

Interactive Volume Rendering of Block Copolymers Defect Formation and Evolution

S. Zhang, D. Porter, J. McDonald, J. Viñals

University of Minnesota

Supercomputing Institute

Nov 16-22, SC13, Denver, CO, USA



Background information

- Challenges in understanding pattern dynamics of block copolymers melts
 - Complicated 3D self-organization process
 - Defects even more complicated
 - Scientifically, not well understood
 - Computationally expensive
 - Graphically, tempo-spatial characterization
- Objective: to develop computing framework for characterizing defects of block copolymers
- Approaches
 - Heterogeneous computing
 - Interactive visualization
 - Characterization of defects

Oscillatory frame of reference

Shearing frame (x y z) related to the normal orthogonal coordinates (x_n y_n z_n) by

$$x = x_n - a(t)z_n$$

$$y = y_n$$

$$z = z_n$$

with $a(t) = \gamma \sin(\omega t)$ being the model's position in the x direction, γ the largest distance away from the initial position and ω the oscillation frequency.

Dimensionless governing equations

$$\frac{\partial \psi}{\partial t} + \mathbf{V} \cdot \nabla \psi = \varepsilon \psi - (\nabla^2 + q_0^2) \psi - \psi^3 = -\mu \quad (1)$$

$$\nabla \cdot \mathbf{V} = 0 \quad (2)$$

$$\mathbf{0} = -\nabla P - \zeta \psi \nabla \mu + \nabla \cdot \boldsymbol{\sigma} \quad (3)$$

$$\boldsymbol{\sigma} = \frac{1}{2} [\nabla \mathbf{V} + (\nabla \mathbf{V})^T] \quad (4)$$

with

$$\nabla = \left[(1 + a^2) \frac{\partial}{\partial x} - a \frac{\partial}{\partial z} \right] \mathbf{x} + \frac{\partial}{\partial y} \mathbf{y} + \left(-a \frac{\partial}{\partial x} + \frac{\partial}{\partial z} \right) \mathbf{z}$$

$$\nabla^2 = (1 + a^2) \frac{\partial^2}{\partial x^2} - 2a \frac{\partial^2}{\partial x \partial z} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$\mathbf{V}(x, y, z, t)$ - velocity vector, $\psi(x, y, z, t)$ the order parameter field
 $P(x, y, z, t)$ the pressure field, ε , q_0 and ζ being bifurcation number,
characteristic wave number and “capillary” number respectively.

Characterization of Defects

Defects – singularities of scalar order parameter field ψ

Two approaches for characterizing the defects

$$MFP(t) = \|\nabla\psi \times \nabla(\Delta\psi)\|^2 \quad (5)$$

$$GP2P2(t) = \psi^2 + \frac{1}{k_l^2} \|\nabla\psi\|^2 \quad (6)$$

ψ is computed on the CPUs whereas MFP and $GP2P2$ are computed and visualized on the GPUs using Matlab, HVR and Amira.

Model description

Simulations:

Case 1: no shear - $\gamma = 0$

Case 2: oscillatory shearing - $\gamma = 0.2$

Other parameters:

$\zeta = 10$, $\varepsilon = 0.2$,

Time increment is 0.035

Shearing frequency of $t=2$ (once every 58 time steps)

Maximal shear velocity 0.022.

Initial condition:

