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

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EXECUTIVE SUMMARY

The overarching goal of this work 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. This will allow simulation of a wide range of technologically and biologically relevant systems such as DNA, RNA, and viral capsids; polymer chains with stiff backbones used in organic electronics (field effect transistors, photovoltaics, thermoelectrics); liquid crystals, where orientation and alignment create ordered phases; and rod-like polymers used in membranes and sensors.

To handle the range of applications, the simulation system is designed to be capable of scaling to large numbers of processors for large, complex systems of semi-flexible polymer systems. It is also designed to use high-throughput simulations for parameter sweeps of smaller or less complex systems. This work has developed tools to meet these goals.

RESEARCH CHALLENGE

An understanding of the morphology of polymers under different conditions aids in materials design and discovery. Self-consistent field theory (SCFT) [1] simulations are a tool for efficiently modeling polymer microstructures. While the method has proven very successful, most SCFT simulations are not designed for scaling to large systems with arbitrary geometries and boundary conditions. They are also not designed to handle polymer systems with semi-flexible chains. This puts limits on the applicability of those simulations. A generic, highly scalable SCFT simulation tool capable of modeling semi-flexible polymers greatly expands the types of polymer systems that SCFT studies can address. These tools will be of great interest to polymer scientists and materials researchers. It will also enable the ultimate goal of studying confinement effects on semi-flexible chains.

METHODS & CODES.

To address the desired goals of highly scalable simulations of systems having arbitrary geometries and boundaries with complex chain models, we utilized a finite element approach with several advanced techniques. Our implementation uses a custom finite element library built upon the Portable, Extensible Toolkit for Scientific Computation (PETSc) [2].

The SCFT method utilizes an evolving chain contour, analogous to a time-dependent problem. To provide enhanced scaling, we use a coupled space-time model in the contour solver. In contrast to typical time-dependent finite element models that solve for each step sequentially, we can utilize a simultaneous solution over the entire contour space. This process enables efficient adaptivity and leads to enhanced scaling as the number of processors increases.

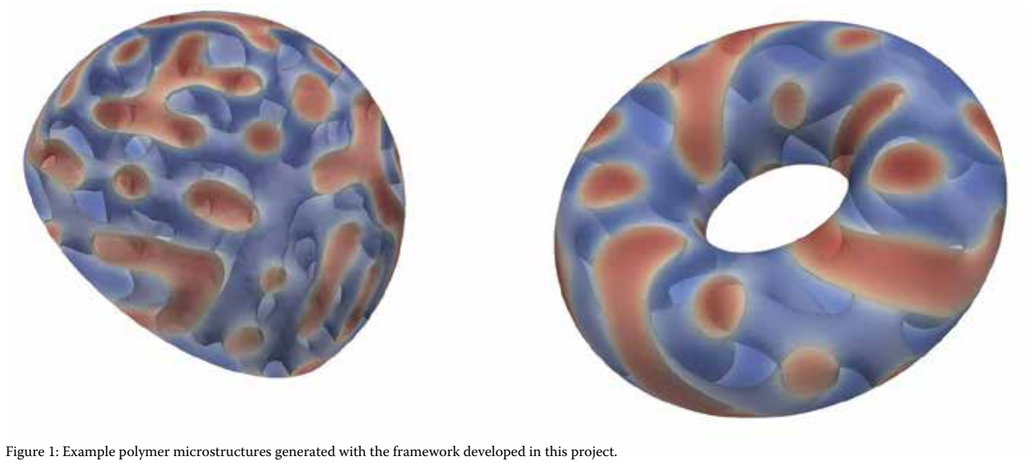

Figure 1: Example polymer microstructures generated with the framework developed in this project.

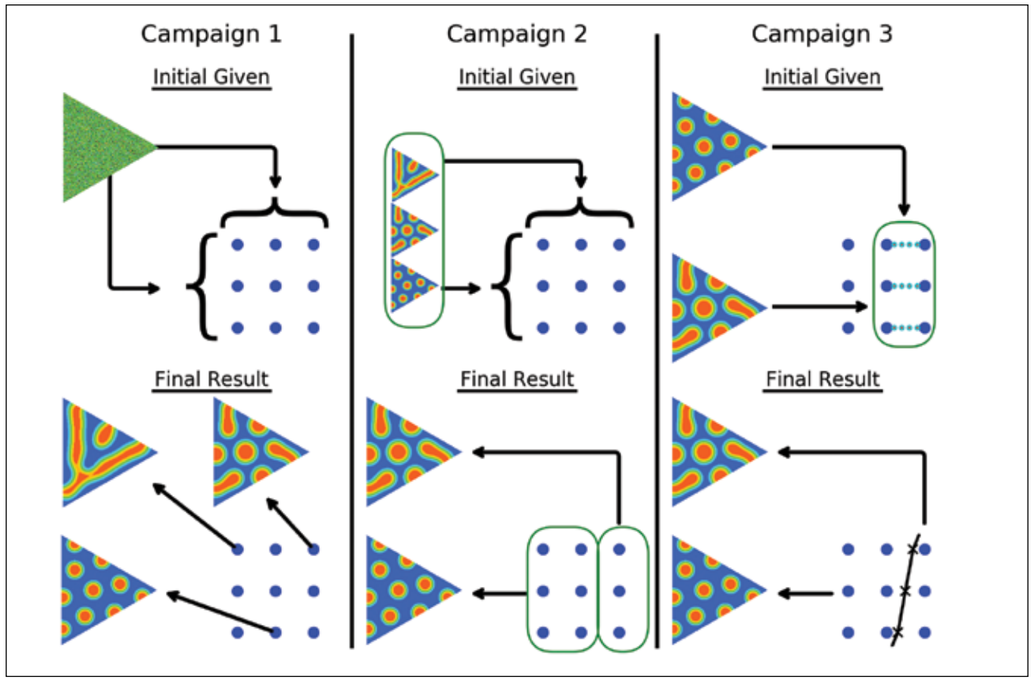

Figure 2: High throughput workflow for polymer phase diagram studies utilizing simulation "campaigns" for identifying equilibrium microstructures across a range of configuration parameters.

To model semi-flexible polymers, we have developed and utilized an approach that formulates this problem in an appropriate finite element space (the product space of spatial discretization and orientation discretization). This uses a two-level finite element method [3]. In this approach, the entire spatial system is a finite element volume mesh. At each nodal point within the volume mesh, a spherical surface mesh handles the orientations. The coupling of the two simulation spaces enables orientationally dependent systems to be simulated.

RESULTS & IMPACT

This work has had three major results: First, the development, testing, and deployment of a scalable finite element SCFT code. This has been utilized in a high-throughput study of polymer confinement and will be used in several future studies. Development of this code included design of an efficient process for the construction of polymer structure phase diagrams.

Second, implementation and testing of a simultaneous space-time finite element method. Access to the Blue Waters supercomputer enabled testing of this system by providing access to numbers of CPU cores unavailable elsewhere. This ensured a full view of the capabilities and limitations of this method. This is invaluable for a method aimed at enhancing scaling.

Third, development of a framework for modeling semi-flexible polymers using SCFT. This enables morphology studies of polymers with complex, orientation-dependent properties. The computational demands of polymer models have limited past work on these types of polymers. The resources of Blue Waters are well suited to the computational demands of this work.

WHY BLUE WATERS

The target systems for this work are polymer systems on a physically relevant scale. 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 for which to solve. For even the smallest problem, this results in billions of unknowns evolving under complex physical processes. Solving for these values yields the polymer structure. The solving process requires significant, sustained computational resources. Solving for a structure in a reasonable time takes even more 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.