

Simple PFC Model

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Model A

Model A systems are systems where the order parameter is not conserved, a common example is the Ising model of a spin system. Throughout the evolution of the system the total number of "up" spins does not need to stay constant. This system can be modelled by the following equations:

$$\phi^{n+1}(i, j) = \phi^n(i, j) + \frac{\Delta \bar{t}}{\Delta \bar{x}^2} \bar{\Delta}^2 \phi^n + 1(i, j) - \Delta \bar{t} \frac{\partial f(\phi^n(i, j))}{\partial \phi}$$

with $\bar{\Delta}^2$ is the discrete Laplacian which may be given by

$$\bar{\Delta}^2 \phi^n(i, j) = \phi^n(i+1, j) + \phi^n(i-1, j) + \phi^n(i, j+1) + \phi^n(i, j-1) - 4\phi^n(i, j)$$

although there are other ways to represent the discrete Laplacian that in some cases may be better suited. Used periodic boundary conditions. The free energy functional may be expressed as a function with two minima, $f(\phi^n(i, j)) = a_1 + \frac{a_2}{2}(\phi^n(i, j))^2 + \frac{a_4}{4}(\phi^n(i, j))^4$ which has the following first order derivative

$$\frac{\partial f(\phi^n(i, j))}{\partial \phi} = a_2(\phi^n(i, j)) + a_4(\phi^n(i, j))^3$$

Notes on variables:

- $i, j = 0..N$ are indices for the ϕ array which represents the phase field of the system.
- N is the size of the array, here the system is assumed to have the same size in x and y directions.
- $n = 0..T$ is the time index of the system.
- T is the final time of the array.
- $\bar{t} = nM\Delta t$, M is the diffusion coefficient
- $\bar{x} = n\frac{\Delta x}{W_o}$, W_o is the interface width (?)
- $\Delta \bar{t} < \frac{1}{4}\Delta \bar{x}$, euler time marching algorithm stability restriction in 2D