Cahn-Hilliard with Constant Mobility

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Direct Solve

We consider the Cahn-Hilliard equation of the following form

$$\frac{\partial \phi}{\partial t} = \nabla^2 \eta(\phi) \tag{1}$$
$$\eta(\phi) = f'(\phi) - \epsilon^2 \nabla^2 \phi \tag{2}$$

where $f(\phi) = (\phi^2 - 1)^2/4$. This can be reorganized as

$$\frac{\partial \phi}{\partial t} = \nabla^2 \left(\phi^3 - \phi - \epsilon^2 \nabla^2 \phi\right) \tag{3}$$
$$= \nabla^2 \phi^3 - \nabla^2 \phi - \epsilon \nabla^4 \phi \tag{4}$$

We will consider a backward Euler method, which can be easily modified into a Crank-Nicoholson scheme later.

$$\phi^n - \phi^{n-1} - \Delta t \left(\nabla^2 (\phi^n)^3 - \nabla^2 \phi^n - \epsilon^2 \nabla^4 \phi^n\right) = 0 \tag{5}$$

Multiplying on the left by a test function φ

$$\langle \varphi, \phi^n \rangle_\Omega - \left\langle \varphi, \phi^{n-1} \right\rangle_\Omega - \Delta t \left(\left\langle \varphi, \nabla^2 (\phi^n)^3 \right\rangle_\Omega - \left\langle \varphi, \nabla^2 \phi \right\rangle_\Omega - \epsilon^2 \left\langle \varphi, \nabla^4 \phi \right\rangle_\Omega \right) = 0 \tag{6}$$

Integrating the more troublesome equations by parts

$$\langle \varphi, \phi^n \rangle_\Omega - \left\langle \varphi, \phi^{n-1} \right\rangle_\Omega + \Delta t \left(\left\langle \nabla \varphi, 3(\phi^n)^2 \nabla \phi^n \right\rangle_\Omega - \langle \nabla \varphi, \nabla \phi^n \rangle_\Omega + \left\langle \nabla^2 \varphi, \nabla^2 \phi^n \right\rangle_\Omega \right) = 0 \tag{7}$$

Assume that ϕ and φ live in the same finite dimensional function space which is spanned by φ_i, then

$$\langle \varphi_i, \varphi_j \rangle_\Omega + \Delta t \left(\left\langle \nabla^2 \varphi_i, \nabla^2 \varphi_j \right\rangle_\Omega - \langle \nabla \varphi_i, \nabla \varphi_j \rangle_\Omega \right) = \langle \varphi_i, \varphi_j \rangle \phi_j^{n-1} - \Delta t \left\langle \varphi_i, 3(\phi^{n-1})^2 \nabla \phi^n \right\rangle_\Omega \tag{8}$$

Constructing the finite element space for this will require second order elements and is particularly expensive. We are better off trying to determine a way of implementing by introducing a dummy variable

Newton with a Dummy

$$\frac{\partial \phi}{\partial t} = \nabla^2 \phi^3 - \nabla^2 \phi - \epsilon^2 \nabla^2 \eta, \tag{9}$$
$$\eta = \nabla^2 \phi \tag{10}$$

We quickly compute the temporal discretization of the problem, substituting k for Δt which is less cumbersome,

$$\phi^n - k(\nabla^2 (\phi^n)^3 - \nabla^2 \phi - \epsilon^2 \nabla^2 \eta^n) = \phi^{n-1}, \tag{11}$$
$$\eta^n = \nabla^2 \phi^n. \tag{12}$$

projecting into the test space gives

$$\langle u, \phi^n \rangle_\Omega - k \left(\left\langle -\nabla u, 3(\phi^n)^2 \nabla \phi^n \right\rangle_\Omega + \langle \nabla u, \nabla \phi^n \rangle + \epsilon^2 \langle \nabla u, \nabla \eta^n \rangle \right) = \left\langle u, \phi^{n-1} \right\rangle_\Omega \tag{13}$$

$$\langle u, \eta^n \rangle_\Omega = \langle \nabla u, \nabla \phi^n \rangle_\Omega \tag{14}$$

To derive the Newton step let $\phi^n = \phi^{n,k} + \delta\phi^n$ then

$$\left\langle u, \phi^{n,k} \right\rangle_\Omega + \langle u, \delta\phi^n \rangle_\Omega - k \left\langle \nabla u, 3(\phi^{n,k} + \delta\phi^n)^2 \nabla(\phi^{n,k} + \delta\phi^n) \right\rangle_\Omega \tag{15}$$

$$+ k \left\langle \nabla u, \nabla(\phi^{n,k} + \delta\phi^n \right\rangle + k\epsilon^2 \left\langle \nabla u, \nabla \eta(\phi^{n,k} + \delta\phi^n) \right\rangle = \left\langle u, \phi^{n-1} \right\rangle_\Omega \tag{16}$$

If we assume that $(\delta\phi^n)^2 \approx 0$ and $\delta\phi^n \nabla(\delta\phi^n) \approx 0$, we obtain

$$\left\langle u, \phi^{n,k} \right\rangle_\Omega + \langle u, \delta\phi^n \rangle_\Omega \tag{17}$$

$$- k \left\langle \nabla u, 3(\phi^{n,k})^2 \nabla(\phi^{n,k}) \right\rangle \tag{18}$$

$$- k \left\langle \nabla u, 3(\phi^{n,k})^2 \nabla(\delta\phi^n) \right\rangle_\Omega \tag{19}$$

$$- k \left\langle \nabla u, 6(\delta\phi^n)\phi^{n,k} \nabla \phi^{n,k} \right\rangle_\Omega \tag{20}$$

