Phase-Field Modeling with Finite Element Method

Xiukun Hu[1,2], *Mallory Lai*[1,3], *Geeta Monpara*[1,4]

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[1] University of Wyoming, [2] Department of Mathematics, [3] Department of Botany [4] Department of Mechanical Engineering

Since the underlying microstructure of a material can affect its physical properties, it is important to understand the processes underlying microstructure formation in order to improve engineered materials.[1] However, modeling microstructure formation is complicated by the fact that the structures are thermodynamically unstable and thus evolve over time.[2] Phase-field modeling has gained popularity as a technique for simulating microstructure evolution due to its ability to incorporate different thermodynamic driving forces into the model. As such, it can be used to simulate the microstructure evolution seen in such processes as solidification, grain growth, and solid-state phase transformations.[2]

When it comes to phase-field modeling, the finite element method (FEM) underlies some of the most efficient and accuracte numerical methods to date.[3] The strength of the finite element method arises from its ability to model irregular shapes, heterogeneous materials, general load conditions, nonlinear behavior, and dynamic effects. Furthermore, once the finite element model is established, it can be modified relatively easily.[4] Finite element analysis involves the conversion of the original partial differential equation (PDE) from its original, strong form, into a weak integral form. The domain is then discretized into elements from which shape functions are used to find an approximate numerical solution.[5]

We present here the Galerkin finite element in 2D. The Galerkin method is an example of a weighted residual method which assumes the same shape functions are used for both the solution and the weights.[5] We begin by identifying the strong form PDE and rearranging to get zero on the right hand side. We then multiply the resulting equation by our shape function, as per the Galerkin method.[6] Finally, we integrate over the domain, accounting for both local and global coordinate systems.

Phase field equation:

$$\frac{\partial \phi}{\partial t} = 2\left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right) - g(\phi)$$

where

$$g(\phi) = a\phi^3 + b\phi^2 + c\phi$$

with

$$a = \frac{-36}{\epsilon^2}$$

$$b = \frac{54}{\epsilon^2} + \frac{6m}{\epsilon}$$

$$and$$

$$c = -\left(\frac{18}{\epsilon^2} + \frac{6m}{\epsilon}\right)$$

$$\Rightarrow \frac{\partial \phi}{\partial t} - 2\nabla \cdot \nabla \phi + g(\phi) = 0$$

Applying the Galerkin method:

$$\int\int [N]^T \{\frac{\partial \phi}{\partial t} - 2\nabla \cdot \nabla \phi + g(\phi)\} dxdy = 0$$

Working in a local coordinate system $(\xi - \eta)$ and distributing:

$$\int_{\Omega_{e_i}} \int \left([N]^T \frac{\partial \phi}{\partial t} - [N]^T 2\nabla \cdot \nabla \phi + [N]^T g(\phi) \right) dxdy$$

First term:

$$\int_{\Omega_{e_i}} \int \left([N]^T \frac{\partial \phi}{\partial t} \right) dxdy$$

$$= \int_{-1}^{1} \int_{-1}^{1} \left([N(\xi,\eta)]^T \frac{\partial \phi(\xi,\eta)}{\partial t} |J| \right) d\xi d\eta$$

$$= \int_{-1}^{1} \int_{-1}^{1} \left([N(\xi,\eta)]^T \frac{\partial ([N(\xi,\eta)][\phi_{e_i}]^T)}{\partial t} |J| \right) d\xi d\eta$$

$$= |J| \int_{-1}^{1} \int_{-1}^{1} \left([N]^T [N] [\dot{\phi}_{e_i}]^T \right) d\xi d\eta$$

$$= \left[|J| \int_{-1}^{1} \int_{-1}^{1} \left([N]^T [N] \right) d\xi d\eta \right] [\dot{\phi}_{e_i}]^T$$

where

$$[\dot{\phi}_{e_i}]^T = \frac{\partial [\phi_{e_i}])^T}{\partial t}$$

$$= \frac{\left[\phi_{e_i}^{n+1}\right]^T - \left[\phi_{e_i}^{n}\right]^T}{\Delta t}$$

First term =

$$[C_{e_i}][\dot{\phi}_{e_i}]^T \tag{i}$$

Second term:

$$\int_{\Omega_{e_i}} \int \left([N]^T 2\nabla \cdot \nabla \phi \right) dxdy$$

Applying Green's theorem/Divergence theorem:

$$= 2\{ - \int_{\Omega_{e_i}} \int \nabla \phi \cdot [N]^T dxdy + \oint N_i \nabla \phi \eta dl \}$$

...
...
...

