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Set 4 - Diffusion and OpenMP

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Question 1: Diffusion in 2D

Heat flow in a medium can be described by the diffusion equation

$$\frac{\partial \rho(x,y,t)}{\partial t} = D\nabla^2 \rho(x,y,t), \tag{1}$$

where $\rho(x,y,t)$ is a measure for the amount of heat at position (x,y) and time t and the diffusion coefficient D is constant.

Lets define the domain Ω in two dimensions as $\{x,y\} \in [-1,1]^2$. Equation 1 then becomes

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

Equation 2 can be discretized with a central finite difference scheme in space and explicit Euler in time to yield:

$$\frac{\rho_{r,s}^{(n+1)} - \rho_{r,s}^{(n)}}{\delta t} = D\left(\frac{\rho_{r-1,s}^{(n)} - 2\rho_{r,s}^{(n)} + \rho_{r+1,s}^{(n)}}{\delta x^2} + \frac{\rho_{r,s-1}^{(n)} - 2\rho_{r,s}^{(n)} + \rho_{r,s-1}^{(n)}}{\delta y^2}\right) \tag{3}$$

where $\rho_{r,s}^{(n)} = \rho(-1 + r\delta x, -1 + s\delta y, n\delta t)$ and $\delta x = \frac{2}{N-1}$, $\delta y = \frac{2}{M-1}$ for a domain discretized with $N \times M$ gridpoints.

We will use open boundary conditions

$$\rho(x,y,t) = 0 \quad \forall\, t \geq 0 \,\text{and}\, (x,y) \notin \Omega \tag{4}$$

and an initial density distribution

$$\rho(x,y,0) = \begin{cases} 1 & |x,y| < 1/2 \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

a) Analyze the stability of the scheme given in Equation 3 using the von Neumann stability analysis.

b) Parallelize your code from Exercise 2a using OpenMP and make both strong and weak scaling plots up to 24 cores. Define the problem size as the number of grid points in the discretization of Ω. Try different problem sizes for the scaling plots, do they affect the scaling? Try using both the gcc OpenMP and the Intel OpenMP libraries. Can you see a difference?

The total amount of heat in the system $N(t)$ and the second moment of the cloud $\mu^2(t)$ at a time t can be computed as

$$N(t) = \int_\Omega dx\, dy\, \rho(x, y, t), \qquad \mu^2(t) = \int_\Omega dx\, dy\, \rho(x, y, t)(x^2 + y^2). \tag{6}$$

c) Make a plot of the time evolution of $N(t)$ and $\mu^2(t)$ for $D = 1, 2, 5$ and $t \in [0, 10]$. What is the effect of the boundary? What is the effect of D?