Small 3D uniformly-random perturbations on ψ

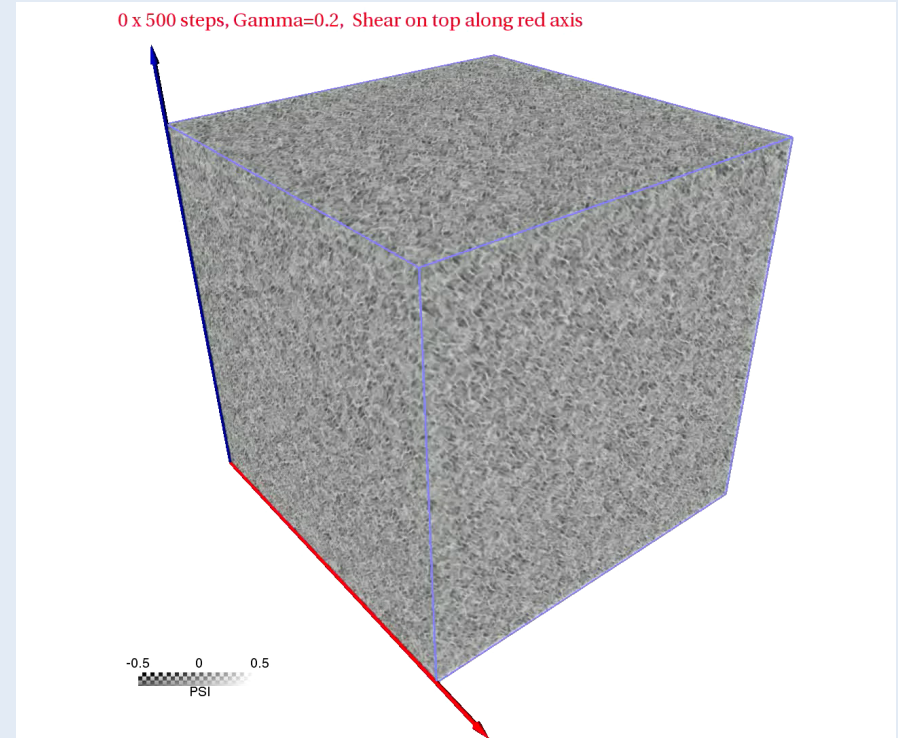
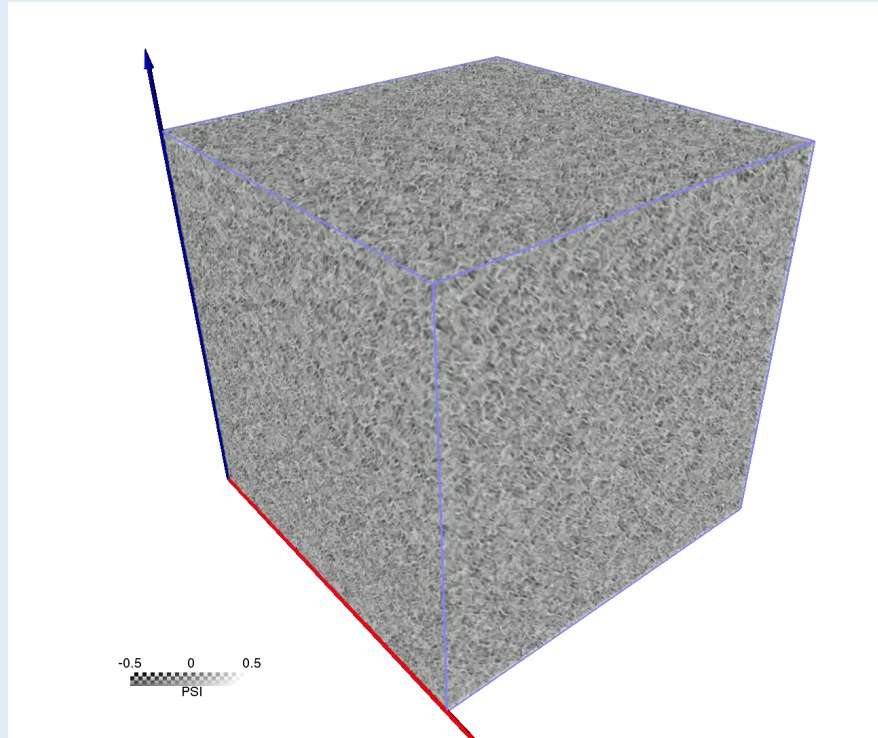
Resolution: 256x256x256 grids

