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Hybrid BD-MC-kMC Framework for Predicting Nanoparticle Easy Axis Dynamics in Hyperthermia

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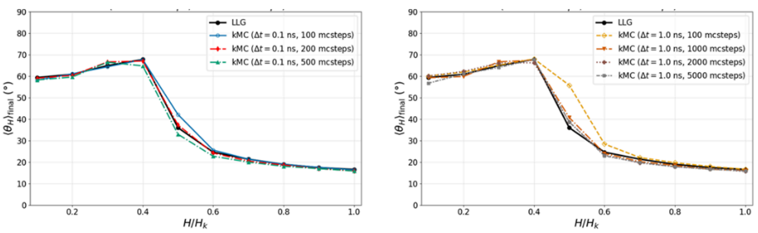
Magnetic nanoparticles (MNPs) display complex dynamics due to the coupling between magnetic moment evolution and particle rotation under applied fields in viscous fluids. Accurate modeling is needed for optimizing biomedical applications like magnetic hyperthermia, targeted drug delivery, and biosensing [1], where particle alignment with the field affects heating efficiency and performance. The Landau-Lifshitz-Gilbert (LLG) equation [2] provides a description of magnetization dynamics but becomes computationally expensive for large systems and long timescales. On the other hand, Monte Carlo (MC) methods [3] are faster but cannot clearly distinguish thermal fluctuations from barrier-crossing events within energy minima. To overcome these limitations, we propose a hybrid Brownian Dynamics–Monte Carlo–kinetic Monte Carlo (BD–MC–kMC) method that separates the different time scales. The kMC handles thermally activated switching [4,5], MC captures fast thermal fluctuations, and BD governs particle rotation in a viscous fluid [5]. A key finding of this work is that the anisotropy torque must be computed using all MC trial moves, including rejected ones. This approach accurately reproduces the dynamics predicted by LLG. In contrast, using only accepted moves introduces systematic error and fails to represent the true physical behavior. We further introduce a barrier-trapping approach to prevent unphysical barrier-crossing events within MC sampling by rejecting moves that flip the moment across the barrier. Without trapping, MC sampling produces artificial switching events. Validations against LLG for particle sizes of 10–50 nm and fields of 0.1–1.0 H_k show strong agreement when appropriate MC sampling is used. With this approach, the average angle $\langle\theta\rangle$ between the easy axis and the applied field agrees well with LLG across particle sizes, field cases, and timesteps. This mechanism confines thermal fluctuations within energy minima while ensuring that true switching occurs only through kMC transition. Overall, the proposed hybrid framework provides an efficient and accurate alternative to micromagnetic simulations, enabling reliable prediction of alignment and dynamics of magnetic nanoparticles for biomedical applications.



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