Abstract Submitted
for the DFD16 Meeting of
The American Physical Society

Rapid Calculation of Thermal Forces in Coarse Grained Simulation of Colloidal Particles JAMES SWAN, ANDREW FIORE, Massachusetts Inst of Tech-MIT, ALEKSANDER DONEV, FLORENCIO BALBOA, New York University Courant Institute — In the presented work, we will demonstrate a spectrally accurate method for calculation of thermal forces in implicit solvent simulations of soft materials such as colloidal dispersions. For implicit solvent models, the stochastic forces must be drawn from a normal distribution whose covariance is a complicated function of the particle configuration. For a system of interacting N particles, drawing a single sample requires $O(N^3)$ operations, if numerically exact techniques from linear algebra are employed. So-called fast methods can approximate the sampling with roughly $O(N^m logN)$ computational complexity, where m is a coefficient greater than one which depends on the configuration of the particles. The computational complexity of the presented approach is $O(N(logN)^{d/(d+3)})$, where d is the fractal dimension of the particulate structures being modeled. Remarkably, this new approach adapts to the structure of the material under study by leveraging the algebraic structure of Ewald summation and balancing the computational effort spent evaluating near-field and far-field contributions to the hydrodynamic interactions among the suspended particles. Applications of this approach to modeling colloidal gelation and particulate suspensions will be discussed.

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Date submitted: 01 Aug 2016 Electronic form version 1.4