ICOM 6025/CIIC 5019 – High Performance Computing
Programming Assignment #2: Open-MP

In the simulation of a collection of soft particles (such as proteins in a fluid), there is a repulsive force between a pair of particles when they overlap. The goal of this assignment is to use parallel computing to accelerate the computation of these repulsive forces, using multiple cores with Open-MP.

In the force repulsion function, the particles are assumed to have unit radius. The particles are in a "simulation box" of dimensions L × L × L. The dimension L is chosen such that the volume fraction of particles is $\phi = 0.3$. The simulation box has periodic (wrap-around) boundary conditions, which explains why we need to use the remainder function to compute the distance between two particles. If the particles overlap, i.e., the distance s between two particles is less than 2, then the repulsive force is proportional to $k(2-s)$ where k is a force constant. The force is along the vector joining the two particles.

1. Write a program that tests the correctness of your code. This can be done by computing the correct forces and comparing them to the forces computed by your optimized code. Give evidence in your report that your program works correctly using your test program.

2. How much faster is your accelerated code compared to the provided baseline code? Include timings for different problem sizes.

3. Use different thread scheduling policies (static, dynamic, guided) and chunk sizes for problems of different sizes (100, 1000, 10000, and 100000 particles). The goal is to find the fastest strategy for different problem sizes. Use graphs to plot your results. You are also free to modify the code any way you wish to try to reduce computation time.

Deliverables (parallel code & report)