Multi-Component Phase Field Modeling in Python

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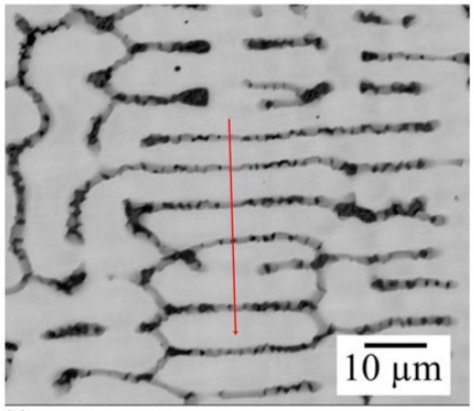
Overview

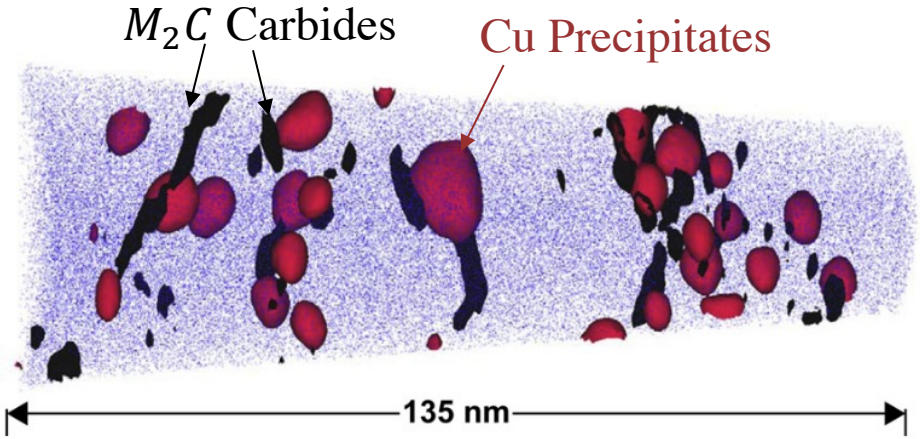
- Motivation
- Phase Field Modeling Equations
- Numerical Methods
- Examples
- Future Work

Motivation

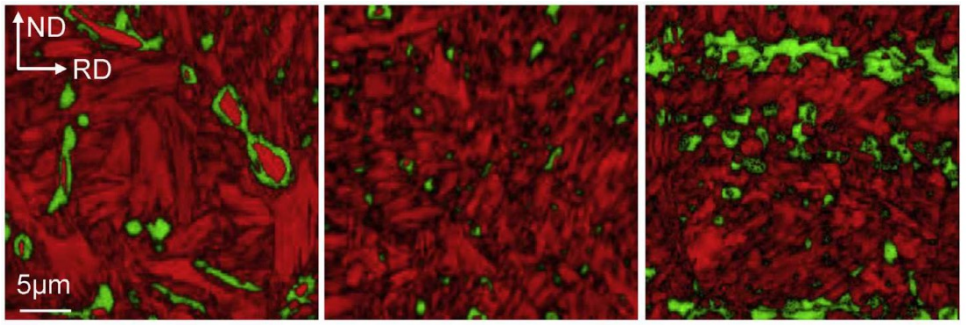
- Steels & other materials derive their properties from their microstructural features
- Phase fraction & morphology both influence the final properties



Zhang 2017



Mulholland 2012

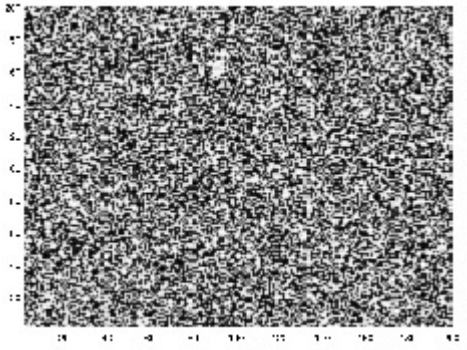


bcc, $M_{23}C_6$ / fcc

Belde 2016

Phase Field Equations

- Conserved parameters (i.e. concentrations) follow the Cahn-Hilliard (1958) Equation
  - Originally developed to explain spinodal decomposition (uphill diffusion)



