## High Performance Computing for Science and Engineering I

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## Tutorial Session: N-body solver with MPI

In this task you will implement an N-body solver describing a system of positively charged inertialess particles with MPI parallelization. The provided skeleton code

- seeds N particles on a unit circle

$$\mathbf{x}_i = (x_i, y_i) = \left(\cos \frac{2\pi i}{N}, \sin \frac{2\pi i}{N}\right), \qquad i = 0, \dots, N - 1;$$

distributing them over P ranks such that each rank takes N/P particles (assume N is divisible by P);

- performs multiple time steps calling functions Step() and PrintStat();
- writes the particle positions to files init.dat and final.dat.
- a) Implement Step() which computes the forces and advances the particles

$$egin{aligned} oldsymbol{f}_i &= \sum_{\substack{j=0\j
eq i}}^{N-1} rac{oldsymbol{x}_i - oldsymbol{x}_j}{|oldsymbol{x}_i - oldsymbol{x}_j|^3}, \ oldsymbol{x}_i^{t+1} &= oldsymbol{x}_i^t + \Delta t \, oldsymbol{f}_i^t, \end{aligned}$$

where  $|\boldsymbol{x}| = \sqrt{x^2 + y^2}$  and  $\Delta t$  is a given time step.

Each rank can make  $\mathcal{O}(P)$  MPI calls<sup>1</sup> and use  $\mathcal{O}(N/P)$  bytes of memory. Your solution will be given more points for overlapping communication and computation. You may use make to build the executable, make run to run it on 2 processors and make plot to create image.png with particle positions as shown in Figure 1.

Notation  $p = \mathcal{O}(q)$  means that p < Mq for a large enough constant M.

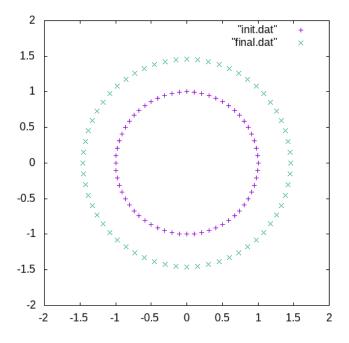


Figure 1: Expected output image.png produced by make plot.

b) Implement PrintStat() which computes and prints the mean and variance of the radial distance  $r_i = |{m x}_i|$ 

$$\mu = \frac{1}{N} \sum_{i=0}^{N-1} r_i,$$
 
$$\sigma^2 = \frac{1}{N} \sum_{i=0}^{N-1} r_i^2 - \mu^2.$$

Expected output after 10 time steps:

mean=1	var=0
mean=1.0672	var=6.6613e-16
mean=1.1261	var=6.6613e-16
mean=1.1791	var=0
mean=1.2274	var=-8.8818e-16
mean=1.272	var=8.8818e-16
mean=1.3135	var=-2.2204e-16
mean=1.3524	var=4.4409e-16
mean=1.3891	var=4.4409e-16
mean=1.4239	var=1.3323e-15
mean=1.4571	var=0

The values may depend on P and the implementation but the absolute difference should be below  $10^{-3}$  for the mean and  $10^{-14}$  for the variance.