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, dy-
namic 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 pa-
per 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, how-
ever some of the extensions available in other libraries such as OmpSs
or StarPU may help with performance for problems similar to Molecu-
lar 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 dynami-
cally, 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 Parallelism has
been added and extended, allowing a standardised way to use task-based parallel-
ism.

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