Tutorial Session: Coding Exercises on MPI

Question 1: Monte Carlo

Monte Carlo integration is a method to estimate the value of an integral as the mean over a set of random variables. For instance,

$$\int_\Omega f(x)\,dx \;\approx\; \frac{|\Omega|}{N}\sum_{i=1}^{N} f(X_i),$$

where X_i are samples from a uniform distribution on the domain Ω. The algorithm can be applied for calculation of volume of arbitrary shapes, in which case the integrand is the indicator function. For a unit circle centered at $(0, 0)$, it has the form

$$f(x,y) = \begin{cases} 1, & x^2 + y^2 < 1, \\ 0, & \text{otherwise.} \end{cases}$$

Therefore, the number π can be estimated as

$$\frac{1}{N}\sum_{i=1}^{N} f(X_i, Y_i) \approx \pi$$

where X_i and Y_i are samples from uniform distribution on the square $[0, 1] \times [0, 1]$. You are given a serial code that computes this integral. Parallelize it with MPI.

Question 2: Quadratic Form

Parallellize with MPI the computation of the quadratic form

$$Q = \sum_{i=0}^{N-1}\sum_{j=0}^{N-1} v_i A_{ij} w_j \tag{1}$$

for a matrix $A \in \mathbb{R}^{N\times N}$ and two vectors $v, w \in \mathbb{R}^N$.

Question 3: Poisson Equation and Jacobi Method

We are interested in solving the Poisson equation

$$\frac{d^2u}{dx^2} = f(x)\ ,\ \ u(0) = u(L) = 0, \tag{2}$$

for a scalar quantity $u : [0, L] \to \mathbb{R}$ and the following right-hand side

$$f(x) = \exp\left[-(x - L/2)^2\right]. \tag{3}$$

To do so, we employ a grid of N points and define

$$u_i = u\left(i\Delta x\right) \quad , \quad f_i = f\left(i\Delta x\right), \tag{4}$$

where $\Delta x = \frac{L}{N-1}$ is the grid spacing. Using this definition and the fact that

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

we discretize eq. (2) as follows

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} = f_i \tag{5}$$

which is valid for the inner points $i = 1, \ldots, N-2$. For the points on the boundary, we set

$$u_0 = u_{N-1} = 0. \tag{6}$$

Equation (5) corresponds to a linear system of $(N-2)$ equations with an equal number of unknowns. We will solve this system with the iterative Jacobi method. First, we rewrite eq. (5) as

$$u_i^{m+1} = \frac{1}{2}\left(u_{i+1}^m + u_{i-1}^m - \Delta x^2 f_i\right) \tag{7}$$

where we simply solved for u_i and added a superscript m. The iterative Jacobi method performs iterations with eq. (7) for $m = 0, 1, \ldots$ until

$$E_m = \sum_{i=0}^{N-1} \left|u_i^{m+1} - u_i^m\right| < \epsilon \tag{8}$$

where $\epsilon = 10^{-6}$ is a user-defined threshold. Note that we set $u_i^0 = 0$.

You are given a skeleton code that solves the Poisson equation with the method described above. Parallelize the code with MPI.