\psi, \chi, \phi; \delta\psi, \delta\chi, \delta\phi) &= \frac{d}{d\tau} R_1(\psi + \tau\delta\psi, \chi + \tau\delta\chi, \phi + \tau\delta\phi) \Big|_{\tau=0} \\ &= \frac{d}{d\tau} \left[\begin{aligned} &\psi_n + \tau\delta\psi_n - \delta t \theta \left[\nabla^2 (\phi_n + \tau\delta\phi_n) + 2(\phi_n + \tau\delta\phi_n) \right. \\ &\quad \left. + (1 + \epsilon + 3(\psi_n + \tau\delta\psi_n)^2) (\chi_n + \tau\delta\chi_n) \right. \\ &\quad \left. + 6(\psi_n + \tau\delta\psi_n) (\nabla (\psi_n + \tau\delta\psi_n))^2 \right] \\ &- \psi_{n-1} - \delta t (1 - \theta) \left[\nabla^2 \phi_{n-1} + 2\phi_{n-1} + (1 + \epsilon + 3\psi_{n-1}^2) \chi_{n-1} + 6\psi_{n-1} (\nabla \psi_{n-1})^2 \right] \end{aligned} \right]_{\tau=0} \\ &= \delta\psi_n - \delta t \theta \left[\nabla^2 \delta\phi_n + 2\delta\phi_n \right. \\ &\quad \left. + (1 + \epsilon + 3\psi_n^2) \delta\chi_n + 6\psi_n \chi_n \delta\psi_n \right. \\ &\quad \left. + 6(\nabla \psi_n)^2 \delta\psi_n + 12\psi_n (\nabla \psi_n) \cdot \nabla \delta\psi_n \right] \\ dR_2(\psi, \chi, \phi; \delta\psi, \delta\chi, \delta\phi) &= \delta\chi_n - \nabla^2 \delta\psi_n \\ dR_3(\psi, \chi, \phi; \delta\psi, \delta\chi, \delta\phi) &= \delta\phi_n - \nabla^2 \delta\chi_n \end{aligned} \quad (11)$$

Given this derivative of the residual, then Newton-Rhapson method in functional space reads:

$$\begin{aligned} dR(\Psi_n)\delta\Psi_n &= -R(\Psi_n) \\ \Psi_{n+1} &= \Psi_n + \delta\Psi_n \end{aligned} \quad (12)$$

where we have defined:

$$\Psi = \begin{bmatrix} \psi \\ \chi \\ \phi \end{bmatrix} \quad (13)$$

R is the vector residual, $\delta\Psi$ is the vector variation of Ψ and:

$$dR(\Psi) = \begin{bmatrix} 1 - \delta t \theta \left[6\psi\chi + 6(\nabla\psi)^2 + 12\psi(\nabla\psi) \cdot \nabla \right] & -\delta t \theta (1 + \epsilon + 3\psi) & -\delta t \theta (\nabla^2 + 2) \\ -\nabla^2 & 1 & 0 \\ 0 & -\nabla^2 & 1 \end{bmatrix} \quad (14)$$

2.3 Space discretization

For this, we introduce a vector test function A :

$$A = \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} \quad (15)$$

Then our linear equation looks like:

$$A^T dR \delta\Psi = -A^T R \quad (16)$$

The left-hand side is given by:

$$\begin{aligned} A^T dR \delta\Psi &= \langle \alpha, \delta\psi_n \rangle - \delta t \theta \left[\langle \alpha, \nabla^2 \delta\phi \rangle + 2 \langle \alpha, \delta\phi_n \rangle \right. \\ &\quad \left. + (1 + \epsilon) \langle \alpha, \delta\chi_n \rangle + 3 \langle \alpha, \psi_n^2 \delta\chi_n \rangle \right. \\ &\quad \left. + 6 \langle \alpha, (\nabla\psi_n)^2 \delta\psi_n \rangle + 12 \langle \alpha, \psi_n (\nabla\psi_n) \cdot \nabla \delta\psi_n \rangle \right] \\ &\quad + \langle \beta, \delta\chi_n \rangle - \langle \beta, \nabla^2 \delta\psi_n \rangle \\ &\quad + \langle \gamma, \delta\phi_n \rangle - \langle \gamma, \nabla^2 \delta\chi_n \rangle \\ &= \langle \alpha, \delta\psi_n \rangle - \delta t \theta \left[-\langle \nabla\alpha, \nabla\delta\phi \rangle + 2 \langle \alpha, \delta\phi_n \rangle \right. \\ &\quad \left. + (1 + \epsilon) \langle \alpha, \delta\chi_n \rangle + 3 \langle \alpha, \psi_n^2 \delta\chi_n \rangle \right. \\ &\quad \left. + 6 \langle \alpha, (\nabla\psi_n)^2 \delta\psi_n \rangle + 12 \langle \alpha, \psi_n (\nabla\psi_n) \cdot \nabla \delta\psi_n \rangle \right] \\ &\quad + \langle \beta, \delta\chi_n \rangle + \langle \nabla\beta, \nabla\delta\psi_n \rangle \\ &\quad + \langle \gamma, \delta\phi_n \rangle + \langle \nabla\gamma, \nabla\delta\chi_n \rangle \end{aligned} \quad (17)$$

