Chapter 9

High Performance and Grid Computing Developments and Applications in Condensed Matter Physics

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ABSTRACT

This chapter introduces applications of High Performance Computing (HPC), Grid computing, and development of electronic infrastructures in Serbia, in the South Eastern Europe region, and in Europe as a whole. Grid computing represents one of the key enablers of scientific progress in many areas of research. Main HPC and Grid infrastructures, initiatives, projects and programs in Europe, Partnership for Advanced Computing in Europe (PRACE) and European Grid Initiative (EGI) associations, as well as Academic and Educational Grid Initiative of Serbia (AEGIS) are presented. Further, the chapter describes some of the applications related to the condensed matter physics, developed at the Scientific Computing Laboratory of the Institute of Physics, University of Belgrade.

INTRODUCTION

Electronic Infrastructures (hereinafter: eInfrastructures) represent key enablers of modern scientific research and development of information society. eInfrastructures effectively consist of underlying computer networks and Distributed Computing Infrastructures (DCIs). Enabling large-scale innovative research, conducted through collaboration of distributed teams of scientist across the European Research Area (ERA), paves the way towards a long-term vision of a sustainable, transparent, ubiquitous electronic infrastructure open to a wide range of scientific user communities.

Numerical simulations in all fields of science are now necessary ingredient in research and development, offering the possibility of virtual, or in silico experiments, which become as important as

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the real experiments. On the other hand, theoretical models of most of complex systems studied today usually require sophisticated numerical simulations in order to compare their predictions with the experimental data. Therefore, computational science (not to be confused with computer science, which deals with algorithms, programming, and architecture of computer systems) that designates research related to numerical simulations and in silico, virtual experiments, is now well-established approach to research, at the equal footing to theory and experiment.

Detailed modelling and testing of realistic theories, as well as processing of huge amounts of data produced in large-scale experiments or derived from complex systems in nature or from social systems present a standing challenge for many decades. The almost exponential development of computer systems, in particular computer power of modern CPUs, had allowed computational science to become a reliable and favoured approach for research and development, now able to tackle realistic systems and to provide critical information in many industrial applications. However, to achieve this, supercomputers or large high performance computing systems are necessary, which can execute highly parallel algorithms, in which case we refer to High Performance Computing (HPC), or provide capacity of simultaneous calculation of huge numbers of independent tasks, in which case we speak about Grid computing. In this chapter we will briefly introduce these topics and describe in more details one application relevant to condensed matter physics.

HIGH PERFORMANCE COMPUTING: SUPERCOMPUTING

A supercomputer (Hoffman & Traub, 1989) is a computer at the frontline of current data processing capacity, particularly related to the speed of calculation. Supercomputers were introduced in the 1960s and at that time were designed primarily by Seymour Cray at Control Data Corporation (CDC), and later at Cray Research. While the supercomputers of the 1970s used only a few processors, in the 1990s, machines with thousands of processors began to appear and by the end of the 20th century, massively parallel supercomputers with tens of thousands of "off-the-shelf" processors were the norm.

Systems with a massive number of processors generally take one of two paths: in one approach, e.g. in Grid computing (Foster & Kesselman, 2004), the processing power of a large number of computers in distributed, diverse administrative domains, is opportunistically used whenever a computer is available. In another approach, a large number of processors are used in close proximity to each other, e.g. in a computer cluster. The use of multi-core processors combined with centralization is an emerging direction. Currently, Japan's K computer is the fastest in the world.

Supercomputers are used for compute-intensive tasks such as problems including quantum physics, weather forecasting, climate research, oil and gas exploration, molecular modelling (computing the structures and properties of chemical compounds, biological macromolecules, polymers, and crystals), and physical simulations (such as simulation of airplanes in wind tunnels, simulation of the detonation of nuclear weapons, and research into nuclear fusion).

Approaches to supercomputer architecture (Hill, Jouppi, & Sohi, 2000) have taken dramatic turns since the earliest systems were introduced in the 1960s. Early supercomputer architectures pioneered by Seymour Cray relied on compact innovative designs and local parallelism to achieve superior computational peak performance. However, in time the demand for increased computational power ushered in the age of massively parallel systems.

Supercomputers of the 21st century usually comprise of over 100,000 processors (some being general purpose graphical processing units) connected by fast computer networks. In such