Chapter 4.7
Grid Computing in 3D Electron Microscopy Reconstruction

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ABSTRACT

Three-dimensional electron microscopy allows scientists to study biological specimens and to understand how they behave and interact with each other depending on their structural conformation. Electron microscopy projections of the specimens are taken from different angles and are processed to obtain a virtual three-dimensional reconstruction for further studies. Nevertheless, the whole reconstruction process, which is composed of many different subtasks from the microscope to the reconstructed volume, is not straightforward nor cheap in terms of computational costs. Different computing paradigms have been applied in order to overcome such high costs. While classic parallel computing using mainframes and clusters of workstations is usually enough for average requirements, there are some tasks which would fit better into a different computing paradigm – such as grid computing. Such tasks can be split up into a myriad of subtasks, which can then be run independently using as many computational resources as are available. This chapter explores two of these tasks present in a typical three-dimensional electron microscopy reconstruction process. In addition, important aspects like fault-tolerance are widely covered; given that the distributed nature of a grid infrastructure makes it inherently unstable and difficult to predict.

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INTRODUCTION

Studying the structure of biological specimens on different levels is of vital importance in understanding their functionality and interactions. Different techniques like X-ray crystallography, nuclear magnetic resonance and electron microscopy (EM) are used for such purposes.

EM relies on the transmission electron microscope to obtain projection images of the specimen under study (Williams & Carter, 2004). Such projections are somewhat similar to the well-known medical radiographs – but with X-rays being substituted by highly energetic electron beams. The projections of the specimen are processed, using complex computational algorithms, to create a three-dimensional (3D) representation of the specimen that can then be thoroughly studied. 3D EM is therefore the result of applying certain computing algorithms to the 2D projections obtained from the specimen under study through the electron microscope (Frank, 2006).

Depending on the nature of the specimen and the problem under consideration, different reconstruction techniques are used. For example, when studying specimens in the cellular range, the so-called electron tomography (ET) is used. On the other hand, specimens in the macromolecular domain are usually studied through electron crystallography and single particle techniques, depending on their structural features (like, for example, symmetry).

The objectives of the work presented here is to develop and test computational tools which cope with high computational demands existing at different steps of a 3D reconstruction process. In particular, grid computing will be the computational platform chosen to tackle two different tasks; parameters optimization in algebraic reconstruction algorithms and the application of such algebraic algorithms in the 3D ET field.

BACKGROUND

Three-Dimensional Electron Microscopy and Computational Demands

A complete reconstruction process, from the rough projections to the reconstructed volume, involves a set of complex subtasks oriented towards reaching as high a resolution as possible. Most such subtasks pose computational challenges. For example, ET studies usually involve a small number of projections - with those normally being of considerable dimensions. Consequently, the reconstructed volume will also be large, resulting in high memory and processing power demands. On the other hand, single particle studies typically comprise a large number of smaller projections and while the required processing power is still huge, because of the large number of projections, memory requirements are, in turn, smaller.

High computational demands have usually been dealt with by using parallel computing techniques like message passing and shared memory. Nevertheless, many research groups do not have unlimited access to parallel computing facilities or available resources are simply insufficient for some problems. Here is where grid computing techniques could play an important role.

Progress of 3D EM techniques goes hand in hand with the development of new, more powerful computational software and hardware. Current studies use up to tens of thousands of projections to reach resolutions between 6 and 10 Angstroms (Valle et al., 2003; Gao et al., 2003; Cheng, Zak, Aisen, Harrison, & Walz, 2004). New, automated techniques for image processing will soon allow the use of hundreds of thousands of projections in a single study (Potter, Zhu, & Carragher, 2004). The final objective of the technique is to reach atomic resolutions (less than 3 Angstroms) (Henderson, 2004). It is estimated that, for this purpose, millions of projections could be needed

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