Parallelization Strategies for Wavepacket Dynamics Using the Quantum Trajectory Method *

Ioana Banicescu
Department of Computer Science and Engineering Research Center
Mississippi State University

The study of quantum mechanics is based on finding the solution to the time-dependent Schroedinger equation (TDSE). One approach to solving the TDSE is the Quantum Fluid Dynamics (QFD) formulation, where wavepacket dynamics are based on the Bohmian formalism [1]. One of several computational approaches for simulating wavepacket dynamics is the algorithm introduced by Lopreore and Wyatt [2]. The algorithm solves the one-dimensional Lagrangian QFD equations of motion using a moving least square (MLS) method. This quantum trajectory method (QTM) is particularly attractive, given its simplicity without sacrifice of accuracy. However, its implementation is computationally-intensive, mainly due to frequent use of the MLS method. Therefore, parallel algorithms are necessary for simulating realistic applications within reasonable amount of time.

This talk will describe our multidisciplinary collaborative research project on the development of parallel versions of the algorithm by Lopreore and Wyatt [2] for shared and distributed memory architectures. Preliminary experiments indicate that the parallel algorithm achieves efficiency values of up to 65% on a 8-processor shared memory machine, and up to 82% on a 32-processor cluster. Further optimization of this algorithm's implementation is expected to result in even higher efficiency values. Adapting the algorithm for two- and three-dimensional problems is expected to lead to load imbalance among processors, and therefore result in performance degradation. In that case, to adequately address this problem, novel loop scheduling techniques will be incorporated in the parallel implementation of the algorithm. The talk will conclude with insights we have gained from this work and future directions of our collaborative research.

References

[1] D. Bohm, Phys. Rev. 85, 166 (1952); 85, 180 (1952)
[2] C. L. Lopreore and R. W. Wyatt, Phys. Rev. Lett. 82, 5190 (1999)
[3] R. G. Brook, P. E. Oppenheimer, C. A. Weatherford, I. Banicescu and J. Zhu, Int. J. Quant. Chem., 00, 1 (2001).

*This work was supported by the National Science Foundation Grants NSF ITR/ACS Award # ACI0081303, NSF CAREER Award # ACI9984465, and Award # EEC-9730381