Term 2 Summary

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During this term we have studied the Phase Field Crystal (PFC) model proposed in [EKHG02]. To connect with our previous work and provide a physical motivation of our model we initially studied a derivation of PFC from the canonical form of density functional theory following the ideas of [EPBSG07]. The motivation for studying PFC theory is that the functional is relatively simple and it is hoped that it will be numerically tractable.

We created a Matlab program that generates a hexagonal lattice using the equations of PFC. The method used in this code follows the techniques of [EW12] using a convex-concave splitting technique to ensure stability and solving in Fourier space and Fourier transforming to greatly increase the speed of calculation. We are currently working on adapting our code to create a hexagonal lattice within a constant density field, which represents a liquid, in the hope this will simulate a phase interface. We also anticipate using our program to create a defect within the lattice and studying the evolution of the system.

References

[EW12] M. Elsey, B. Wirth A simple and efficient scheme for phase field crystal simulation, pre-print, (2012).

[EKHG02] K.R. Elder, M. Katakowski,M. Haataja, M. Grant Modeling Elasticity in Crystal Growth, Physical Review Letters 88 :24, 235701, (2002).

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