Modeling the motion of a nanocarrier for targeted drug delivery

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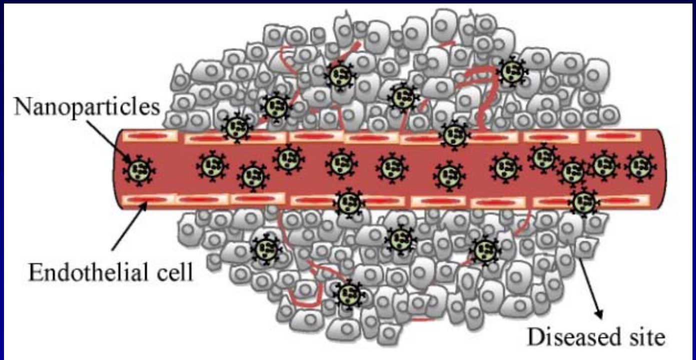
• Clinical optimization of drug transport requires accurate description of carrier motion in the blood stream and near endothelial cells.



• Synergistic computational approach is required to determine the translational and rotational motions of a nanocarrier.

• Formalism considers situations where both the Brownian motion and hydrodynamic interactions are important.

• A direct numerical simulation adopting an arbitrary Lagrangian-Eulerian based finite element method is employed to simulate the motion of a spherical nanocarrier in a quiescent fluid medium or Poiseuille flow in a tube.

• Thermal fluctuations are implemented using two different approaches:
(1) Fluctuating Hydrodynamics (2) Generalized Langevin Dynamics (Mittag-Leffler noise).

• At thermal equilibrium, the results are validated by comparing the predictions of particle temperatures with that obtained from the equipartition theorem. The nature of the hydrodynamic interactions is verified by comparing the velocity autocorrelation functions and mean square displacements with analytical and experimental results.

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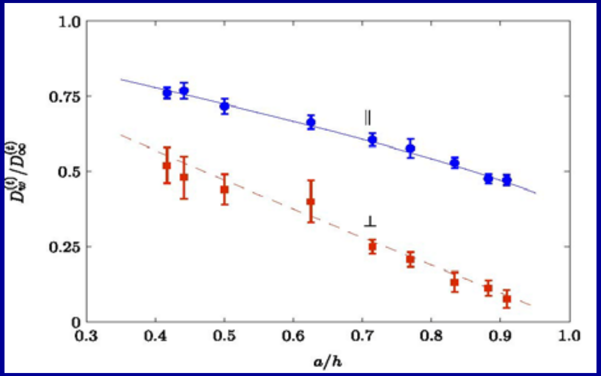
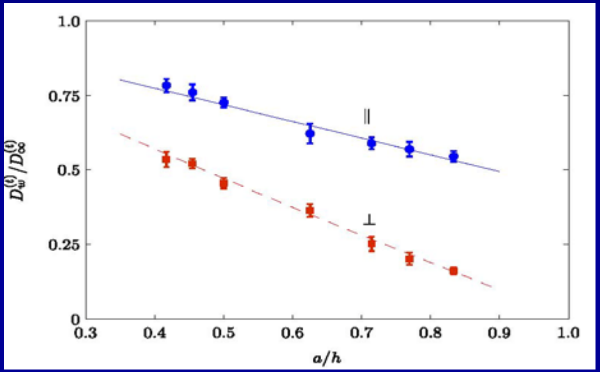
I. Fluctuating Hydrodynamics

- Thermal fluctuations from the fluid are added as random stress tensor in the fluid equation, that depends on the temperature and viscosity of the fluid.
- Equipartition theorem is satisfied. The particle mass is augmented by an added mass to account for compressibility.
- In the diffusive regime, translational and rotational MSDs obey Stokes-Einstein and Stokes-Einstein-Debye relations, respectively.

Quiescent Fluid



Poiseuille Flow



II. Generalized Langevin Dynamics with Mittag-Leffler Noise

- Thermal fluctuations from the fluid are added as random force and torque in the particle equations of motion, that does not depend on position or shape of the particle.
- Equipartition theorem is satisfied. When the thermostat adheres to the equipartition theorem, the characteristic memory time in the noise is consistent with the inherent time scale of the memory kernel.
- In the diffusive regime, translational and rotational MSDs obey Stokes-Einstein and Stokes-Einstein-Debye relations, with scaling factors (as thermostat alters the dynamics).

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