1109-65-263 **Bobby Philip*** (philipb@ornl.gov) and **Rajeev Kumar** (kumarr@ornl.gov). *Iterative Methods for Nonlinear Systems Arising in Diblock CoPolymer Systems.*

Over the past four decades, extensive scientific research has been directed towards developing a molecular level understanding of micro-phase separation in diblock copolymers. 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 and field theoretic approaches such as the self-consistent field theory (SCFT) have been used to predict the thermodynamic stability of these polymers.

We describe the SCFT model for a diblock copolymer system posed in terms of field potentials. The resulting nonlinear SCFT equations are solved using a nonlinear Krylov accelerator solver. The outer nonlinear solver requires computing the nonlinear residual at each iteration. For the SCFT systems this is extremely expensive as it requires 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. We describe the full solution process and some initial results and conclude with a description of the challenges to be tackled in future. (Received February 02, 2015)