Purpose: to show some characteristics of unknown defects

3D self-organization of order parameter field ψ

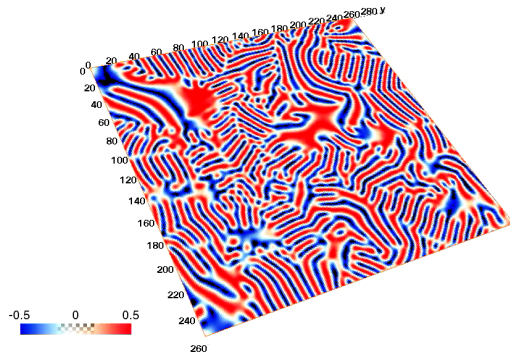
$\gamma=0$

$\gamma=0.2$

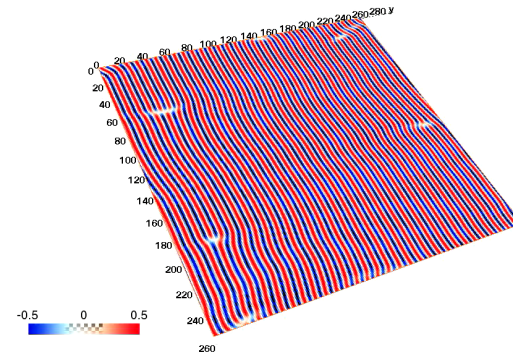


Singularities in order parameter field ψ at a fixed time

Gamma=0, 50001 time steps

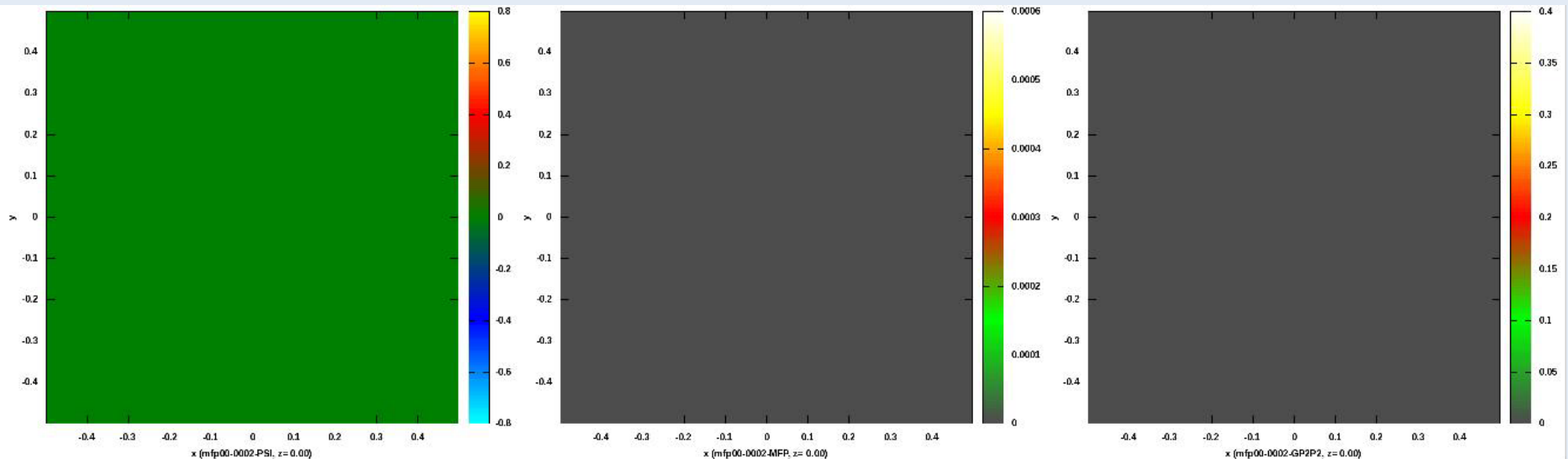


Gamma=0.2, 50001 time steps



How to localize the 3D singularities? How are they evolving in the order parameter field?

Characterization of defects ($\gamma=0.2$)

