Task Based Parallelism with OpenMP: A Case Study with DL_POLY_4

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Abstract

When performing computations where load balancing is complex, dynamic load balancing is becoming increasingly necessary. In this paper we examine one of these methods, Task-Based Parallelism.

Many libraries implement Task-Based Parallelism, however in this paper we examine the OpenMP standard and implementations, and apply it to the Classical Molecular Dynamics code, DL_POLY_4, focusing on the two body force calculations that make up a large percentage of the compute in many simulation runs.

Our results show reasonable performance using OpenMP tasks, however some of the extensions available in other libraries such as OmpSs or StarPU may help with performance for problems similar to Molecular Dynamics, where avoiding race conditions between tasks can have a substantial scheduling overhead.

Keywords. Task-Based parallelism, OpenMP 4.5, Molecular Dynamics

1. Introduction

Task-Based Parallelism is a method for shared memory parallel programming in which a program is split into a series of tasks, which are picked up and executed by a set of cores in parallel until the computation is completed. To avoid concurrency issues, the *dependencies* between tasks need to be considered, i.e. if there are 2 tasks, A and B, where task A produces a result needed to compute task B, we say B is dependent on A, or A *unlocks* B. The tasks and their dependencies form a Directed Acyclic Graph (DAG).

Task-Based Parallelism has two major advantages over traditional parallel processing techniques. Firstly, since the tasks are assigned to the cores dynamically, the work is automatically load balanced. Secondly, the task dependencies avoid the need for explicit synchronisation between the cores.

In the OpenMP 3.0, 4.0 and 4.5 specifications, Task-Based Paralellism has been added and extended, allowing a standardised way to use task-based parallelism.

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