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Iterative Methods for Nonlinear Systems Arising in Diblock CoPolymer Systems

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Over the past four decades, extensive scientific research has been directed towards developing a molecular level understanding of micro-phase separation in diblock copolymers. Various novel applications such as the development of advanced materials for thermoplastic elastomers, nano lithography, fuel cells and supercapacitors have made these systems a major focus in soft matter research worldwide. Field theoretic approaches such as the self-consistent field theory (SCFT) have been used to predict thermodynamic stabilities of various polymer morphologies such as the lamellae, spheres, cylinders, gyroid etc.

In this talk the SCFT model for a diblock copolymer system is first described. The resulting set of nonlinear SCFT equations is solved in 3D using a nonlinear Krylov accelerator solver. Issues encountered in using potentially more efficient Jacobian Free Newton Krylov (JFNK) solvers and the performance of less efficient simple mixing algorithms are also detailed. The outer nonlinear solver requires computing the nonlinear residual at each iteration. For the SCFT systems this turns out to be extremely expensive as it requires time integration of a set of diffusion equations at each iteration. These equations are integrated using an implicit BDF4 method with multigrid solvers at each time step. After describing the full solution process some initial results in 3D will be presented with a description of the challenges to be tackled for future work.