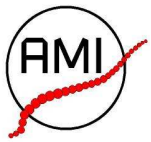
Applied Mathematics Institute



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PIMS / AMI Seminar

Tuesday, March 1, 2011
3:30 p.m.
CAB 657

"A mixed Brownian dynamics - SPH method for the simulation of flows of polymer solutions in confined geometries with hydrodynamic interaction"

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Abstract

A new coupled Brownian dynamics-smoothed particle hydrodynamics (SPH) method for the computation of confined flows of polymer solutions with full hydrodynamic interaction and excluded volume forces is presented. The starting point for the algorithm is the system of coupled Langevin equations for polymer and solvent (CLEPS) (see Oono and Freed (1981) and Öttinger and Rabin (1989), for example) describing, in the present case, the microscopic dynamics of a flowing polymer solution with a bead-spring representation of the macromolecules. Of crucial importance to the success of our numerical scheme is the manner in which bead forces are transmitted to the fluid. We adopt an approach which is reminiscent of the method of regularized Stokeslets (Cortez (2001)). Numerical tests of some two-dimensional channel flows reveal that use of a second-order projection scheme coupled with fixed SPH quadrature points leads to second-order velocity convergence and almost second-order pressure convergence, provided that the solution is sufficiently smooth. In the case of large-scale dumbbell and bead spring chain calculations, an appropriate scaling of the number of grid points as a function of the number of beads N ensures, in the absence of excluded volume forces, that the cost of our algorithm is O (N) flops.

Refreshments will be served in CAB 649 at 3:00 p.m.