$$+ k \left\langle \nabla u, \nabla \phi^{n,k} \right\rangle_\Omega \tag{21}$$

$$+ k \langle \nabla u, \nabla \delta\phi^n \rangle_\Omega \tag{22}$$

$$+ k\epsilon^2 \left\langle \nabla u, \nabla \eta(\phi^{n,k}) \right\rangle_\Omega \tag{23}$$

$$+ k\epsilon^2 \left\langle \nabla u, \nabla \eta(\phi^{n,k}) \right\rangle \tag{24}$$

$$+ k\epsilon^2 \left\langle \nabla u, \nabla \eta'(\phi^{n,k})\delta\phi^n) \right\rangle_\Omega \tag{25}$$

$$= \left\langle u, \phi^{n-1} \right\rangle_\Omega \tag{26}$$

Constructing the linear system for $\delta\phi^n$ we find that

$$\langle \varphi_i, \varphi_j \rangle \delta\phi_j^n \tag{27}$$

$$- k \left\langle \nabla\varphi_i, 3(\phi^{n,k})^2 \nabla\varphi_j \right\rangle \delta\phi_j^n \tag{28}$$

$$- k \left\langle \nabla\varphi_i, (6\phi^{n,k} \nabla\phi^{n,k})\varphi_j \right\rangle \delta\phi_j^n \tag{29}$$

$$+ k \langle \nabla\varphi_i, \nabla\varphi_j \rangle \delta\phi_j^n \tag{30}$$

$$+ k\epsilon^2 \left\langle \nabla\varphi_i, \nabla\eta'(\phi^{n,k})\varphi_j \right\rangle \delta\phi_j^n \tag{31}$$

$$= \left\langle \varphi_i, \phi^{n-1} \right\rangle \tag{32}$$

$$- \langle \varphi_i, \varphi_j \rangle \phi_j^{n,k} \tag{33}$$

$$+ k \left\langle \nabla\varphi_i, 3(\phi^{n,k})^2 \nabla\phi^{n,k} \right\rangle \tag{34}$$

$$- k \langle \nabla\varphi_i, \nabla\varphi_j \rangle \phi_j^{n,k} \tag{35}$$

$$- k\epsilon^2 \left\langle \nabla\varphi_i, \eta(\phi^{n,ki}) \right\rangle \tag{36}$$

By inverting the linear system we can find $\delta\phi^n$ and define our update $\phi^{n,k+1} = \phi^{n,k} + \alpha\delta\phi^n$; however, this raises an obvious question, what the heck is $\eta'(\phi^{n,k})$? Being entirely unrigourous, in part because the last time I saw this sort of functional analysis was several years ago we have something like this

$$\eta(\phi + \delta\phi) = \nabla^2\phi + \nabla^2\delta\phi \tag{37}$$

$$= \eta(\phi) + \eta'(\phi)\delta\phi \tag{38}$$

The take away being that ∇^2 is a linear operator, so it's linearization is itself.

$$\langle \varphi_i, \varphi_j \rangle \delta\phi_j^n \tag{39}$$
$$- k \left\langle \nabla\varphi_i, 3(\phi^{n,k})^2 \nabla\varphi_j \right\rangle \delta\phi_j^n \tag{40}$$
$$- k \left\langle \nabla\varphi_i, (6\phi^{n,k}\nabla\phi^{n,k})\varphi_j \right\rangle \delta\phi_j^n \tag{41}$$
$$+ k \left\langle \nabla\varphi_i, \nabla\varphi_j \right\rangle \delta\phi_j^n \tag{42}$$
$$+ k\epsilon^2 \left\langle \nabla\varphi_i, \nabla^3\varphi_j \right\rangle \delta\phi_j^n \tag{43}$$
$$= \left\langle \varphi_i, \phi^{n-1} \right\rangle \tag{44}$$
$$- \langle \varphi_i, \varphi_j \rangle \phi_j^{n,k} \tag{45}$$
$$+ k \left\langle \nabla\varphi_i, 3(\phi^{n,k})^2 \nabla\phi^{n,k} \right\rangle \tag{46}$$
$$- k \left\langle \nabla\varphi_i, \nabla\varphi_j \right\rangle \phi_j^{n,k} \tag{47}$$
$$- k\epsilon^2 \left\langle \nabla\varphi_i, \eta(\phi^{n,ki}) \right\rangle \tag{48}$$

integrating by parts we are actually left in the same situation as before

$$\langle \varphi_i, \varphi_j \rangle \delta\phi_j^n \tag{49}$$
$$- k \left\langle \nabla\varphi_i, 3(\phi^{n,k})^2 \nabla\varphi_j \right\rangle \delta\phi_j^n \tag{50}$$
$$- k \left\langle \nabla\varphi_i, (6\phi^{n,k}\nabla\phi^{n,k})\varphi_j \right\rangle \delta\phi_j^n \tag{51}$$
$$+ k \left\langle \nabla\varphi_i, \nabla\varphi_j \right\rangle \delta\phi_j^n \tag{52}$$
$$- k\epsilon^2 \left\langle \nabla^2\varphi_i, \nabla^2\varphi_j \right\rangle \delta\phi_j^n \tag{53}$$
$$= \left\langle \varphi_i, \phi^{n-1} \right\rangle \tag{54}$$
$$- \langle \varphi_i, \varphi_j \rangle \phi_j^{n,k} \tag{55}$$
$$+ k \left\langle \nabla\varphi_i, 3(\phi^{n,k})^2 \nabla\phi^{n,k} \right\rangle \tag{56}$$
$$- k \left\langle \nabla\varphi_i, \nabla\varphi_j \right\rangle \phi_j^{n,k} \tag{57}$$
$$- k\epsilon^2 \left\langle \nabla\varphi_i, \eta(\phi^{n,ki}) \right\rangle \tag{58}$$