Assignment - 2

Assigned: 2^{nd} April 2024 Due: 12^{th} April 2024 Max. marks: 100

General Instructions

- Submit a hard-copy of the solutions either in-class or in TAs office NAC-1, Room no. 322.
- Upload a scanned copy of the solutions and the codes you have developed as a single zipped folder on Moodle.
- Do not email your solutions/codes. Emailed submissions will not be graded.

Programming Questions

1. (40 points) Consider the following one-dimensional first-order traveling wave equation that convects to the right,

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0, \tag{1}$$

with $c = 1.0$ in a domain of length $L = 2.0$. The initial condition for the wave is given as follows,

$$u(x, t = 0) = u_0(x) = \left\{ \begin{array}{ll} \sin(4\pi x), & \text{for } 0 \le x \le 0.5 \\ 0, & \text{for } 0.5 \le x \le 2.0 \end{array} \right\}.$$

The exact solution at any time instant, t, is given by $u(x,t) = u_0(x - ct)$. Consider the numerical solution of this equation using Euler explicit time integration method and two different spatial discretization schemes (i) first-order upwind scheme and (ii) third-order accurate QUICK scheme. The Euler explicit time discretization is given as follows:

$$\frac{\partial u}{\partial t} \approx \frac{u_i^{n+1} - u_i^n}{\Delta t}, \tag{2}$$

and the first-order upwind scheme is given by,

$$\frac{\partial u}{\partial x} \approx \frac{u_i^n - u_{i-1}^n}{\Delta x}, \tag{3}$$

and the QUICK scheme is given by,

$$\frac{\partial u}{\partial x} \approx \frac{1}{\Delta x}\left(\frac{3}{8}u_i^n - \frac{7}{8}u_{i-1}^n + \frac{1}{8}u_{i-2}^n + \frac{3}{8}u_{i+1}^n\right) \tag{4}$$

where Δx is the grid spacing and Δt is the time-step and they can be taken as $\Delta x = 0.002$ and $\Delta t = 0.0001$. The boundary conditions on the left and right-ends of the domain are given as $u(x = 0, t) = 0$ and $u(x = L, t) = 0$. Use upwind scheme for the near boundary point ($x = \delta x$) where QUICK scheme cannot be applied.

   (a) Develop a serial program to solve this problem using upwind and QUICK schemes. Plot the analytical solution and the numerical solution obtained at several times $t = 0, 0.5, 1.0$ in the same graph.

   (b) Develop an MPI program to solve this problem using both the spatial discretization schemes as above. Plot the analytical solution and the numerical solutions at times $t = 0, 0.5, 1.0$ in the same graph for number of threads $p = 2$ and 4. Use appropriate number of halo/virtual points on both sides of the parallel domains.

   (c) Comment on the differences observed between the solutions for upwind and QUICK schemes.

2. (60 points) Consider the solution of the following Poisson equation,

$$\nabla^2\phi = -q; \quad q = (x^2 + y^2); \tag{5}$$

in the domain shown in Figure 1 and the boundary conditions are as specified in the figure. The discretized equation using Jacobi or Gauss-Seidel method can be written as follows,

$$\phi_{i,j}^{(k+1)} = \frac{1}{4}\left[\phi_{i+1,j}^{(k)} + \phi_{i-1,j}^{(k),(k+1)} + \phi_{i,j+1}^{(k)} + \phi_{i,j-1}^{(k),(k+1)}\right] + \frac{\Delta^2}{4}q_{i,j} \tag{6}$$

where $\Delta = \Delta x = \Delta y$. Consider an initial guess of $\phi(x, y) = 0$ everywhere. Use double precision arithmetic. On the $x = 1$ boundary, approximate the first derivative $\frac{\partial\phi}{\partial x}$ using the second-order accurate one-sided formula as given below,

$$\phi_i = \frac{4\phi_{i-1} - \phi_{i-2}}{3} \tag{7}$$

(a) Develop a serial program using Jacobi iterative method. Test your program using $\Delta = \Delta x = \Delta y = 0.1$ (that is 21 points along each of the directions). Report the number of iterations for the solution between successive iterations to converge to 10^{-4}, using any norm. Plot the numerical solution of ϕ vs x for $y = 0.0$ and ϕ vs y for $x = 0.0$.

(b) Develop an MPI program using Jacobi iterative method. Test your program using $\Delta = \Delta x = \Delta y = 0.01$ (that is 201 points along each of the directions). Report the number of iterations for the solution between successive iterations to converge to 10^{-4}, using any norm. Plot the numerical solution obtained using the Jacobi iterative method run on parallel system using $p = 2, 4, 8$ for ϕ vs x for $y = 0.0$ and ϕ vs y for $x = 0.0$. Use a one-dimensional domain decomposition (either row-wise block decomposition or column-wise block decomposition on the two-dimensional mesh) only. In the same plots compare the parallel solution obtained with the serial solution for the same grid sizes of 0.01.

(c) Repeat the above step using Gauss-Seidel red-black coloring approach. Comment on the number of iterations required by Gauss-Seidel when compared the Jacobi method.

(d) Run parallel versions of the Jacobi and Guass-Seidel methods for $\Delta = 0.005$ using $p = 2, 4, 8$ and 16 threads. Plot the speed-up, $\psi(n, p)$, obtained by each of the methods as a function of the number of processors. Do you see any improvement in performance? Which method is better? Comment on the speedup obtained as the problem size is increased.

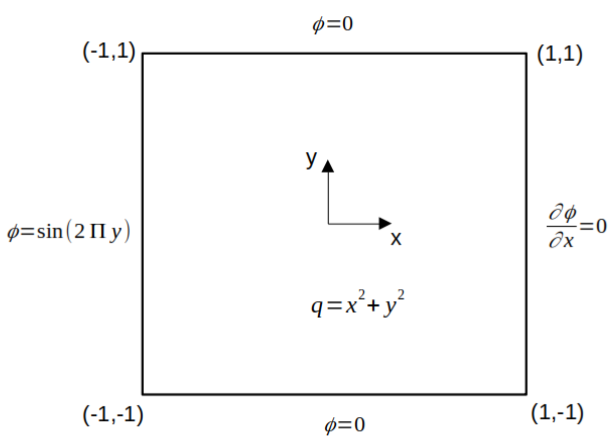

Figure 1: Domain and boundary conditions for Poisson equation