Performance Programming Coursework: Serial Optimization of a Molecual Dynamics Program

Abstract

Keywords: Scientific programming, serial optimization, molecular dynamics, Fortran

1. Introduction

This paper documents the serial performance optimization conducted for a molecular dynamics program written in the Fortran programming language. The program reads data from n molecules as its input and iterates a predefined amount of steps. Each step the data of the molecules (e.g. force, position in a three dimensional space, velocity) is updated. The program counts collisions between molecules and writes the data for each molecule of the simulation out at certain, also predefined, intervals. The original version of the program is not optimized for computational efficiency.

This paper describes, documents and discusses the process of optimizing the original version of the program serially. The program was optimized for the Cirrus supercomputer, a tier-2 UK national supercomputer of the engineering and physical sciences research council, which is hosted and maintained by the EPCC (EPCC, 2020). The compiler used was Intel's Fortran compiler `ifort`, version 18.0.5 (Intel, 2018). The conducted optimizations range from choosing the appropriate compiler flags over rewriting performance critical sections of the program to hardware specific optimizations, like leveraging vectorization and cache optimizations. Since raw performance benefits are not all that is important for writing well performing and good programs, the maintainability and portability of the program are also looked at and discussed.

This paper continues in Section 2 with describing the molecular dynamics program in detail. Section 3 describes Cirrus and how the correctness of the program is tested with a regression test suite. Also the benchmark suite used for assessing the performance benefits of an optimization is outlined. Section 4 lists, describes and discusses all optimizations tested with their performance benefits. Afterwards, the results are discussed in Section 5. At least a conclusion is given in Section 6.

2. Molecular Dynamics Program

This section describes what the molecular dynamics program, which is optimized, does.

3. Setup

4. Optimizations

5. Discussion

6. Conclusion

References

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Intel. Intel Fortran Compiler 18.0 for Linux, 2018. URL https://software.intel.com/en-us/articles/intel-fortran-compiler-180-for-linux-release-notes-for-intel-parallel-studio-xe-2018.