Homework 5
2D Diffusion MPI

HPCSE I
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CSE**lab**
Computational Science & Engineering Laboratory
http://www.cse-lab.ethz.ch

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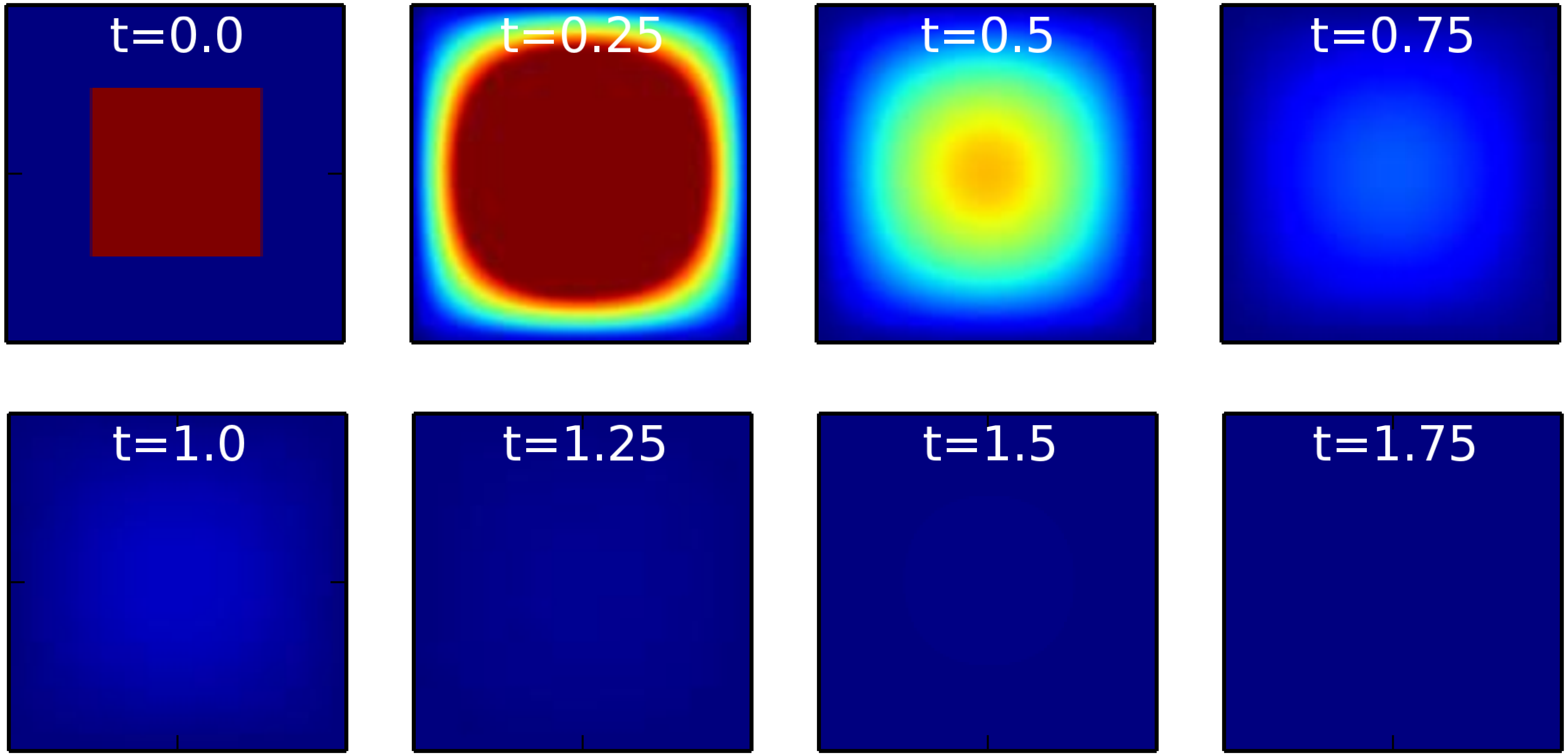
Question 1: Diffusion

Given:
- Initial concentration in a 2-D plate.
- Boundary conditions along the boundaries of the plate.

Find:
- Concentration in the plate as a function of **time** and **position**.

