CSCI653 Assignment 2—Fast Multipole Method

Due: 11:59 pm, Monday, September 15, 2025

The purpose of this assignment is to acquire a good sense of computational complexity and floating-point performance, which are central to high performance computing (HPC), using the N-body problem and fast multipole method (FMM) [*Journal of Computational Physics* **73**, 325 (1987)] as an example. Use the program fmm2d.c (https://aiichironakano.github.io/cs653/src/FMM), which evaluates the electrostatic potential at all particles' positions for a 2-dimensional system of charged particles using both $O(N)$ FMM and $O(N^2)$ direct sum. For this assignment, you can use any computer, which has a C compiler.

1. ***Computational complexity*:** Perform a series of runs of the original fmm2d.c, in which the problem size (*i.e.*, the number of particles) is changed systematically: $N_{\text{par}} = 4{,}000\times4^{L-5}$, where the quadtree height L = 5, 6, 7 (*i.e.*, corresponding N_{par} = 4,000, 16,000, 64,000). Plot the elapsed wall-clock time T as a function of N_{par}. Fit the measured T to the formula, $T = C\times N_{\text{par}}^{p}$, and find the power p for both FMM and direct calculations (C is the other fitting parameter). Explain the observed power in the light of computational complexity.

   Submit the plot, fitted power and your explanation.

2. ***Flop/s Performance*:** Performance of a program is often measured in Gflop/s (gigaflop/s = billion floating-point operations per second). Modify fmm2d.c so as to count the number of floating-point operations (+, −, *, /) executed separately for FMM and direct calculations. Though it is difficult find how many operations are performed within math-library functions, for simplicity, here let us count *sqrt*(), *log*() and *atan*() functions as *FSQRT* = 10, *FLOG* = 10 and *FATAN* = 10 operations. Run the modified program for L = 6 and $N_{\text{par}} = 4{,}000\times4^{6-5}$ = 16,000. Divide the resulting number by the elapsed time (in seconds), then divide that number further by 10^9, to obtain the Gflop/s performance for both FMM and direct calculations.

   Submit the modified program and the measured Gflop/s performance along with the machine information (processor, clock speed, etc.).