Connecting Phase Field modeling to Dislocation Dynamics

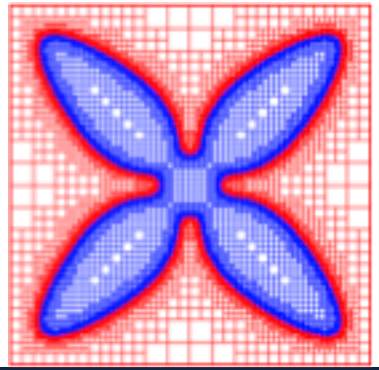
Feb 19

Chaoming Yang, Liang Qi

Phase Field to Dislocation Dynamics

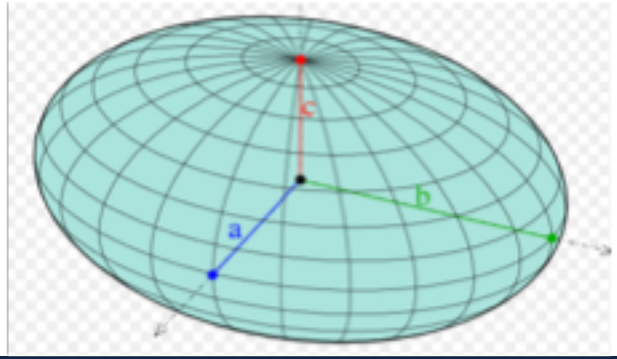
PRISM Phase field packages
Output data in **vtk** format. They are **Discretized data.**

For example:
At 200 x 200 mesh points
Point (10, 15) has value 0.7 => it's in precipitates
Point (3, 15) has value 0.0 => it's in matrix



Dislocation Dynamics (Paradis) treat precipitate in **geometry** due to calculation requirements

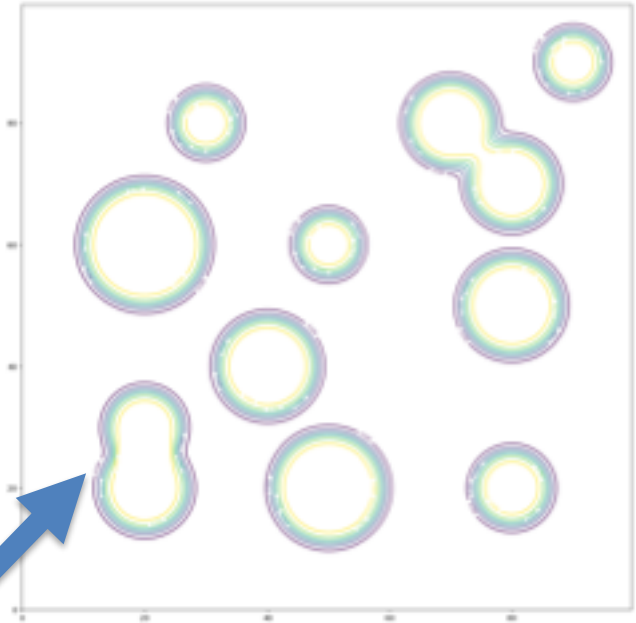
Each single precipice is treated as an ellipsoid
⇒ Center position (x, y, z)
⇒ Radius (a, b, c)
⇒ Rotation angles (matrix)



Phase Field to Dislocation Dynamics (PF2DD)

We make a simple package, **PF2DD,** that converts the data generated by Phase Field to the data required by Paradis.

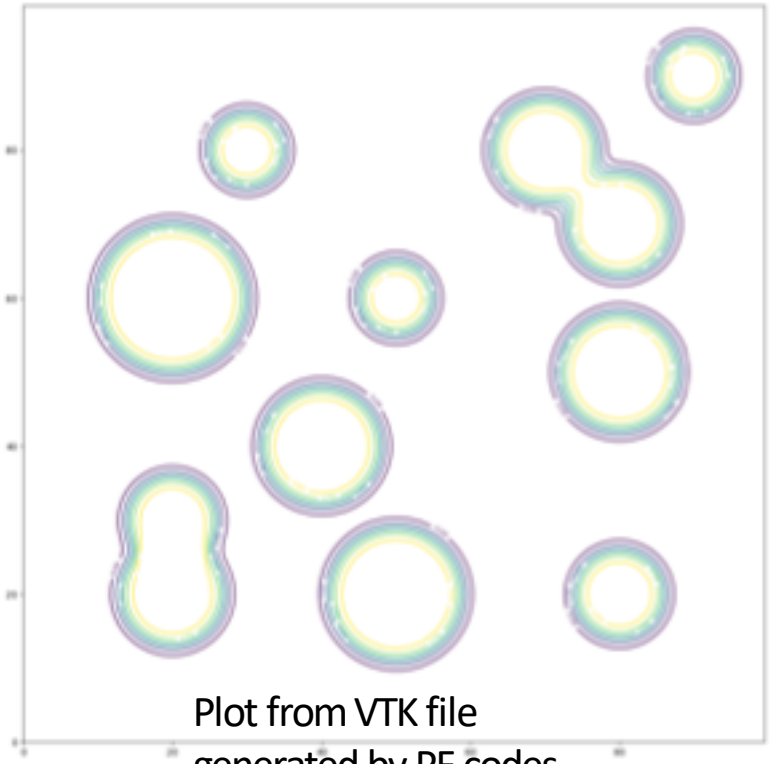
- First applies **Breath first search (BFS)** to find where is the "**precipitate group**", which may contain one or more single precipitate (in C++)
- Apply **genetic algorithm** to find the geometry of precipitates inside the "precipitate group" (in C++)
- Collect the geometry info of precipitates to plot and prepare inputs of Paradis (in Python)