Wikipedia

Concentration

Free Energy

$$\frac{\partial c_i}{\partial t} = M_i \nabla^2 \left[\frac{dF}{dc_i} - \varepsilon \nabla^2 c_i \right]$$

Mobilities

Gradient Coefficients

$$F(\boldsymbol{c}) = \frac{\boldsymbol{c}^2 \cdot \boldsymbol{I}(1-\boldsymbol{c})^2}{p} + \Sigma_{i<j} \beta_{ij} c_i c_j$$

# of Components

Interaction Coefficients

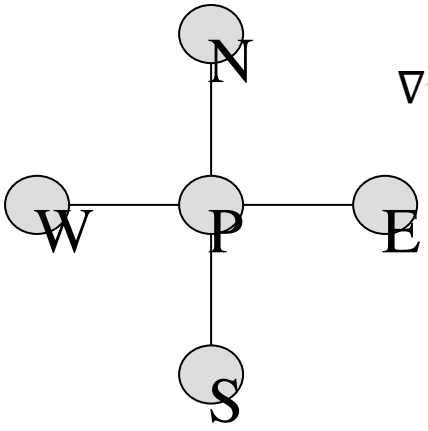
$$\frac{dF}{dc_i} = \frac{1}{p}\left[2c_i(1-c_i)^2 - 2c_i^2(1-c_i)c_i\right] + \Sigma_{j \neq i} \beta_{ij} c_j$$

Numerical Methods - Explicit

- Cahn-Hilliard:

$$\frac{\partial c_i}{\partial t} = M_i \nabla^2 \left[\frac{dF}{dc_i} - \varepsilon \nabla^2 c_i \right]$$

- Solved in 2D w/ periodic boundary conditions
- Laplace operator (∇^2) was implemented as a 5 point FD stencil



$$\nabla^2 c = \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \qquad \nabla^2 c \approx (c_N + c_S + c_W + c_E - 4c_p)/\Delta h^2$$

$$c_i^{n+1} = c_i^n + \Delta t M_i \nabla^2 \left[\left(\frac{dF}{dc_i} \right)^n - \varepsilon \nabla^2 c_i^n \right]$$

Numerical Methods - Spectral

- $\{\cdot\}$ represents fourier transform
- $\left\{\frac{\partial^n u}{\partial x^n}\right\} = (ik)^n\{u\}$
- Can be used to derive a semi-implicit scheme where the non-linear terms are explicit (avoiding a non-linear solve)
- Solution is stable with large Δt, but error still grows

$$\left\{\frac{\partial c_i}{\partial t}\right\} = \left\{\nabla^2 M_i \left[\frac{dF}{dc_i} - \varepsilon\nabla^2 c_i\right]\right\}$$

