Abstract

Molecular dynamics simulates behavior of atoms and molecules. Molecular dynamics Simulation demonstrates and derives macroscopic properties by atomic interactions.

In this experiment we have redesigned Molecular Dynamics (MD) Simulation by applying different parallel design pattern. Redesigned MD Simulation focuses on adaptability to different architectures and scalability to use with large number of atoms and long duration simulation. The paper demonstrates performance of MD on different architectures.

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Index Terms

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