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:

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

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

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

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:

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

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:

$$\frac{\partial \psi}{\partial t} = \nabla^2 \frac{\delta F}{\delta \psi} \tag{4}$$

Writing this out explicitly gives:

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

2 Finite element method

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

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

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

$$\chi \coloneqq \nabla^2 \psi, \quad \phi \coloneqq \nabla^2 \chi = \nabla^4 \psi \tag{7}$$

Substituting these auxiliary variables into our original equations yields:

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

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:

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

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:

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

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:

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

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

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

where we have defined:

$$\Psi = \begin{bmatrix} \psi \\ \chi \\ \phi \end{bmatrix} \tag{13}$$

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

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

2.3 Space discretization

For this, we introduce a vector test function A:

$$A = \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} \tag{15}$$

Then our linear equation looks like:

$$A^T\, dR\, \delta\Psi = -A^T\, R \tag{16}$$

The left-hand side is given by:

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

and the right-hand side is given by:

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

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:

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

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

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

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:

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

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:

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

Additionally, we get:

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

Substituting this back into the first equation yields:

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

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):

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

Rewriting as a linear equation gives:

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

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). However, ψ is real so that we must only take the real part of the equation to get:

$$\psi\left(\mathbf{r}\right) = \psi_0 + \sum_n A_0 \cos\left(\mathbf{q}_n \cdot \mathbf{r}\right) \tag{30}$$

The other fields are then given as:

$$\chi(\mathbf{r}) = \nabla^2\psi(\mathbf{r}) = -A_0 \sum_n q_n^2 \cos(\mathbf{q}_n \cdot \mathbf{r}) = -A_0 \sum_n \cos(\mathbf{q}_n \cdot \mathbf{r}) \tag{31}$$

and

$$\phi(\mathbf{r}) = \nabla^2\chi(\mathbf{r}) = A_0 \sum_n q_n^4 \cos(\mathbf{q}_n \cdot \mathbf{r}) = A_0 \sum_n \cos(\mathbf{q}_n \cdot \mathbf{r}) \tag{32}$$

because each $\mathbf{q}_n$ is a unit vector.