

Improving Particle Methods

Robert Krasny, University of Michigan

Particles are used in several different ways in computational physics. For example one can study systems of point masses, point charges, and point vortices. However another approach considers the particles as a discretization of a continuous problem; in this case one is dealing with a particle method, as an alternative to other discretization methods such as finite-difference, finite-element, and spectral methods. Here we consider particle methods in two areas, (1) electrostatics of solvated proteins, where the particles are nodes in a triangulation of the molecular surface, and (2) incompressible fluid dynamics, where the particles represent the flow map and carry vorticity. We discuss the challenges facing particle methods and some techniques that improve their accuracy and efficiency, including adaptive refinement, extrapolation, remeshing, and treecode-acceleration.