

# Modelling and Visualizing the Cahn-Hilliard-Cook Equation

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## Introduction

The Cahn-Hilliard-Cook equation[1] was developed to describe the phase separation of two fluids or atomic species in an alloy. This equation is non-linear and thus can only be solved as a numerical simulation. Using the Runge-Kutta integration method and finite-difference representations of the Laplace operator this equation can be discretised in terms of both time and space. The equation has been simulated and visualised in 1, 2 and 3 dimensions. Using this simulation technique in conjunction with various visualisation methods we can study the system's spatial structure as it evolves in time.

"Cahn-Hilliard-Cook theory is essentially a mean-field approximation to the time-dependent Ginzburg-Landau equation for the free energy of a binary system." [2]

$$\frac{\partial \phi(\mathbf{r}, t)}{\partial t} = m \nabla^2 \left( \frac{\partial f(\phi(\mathbf{r}, t))}{\partial \phi} \Big|_T - K \nabla^2 \phi(\mathbf{r}, t) \right) + \zeta(\mathbf{r}, t) \quad (1)$$

It is possible to discretise this field by representing continuous space with a number of discrete cells. Each cell in the simulation represents a spatial area containing varying concentrations of each fluid or atoms. The concentration is in the range  $[-1, 1]$  where  $-1$  represents a cell containing only "B-type atoms" and  $1$  represents a cell containing only "A-type atoms". Using the appropriate Laplace operator we can find a formula for the instantaneous change in concentration of each cell and using the Runge-Kutta 4th order integrator we can find the change in concentration over a discrete time-step. In order to apply these methods we can approximate the term  $\frac{\partial f(\phi(\mathbf{r}, t))}{\partial \phi} \Big|_T$  with a polynomial, giving the equation:

$$\frac{\delta \phi}{\delta t} = m \nabla^2 (-b\phi + u\phi - K \nabla^2 \phi) + \zeta(\mathbf{r}, t) \quad (2)$$

### 1-Dimension

A 1-dimension discrete simulation of the Cahn-Hilliard-Cook equation can be thought of as string or line of individual cells, each cell interacting with the cells either side of it. The Laplace operator  $\nabla^2$  we apply to the equation for 1-dimension is  $(+1 -2 +1)$ , thus the general form of the equation becomes:

$$P_j^{(n)} = \frac{M_j}{\Delta x^2} (-b\phi_{j-1}^{(n)} + 2b\phi_j^{(n)} - b\phi_{j+1}^{(n)} + u\phi_{j-1}^{(n)3} - 2u\phi_j^{(n)3} + u\phi_{j+1}^{(n)3}) + \frac{1}{\Delta x^2} [-K\phi_{j-2}^{(n)} + 4K\phi_{j-1}^{(n)} - 6K\phi_j^{(n)} + 4K\phi_{j+1}^{(n)} - K\phi_{j+2}^{(n)}] + \zeta_j^{(n)} \quad (3)$$

This equation can be used to calculate the change in field concentration of each cell for each step. The Runge-Kutta method is used to perform the time integration.

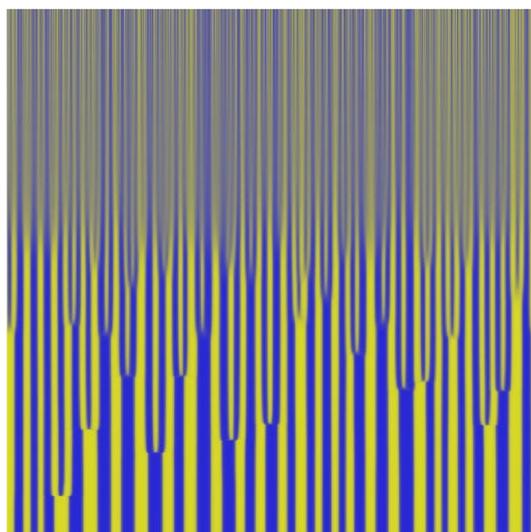


Figure 1: Logarithmic time 1-Dimension CHC simulation

Figure 1 shows the time evolution of a 1-dimensional system with space ( $X$ ) horizontally and time ( $t$ ) shown vertically. The random thermal mixture separates out into groups of similar components.

Considering the random simulated annealing term  $\zeta(\mathbf{r}, t)$  the field simulation should converge to two domains. It can be easily seen that the 1-Dimensional simulation can get stuck with multiple domains and timescale well beyond the stability of the simulation would be required for it to converge. In 2D and 3D however we can easily see that due to the extra dimensions, they converge into two domains significantly faster.