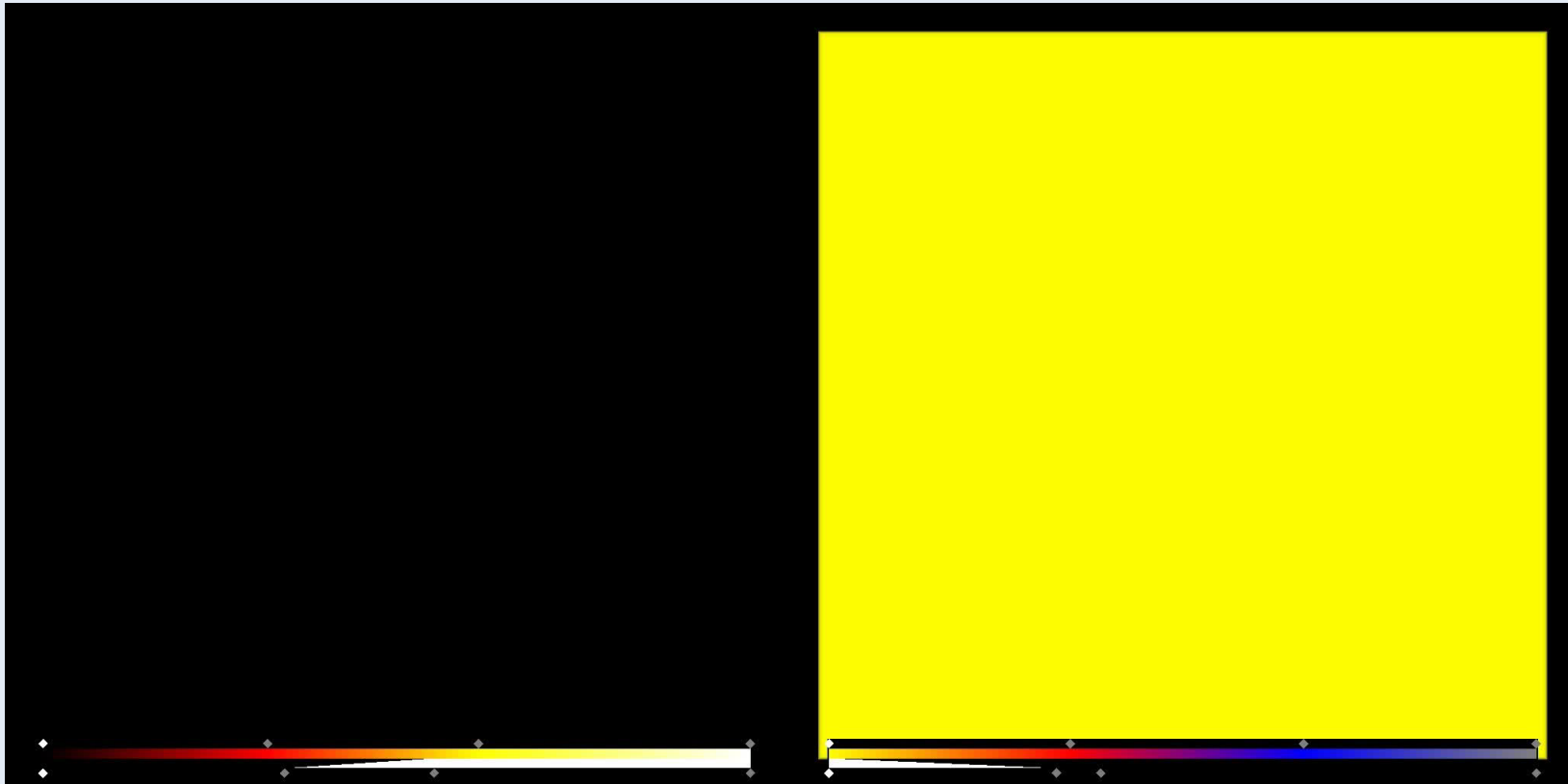


Defect localized by MFP (middle), P2DP2(right) for the order parameter field (the left) as a function of time showing the usefulness of both approaches

Volume rendering of defects ($\gamma=0.2$)

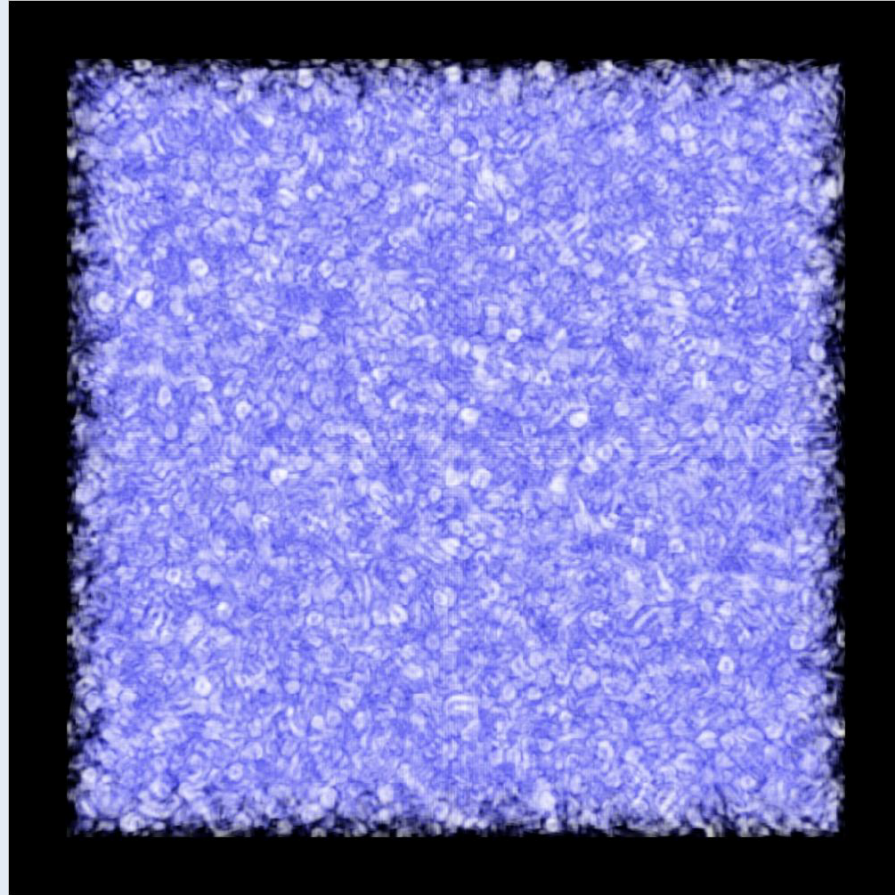
MFP

P2DP2



Volume rendering of defects ($\gamma=0$)

P2DP2



Discussion and Conclusions

- **A success in heterogeneous computing**
- **Interactive visualization**
 - important to capture complicated transient structures
 - helpful to quickly explore parameter space of interest
- **Roughly uniform patterns over sufficiently large scale have been generated in the model.**
- **Two methods are derived for characterizing the “defects”.**
- **Both are capable of identifying their spatial locations.**
- **Same morphological characteristics of 1st order structures.**
- **Differences in the high-order features requires a further improvement in characterizing the defects.**