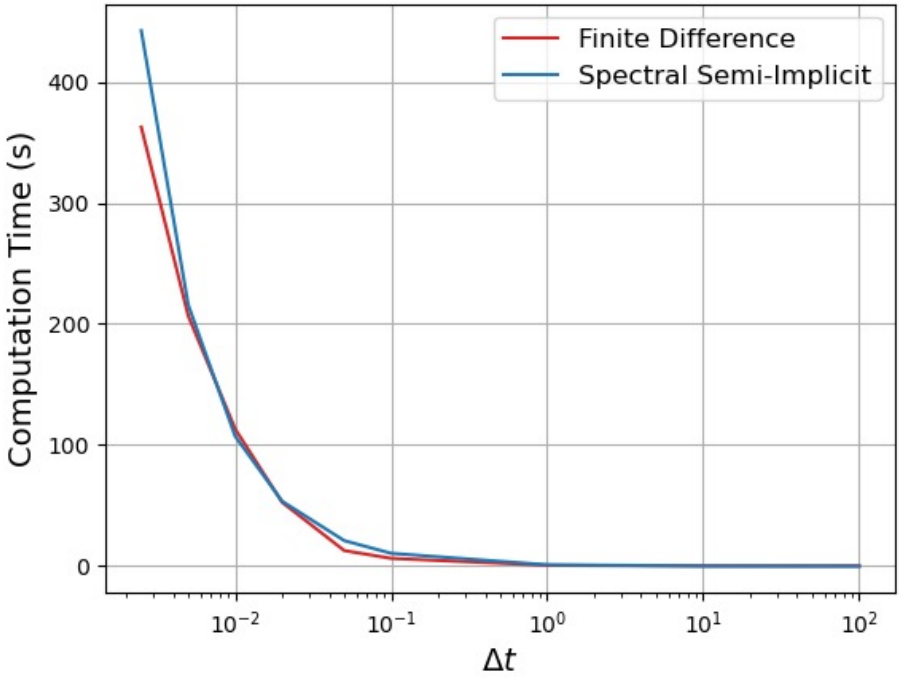
$$\left\{\frac{\partial c_i}{\partial t}\right\} = -k^2 M_i \left(\left\{\frac{dF}{dc_i}\right\} + \varepsilon k^2\{c_i\}\right)$$

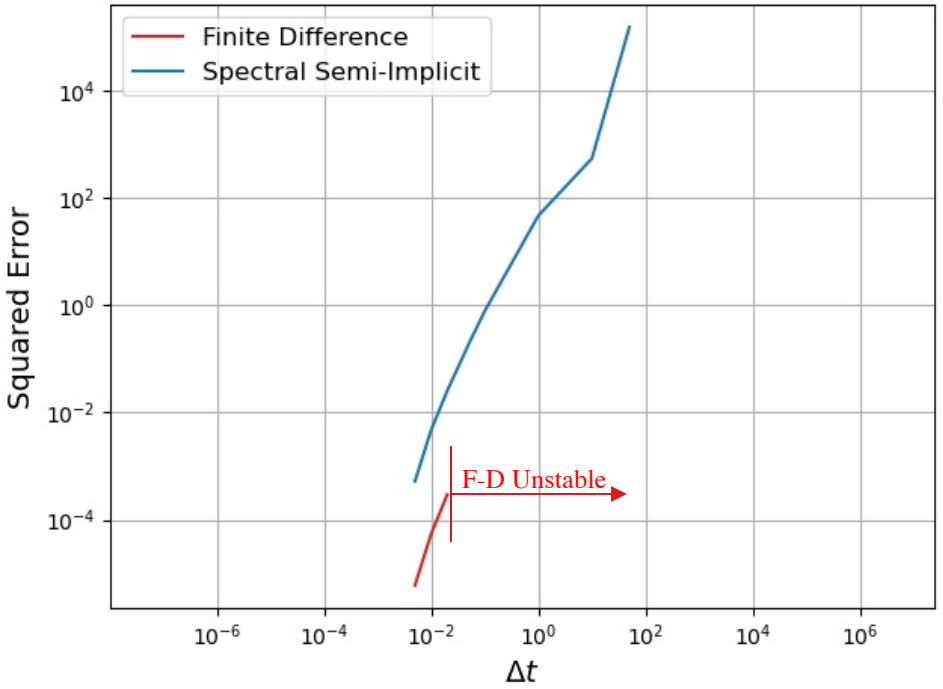
$$\{c_i^{n+1}\} - \{c_i^n\} = \Delta t M_i \left(-k^2\left(\left\{\frac{dF}{dc_i}\right\}\right)^n - \varepsilon k^4\{c_i^{n+1}\}\right)$$

$$\{c_i^{n+1}\} = \frac{\{c_i^n\} - \Delta t M_i k^2\left\{\left(\frac{dF}{dc_i}\right)^n\right\}}{1 + \Delta t M_i \varepsilon k^4}$$