Third term:

$$\int_{\Omega_{e_i}} \int \left([N]^T g(\phi)\right) dxdy$$

$$I_1 = \int_{\Omega_{e_i}} \int \left([N]^T \phi\right) dxdy$$

$$I_1 = \int \int \left([N]^T [N][\phi_{e_i}]^T\right) dxdy$$

$$= \int_{-1}^{1} \int_{-1}^{1} \left([N]^T [N][\phi_{e_i}]^T |J|\right) d\xi d\eta$$

$$\Rightarrow \phi = [N][\phi_{e_i}]^T \Rightarrow [N]^T \phi = [C_{e_i}[\phi_{e_i}]]$$

$$\Rightarrow \phi^2 = \left([N][\phi_{e_i}]^T\right)^2$$

$$= [\phi_{e_i}][N]^T [N][\phi_{e_i}]^T$$

$$= [\phi_{e_i}][C_e][\phi_{e_i}]^T$$

where:

$$[C_e] = [N]^T [N]$$

$$\Rightarrow \phi^3 = \left([N][\phi_{e_i}]^T\right)^3$$

$$= [N][\phi_{e_i}]^T [\phi_{e_i}][N]^T [N][\phi_{e_i}]^T$$

$$= [N][\phi_{e_i}]^T [\phi_{e_i}][C_e][\phi_{e_i}]^T$$

$$= [\phi_{e_i}]^T [\phi_{e_i}] \underbrace{[N][C_{e_i}]}_{[D_{e_i}]} [\phi_{e_i}]^T$$

$$= [\phi_{e_i}]^T [\phi_{e_i}][D_{e_i}][\phi_{e_i}]^T$$

$$[N]^T \phi^3 = [\phi_{e_i}]^T [\phi_{e_i}][C_{e_i}]^2 [\phi_{e_i}]^T$$

Hence,

$$\int_{\Omega_{e_i}} \int \left([N]^T g(\phi)\right) dxdy$$

$$= \int_{-1}^{1} \int_{-1}^{1} \left([N]^T (a\phi^3 + b\phi^2 + c\phi)|J|\right) d\xi d\eta$$

$$= \left[a \int_{-1}^{1} \int_{-1}^{1} \left([\phi_{e_i}]^T [\phi_{e_i}] [C_{e_i}]^2 |J| \right) d\xi d\eta + b \int_{-1}^{1} \int_{-1}^{1} \left([N]^T [\phi_{e_i}] [C_{e_i}] |J| \right) d\xi d\eta + \underbrace{c \int_{-1}^{1} \int_{-1}^{1} \left([C_{e_i}] \right) d\xi d\eta}_{G_e} \right] [\phi_{e_i}]^T$$

Writing phase-field equation in terms of matrices:

$$= |J| \left[\int_{-1}^{1} \int_{-1}^{1} [C_e] d\xi d\eta \right] [\dot{\phi}_{e_i}]^T$$

$$= 2[K_e][\phi_{e_i}]^T - [G_e][\phi_{e_i}]^T$$

Where,

$$[C_{e_i}] = [N]^T [N]$$

Methods

In order to implement the FEM, we began by considering the equation without $g(\phi)$. By witholding $g(\phi)$, we can then compare our results to the heat equation. Be began with a triangular mesh generating code written in Matlab by John Burkardt.[7] From here, we modified the code to fit our model. This involved changing _____. We started with very simple initial conditions, letting a square within our rectangular domain represent a solid phase with $\phi = 1$ and elsewhere a liquid phase with $\phi = 0$. Neumann, Dirichlet, and Periodic boundary conditions were imposed.

After successful implementation of all three boundary conditions without $g(\phi)$, we added $g(\phi)$ to our modified code. Instead of a square domain, we produced a rectangular strip. We varied ϵ to see if changes in the diffusion of the interface could be detected. Then we varied m to see if changes in direction and speed at the interface could be seen. We compared our results with those seen in Nestler[1].

Results

Modification of our code without $g(\phi)$ produced results aligning with those of the heat equation.

Discussion

Insert error analysis stuff

Future work should center around speeding up the current code. Converting the code from Matlab to C, and using techniques for sparse matrices, we believe the code could be sped up considerably.

