

# Chapter 13

## Grids, Clouds, and Massive Simulations

**Levente Hajdu**

*Brookhaven National Laboratory, USA*

**Jérôme Lauret**

*Brookhaven National Laboratory, USA*

**Radomir A. Mihajlović**

*New York Institute of Technology, USA*

### ABSTRACT

*In this chapter, the authors discuss issues surrounding High Performance Computing (HPC)-driven science on the example of Peta science Monte Carlo experiments conducted at the Brookhaven National Laboratory (BNL), one of the US Department of Energy (DOE) High Energy and Nuclear Physics (HENP) research sites. BNL, hosting the only remaining US-based HENP experiments and apparatus, seem appropriate to study the nature of the High-Throughput Computing (HTC) hungry experiments and short historical development of the HPC technology used in such experiments. The development of parallel processors, multiprocessor systems, custom clusters, supercomputers, networked super systems, and hierarchical parallelisms are presented in an evolutionary manner. Coarse grained, rigid Grid system parallelism is contrasted by cloud computing, which is classified within this chapter as flexible and fine grained soft system parallelism. In the process of evaluating various high performance computing options, a clear distinction between high availability-bound enterprise and high scalability-bound scientific computing is made. This distinction is used to further differentiate cloud from the pre-cloud computing technologies and fit cloud computing better into the scientific HPC.*

### INTRODUCTION

Modern science is hard to imagine without massive computing support. Almost all recent significant discoveries were in a way a consequence of

great computation effort. Times of external wise Aristotelian observation and insightful scientific postulates, based on minimal measurements, are mostly a thing of the past. Scientific work and discoveries of Archimedes, Isaac Newton or Galileo, based on a few manual computations we may consider as legacy science.

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Throughout the later history of science, computing and computing machines have gradually crept into the scientific process. For instance, early sixteenth century astronomer Nicolaus Copernicus, in search of heavenly body trajectories, or nineteenth century geneticist Gregor Mendel, who was crossbreeding pea plants and describing their inherited traits, used pen and paper and abacus' to perform numerical processing of their measurement data. The mechanical calculators of the day, more sophisticated than the abacus, have started to emerge as scientific tools about the time of European renaissance. The seventeenth century has brought mechanical computing devices such as: multiplying bones, John Napier's bones, the slide rule, Pascaline, and Leibniz stepped-drum (Redin, 2012). Charles Xavier Thomas's arithmometer J. H. Muller's difference engine, Charles Babbage's analytical engine, and Thomas Fowler's ternary calculator of 1875, have followed, with much higher calculating power and even rudimentary programmability. One hundred years later, James D. Watson and Francis Crick have discovered the structure of DNA, and in 1990 the Human Genome Project has started identifying and mapping the three billion chemical base pairs that make up human DNA. DNA and genomic research tasks would not have been conceivable without modern electronic computing technology.

Geneticists were fortunate in as much as the computing technology required for the field has become available before the need for it emerged, or maybe, the research necessity has caused the introduction of adequate electronic computing. One may state that geneticists with their marvelous discoveries are standing on the shoulders, not of great biologist of the past, but on the shoulder of Babbage, Turing, von Neumann, and all others that have made modern electronic computing possible. This statement applies to almost all modern scientific disciplines, as a sort of meta science, computing science serves as a driving force propelling modern science in general. Among all scientific fields, the most prominent one, the

true field from which necessity has promoted the greatest computing discoveries, is physics, or more precisely, high energy and nuclear physics.

Working on the famous Manhattan Project (Manhattan Project Hall of Fame Directory, 2005), John von Neumann (in whose honor the Von Neumann computer architecture is named), Stanislaw Ulam, and others, faced the problem of how far a neutron would travel through a material before colliding with an atomic nucleus. The geometry was known along with all of the base data for the problem, however no deterministic mathematical solution could be found. Consequently, a quite unusual statistical technique was envisioned by Stan Ulam (Metropolis & Ulam, 1949). Since it required huge computational support, available only on electronic computers of that time, the implementation of the technique was delegated to Von Neumann. Due to the intense computations needed, one of the rare experts on electronic computing in the early 1940's, the key innovator in the field, John Von Neumann was invited to handle the problem. In March, 1945, at the Moore School of Electrical Engineering at the University of Pennsylvania, John von Neumann, nick named Johnny, also known as the first computer hacker ever (Myhrvold, 1999), professor of Mathematics at the Institute for Advanced Study and a consultant to Los Alamos Nuclear Center, with several associates, has initiated on the ENIAC machine, the first computer simulation project ever. The code name for the project was "Monte Carlo" (Metropolis, 1987). The method used in the project, also named "Monte Carlo" is still used today in a wide range of fields, from nuclear research, particle physics, modeling the flows of fluids, complex systems engineering to even finance and financial engineering.

This chapter is dedicated to the tight coupling relationship between high performance computing (HPC), massive computing simulations of the Monte Carlo type and high energy physics. By presenting an abbreviated historical background and some experience gained at Brookhaven Na-

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