Wavelet Monte Carlo dynamics: hydrodynamics without the calculation

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Probing the dynamical properties of large, hydrodynamically interacting soft-matter systems remains a challenge in simulations because of the computational cost of either evolving all the solvent molecules in explicit solvent methods such as Lattice Boltzmann (LB), or the decomposition of the diffusion matrix in Brownian dynamics (BD). We have recently developed the Wavelet Monte Carlo dynamics (WMCD) algorithm to approach this problem with an implicit solvent Monte Carlo method [1], which faithfully replicates the correct hydrodynamic interactions in the low Reynolds number regime without needing any calculation involving the diffusion matrix.

This is achieved using the wavelet representation of the diffusion matrix, from which we find the probability distributions of wavelet parameters to generate the correct correlated motion when these wavelets are taken as the Monte Carlo moves in the simulation. Further to this, occasional plane wave moves are included to supply long-range correlations that the wavelets omit for computational efficiency. These can be tailored for either periodic or unbounded systems, adding a negligible cost in both cases. Thus WMCD removes the largest contributions to the cost in established algorithms, leading to cost with the number of particles, N, scaling at worst as NlnN. Comparisons against LB and BD simulations of identical polymeric systems have shown the constant prefactor for this cost to be very competitive, even for an unoptimised implementation of WMCD, owing to the simplicity of the Monte Carlo method [1-3].

Correct equilibrium and dynamical behaviour has been verified in simulations of simple polymeric systems, with the relaxation of chain size and centre-of-mass diffusivity both exhibiting expected behaviour and absolute values matching those from previous work. Finally, we have collected higher accuracy data to observe the difference between long- and short-time centre-of-mass diffusivity and to quantify the effect of using a finite time step size on the dynamics observed.

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