Title: Dynamical simulation of disordered micelles in a diblock copolymer melt with fluctuations

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Abstract: By including composition fluctuations in our dynamical simulation of the time-dependent Landau-Brazovskii model for a diblock copolymer melt we find that disordered micelles form above the order-disorder transition to a BCC phase. At high-temperatures the micelle number density and volume fraction are effectively zero and the melt is disordered at the molecular level. As we lower the temperature the micelle number density increases gradually and approaches the number density in the BCC phase. If we increase the strength of the fluctuations the temperature range over which disordered micelles exist broadens and the onset of BCC order is suppressed. By tracking trajectories we also investigate the dynamical behaviour of individual micelles in an environment of disordered micelles We find diffusive behaviour which we investigate as a function of temperature and micelle volume fraction.

# Dynamical Simulation of Disordered Micelles in a Diblock Copolymer Melt with Fluctuations

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Fondation canadienne pour l'innovation

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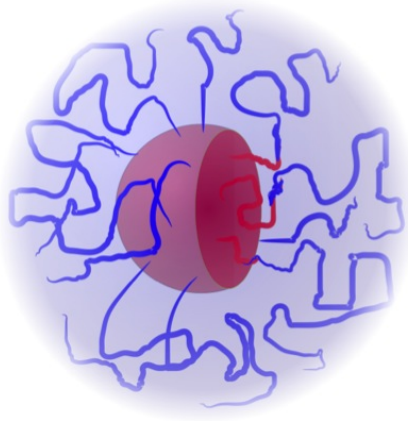
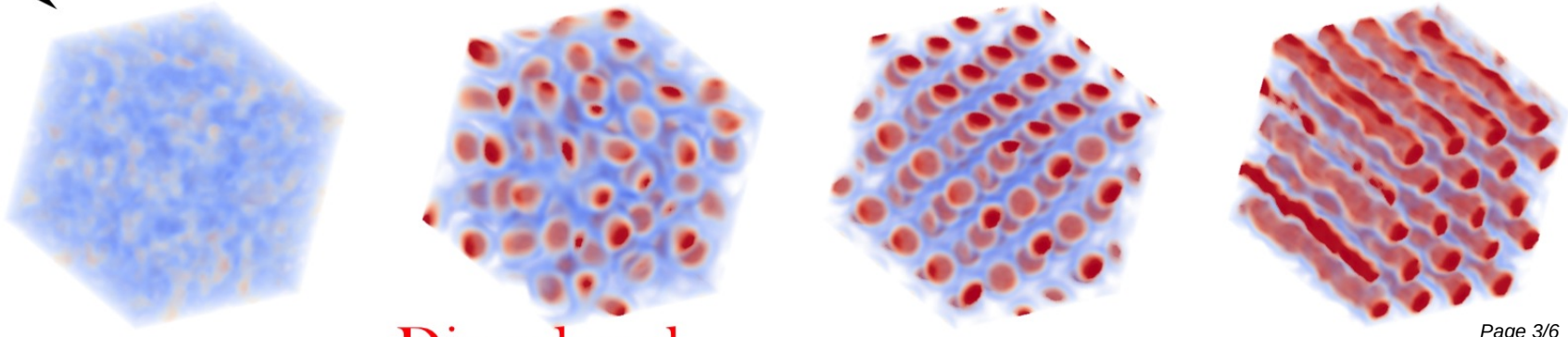
# Order-Disorder Transition with Disordered Micelles



- Do we see disordered micelles in simulations?
- How do disordered micelles join the disordered phase?
- How do disordered micelles behave dynamically?
- We study disordered micelles using the time-dependent Landau-Brazovskii model

$$\frac{\partial \phi}{\partial t} = \nabla^2 \left[ \xi^2 (\nabla^2 + 1)^2 \phi + \tau \phi - \frac{\gamma}{2} \phi^2 + \frac{1}{3!} \phi^3 \right] + \eta(\vec{r}, t)$$

Temperature



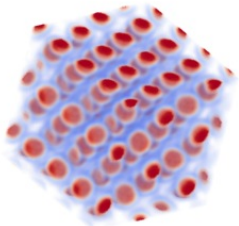
DIS

Disordered Micelles (DM)

