Super-Resolution Simulations: Reconstructing Atomic Details in Polymer Models

Scientific Achievement

A CINT User Team developed a "super-resolution" AI framework that reconstructs high-fidelity polymer structures from low-fidelity simulations. By compressing complex chain conformations into a shared "latent space," this work overcomes the historical trade-off between computational speed and atomic-scale detail.

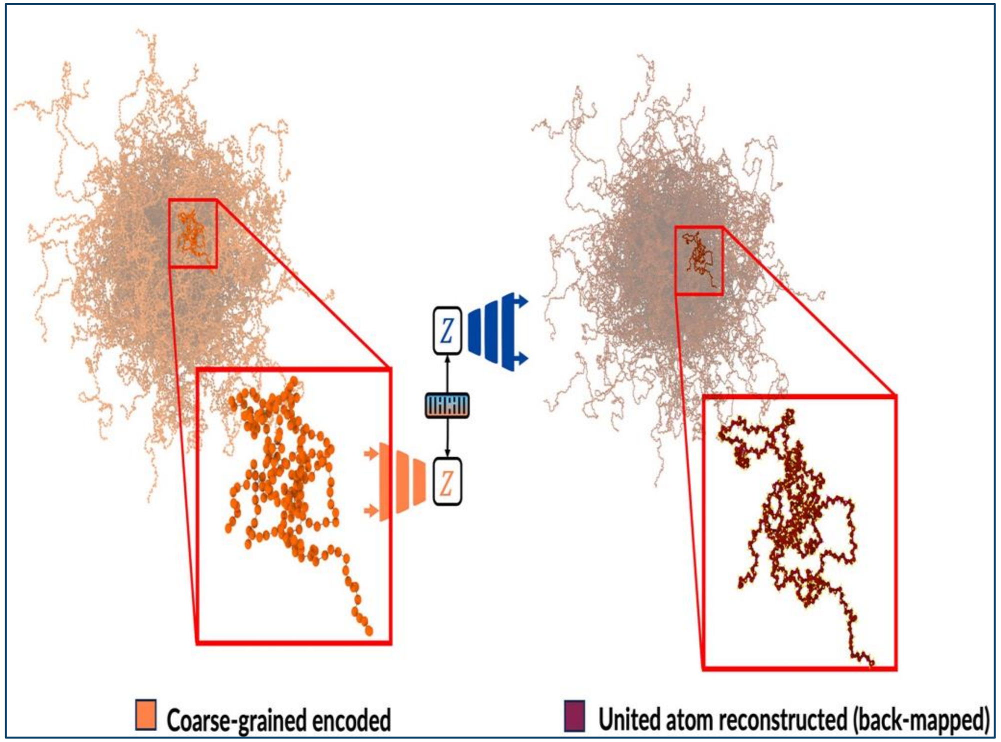

Figure: Back-mapped polymer melt, with magnified views of a single coarse-grained and united-atom back-mapped chain.

Significance and Impact

This work enables on-demand "fidelity switching," allowing scientists to model long-term processes like polymer curing or crystallization while retaining the high-fidelity detail needed for property evaluation.

Research Details

- Compressed high-dimensional polymer chains into compact "latent representations" using linear (SVD) and nonlinear (autoencoder) methods.
- Reconstructed atomistic structures from coarse data, then used brief molecular dynamics relaxation to restore 100% of structural and mechanical accuracy.

Desai, S.; Wilson, M.; Liu, S.; Kounouho, S.; O'Connor, T.; Dingreville, R. Learning Latent Representations to Bridge Coarse-Grained and Atomistic Resolutions in Polymer Simulations. *Journal of Chemical Theory and Computation.* 2026.

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