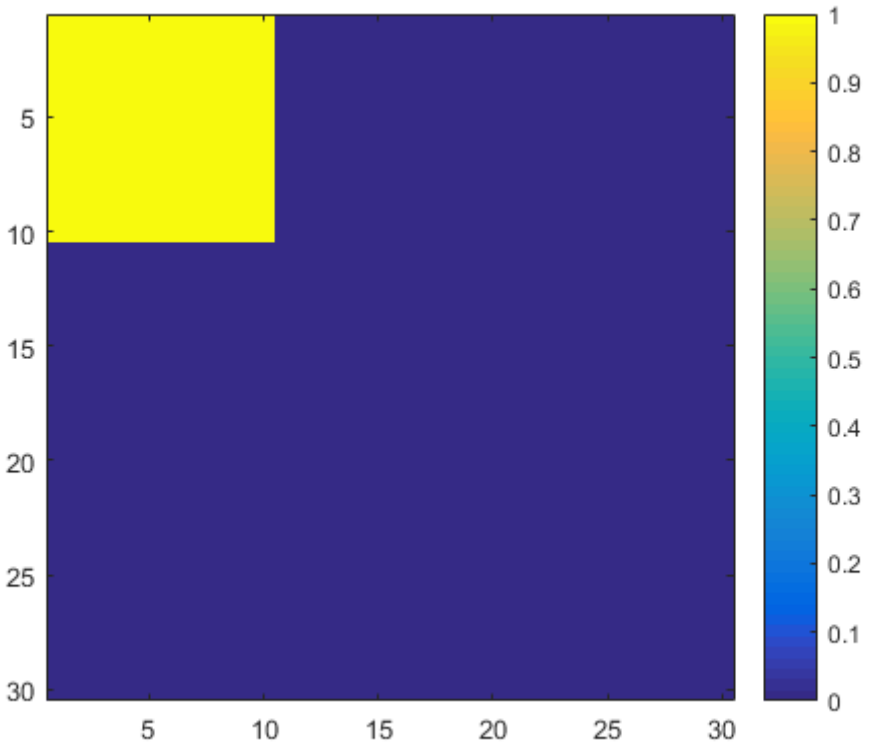

Figure 1: Initial conditions for our PFM. The rectangular region represents $\phi = 1$ and elsewhere $\phi = 0$.

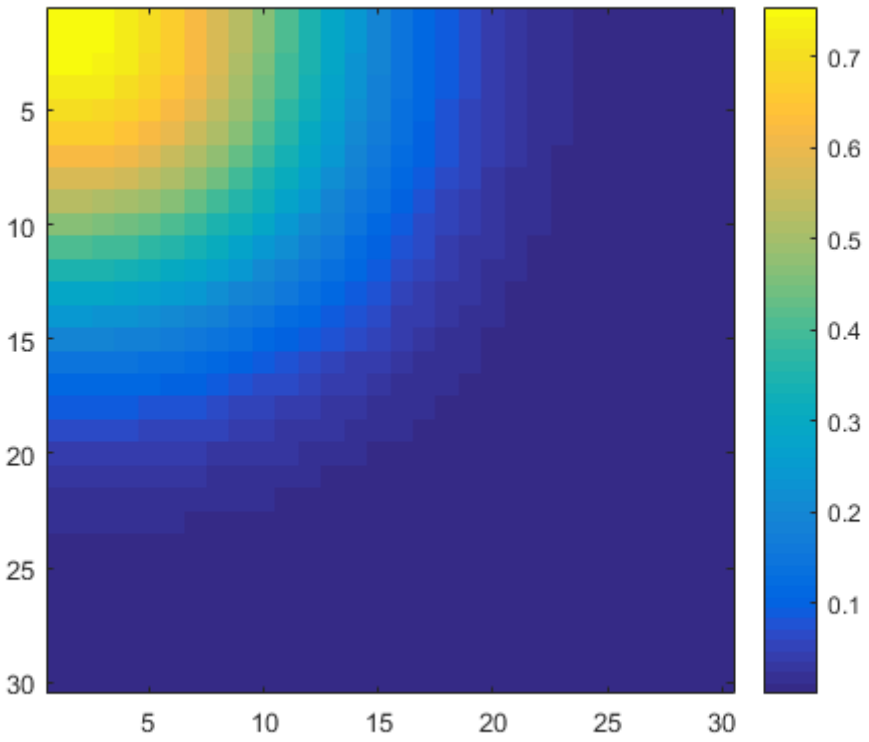

Figure 2: Neumann boundary conditions for our PFM without $g(\phi)$.