### 2-Dimensions

The 2-dimensional CHC simulation can be thought of as a square mesh of cells each interacting with its nearest-neighbours. In 1-dimension the Laplace operator  $\nabla^2$  is just represented as  $(+1 -2 +1)$  as shown in equation 3, whereas in 2-dimensions we the finite-difference weights:

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

By applying this centred-difference operator to the CHC equation we can get a formula for the change in concentration for any cell in a 2-dimensional simulation. The same time integration methods as the 1-dimensional simulation are used for the 2-dimensional version. Using this simulation we can create a video of the 2-dimensional simulation running over time. Some stills are shown below:

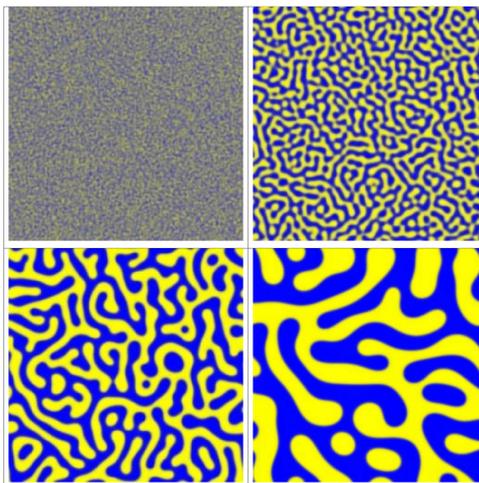


Figure 2: 2-Dimensional CHC simulation at  $t = 0$  (top left),  $t = 100$  (top right),  $t = 1000$  (lower left) and  $t = 10000$  (lower right)

The domain coarsening structures and domain formation behaviour is apparent in 1-, 2- and 3-dimensions.

A number of macroscopic properties of the CHC system can be measured to characterise system bulk behaviour. Domains can be counted using a graph labelling technique and [3] averaging over multiple sample random starting conditions and different temporal trajectories we can obtain a meaningful fit to the number of domains  $N_D(t)$  as it varies with time. Figure 4 shows the number of distinct domains in different dimensional systems plotted against time. As can be seen from the log-log plots the system is quite well approximated by a power law in time  $N_D \approx t^d$ , where  $d \equiv 2$  is the critical dimension.

### 3-Dimensions

The 3-dimensional CHC Simulation can be most easily thought of as a large cube made up of smaller cubes where each small cube represents a single cell. Each cell will now interact with its neighbours in all 3-dimensions. To get the equation for the change in concentration of each 3-dimension cell we apply the 3-dimensional Laplace operator to the CHC equation, the laplace operator in 3-dimensions is:

$$\begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & -6 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

As a 3-dimensional cube cannot be visualised easily using simple 2-dimensional methods, JOGL [4] was used to render the cube using transparent spheres to allow the values of concentration field values within the cube to be seen.

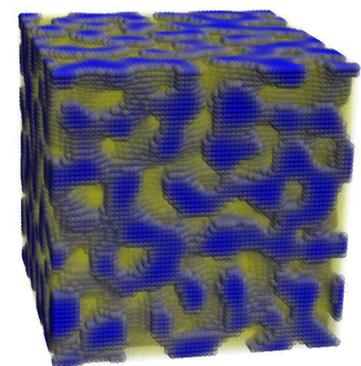


Figure 3: 3D CHC Simulation

Figure 3 shows the visualisation of a 3-dimensional CHC simulation represented as a coloured cube at different time steps.

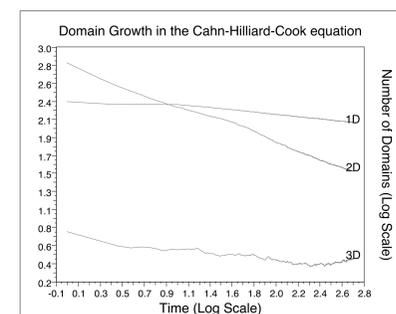


Figure 4: CHC domains

## Conclusions

We have presented results from some numerical experiments on the Cahn-Hilliard-Cook equation and investigated the relative merits of different integration algorithms. While it is possible to use an adaptive step size method for time integration we find the fixed-step size fourth-order Runge-Kutta algorithm entirely adequate and indeed more useful for studying regular time spaced samples. Graphics libraries such as JOGL[4] provide a manageable interface to an interactive simulation system and we have been able to study interactively the early stages of the three dimensional system for relatively interesting mesh resolutions. Further details are given in Technical Note CSTN-049[5] - see [www.massey.ac.nz/kahawick/cstn/049](http://www.massey.ac.nz/kahawick/cstn/049).

## References

- [1] J.W.Cahn and J.E.Hilliard, "Free energy of a non-uniform system III. Nucleation in a two point compressible fluid," *J.Chem.Phys.*, vol. 31, pp. 688-699, 1959.
- [2] K. A. Hawick, *Domain Growth in Alloys*. PhD thesis, Edinburgh University, March 1991.
- [3] M. Sonka, V. Hlavac, and R. Boyle, *Image Processing, Analysis and Machine Vision*, ch. 6, pp. 232-234. PWS Publishing, Pacific Grove, 2 ed., 1999.
- [4] "Jogl." Available from <https://jogl.dev.java.net/>, January 2008.
- [5] K. Hawick and D. Playne, "Modelling and visualising the cahn-hilliard-cook equation," tech. rep., Computer Science, Massey University, 2008. CSTN-049.