Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

A Particle-Field Hybrid Simulation Method for Studying Strong Correlations in Polymeric Systems[1] DONG MENG, JING ZONG, Mississippi State Univ — The presence of strongly correlated interactions in polymeric materials, such as hydrogen bonding, ionomers, and coordinative bonds, can drastically alter materials' mesoscale structural and dynamical properties. Examples include supramolecular polymeric assemblies and micro-phase separation of ion-containing block copolymers, etc. Understanding of such materials demands computational methods that can faithfully capture strongly correlated interactions, and have also access to materials' mesoscopic behaviors. Among existing approaches, particle-based methods tend to be highly computationally demanding, while field-based methods tend to undercount essential correlations and fluctuations. With these limitations in mind, here we propose a new simulation formalism that is based on expanding the single chain in mean field (SCMF) scheme [1]. As a hybrid particle-field method, the new formalism offers the degree of freedom of separating interactions into ones to be treated using mean-field representations, and those to be preserved in particle-based representations. By doing so, the formalism combines the strength of both approaches via efficient calculation of interactions in dense systems, while being able to capture correlation and fluctuation effects due to interactions of particular interests. We illustrate the approach in the context of two examples. The accuracy and computational advantage of the new formalism are assessed by direct comparisons with Monte Carlo simulations. [1] J. Chem. Phys., 125, 184904 (2006).

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Date submitted: 11 Nov 2016 Electronic form version 1.4