P. Koumoutsakos
ETH Zentrum, CLT E 13
CH-8092 Zürich

Fall semester 2019

Set 6 - 2D Diffusion Processes with Structured Grids and Particles

Issued: December 6, 2019
Hand in (optional): December 20, 2019 08:00am

Question 1: Diffusion in 2D using ADI scheme (50 points)

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

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

where $\phi(x,y,t)$ is a measure for the amount of heat at position $\boldsymbol{r}$ and time t. The diffusion coefficient D describes how fast heat can spread in the medium and is constant for this task. You can think of D in a similar way as you would for the kinematic viscosity of a fluid, which describes whether a fluid behaves more like honey or water, for example. We define the domain Ω for two dimensions as $x, y \in [-1,1]$. The boundary conditions are:

$$\phi(x,y,t) = 0 \quad \forall\, t \geq 0 \,\text{and}\, (x,y) \in \partial\Omega, \tag{2}$$

and the initial condition is:

$$\phi(x,y,0) = \begin{cases} 1 & |x,y| < 1/2 \\ 0 & \text{otherwise.} \end{cases} \tag{3}$$

a) (15 points) Discretize Eq. (1) using the Alternating Direction Implicit (ADI) scheme. Write down the resulting system in matrix form. What do you observe? Comment on your choice of method/algorithm for the solution of the resulting implicit scheme and explain why this choice is justified.

b) (20 points) Use the provided skeleton code (`diffusionADI.cpp`) to solve the 2D diffusion problem on a uniform grid. Implement the missing code parts in all sections marked by `TODO`. Use Thomas algorithm for the solution of the implicit systems resulting from the ADI scheme.

c) (10 points) Parallelize your code using OpenMP. Comment on any complexity that would arise if you chose to parallelize the ADI scheme with MPI.

d) (5 points) Compute an approximation to the integral of ϕ over the entire domain in `compute_diagnostics` and plot the result as a function of time using the parameters $D = 1$, $L = 2$ and $N = 256$. Generate three plots on top of each other for the time step size $\Delta t = 0.1$, $\Delta t = 0.01$ and $\Delta t = 0.001$. Explain what you observe.

Question 2: Diffusion with Particle Strength Exchange (50 points)

Consider again a scalar two-dimensional field $\phi(x, y, t)$ now defined on a periodic domain $(x, y) \in [0, 1)^2$. We want to utilize the Particle Strength Exchange (PSE) method to solve the diffusion equation in Eq. (1) for a given initial condition $\phi(x, y, t = 0)$.

Instead of discretizing the field ϕ on a grid as in the previous task, we will use a collection of N particles. A particle represents a small "volume" of the field, and is defined by its position $\mathbf{x}_i$ and field value $\phi_i = \phi_i(t)$. In this exercise we assume the volume of each particle is equal ($V_i = V_{\text{total}}/N = 1/N$).

We utilize the PSE method and rewrite Eq. (1) as a system of ODEs on particles:

$$\frac{\mathrm{d}\phi_i}{\mathrm{d}t} = \frac{D}{\varepsilon^2} \sum_j V_j \left(\phi_j - \phi_i\right) \eta_\varepsilon(\mathbf{x}_j - \mathbf{x}_i), \tag{4}$$

where $\eta_\varepsilon(\mathbf{r})$ is a kernel representing the Laplacian operator, and ε a scale constant. In this exercise we consider the following kernel:

$$\eta_\varepsilon(\mathbf{r}) = \frac{1}{\varepsilon^2}\eta\left(\mathbf{r}/\varepsilon\right), \qquad \eta(\mathbf{r}) = \frac{4}{\pi}e^{-|\mathbf{r}|^2}. \tag{5}$$

You are given a skeleton code that initializes the particle positions and values. As a placeholder for the final timestep, the skeleton code simply decays the values ϕ_i in time. Get familiar with the skeleton code. Use `make run` and `make plot` to run the code and test the plotting script.

Hint: The plotting script requires numpy, matplotlib and ffmpeg.

a) (20 points) We assume a one-dimensional field $\phi(x, t)$ for this sub-task. Derive Eq. (4) by using the method of Particle Strength Exchange.

b) (20 points) Extend the provided skeleton code to compute the right-hand side of Eq. (4) using Eq. (5) for the kernel η_ε. Account for a periodic domain when computing the distance between two particles!

c) (10 points) Implement the forward Euler scheme for the integration of the Eq. (4).