

Set 5 - MPI Part II

Issued: November 23, 2022

Hand in (optional): December 6, 2022 08:00

Grading: To get full credits solve any two of the questions.

Question 1: Diffusion (100 points)

The diffusion of a substance can be described by the equation

$$\frac{\partial c(x, y, t)}{\partial t} = D \left(\frac{\partial^2 c(x, y, t)}{\partial x^2} + \frac{\partial^2 c(x, y, t)}{\partial y^2} \right),$$

where c is the concentration of the substance at position (x, y) and at time t , and D is the diffusion constant. The diffusion process happens in the domain $|x| < L/2$ and $|y| < L/2$. The concentration is zero on the boundaries of the domain. The initial concentration is

$$c(x, y, 0) = \begin{cases} 1, & \text{if } |x| < L/4 \text{ and } |y| < L/4, \\ 0, & \text{otherwise.} \end{cases}$$

- a) The skeleton code solves the equation on a uniform grid using a central finite difference scheme in space and forward Euler time integration. Parallelize the code by filling parts marked by `TODO` in the functions `advance` and `main`. Use a tiling decomposition scheme (i.e., distribute the rows evenly to the MPI processes). How to run the code:
- make to compile the code
 - make run to run single core (please not in the login node on euler!). If not locally on the laptop, use `sbatch launch_single.sh` to submit a job via slurm.
 - to run multicore use: `mpirun -n x ./diffusion D L N`. You can also use `sbatch launch_single.sh` to submit a job via slurm.
- b) For a given time compute the integral of $c(x, y, t)$ over the domain (total ammount of the substance). Fill the missing MPI parts in `compute_diagnostics`, and plot the result as a function of time using $D = 1$, $L = 2$ and $N = 100$. When run correctly, the code will output file called `diagnostics.dat`. To plot this data use `python plot_diagnostics.py` (module load python).
- c) For a given time compute the histogram of $c(x, y, t)$ in the function `compute_histogram` by implementing the missing MPI parts marked by `TODO`, and plot or print the resulting histogram for $t = 0.5$ using $D = 1$, $L = 2$ and $N = 100$.

- d) Suggest other ways to divide the real-space domain between processes with the aim of minimizing communication overhead. Prove your argument by computing the message communication size for the tiling domain decomposition and for your suggestion.
- e) Make a strong and weak scaling plot up to 48 cores. Justify what is happening in your plots. Make at least five different numbers of cores runs (e.g. [1, 12, 24, 36, 48] or [1, 2, 4, 8, 16]). For the strong scaling plot use: $N = \{1024, 2048, 4096, 8192\}$, in other words, plot at least four lines (if too slow use smaller N 's). For the weak scaling plot, use $N = 1024$ and $N = 2048$ (if those are taking too long use smaller N 's). Use $D = 1$, $L = 2$ and modify the number of timesteps $\text{step} = 100$. Do not forget to state which CPU you ran the tests on! You can use the `run.sh` script to run for different number of cores. On euler use `run.sh` via `sbatch launch.sh`. Draw the plots either directly on the paper (which is the way you will do it on the exam). Or use any desired plotting scripts.