A demo of computing phase diagrams

Wei Si, Kai Jiang

School of Mathematics and Computational Science, Hunan Key Laboratory for Computation and Simulation in Science and Engineering, Xiangtan University, Xiangtan, Hunan, China, 411105.

Abstract

We use the Landau-Brazovskii (LB) model as an example to show the performance of our code in computing phase diagrams.

1. Landau-Brazovskii (LB) model

We consider the LB model with the following form

$$E[\phi] = \frac{1}{2}\int \left[(\Delta + 1)\phi(\mathbf{r})\right]^2 d\mathbf{r} + \int \left\{\frac{\tau}{2}\phi(\mathbf{r})^2 - \frac{\gamma}{3!}\phi(\mathbf{r})^3 + \frac{1}{4!}\phi(\mathbf{r})^4\right\} d\mathbf{r}. \tag{1}$$

2. Iteration method

In this code, we adopt the adaptive accelerated Bregman proximal gradient (AA-BPG) methods. More detail can be found in "Jiang, Si, Chen, and Bao, Efficient Numerical Methods for Computing the Stationary States of Phase Field Crystal Models, SIAM Journal on Scientific Computing, 2020, 42, B1350-B1377".

3. Demo

*Corresponding author. Email: kaijiang@xtu.edu.cn

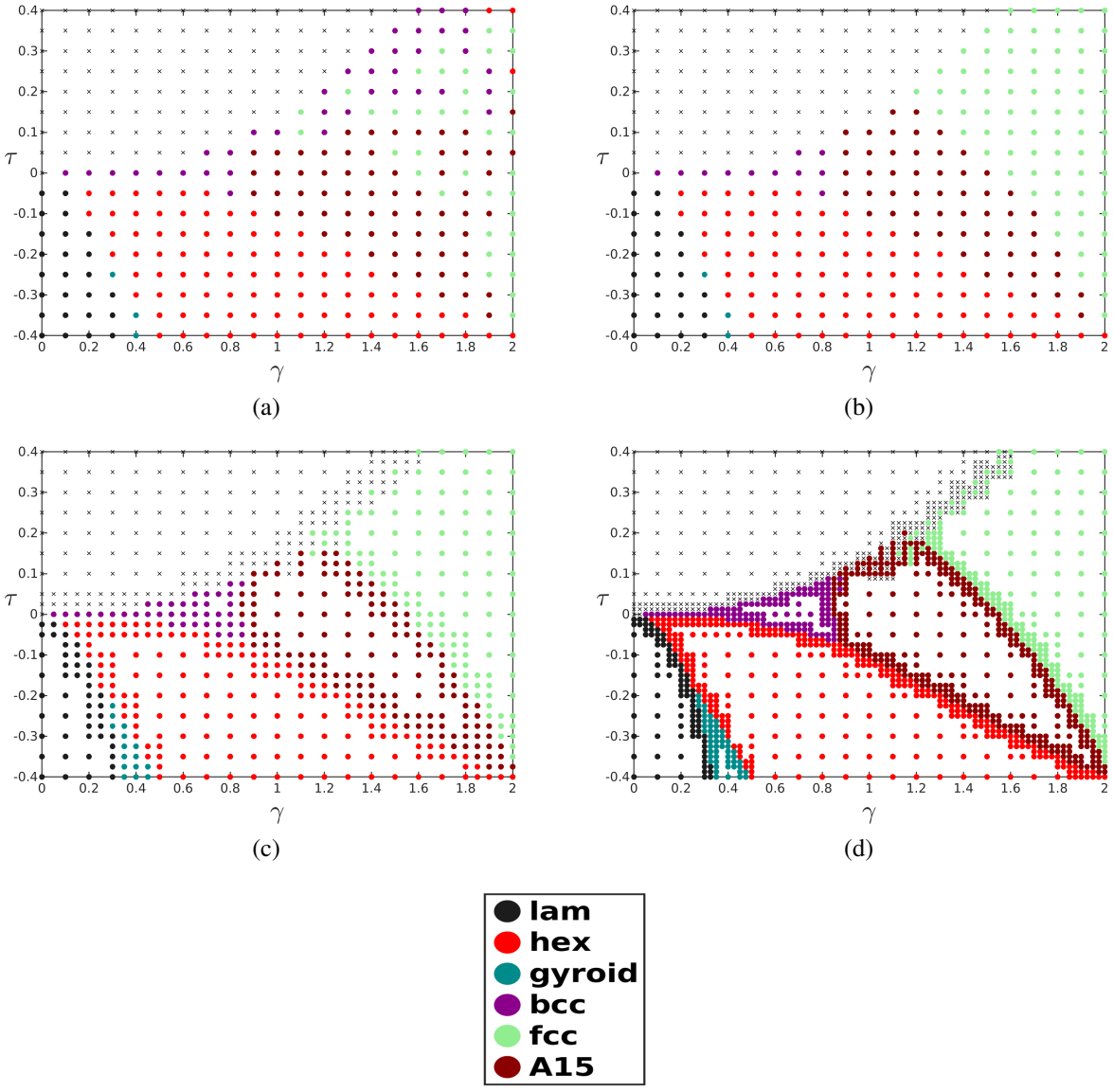

Figure 1: (a) the phase diagrams with our given initial values; (b) the phase diagrams using the adjacent convergent solutions as the initial values; (c) the phase diagrams after refining the diagram grid; (d) the phase diagrams after refining the diagram grid based on (c).