Applied Mathematics

CRM-McGill Applied Mathematics Seminar

Nov. 13, 2006, 2:35 pm Monday
At McGill, Burnside Hall 1205

"The Fastest N-Body Solver (for Molecular Dynamics) "

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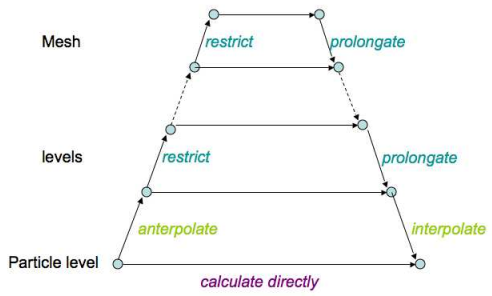
Coffee and refreshments will be served after the seminar

Abstract: The computing time needed to calculate 2-body interactions between N particles grows as N^2. Fast N-body solvers calculate approximations in a time proportional to $N \log N$ or N, for potentials that become more slowly varying as distance increases. Two types of algorithms can be distinguished: hierarchical clustering algorithms, such as the celebrated fast multipole method, and potential splitting algorithms, such as the popular particle–mesh Ewald method. By formulating the problem as that of computing a matrix–vector product, the basic structure of these algorithms is elucidated. Additionally, evidence is presented indicating that potential splitting algorithms are much to be preferred for molecular dynamics and that the virtually unknown *multilevel summation method* of Brandt and Lubrecht is the best among these. This method uses hierarchical interpolation of interaction potentials on nested grids to calculate energies and forces in linear time for both periodic and nonperiodic boundary conditions. This is joint work with David J. Hardy.



Schematic of fast-summation technique.