BLUE WATERS
SUSTAINED PETASCALE COMPUTING

Example polymer microstructures generated with the framework developed in this project.

EXPLORING CONFINEMENT VS. ORIENTATION EFFECTS IN RIGID AND SEMI-FLEXIBLE POLYMERS USING A MASSIVELY PARALLEL FRAMEWORK
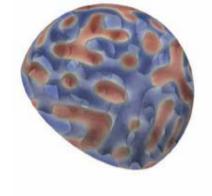
Research Challenge

The research goal is to develop and utilize a highly parallel computational framework to model equilibrium structures of semi-flexible polymers efficiently in complex, confined, non-periodic geometries. The simulation system is designed to be capable of scaling to large numbers of processors for large, complex systems of semi-flexible polymer systems. These tools will enable the ultimate goal of studying confinement effects on semi-flexible chains.

Methods & Codes

We built a custom finite element library from the Portable, Extensible Toolkit for Scientific Computation (PETSc). We use a simultaneous solution over the evolving chain contour space that enables efficient adaptivity and scaling. To model semi-flexible polymers, we use a two-level finite element method in which the entire spatial system is a finite-element volume mesh. Coupling the simulation spaces enables orientationally-dependent systems to be simulated.

Results & Impact

The development of a scalable finite element SCFT code utilized in a high-throughput study of polymer confinement, which will be used in several future studies.

The implementation of a simultaneous space–time finite-element method which is invaluable for a method aimed at enhancing scaling.

The development of a framework for modeling semi-flexible polymers which enables morphology studies of polymers with complex, orientation-dependent properties.

Why Blue Waters

The finite-element framework has been designed to model systems with large numbers of nodal points. At each finite-element nodal point there are 100 or more degrees of freedom to solve. For even the smallest problem, this results in billions of unknowns evolving under complex physical processes. The process requires significant, sustained computational resources. Utilizing a highly scalable framework and thousands of nodes makes these structure determinations feasible. The processing resources are not available outside the Blue Waters system.