Foundations of MHPC, 2020/2021

Additional project required to access the oral examination for students that did not complete the course assignments

The candidate must submit the code developed to solve the following problem within 30 days from receiving it, following the instruction given by the instructors.

The candidate is required to develop a parallel code that computes the local density of a given 3D distribution of points. Both an MPI and an OpenMP version must be delivered (or a hybrid MPI+OpenMP version).

The input distribution is acquired from an external binary file whose format is specified below. 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 points 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.

The code must be able to generate a random points distribution in case that no external input file is provided. Then, the code must require this 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 of points contained in the file. Following, 3 single-precision floating-point coordinates follows for each point. 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
The output required is a binary file that contains the value of the density at each grid point. The first 4 bytes must be an integer that specifies the grid number N. The file will 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 coordnate changing is the z:
$(0,0,0),\ (0,0,1),\ \cdots, (0,0,N-1),\ (0,1,0),\ \cdots,\ (0,1,N-1),\ \cdots.$

Additional requirements

1. The candidate must assess the behviour 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 of input points *n* grows (hint: let R vary as a function of the mean inter-point separation $1.0/n^{1/3}$);
    - when the number of points *n* 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`.

At the moment of submission, the code provided by the candidate will be tested against a points distribution whose result is known.