Numerical Methods - Comparison

$ue = c_{final}(\Delta t = 0.0025)$





- Computation Times were similar

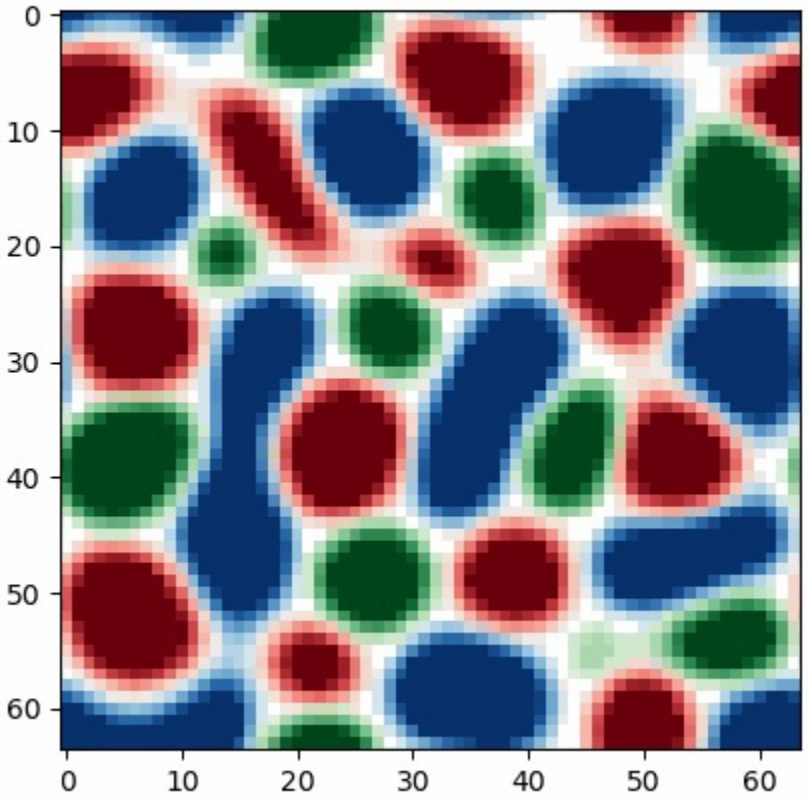
- Convergence $O(\Delta t^2)$
- FD unstable for $\Delta t > 0.025$ for $\Delta x = 1$

Examples

- Various combinations of initial concentrations, gradient and interaction coefficients were tested
- Finite Difference w/$\Delta t = 0.01$ was used

