Abstract

We present the new approach to utilize all heterogeneous resources like CPU cluster, GPU cluster in multi core and multi GPU environment. MD simulation are used for deeper understating of fluid flows, chemical reaction, and other phenomena due to molecular interaction. The main drawback in the MD simulation is that it require computationally demanding more resource because of its amount of O(n^2). The use of heterogeneous resources is an attractive solution and has been applied to MD problems. However, such heterogeneous resources cause load imbalances between CPUs and GPUs and they were not utilize all available computation resources.

References


Tavel, P. 2007 Modeling and Simulation Design. AK Peters Ltd.


16. Takuro Udagawa and Masakazu Sekijima, “GPU Accelerated Molecular Dynamics with Method of Heterogeneous Load Balancing,” 2015 IEEE International Parallel and Distributed Processing Symposium Workshops

**Index Terms**

Computer Science  
Parallel Computing

**Keywords**

Molecular Dynamics Simulation, GPU, CPU, Heterogeneous Resources