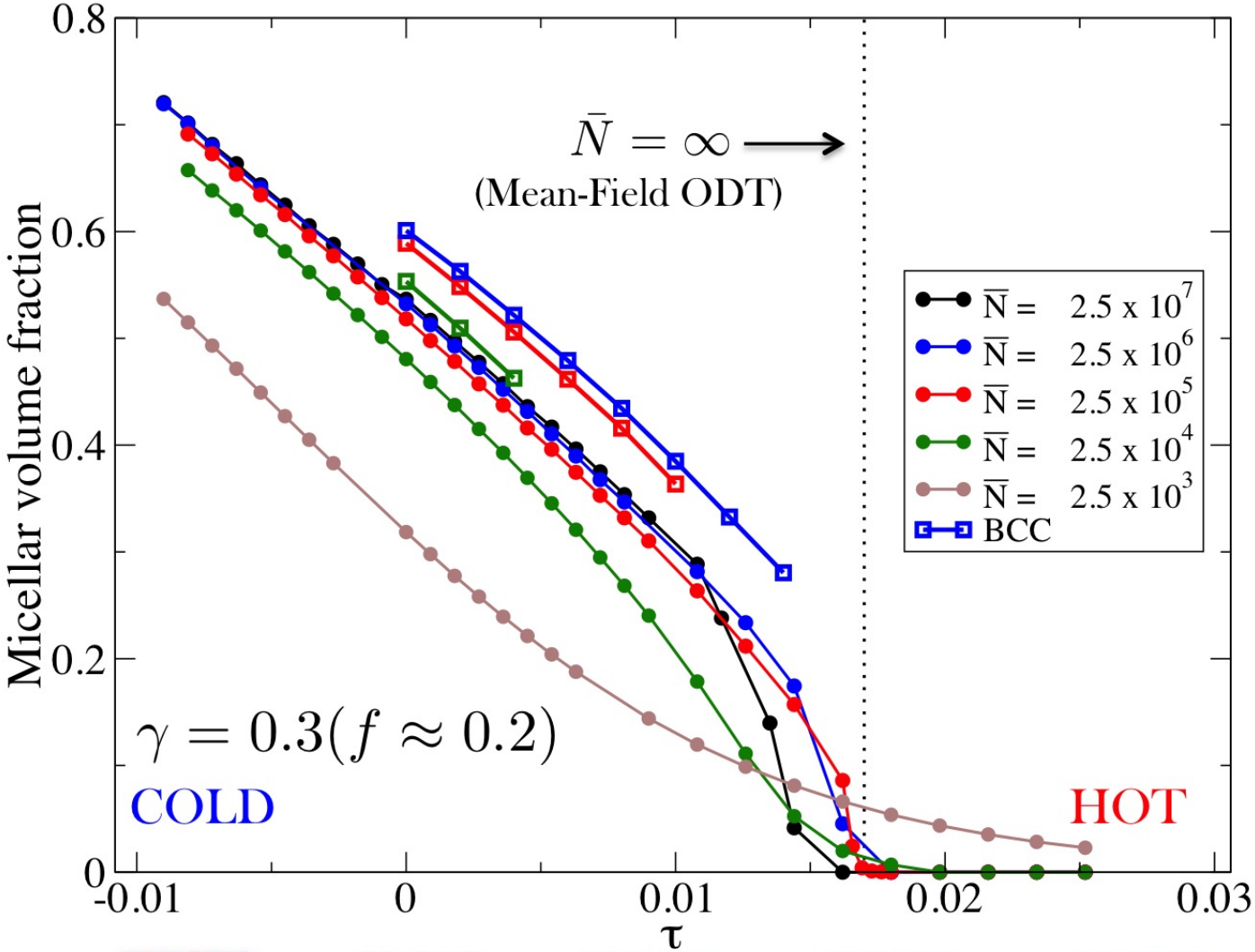
BCC

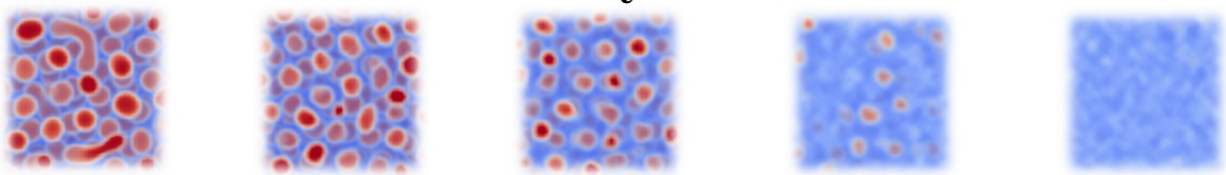
HEX

# Temperature-dependence of Micelle Volume Fraction