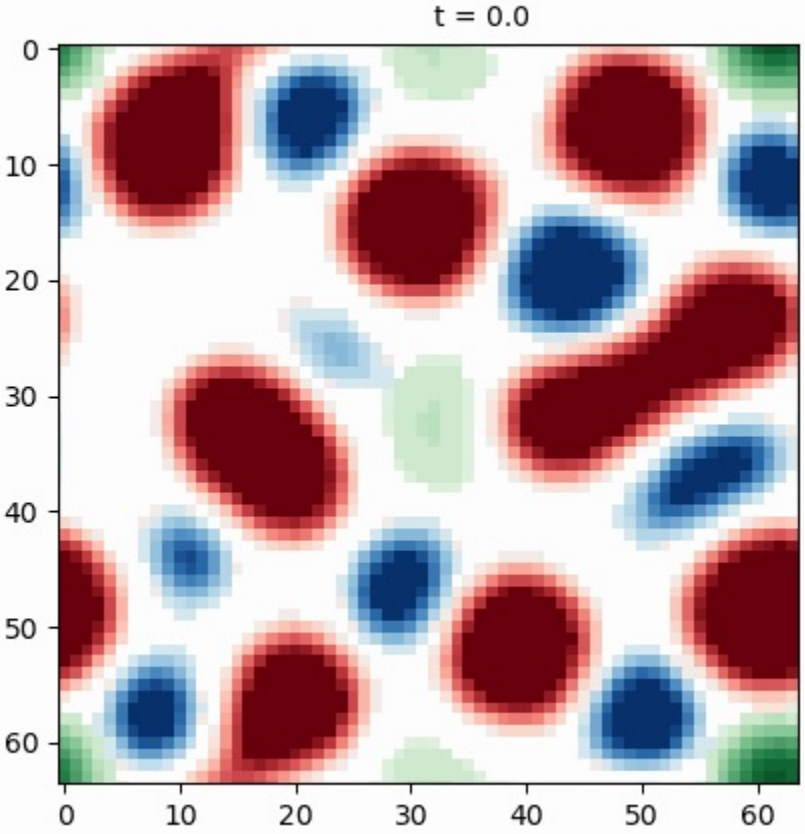
Examples

$$c_0 = [0.3,0.2,0.1], M = [1,1,1], \varepsilon = [1,1,1], \beta_{ij} = \begin{bmatrix} 0.3 & 0.3 & 0.3 \\ 0.3 & 0.3 & 0.3 \\ 0.3 & 0.3 & 0.3 \end{bmatrix}$$



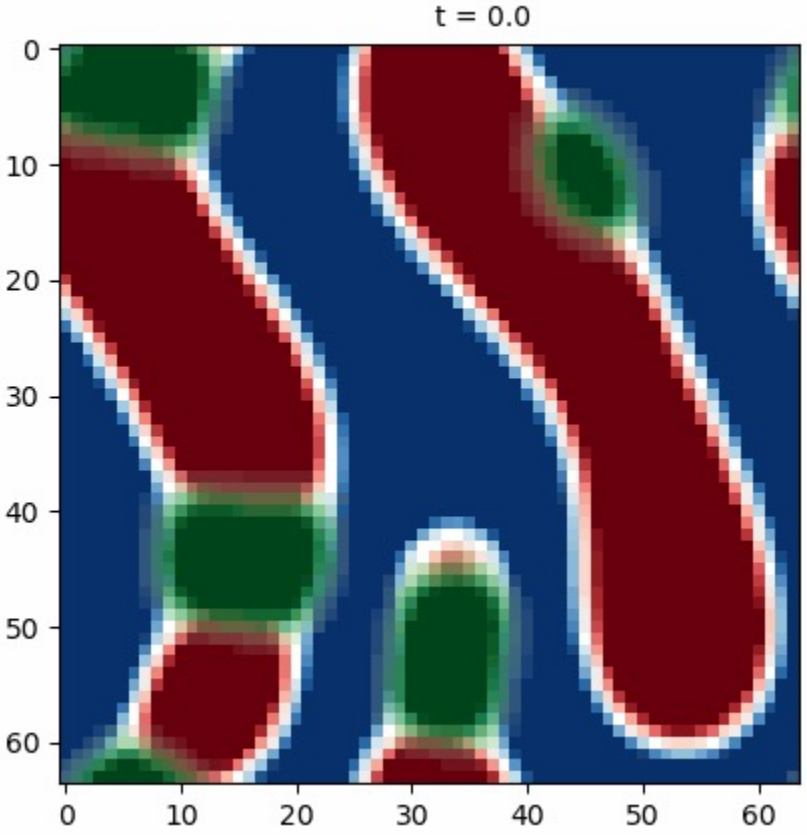
Examples

$$c_0 = [0.1,0.3,0.05], M = [0.5,1,2], \varepsilon = [1,1,3], \beta_{ij} = \begin{bmatrix} 0.3 & 0.3 & 0.3 \\ 0.3 & 0.3 & 0.3 \\ 0.3 & 0.3 & 0.3 \end{bmatrix}$$



Examples

$$c_0 = [0.3,0.2,0.1], M = [1,1,1], \varepsilon = [1,1,1], \beta_{ij} = \begin{bmatrix} 0.3 & 0.6 & 0.3 \\ 0.6 & 0.3 & 0.3 \\ 0.3 & 0.3 & 0.3 \end{bmatrix}$$



Future Work

- Connect my phase-field code to ThermoCalc Mobility and Energy database to start simulating real materials
- Investigate non-linear solvers in case large time steps are desired
- Add in Allen-Cahn equation for non-conserved parameters (i.e. crystallography)
- More parameter studies

Thank You!

References

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Additional Slides

Numerical Methods - Spectral