PARALLELIZATION OF DYNAMIC ALGORITHMS

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1. Background

Parallel computing is increasingly important. There is a growing need for easy-to-use programming models for high performance computing. The de facto standard for distributed computing, the message passing interface (MPI), is more than 20 years old and although the interface has been upgraded the fundamental programming model remains essentially unchanged. Development of applications within the message passing parallel programming paradigm is difficult and costly. In particular, parallelization of dynamic algorithms, with a priori unknown and/or dynamically changing distributions of work and data, often represents a formidable challenge. At the same time, many problems are such that dynamic algorithms would be the natural and appropriate choice if only suitable parallelization tools were available. Consider for example adaptive mesh refinement to capture moving fronts or other time-dependent processes. This proposal targets the development of parallelization strategies (programming models, interfaces, and tools) for dynamic algorithms.

2. Project

This project presents an opportunity to participate in the development of a new programming model that simplifies the development of parallel programs in general and the parallelization of dynamic hierarchical algorithms in particular. Our programming model is named the Chunks and Tasks programming model and has recently been presented in [1] and library implementations are publicly available at www.chunks-and-tasks.org.

In future work we intend to 1) make improvements to the model, 2) develop and implement efficient strategies for scheduling of tasks and distribution of data, and 3) demonstrate the performance for realistic applications that represent a variety of use cases. This work was motivated by the need to parallelize hierarchical dynamic algorithms occurring in large-scale electronic structure calculations. We plan to use the Chunks and Tasks model to parallelize our electronic structure program Ergo (www.ergoscf.org).

We are looking for a candidate that has skills, experience and/or interest in

- programming, in particular C++,
- parallel computing, in particular MPI and pthreads, and
- scientific and high performance computing in general.

References