and the right-hand side is given by:

$$\begin{aligned}
-A^T R = & -\langle \alpha, \psi_n \rangle + \delta t \theta [\langle \alpha, \nabla^2 \phi_n \rangle + 2 \langle \alpha, \phi_n \rangle + (1 + \epsilon) \langle \alpha, \chi_n \rangle \\
& + 3 \langle \alpha, \psi_n^2 \chi_n \rangle + 6 \langle \alpha, \psi_n (\nabla \psi_n)^2 \rangle] \\
& + \langle \alpha, \psi_{n-1} \rangle + \delta t (1 - \theta) [\langle \alpha, \nabla^2 \phi_{n-1} \rangle + 2 \langle \alpha, \phi_{n-1} \rangle + (1 + \epsilon) \langle \alpha, \chi_{n-1} \rangle \\
& + 3 \langle \alpha, \psi_{n-1}^2 \chi_{n-1} \rangle + 6 \langle \alpha, \psi_{n-1} (\nabla \psi_{n-1})^2 \rangle] \\
& - \langle \beta, \chi_n \rangle + \langle \beta, \nabla^2 \psi_n \rangle - \langle \gamma, \phi_n \rangle + \langle \gamma, \nabla^2 \chi_n \rangle \\
= & -\langle \alpha, \psi_n \rangle + \delta t \theta [-\langle \nabla \alpha, \nabla \phi_n \rangle + 2 \langle \alpha, \phi_n \rangle + (1 + \epsilon) \langle \alpha, \chi_n \rangle \\
& + 3 \langle \alpha, \psi_n^2 \chi_n \rangle + 6 \langle \alpha, \psi_n (\nabla \psi_n)^2 \rangle] \\
& + \langle \alpha, \psi_{n-1} \rangle + \delta t (1 - \theta) [-\langle \nabla \alpha, \nabla \phi_{n-1} \rangle + 2 \langle \alpha, \phi_{n-1} \rangle + (1 + \epsilon) \langle \alpha, \chi_{n-1} \rangle \\
& + 3 \langle \alpha, \psi_{n-1}^2 \chi_{n-1} \rangle + 6 \langle \alpha, \psi_{n-1} (\nabla \psi_{n-1})^2 \rangle] \\
& - \langle \beta, \chi_n \rangle - \langle \nabla \beta, \nabla \psi_n \rangle - \langle \gamma, \phi_n \rangle - \langle \nabla \gamma, \nabla \chi_n \rangle
\end{aligned} \tag{18}$$

Now our shape functions are vector-valued, composed like:

$$\eta_i = \begin{bmatrix} \eta_{i,\psi} \\ \eta_{i,\chi} \\ \eta_{i,\phi} \end{bmatrix} \tag{19}$$

Note that, for primitive elements like we will use, only one component will be nonzero for any particular i . In any case, supposing we assume our solution vector can be written as a linear combinations of primitive test functions, and stipulating that the equation hold for any test function, we get the following left-hand side:

$$\begin{aligned}
A^T dR \delta \Psi = \sum_j \left[\langle \eta_{i,\psi}, \eta_{j,\psi} \rangle - \delta t \theta [-\langle \nabla \eta_{i,\psi}, \nabla \eta_{j,\phi} \rangle + 2 \langle \eta_{i,\psi}, \eta_{j,\phi} \rangle \right. \\
+ (1 + \epsilon) \langle \eta_{i,\psi}, \eta_{j,\chi} \rangle + 3 \langle \eta_{i,\psi}, \psi_n^2 \eta_{j,\chi} \rangle \\
+ 6 \langle \eta_{i,\psi}, (\nabla \psi_n)^2 \eta_{j,\psi} \rangle + 12 \langle \eta_{i,\psi}, \psi_n (\nabla \psi_n) \cdot \nabla \eta_{j,\psi} \rangle] \\
+ \langle \eta_{i,\chi}, \eta_{j,\chi} \rangle + \langle \nabla \eta_{i,\chi}, \nabla \eta_{j,\psi} \rangle \\
\left. + \langle \eta_{i,\phi}, \eta_{j,\phi} \rangle + \langle \nabla \eta_{i,\phi}, \nabla \eta_{j,\chi} \rangle \right] \delta \Psi_j
\end{aligned} \tag{20}$$

