Assignment01: Modeling and simulation methods in materials science (MT218)

September 11, 2014

1 Numerical methods

- Using the taylor series expansion work out an fourth order accurate in space operator for $\frac{\partial^2}{\partial x^2}$.
- Utilizing this solve the simple diffusion equation in an *explicit manner*: $\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$
- How many boundary points would you require in this discretization?
- Compare the solutions as functions of time with discretization used in class that was second order accurate in space.
- Write down the system of equations that you would require to solve in a *implicit* discretization.
- Solve the system of equations using a Jacobi/Gauss-siedel methods
- Again compare the solutions against those obtained with the explicit/implicit discretizations which are second order accurate.
- Can you think of a scheme of discretization which is second order accurate in space and time? Will the memory usage of this scheme be higher/lower compared to a simple Euler scheme?

2 Cahn-Hilliard equation

- In the example discussed in class, can you work out the evolution for the different sinusoidal modes as a function of time. Do all modes grow similarly?
- Construct a different symmetric function and work out the equilibrium profiles both numerically and analytically and compare them as was performed in the class? What is the least order of the function that would give you phase separation?
- In the equations discussed in class, if the mobility (M) were a function of composition, how would you modify the discretization?

- Using this impose variable mobilities in the phases(different compositions) and see how the evolution of the compositions change with respect to equal mobilities

- Add a temperature dependent term $(T - T_M)$*f(c), to the free-energy $c^2\left(1-c^2\right)$ in order to tilt the wells energetically. Does a linear function $f(c)$ modify the equilibrium points at all? Construct higher order functions which perform this tilting function.

- How do you find the equilibrium compositions of the two phases at a given temperature?

- If you were to initialize the compositions of the phases corresponding to $T-T_M=0$, and then change the temperature to lower and higher values, what happens with respect to the motion of the interface?

- Is there a limit, beyond which the system becomes unstable to phase separation? Numerically evaluate this limit. Can you compute it also analytically?

- Perform simulations at different temperatures in the stable regime (no phase separation)

- Can you device a scheme for measuring the velocities at the interface?

- Plot the variation of the velocities for different values of the temperature.

- Try an extension of the formulation to two dimensions. Impose perturbations on the system and see whether you get some interesting looking patterns.

- If you were to extend the formulation to having three components how many additional equations will you need to solve. Can you hypothetically think of extending the formulation of $c^2\left(1-c^2\right)$ to $c_A^2\left(1-c_A^2\right)+c_B^2\left(1-c_B^2\right)+c_C^2\left(1-c_C^2\right)$, A,B,C being the components. Plot the function and make a decision.