Abstract Submitted
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A massively parallel space-time formulation for SCFT DAVID
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present a massively parallel, scalable Self Consistent Field Theory framework for
modeling multi block copolymers. This is based on a finite-element based real-
space implementation - which enables investigating complex, non-periodic domains
- integrated into a space-time formulation. A space time formulation allows the
implementation of a posteriori error analysis to ensure rigorous error bounds on the
propagator. The space-time formulation increases the computation problem size but
dramatically enhances the scalability of the problem. We show scaling up to 45,000
processors. The system remains tractable through the use of high order integration
schemes which allow a coarser chain model while retaining accuracy of lower order
schemes. This framework is applied to rod-coil diblock copolymers utilizing a worm-
like chain model. Results of this modeling on complex surfaces (spheres, tori) are
presented.

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