Abstract Submitted
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A finite element method for simulating thermally fluctuating Brownian particles: Random force vs Random stress[1] UMA BALAKRISHNAN, T.N. SWAMINATHAN, R. RADHAKRISHNAN, D.M. ECKMANN, P.S. AYYASWAMY, University of Pennsylvania — Targeted nanocarrier drug delivery holds promise for personalized medicine, but its optimization requires an accurate description of carrier motion. Our computational approach is aimed at situations where both Brownian motion and the hydrodynamic interactions are important. We consider two ways of assessing this motion: (a) time-correlated random forces (colored noise) acting on the particles, (b) hydrodynamic random stresses in the fluid equations (white noise). The first approach is geometry dependent, the number of random numbers (R_n) generated per step is equal to the number of particles. However, the second approach is geometry independent and requires R_n to be equal to the number of mesh points. Both the approaches have been investigated and the results are validated by comparing the calculated temperature of the system, with that determined from the equipartition theorem, and by comparing the predicted mean square displacement with that calculated from Einstein's formula. While both approaches yield comparable accuracies, the random stress approach appears to be more robust and readily generalizable to complex particle as well as flow geometries.

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