**Assignment – PHASETREE**

**Task to develop and model the phase filed simulation capabilities with given paper.**

I have solved the Cahn-Hillard PF model presented in the paper as follows:

A black and white image of a circle with a triangle and a triangle

AI-generated content may be incorrect.

I have implemented the computational model for different free energy expressions from the paper in the Opensource gihub page PRISMS-PF v2.4.0

The model implementation and the updated code can be found in ***application/phaseTreeAssg*** folder.

The code structure is as follows:

1. main C++ code to run is equations.cc
2. ICs\_and\_BCs.cc is used to define the initial spinodal decomposition of the phase to start with
3. Postprocess.cc is used to postprocess the output for visualization of any variable
4. Finally, the “customPDE.h” is the definition file of all the variables used or initiate in any of the code above.
5. parameters.prm is used to define the parameter of the model such as M, K, c -range, domain size, iteration time, steps and the material parameters.

To execute the code, do the following

1. $ cmake .
2. $ make -j <num of available processor>
3. $ mpirun -n <num of available processor> main

This is start running and provide the results file in solutions-iteraions-number.vtu. This is visualized in paraview.

Initially, the implementation was not converging with material parameters of the paper stiffness matrix components. Therefore, the execute the same model equation of the paper I have used an isotropic elastic material with material parameters given in parameters.prm

However, the model equation is same as the reference paper.

**Additional:**

MATLAB code is written to calculate the stiffness matrix components to populate into the equations.cc and postprocess.cc

The results output from time (0, 1000, 5000, 10000 > clockwise) are as follows:

A screenshot of a computer

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Presently, there are some assumptions of ordered parameters orientation, and the stress-free transformation strain are sued to model the Allen-Cahn dynamics together with Cahn-Hilliard dynamics. I haven’t got much time to remove those model parts but, in a week, I will be able to do that.

However, presently, I have used mobility term corresponding to the order parameter n1, n2 and n3 set to zero.

**DISCLAIMER**

*It is worth noting that while executing the cmake and make -j <nprocs> in the main phase-field folder after git clone, It is very much necessary to install and update Install CMake, p4est, and deal.II (version 9.6.0 or above required).*

*I had a lot of trouble to install deal.II and make work with ninja due to my computer does not have right amount of swap memory in WSL ubuntu. I spent almost 2-3 days to make things clear then work on the PRISMS-PF modules.*

*#### These are few tips to make things work while installing deal.II*

*rm -rf build/*

*mkdir build*

*cd build*

*cmake -DDEAL\_II\_DIR=/path/to/dealii ..*

*make -j$(nproc)*

*#### You can increase swap size temporarily (example for 8GB swap):*

*sudo dd if=/dev/zero of=/swapfile bs=1M count=8192*

*sudo mkswap /swapfile*

*sudo swapon /swapfile*