ENGN 2912B – Course Project Rundown

In the paper, the authors have simulated a ternary compound (having 3 components namely A,B and C) which undergoes 'Spinodal Decomposition'. Spinodal Decomposition happens to be a type of phase evolution where a mixed system happens to be unstable thermodynamically at the temperature of interest (which is governed by the parameter X (actually Psi in greek).

In such a case, typically the rich become richer and the poor becomes poorer in a sense that from the mixed alloy if there is a slight perturbation in composition, the elements of same type cluster together (note that such a behavior is not very commonplace, where in general systems tend to get more random in stead of clustering among like atoms). The authors have modeled the free energy based on the Cahn-Hilliard equation and then have minimized it which resulted into the evolution equations. These time dependent evolution equations are then solved at each time to see how the 'phase separation/phase evolution' occurs.

By minimizing the free energy functional (cahn hilliard), we get PDE's in time. Since the intention is to model bulk properties, the boundary condition used is periodic boundary condition (which is that if we discretized the system into grid points starting from 0 to n in each direction, then the value at grid point -1 is the same as the value as grid point n). This allowed them to use Fourier Transforms (since the functions are now periodic).

On using semi-implicit finite difference method on the equation, we can convert the PDE's into a set of ODE's for each timestep that are to be solved. Now the advantage of using fourier transform is that we can easily calculate the differential in real space by taking the variables in reciprocal space (by fourier transforming it), solving the set of equation in the reciprocal space and then inverse fourier transforming them in real space. The values of the composition of each element in each time step can then be recorded and plotted. For this particular paper, they have also played with the interfacial energy parameter to observe it's effect on the morphology of the phases as they evolve with time.

This paper has certain key elements which we believe match the criteria of a typical project expected in this course. It involves math libraries such as random number generator, complex numbers, fourier transforms and solving simultaneous linear equations. Also, he results can be visualized using a visualization tool such as gnuplot. Now this paper has shown phase evolution in 2D which we plan to extend to 3D. Also we plan to parallelize the process.