Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Exponential Time Differencing Methods for Numerical Self-Consistent Field Theory[1] YI-XIN LIU, HONG-DONG ZHANG, Fudan Univ — We present a fast and accurate numerical method for self-consistent field theory (SCFT) studies of polymer systems. For polymers in bulk, periodic boundary conditions are used. For confined polymers, the confining walls with or without preferential interactions with polymers, are modeled by appropriate non-periodic boundary conditions, which avoids the use of surface field terms and the mask technique in a conventional approach. Then the modified diffusion equations subject to these boundary conditions are solved by an exponential time differencing method with Fourier collocation and Chebyshev collocation for periodic and non-periodic boundary conditions, respectively. It exhibits fourth-order accuracy in time and spectral accuracy in space. The performance of this method is examined in comparison with the operator splitting pseudospectral methods. Numerical experiments show that the time differencing method is more efficient than the operator splitting methods in high accuracy SCFT calculations. Applications of this method to polymer brushes, block copolymers both in bulk and under confinement are demonstrated.

[1]This work is supported by the National Natural Science Foundation of China (Grant 21004013), the Fundamental Research Funds for the Central Universities, and the National Basic Research Program of China (Grant 2011CB605701).

Yi-Xin Liu
Fudan Univ

Date submitted: 15 Nov 2013 Electronic form version 1.4