CS267 Assignment 0

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1 About Me

I am a second-year Ph.D. student in Prof. Sayeef Salahuddin's group. My research is focused on applying density functional theory and other *ab-initio* physical methods to the study of semiconductor materials and other structures for use in emerging electronic device technologies. I currently use a number of off-the-shelf packages including Quantum Espresso and VASP to perform my calculations on large parallel computers. I am interested in taking the course to learn how to better write my own simulation tools in such a way that they take full advantage of the hardware.

2 Application of Parallel Computing: Nuclear Weapons Simulation

2.1 Background

In 1992, the United States ended the testing of all nuclear weapons. Since then, several international treaties have been signed codifying this test ban into law. The United States Department of Energy (DOE) is responsible for ensuring the reliability of the nuclear arsenal. With the impossibility of continuing to detonate real nuclear warheads, the National Nuclear Security Administration (NNSA, part of DOE) employs massive supercomputers to simulate the nation's weapons stockpile [2]. While many of the details surrounding this program are highly classified, there is enough publicly available information to piece together a rough picture of what is going on.

2.2 Computer Systems

Nuclear weapons simulation in recent years has been a driving force behind the acquisition of a number of very high performance supercomputers. Near the beginning of the Advanced Simulation and Computing Program (ASC) in 2001, four ASC machines were listed in the top eight machines on the Top500 list [3]. Even today when more general-purpose scientific computing has become more mainstream, NNSA still has several machines near the top of the list [5]. Sequoia, an IBM BlueGene/Q machine at Lawrence Livermore National Laboratories with 1572864 cores and a performance of over 16 petaflops, is currently the second most powerful computer in the world. Cielo, a Cray XE6 machine very similar to the Hopper computer used in class, is currently at position 18. Finally, Roadrunner, a hybrid Opteron/PowerXCell machine, is at position 22.

Though the codes running on the machines are classified, it can be assumed that they scale fairly well given that NNSA continues to request such large machines. While no actual nuclear weapons code is public, Sandia National Laboratories maintains a package called Trilinos which incorporates many tools used for building large robust scientific applications. Some of the capabilities of the Trilinos [1] package include: scalable linear algebra, linear and eigen solvers, meshing, load balancing, and I/O support. Given that the ASC logo is on the Trilinos homepage, it is very likely that this functionality mirrors what is used internally in classified code.

2.3 Examples of Involved Scientific Problems

2.3.1 Materials

According to the ASC history page [4], an example of a problem solved on large supercomputers is examining the effect of defects in the plastic-bonded explosive used to provide the intense heat and pressure required to initiate a fission reaction. If there are not enough defects, the explosive called HMX will not explode, rendering the device useless. If there are too many defects, the compound will be unstable and could lead to an accidental detonation.

2.3.2 Explosions

No publicly available information is available about actually simulating nuclear detonations, but it is easy to guess some of the variables studied. Most non-nuclear explosion simulations are based around some sort of continuum mechanics models that describe the compression and heating of the air around the explosion. Obviously the effect of radiation will come into play, but many simulation techniques are likely very similar to those used in traditional computational fluid dynamics.

References

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[2] Alex R. Larzelere II. Delivering insight: The history of the accelerated strategic computing initiative (asci). https://asc.llnl.gov/asc_history/Delivering_Insight_ASCI.pdf, 2002.

[3] Lawrence Livermore National Laboratory. The mission of the advanced simulation and computing program. https://asc.llnl.gov/asc_history/asci_mission.html, 2002.

[4] Lawrence Livermore National Laboratory. The role of asc in stockpile stewardship. https://asc.llnl.gov/asc_history/asci_role.html, 2002.

[5] Top500. Top 500 supercomputer sites. http://www.top500.org/, 2012.