Chapter XIX
Grid-Based Nuclear Physics Applications

Frans Arickx
University of Antwerp, Belgium

Jan Broeckhove
University of Antwerp, Belgium

Peter Hellinckx
University of Antwerp, Belgium

David Dewolfs
University of Antwerp, Belgium

Kurt Vanmechelen
University of Antwerp, Belgium

ABSTRACT
Quantum structure or scattering calculations often belong to a class of computational problems involving the aggregation of a set of matrices representing a linear problem to be solved. We discuss a number of approaches based on cluster and grid computing, and discuss the implementations and the respective merits and shortcomings. We consider MPI-based cluster computing in a self-scheduling paradigm, CoBRA (a cpu-harvesting desktop grid) in a farmer-worker paradigm, and a batch-computing paradigm on BEGrid (the Belgian research grid facility). It is observed that for all paradigms an efficient implementation is possible, yielding results within a comparable time frame.
INTRODUCTION

Many computational problems belong to a class involving the aggregation of a set of matrices, representing a linear problem to be solved, and which represents a sizeable or major portion of the total computational load.

Microscopic quantum nuclear physics calculations are usually computationally intensive because of a multitude of degrees of freedom. The main aim in such calculations is to obtain a solution for bound or scattering states of the so-called Schrödinger equation. Exact solutions are impossible to obtain except for simplified model problems. A popular technique approximates the solution as an expansion in a complete basis. Such a basis is usually characterized by a multidimensional parameter space. This leads to extensive, but often highly parallelizable calculations of the class mentioned above.

In this paper we consider as an example of the matrix aggregation class of problems, and as a representative for many theoretical nuclear calculations, a description of light nuclei in a microscopic three-cluster model. As is often the case, we start from existing legacy code originally written in Fortran 90. This code is easily parallelizable into a large set of individual subcalculations. We then distribute the calculations on both a cluster (Beowulf) and a Grid (BEgrid) configuration. To solve the distribution of tasks we use 2 distinct approaches on the Beowulf (Gropp et al., 2003) system: task submission using the CoBRA middleware, and a self-scheduling approach based on MPI. On the BEgrid we take a scripting approach to properly submit the individual tasks.

We discuss the timing characteristics of the implementations, and discuss merits and shortcomings. Because of the differences in platforms and middleware, direct comparisons are difficult, but we then compare qualitatively. It is shown that for each of the distribution approaches an efficient implementation is possible within a comparable time frame.

BACKGROUND

Before focusing on the actual distribution, more insight into the actual problem and the possible distribution mechanisms is essential. This section discusses the actual nuclear physics problem and gives a brief introduction to each of the used distribution mechanisms (CoBRA, BeGrid and MPI)

The Nuclear Physics Problem

To obtain physical properties of quantum systems, such as atoms, nuclei or molecules, one needs to solve the Schrödinger equation. In order to solve it, proper boundary conditions must be chosen. The solutions, the so-called wave-functions, then allow for the calculation of physical quantities. The equation and its boundary conditions are usually too complex to be solved exactly for many-body systems (e.g. a nucleus), and approximations have to be introduced. One approach is to expand the wave-function on a discrete, infinite-dimensional, set of basis states. Substitution of this approximation in the equation and boundary conditions leads to a much simpler matrix equation in the expansion coefficients to be solved. The matrix formulation can be further simplified by choosing expansion bases with specified properties. The Modified J-Matrix model (Broeckhove et al., 2004) is such an approach, and has been applied to three-cluster nuclear systems (Vasilevsky et al., 2001). We consider it here to obtain scattering results for a three-particle configuration of a triton and two neutrons of $^5\text{H}$. The calculations essentially consist of two steps: (1) a CPU intensive calculation of the matrix elements in the matrix equation, and (2) the solution of the matrix equation. As step 2 can be obtained sequentially on a single node, we will only consider the distribution of step 1. The expansion basis for the solution of a three-cluster problem is enumerated by a set of indices. These are the hypermoment $K$, describing the three
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