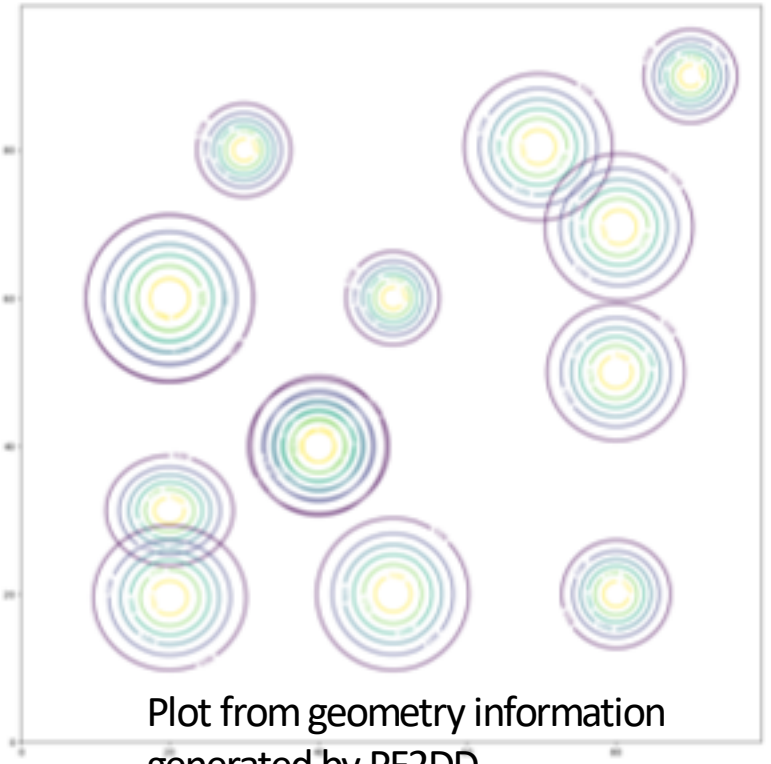
We need to use geometry to describe cases like this

A 2D phase field example data (from Stephen)

PF2DD Example (Plots)

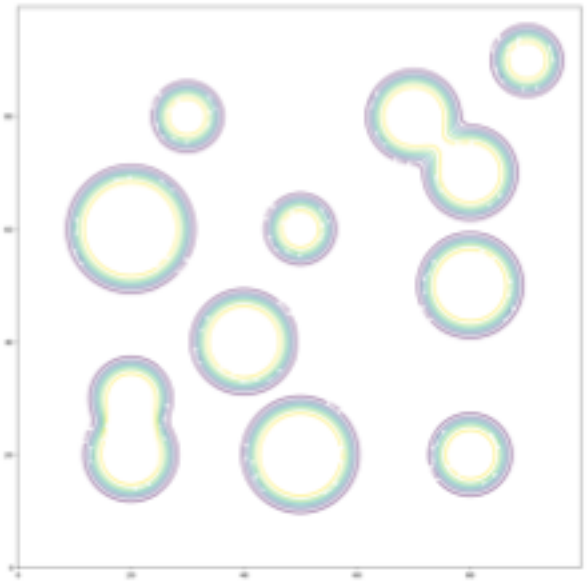


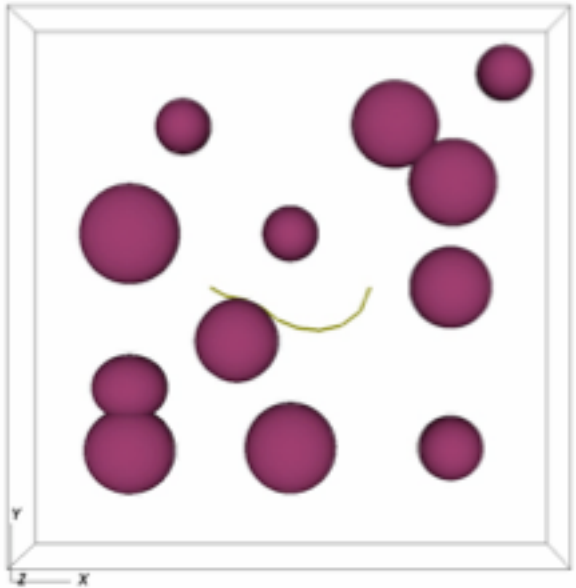
Plot from VTK file
generated by PF codes



Plot from geometry information
generated by PF2DD

PF2DD Example (DD simulations)





It passes 2D test cases, will be testted for 3D.

It's on GitHub: **https://github.com/chaomy/PF2DD**