Simulation of elastic light scattering on distributed memory machines: abstract

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Simulation of elastic light scattering (ELS) on distributed memory machines. A.G. HOEKSTRA, L.O. HERTZBERGER, P.M.A. SLOOT, dep. Computer Systems, Univ. Amsterdam. --- We have implemented the Coupled Dipole (CD) method of ELS on a distributed memory computer. The computational kernel of the CD method comprises a large set of 3N linear equations of 3N complex numbers. The resulting system of equations is solved efficiently by iterative methods, such as Conjugate Gradient (CG), Successive Over Relaxation (SOR) or Jacobi. From a numerical point of view, CG and SOR are preferred to the Jacobi iteration, because of much better convergence properties. However, there are two overlooked reasons to choose for the Jacobi method; it can be shown that each iteration step in the Jacobi method can be identified with a multiple scattering event within the particle, and that the Jacobi method is inherently parallel (in contrast to e.g.. SOR). Therefore, the total elapsed computing time of the Jacobi method, implemented on a parallel computer, can be significantly shorter than for SOR. We will present typical results for the Jacobi method, compared to SOR. In the context of this example we will provide arguments that the development of applications on parallel machines should imply a thorough reconsideration of the algorithms that are commonly used, since in many cases parallelizing existing sequential code will be extremely inefficient.

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