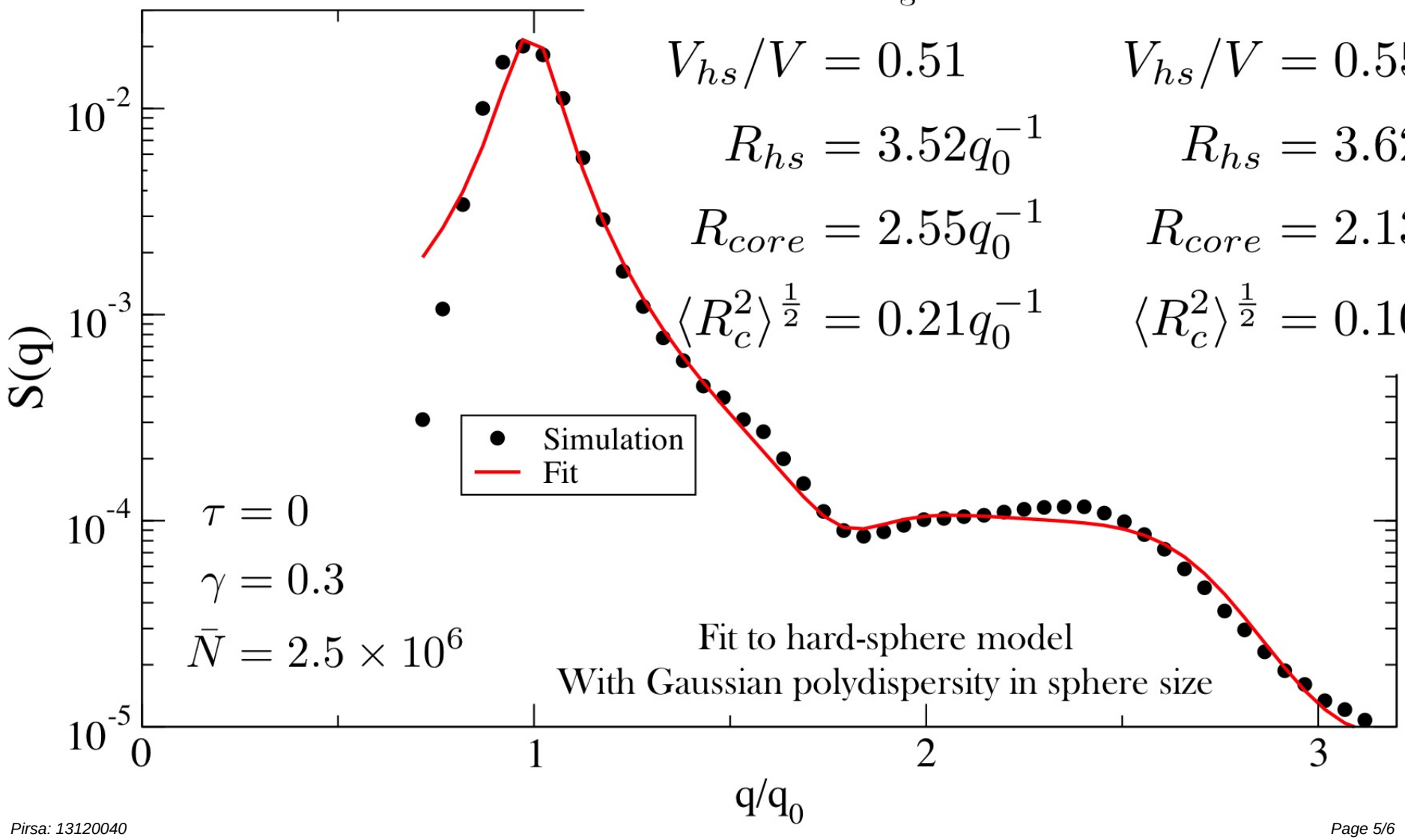


BCC



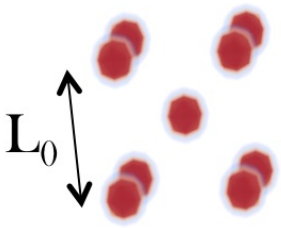
# Structural Properties from Simulated Scattering Function