Finally, we may write our right-hand side as:

$$\begin{aligned}
-A^T R = & -\langle \eta_{i,\psi}, \psi_n \rangle + \delta t \theta [-\langle \nabla \eta_{i,\psi}, \nabla \phi_n \rangle + 2 \langle \eta_{i,\psi}, \phi_n \rangle + (1 + \epsilon) \langle \eta_{i,\psi}, \chi_n \rangle \\
& + 3 \langle \eta_{i,\psi}, \psi_n^2 \chi_n \rangle + 6 \langle \eta_{i,\psi}, \psi_n (\nabla \psi_n)^2 \rangle] \\
& + \langle \eta_{i,\psi}, \psi_{n-1} \rangle + \delta t (1 - \theta) [-\langle \nabla \eta_{i,\psi}, \nabla \phi_{n-1} \rangle + 2 \langle \eta_{i,\psi}, \phi_{n-1} \rangle + (1 + \epsilon) \langle \eta_{i,\psi}, \chi_{n-1} \rangle \\
& + 3 \langle \eta_{i,\psi}, \psi_{n-1}^2 \chi_{n-1} \rangle + 6 \langle \eta_{i,\psi}, \psi_{n-1} (\nabla \psi_{n-1})^2 \rangle] \\
& - \langle \eta_{i,\chi}, \chi_n \rangle - \langle \nabla \eta_{i,\chi}, \nabla \psi_n \rangle - \langle \eta_{i,\phi}, \phi_n \rangle - \langle \nabla \eta_{i,\phi}, \nabla \chi_n \rangle
\end{aligned} \tag{21}$$

Finally, note that our matrix can be written in block form as:

$$\begin{bmatrix} B & C & D \\ L_\psi & M_\chi & 0 \\ 0 & L_\chi & M_\phi \end{bmatrix} \begin{bmatrix} \delta \psi \\ \delta \chi \\ \delta \phi \end{bmatrix} = \begin{bmatrix} F \\ G \\ H \end{bmatrix} \tag{22}$$

where F , G , H are the different components of $-A^T R$, $\delta\psi$, $\delta\chi$, $\delta\phi$ are the finite element vectors for each of the variations, and then:

$$\begin{aligned}
B_{ij} &= \langle \eta_{i,\psi}, \eta_{j,\psi} \rangle - 6\delta t \theta \left[\langle \eta_{i,\psi}, (\nabla \psi_n)^2 \eta_{j,\psi} \rangle + 2 \langle \eta_{i,\psi}, \psi_n (\nabla \psi_n) \cdot \nabla \eta_{j,\psi} \rangle \right] \\
C_{ij} &= -\delta t \theta \left[(1 + \epsilon) \langle \eta_{i,\psi}, \eta_{j,\chi} \rangle + 3 \langle \eta_{i,\psi}, \psi_n^2 \eta_{j,\chi} \rangle \right] \\
D_{ij} &= -\delta t \theta \left[-\langle \nabla \eta_{i,\psi}, \nabla \eta_{j,\phi} \rangle + 2 \langle \eta_{i,\psi}, \eta_{j,\phi} \rangle \right] \\
L_{ij} &= -\langle \nabla \eta_i, \nabla \eta_j \rangle \\
M_{ij} &= \langle \eta_i, \eta_j \rangle
\end{aligned} \tag{23}$$

where L is something like the Laplacian operator, and M is the mass matrix.

2.4 Preconditioning

Given the block structure, we may try to get a nicer preconditioner as follows:

$$\begin{aligned}
L_\chi \delta\chi + M_\phi \delta\phi &= H \\
\implies \delta\phi &= M_\phi^{-1} (H - L_\chi \delta\chi)
\end{aligned} \tag{24}$$

Additionally, we get:

$$\begin{aligned}
L_\psi \delta\psi + M_\chi \delta\chi &= G \\
\implies \delta\chi &= M_\chi^{-1} (G - L_\psi \delta\psi)
\end{aligned} \tag{25}$$

Substituting this back into the first equation yields:

$$\delta\phi = M_\phi^{-1} (H - L_\chi M_\chi^{-1} (G - L_\psi \delta\psi)) \tag{26}$$

The first component of the matrix equation reads:

$$B\delta\psi + C\delta\chi + D\delta\phi = F \tag{27}$$

We may substitute eqs. (24) and (25) into eq. (27):

$$B\delta\psi + C M_\chi^{-1} (G - L_\psi \delta\psi) + D M_\phi^{-1} (H - L_\chi M_\chi^{-1} (G - L_\psi \delta\psi)) = F \tag{28}$$

Rewriting as a linear equation gives:

$$\left(B + \left(D M_\phi^{-1} L_\chi - C \right) M_\chi^{-1} L_\psi \right) \delta\psi = F - C M_\chi^{-1} G - D M_\phi^{-1} (H - L_\chi M_\chi^{-1} G) \tag{29}$$

Then the scheme is to solve eq. (29), then (25) and (24) are straightforward, in that one only has to invert the mass matrix which is generally well-conditioned and symmetric. We may try to come up with a more efficient preconditioner for eq. (29) at some point, but for now we will do a direct solve just to make sure everything is working correctly.

3 Initializing hexagonal lattice

For this, we need to initialize ψ , χ , and ϕ . ψ is given in eq. (1). We calculate as follows:

$$\chi(\mathbf{r}) = \nabla^2 \psi(\mathbf{r}) = A_0 \sum_n q_n^2 e^{i\mathbf{q}_n \cdot \mathbf{r}} \tag{30}$$

and

$$\phi(\mathbf{r}) = \nabla^2 \chi(\mathbf{r}) = A_0 \sum_n q_n^4 e^{i\mathbf{q}_n \cdot \mathbf{r}} \tag{31}$$