Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Accurate, efficient, and scalable parallel simulation of mesoscale electrostatic/magnetostatic problems accelerated by a fast multipole method.[1] XIKAI JIANG, Argonne National Laboratory, DMITRY KARPEEV, JIYUAN LI, JUAN DE PABLO, University of Chicago, JUAN HERNANDEZ-ORTIZ, National University of Colombia, OLLE HEINONEN, Argonne National Laboratory — Boundary integrals arise in many electrostatic and magnetostatic problems. In computational modeling of these problems, although the integral is performed only on the boundary of a domain, its direct evaluation needs $O(N^2)$ operations, where N is number of unknowns on the boundary. The $O(N^2)$ scaling impedes a wider usage of the boundary integral method in scientific and engineering communities. We have developed a parallel computational approach that utilize the Fast Multipole Method to evaluate the boundary integral in O(N) operations. To demonstrate the accuracy, efficiency, and scalability of our approach, we consider two test cases. In the first case, we solve a boundary value problem for a ferroelectric/ferromagnetic volume in free space using a hybrid finite element-boundary integral method. In the second case, we solve an electrostatic problem involving the polarization of dielectric objects in free space using the boundary element method. The results from test cases show that our parallel approach can enable highly efficient and accurate simulations of mesoscale electrostatic/magnetostatic problems.

[1]Computing resources was provided by Blues, a high-performance cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory. Work at Argonne was supported by U. S. DOE, Office of Science under Contract No. DE-AC02-06CH11357.

Xikai Jiang
Argonne National Laboratory

Date submitted: 06 Nov 2015 Electronic form version 1.4