Consistent micelle description found by indirect and direct methods

# Dynamics of Disordered Micelles

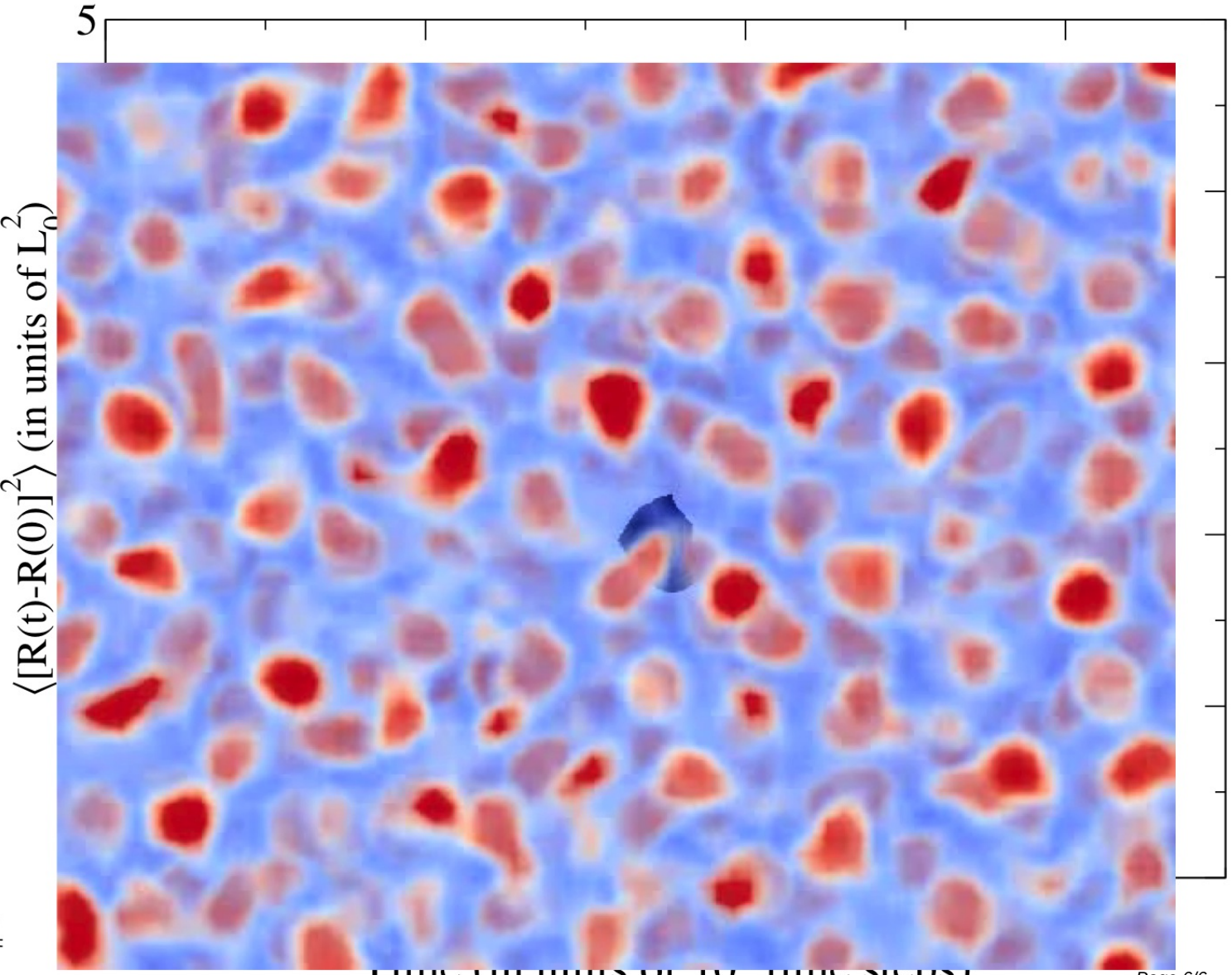



Particle tracking:
Crocker-Grier
(1996) 5000
frames
(2012)

$\gamma = 0.3$

$(f \approx 0.2)$

$\bar{N} = 2.5 \times 10^4$




$\langle [R(t) - R(0)]^2 \rangle$ is linear in time suggesting diffusion of micelles $= 0.009$