Foundations of HPC

@ Data Science and Scientific Computing 2021-2022

Assignment B, to be done by students that did not submit the partial assignment in due date.

Note: you can choose either this assignment A or the other assignment B that you find in ../1/

In this assignment you are requested either to
A) **implement the solution to the proposed problem both a MPI and a OpenMP code.* (so, we do expect 2 codes).**
B) **Implement the solution with an hybrid MPI+OpenMP code.**

The candidate is required to develop a parallel code that

1. Computes the **local density** ρ of a given 3D distribution of N_p particles.
   The local density is calculated at the node points of a regular 3D grid with grid number N, and it is defined as the number of particles that lie within a sphere of radius R centred at every grid node point; the grid number N and the radius R are parameters acquired at the command line.
2. Evaluate a **"potential-like function"** at every point's coordinates for all the N_p particles.
   The V_i function is defined as

$$V_i = \sum_{j=0, j\neq i}^{N_p} \frac{1}{r_{ij}}$$

   where r_{ij} is defined as the distance between particles i and j, $r_{ij} = \|\mathbf{r}_i - \mathbf{r}_j\|$.

The input distribution is acquired from an external binary file whose format is specified below. The code must be able to generate a random distribution of particles in case that no external input file is provided.
The code must have a the following command line: `executable N R [input file]`.

Format of the input file

The input file is a binary file whose first 4 bytes are an integer that specifies the number N_p of particles contained in the file. Following, 3 single-precision floating-point coordinates are present for each particle. The coordinates are the *x*, *y* and *z* position of the point in space and the condition $0 \leq x, y, x < 1$ holds, i.e. points are all generated in a cubic box of side 1 with one vertex in the origin.

Required output
Two output files are required, one for the density values and one for the potential values.
Density file
The first 4 bytes must be an integer that specifies the grid number N. The file will then contain N^3 single-precision floating-points. The grid points are supposed to be written in row-major

order; i.e. starting from the grid point $(0,0,0)$ the fastest coordinate changing is the z: $(0,0,0),\ (0,0,1),\ \cdots,(0,0,N-1),\ (0,1,0),\ \cdots,\ (0,1,N-1),\ \cdots$.

Potential file

The first 4 bytes must be an integer that specifies the number N_p of points. Then a quadruplet $\{x_i, y_i, z_i, V_i\}$ will follow for each point with single-precision floating-point numbers.

Additional requirements

1. The candidate must assess the behaviour of the code when the *size* of the problem changes while the number of MPI tasks / OpenMP threads is fixed. Specifically, he/she must assess the behaviour of the code for a random distribution:
    - when the grid number N is fixed and the number N_p of input particles grows (hint: let R vary as a function of the mean inter-point separation $1.0/N_p^{1/3}$);
    - when the number N_p of particles and the value of R are fixed and the grid number N grows.
2. The candidate should provide either a Makefile or a shell script named `compile` to compile the code whose executable name must be `density`.