Chapter 6

Further Development of an Application Framework for Computational Chemistry (AFCC) Applied to New Drug Discovery

J. Tindle  
University of Sunderland – St. Peter’s Campus, UK

R.L. Warrender  
University of Sunderland – St. Peter’s Campus, UK

M. Gray  
University of Sunderland – City Campus, UK

K. Ginty  
University of Sunderland – St. Peter’s Campus, UK

P.K.D. Dawson  
University of Sunderland – City Campus, UK

ABSTRACT

This chapter describes the performance of a compute cluster applied to solve Three Dimensional (3D) molecular modelling problems. The primary goal of this work is to identify new potential drugs. The chapter focuses upon the following issues: computational chemistry, computational efficiency, task scheduling, and the analysis of system performance. The philosophy of design for an Application Framework for Computational Chemistry (AFCC) is described. Eighteen months after the release of the original chapter, the authors have examined a series of changes adopted which have led to improved system performance. Various experiments have been carried out to optimise the performance of a cluster computer, the results analysed, and the statistics produced are discussed in the chapter.

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1. INTRODUCTION

Computational methods have been developed that allow researchers to carry out comprehensive investigation of molecules and their reactions. Molecular modelling allows the researcher to observe biological reactions and the associated dynamics providing highly accurate descriptions of the relevant interatomic forces. In most cases it is computationally expensive to solve the high level quantum chemistry models.

Chemists are now able to investigate the properties of chemical structures at the molecular level. The aim of the research described in this paper is to discover new drugs that target particular cells and cure diseases at the cellular or genetic level.

This paper describes the performance of a compute cluster applied to solve a large number of molecular models. The paper considers factors such as the computational chemistry and molecular modelling, computational efficiency, task scheduling and the analysis of cluster system performance. The updated design of an application framework for computational chemistry (AFCC) research is discussed (Tindle, Gray, Warrender, Ginty & Dawson, 2012).

The University of Sunderland installed and commissioned a general purpose high performance compute cluster in the Computing department. This development is based upon Microsoft High Performance Computing HPC Servers and the Compute Cluster Pack (“What is Microsofts High Performance Computing HPC Server,” 2014; “Microsoft Compute Cluster Pack,” 2014). The design of the cluster computer was completed by University of Sunderland (UoS) and Dell engineers (Ginty, Tindle, & Tindle, 2009; “Eco-Friendly Super Computing,” 2014), refer to Appendix 1. A more detailed description of the cluster system hardware and software configuration may be found in the paper by Ginty (2009). The UoS cluster computer has been used in areas such as 3D computer graphics (CG) modelling projects (Tindle, Ginty & Tindle, 2009), as well as crash analysis simulation using finite element modelling software. Staff employed within the departments of Computing and Pharmacy collaborated upon this research.

2. MOLECULAR MODELLING

Molecular modelling software allows the user to select atoms from the periodic table and to place them in a three dimensional workspace. In most modelling systems it is possible to build a three dimensional molecular structure by using a colour graphics user interface (GUI), refer to Figure 1. The initial position of the atoms is normally determined by the user calling upon common sense and experience. In all cases the actual position that the atoms assume in the real world is determined by the Laws of Physics. Computational chemistry is a general name for computer based algorithms that may be used to solve this type of problem. There are numerous algorithms that may be deployed and normally this involves computing the minimum value of an energy function to find the optimum solution.

For complex structures in many cases the rate of convergence is relatively slow and it is therefore often necessary to employ high performance computing methods to produce solutions in a reasonable period of time.

2.1 Model Convergence Time

There are three principle factors that influence the time required to produce an acceptable solution.

- The initial position of the atoms selected by the user. This initial set of atomic positions is the seed for the numerical solver algorithm embedded in Gaussian 09.
- The number of heavy atoms in the model of the molecular structure.
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