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Modeling Lubrication Forces From First Principles

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Summary

The objective of this research is determine the lubrication force in the limit were the gap size is of molecular dimensions. It is well-known that the commonly used continuum approximations must break down when these dimensions are approached, but the outstanding challenge is to provide a replacement that is both firmly based in molecular science (statisticsal mechanics), and can be combined smoothly with the existing continuum solvers. By performing molecular dynamics and developing ways to extract the observables relevant to continuum dynamics we seek to fill the gap of knowledge at the molecular scale and bridge the gap to the continuum scale with a sound and systematic approach.

Consider a colloidal sphere steadily approaching a flat substrate ("a wall"). As the gap between the sphere's leading surface and the wall becomes sufficiently small a repulsive force is observed. Brenner [1] has shown that in a continuum description this force, due to the sphere squeezing out the fluid between its apex and the wall, ultimately diverges as 1/h, in the limit that h vanishes. A similar, but weaker divergence is predicted by fluid dynamics for other well-defined elementary motions (shear and rotations.)However, such a divergence must be absent as molecular dimensions are approached. At such small lengthscales both atomic force microscopy experiments and modeling have shown that there exists a force (a so-called solvation force) of equilibrium thermodynamic origin acting between wo opposing surfaces even in the absence of any surface movement. This force is one indication that the ccontinuum approximation breaks down at the nanometer length scale.

To provide insight into the forces at small distance,and to elucidate the fundamental questions associated with the breakdown of the continuum approximation we embarked on molecular dynamics simulations of a sphere falling at constant velocity through a particulate fluid. The density profiles and velocity proofiles are illustrated in Figure 1. The forces calculated on the sphere clearly showed the strong coupling between dynamic and equilibrium ("static") forces. To disentangle the two contributions we have introduced a novel approach based on a symmetry argument [2]. The dynamic force that results of such a decoupling is shown in Figure 2, where we compare several simulation results with Brenner's Force. Although the molecular dynamics force result clearly differs from the contiinuum prediction, we do find that, like the continuum prediction, the force is a universal function in the sense that once divided by the Stokes force (infinite gap) the result is independent of the type of fluid. We have shown this for different interaction

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models, temperature and densities (see Figure 2.)

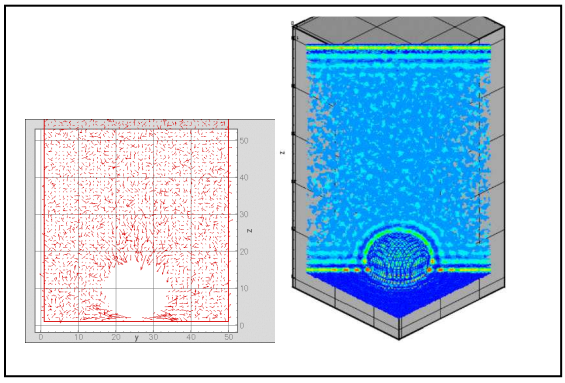

Figure 1. *Density profiles(right) and velocity profiles for a smooth sphere moving through a molecular fluid. The density variations near the flat wall and the smooth sphere reflect molecular packing. The velocity profiles represent a slice through a 3D array. Each vector shows the average velocity vector of a fluid element of cubic fluid element two molecular diamters wide.*

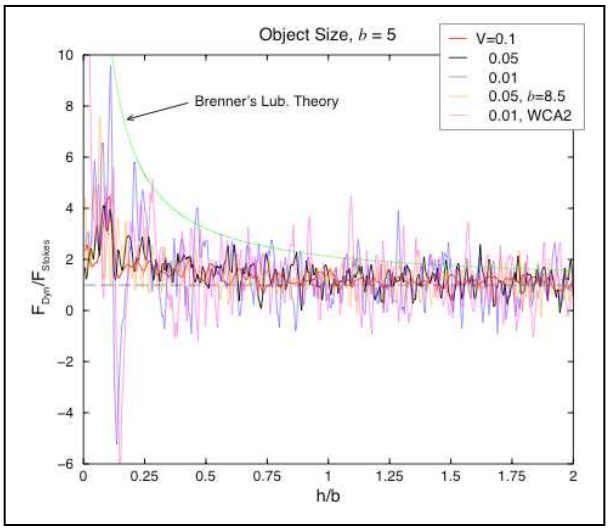

Figure 1. *The ratio of the dynamic drag force over the Stokes force for a variety of velocities (v), different sphere diameters and a different fluid ("WCA").*

We are currently developing a method to caluclate a 3D stress profile and tractions on the sphere which will be used in the boundary element method. In addition, we will implement a buffer region which will bridge the junction between a molecular dynamics regime and a continuum method.

Acknowledgments

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References

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