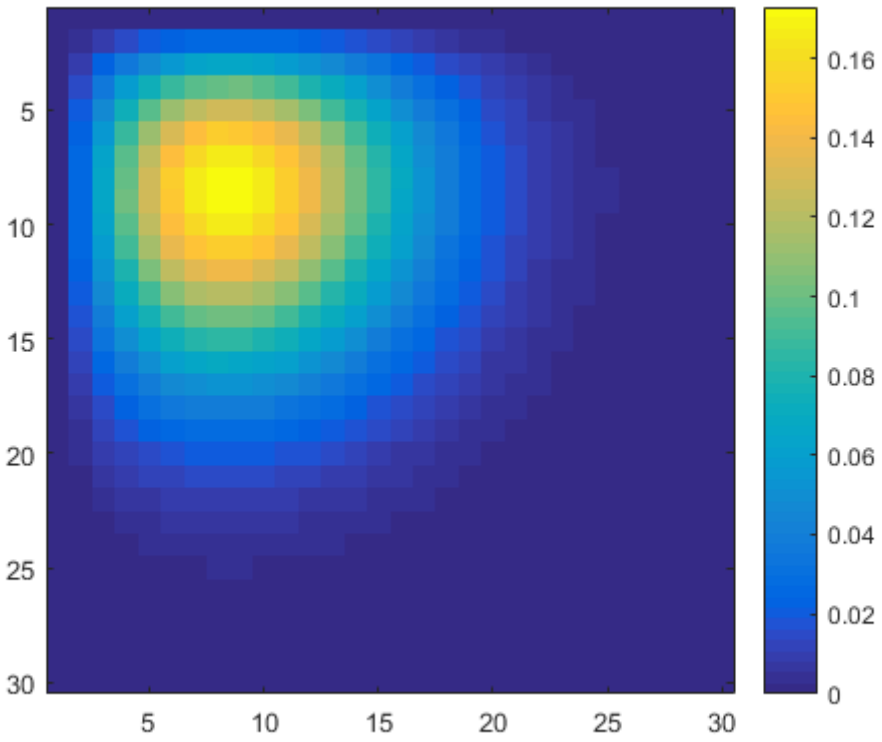

Figure 3: Dirichlet boundary conditions for our PFM without $g(\phi)$.

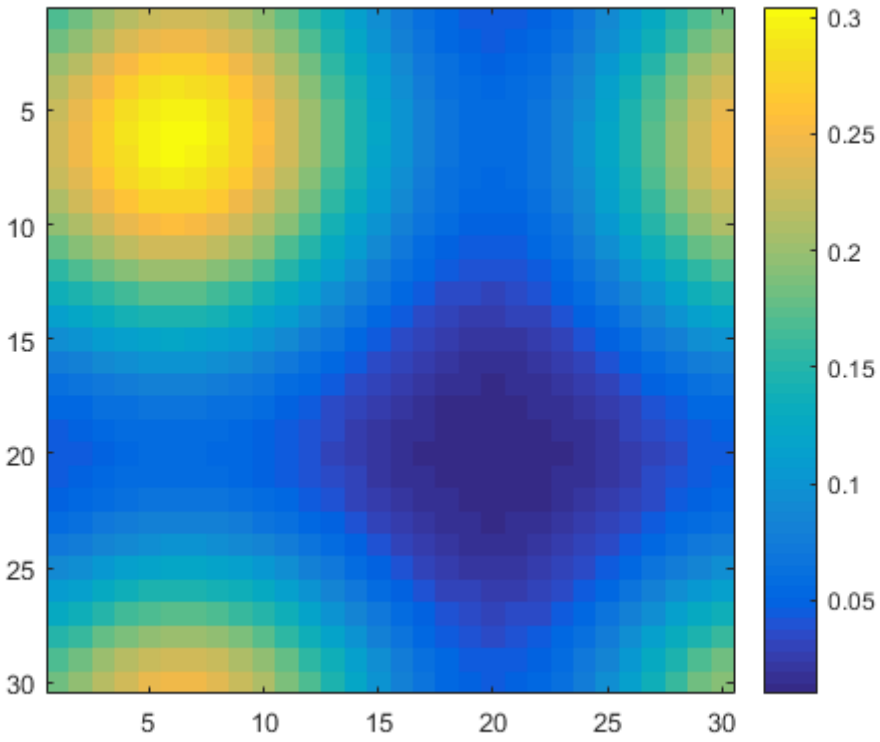

Figure 4: Periodic boundary conditions for our PFM without $g(\phi)$.

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