IMPROVING THE PERFORMANCE OF A PARALLEL COMPUTATIONAL PHYSICOCHEMICAL HYDRODYNAMICS CODE IN AN HETEROGENEOUS BEOWUF CLUSTER

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We report a significant performance improvement of a parallel 3D computational physicochemical hydrodynamics code on a Beowulf heterogeneous cluster under Linux and MPI. The parallel computational code solves the 3D Nernst-Planck equations for ion transport, the Poisson equation for the electric field and the Navier-Stokes equations for the fluid flow, using finite differences and domain decomposition techniques with a strongly implicit iterative scheme. The improvement of the parallel code is attained through: i) a semi-dynamic load balancing without need for "a priori" knowledge of cluster characteristics, ii) a reordering of the iterarion process to support overlapping of interprocessor communication with useful computation for reducing idle time and waiting time among processes, and iii) a judicious blend of the use of non-blocking communications with different buffer quantities and buffer sizes and different MPI implementations. With these strategies a performance improvement of around 40%, as compared with standard parallel versions, was obtained. Moreover, for some cases, scalability with efficiencies close to unity were attained. The optimized parallel code was used in the study of a complex 3D electrochemical problem for scales not yet attained with standard codes.

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