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Parallel framework for wormlike chains using self consistent field theory DAVID ACKERMAN, BASKAR GANAPATHYSUBRAMANIAN, Iowa State University — The Gaussian chain model commonly used in Self Consistent Field Theory (SCFT) has enabled study of a wide range of macromolecule systems; however, the flexible nature of the model makes it unsuitable for many biomolecules and systems such as liquid crystals where alignment effects are critical. The orientations accounted for in a wormlike chain model can correctly capture the physics of these systems. The primary problem with a wormlike chain model is the computational cost of implementation, which far exceeds that of the Gaussian chain model. We address this problem though a parallel SCFT framework for wormlike chains incorporating orientation interactions. The framework can scale to 10s of thousands of processors using an efficient finite element (FE) approach. Orientations are treated with an FE in FE method which overlays a surface orientation mesh on top of the spatial geometry mesh. The finite element approach allows use of arbitrarily shaped systems and is ideal for studying confinement effects. We explore how this framework works on a few examples for polymers confined to a sphere.

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