CSCI596 (Scientific Computing and Visualization) Assignment 1—Molecular Dynamics
Due: September 8 (Fri), 2017, 11:59 pm

The purpose of this assignment is to familiarize yourself with the simple molecular dynamics (MD) program, md.c (and its linked-list cell variant, lmd.c). Note that, later in this course, you will need to be able to modify the programs in various projects such as visualization and parallelization. You will also perform basic scaling and performance measurements of the programs.

1. **(Scaling)** Perform a series of runs of the original md.c, in which the number of atoms is changed systematically. Note that the number of atoms is $nAtom = 4 \times InitUcell[0] \times InitUcell[1] \times InitUcell[2]$. Try a sequence, $InitUcell[] = \{4,4,4\}$, $\{5,5,5\}$, ..., $\{10,10,10\}$, for which $nAtom = 256, 500, ..., 4000$. (Set StepLimit = 10 and StepAvg = 11, and make sure the constant $NMAX$ in md.h is set larger than $nAtom$.) Plot the elapsed time per MD step as a function of the number of atoms. Fit the measured elapsed time T to the formula, $T = C \times nAtom^p$, and find the power p (C is the other fitting parameter). Is your measured scaling, $T = O(nAtom^p)$, close to $O(nAtom^2)$?

    Also perform the same measurement for lmd.c. Is your measured scaling now close to $O(nAtom)$?

2. **(Flop/s Performance)** Performance of a program is often measured in MFlop/s (megaflop/s = million floating point operations per second). Let's choose $InitUcell = \{10,10,10\}$ (or $nAtom = 4000$) and measure the elapsed time of lmd.c. Count the number of floating point operations ($+$, $-$, $*$, $/$) executed (for simplicity, count $sqrt()$ as 1 operation). Divide the resulting number by the elapsed time (in seconds) to obtain the program's Mflop/s performance (also do not forget to divide the number by 10^6). Submit the Mflop/s performance as well as the machine information (processor, clock speed, *etc.*).

*   For the explanation of input parameters such as *StepLimit* and *DeltaT*, read the include file md.h. Leave all input parameters, which are not explicitly mentioned above, unchanged from the default values in the md.in at the course home page.