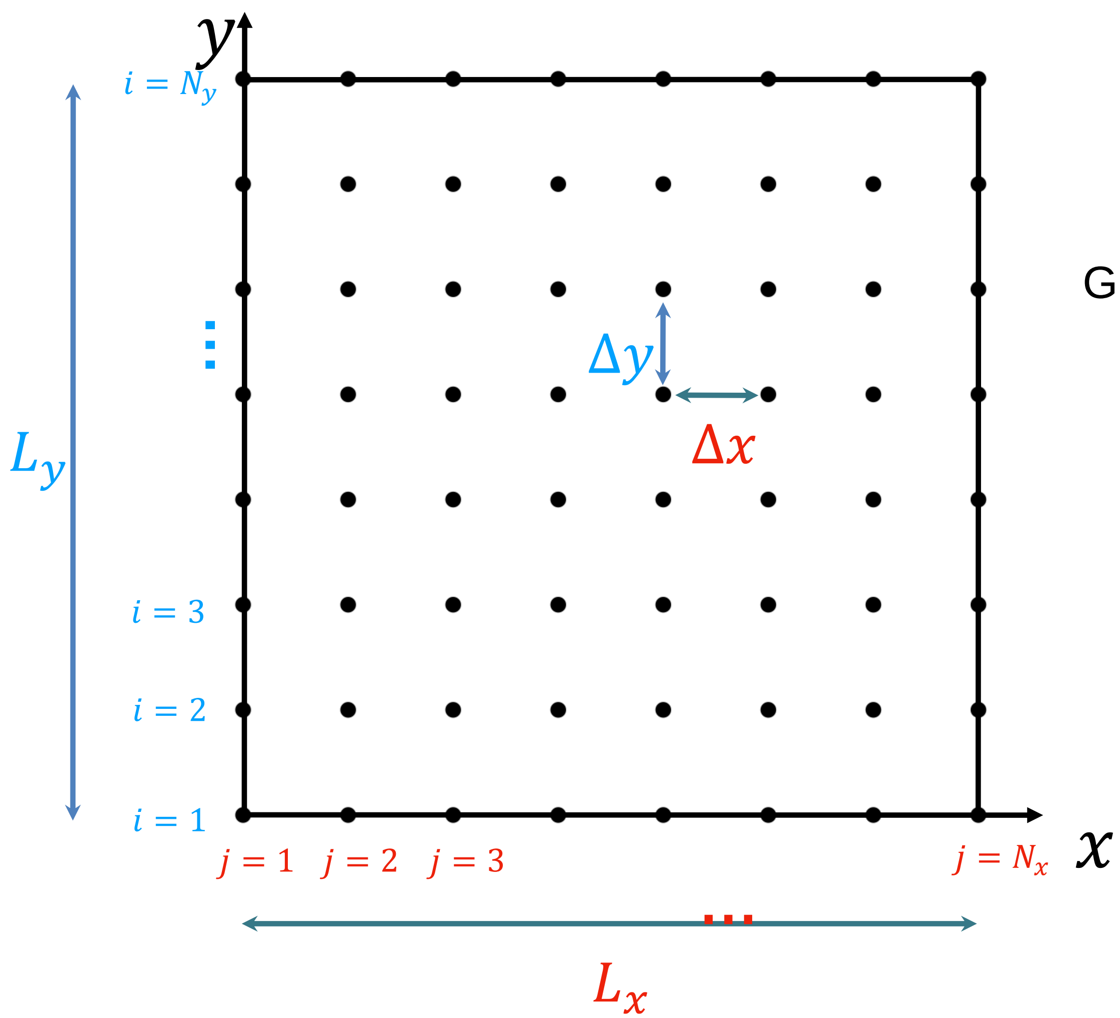
Initial Condition



Fully homogeneous material

Discretizing a 2D Space - Grids

1. Spatial discretization



Grid spacing:

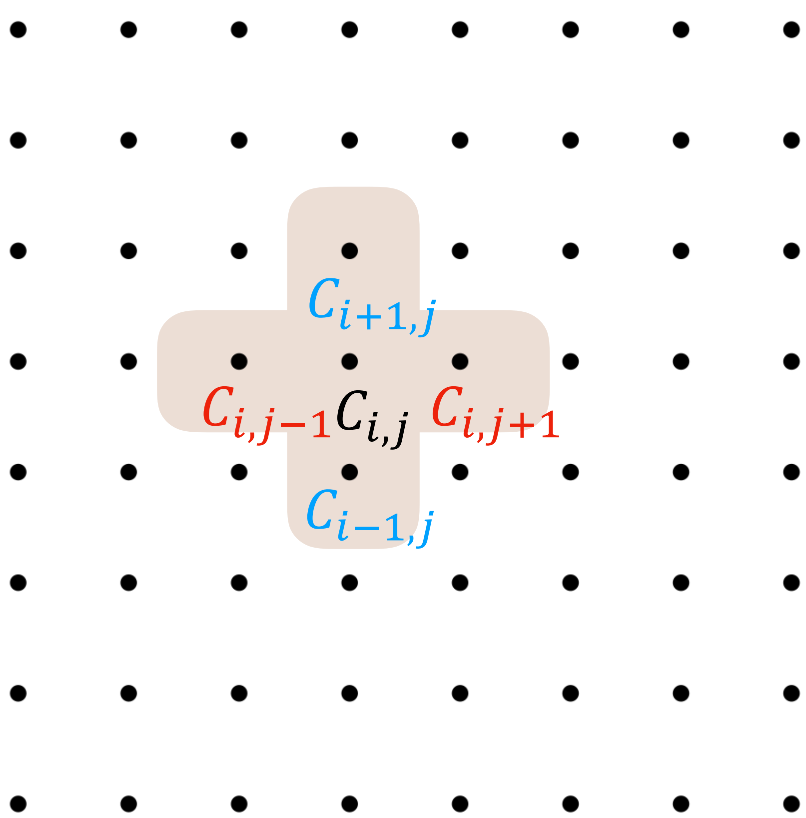
$$\Delta x = \frac{L_x}{N_x - 1}$$

$$\Delta y = \frac{L_y}{N_y - 1}$$

Spatial discretization: Central finite differences

1. Spatial discretization: using *central finite difference* scheme.

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



$$\approx D\left(\frac{C_{i,j-1} - 2C_{i,j} + C_{i,j+1}}{\Delta x^2} + \frac{C_{i-1,j} - 2C_{i,j} + C_{i+1,j}}{\Delta y^2}\right)$$

Time discretization: explicit Euler

2. Time discretization: using *explicit Euler* scheme.

$$\boxed{\frac{\partial C(x,y,t)}{\partial t}} = D\nabla^2 C(x,y,t)$$

time index

$$\frac{\partial C(x,y,t)}{\partial t} \approx \frac{C^{n+1} - C^{n}}{\Delta t}$$

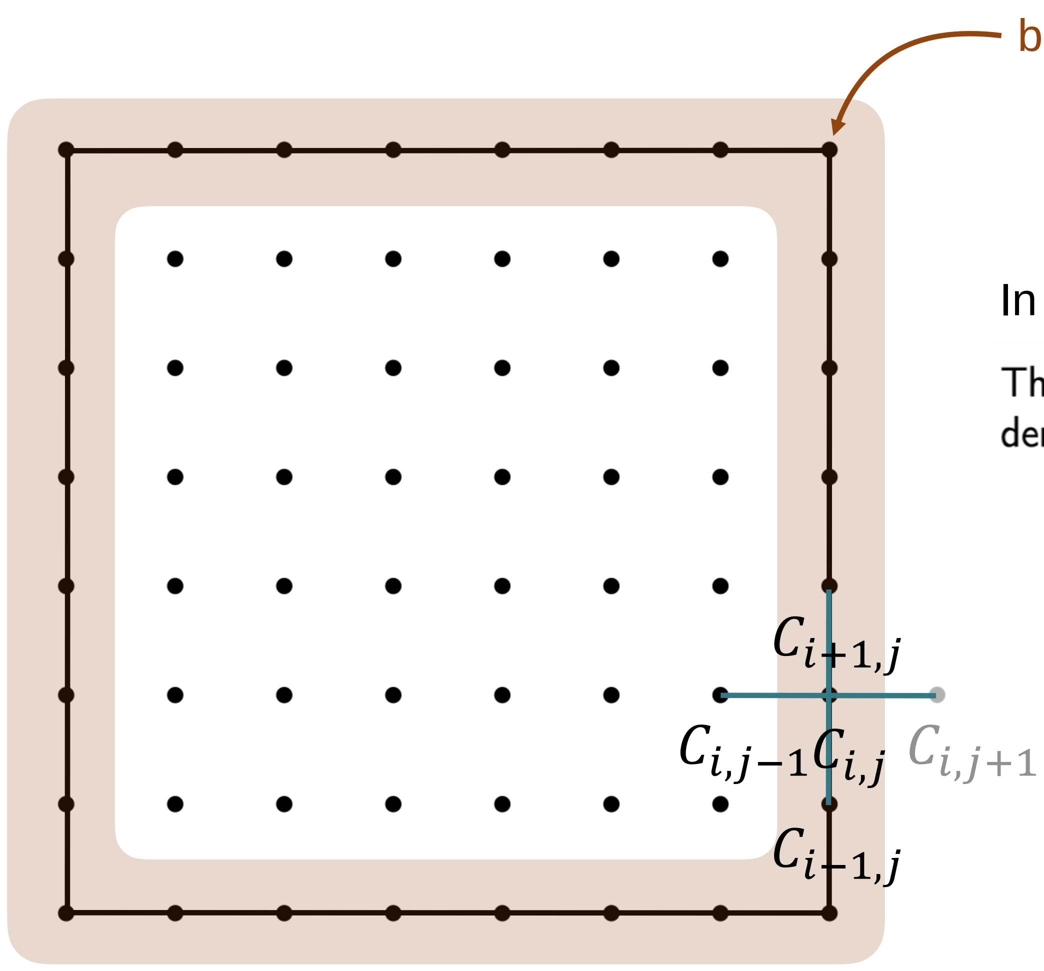
Combining all together:

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} = D\left(\frac{C_{i,j-1}^{n} - 2C_{i,j}^{n} + C_{i,j+1}^{n}}{\Delta x^2} + \frac{C_{i-1,j}^{n} - 2C_{i,j}^{n} + C_{i+1,j}^{n}}{\Delta y^2}\right)$$

taking: $\Delta x = \Delta y = \Delta r$

Boundary Condition

3. Boundary nodes: application of the Boundary Condition

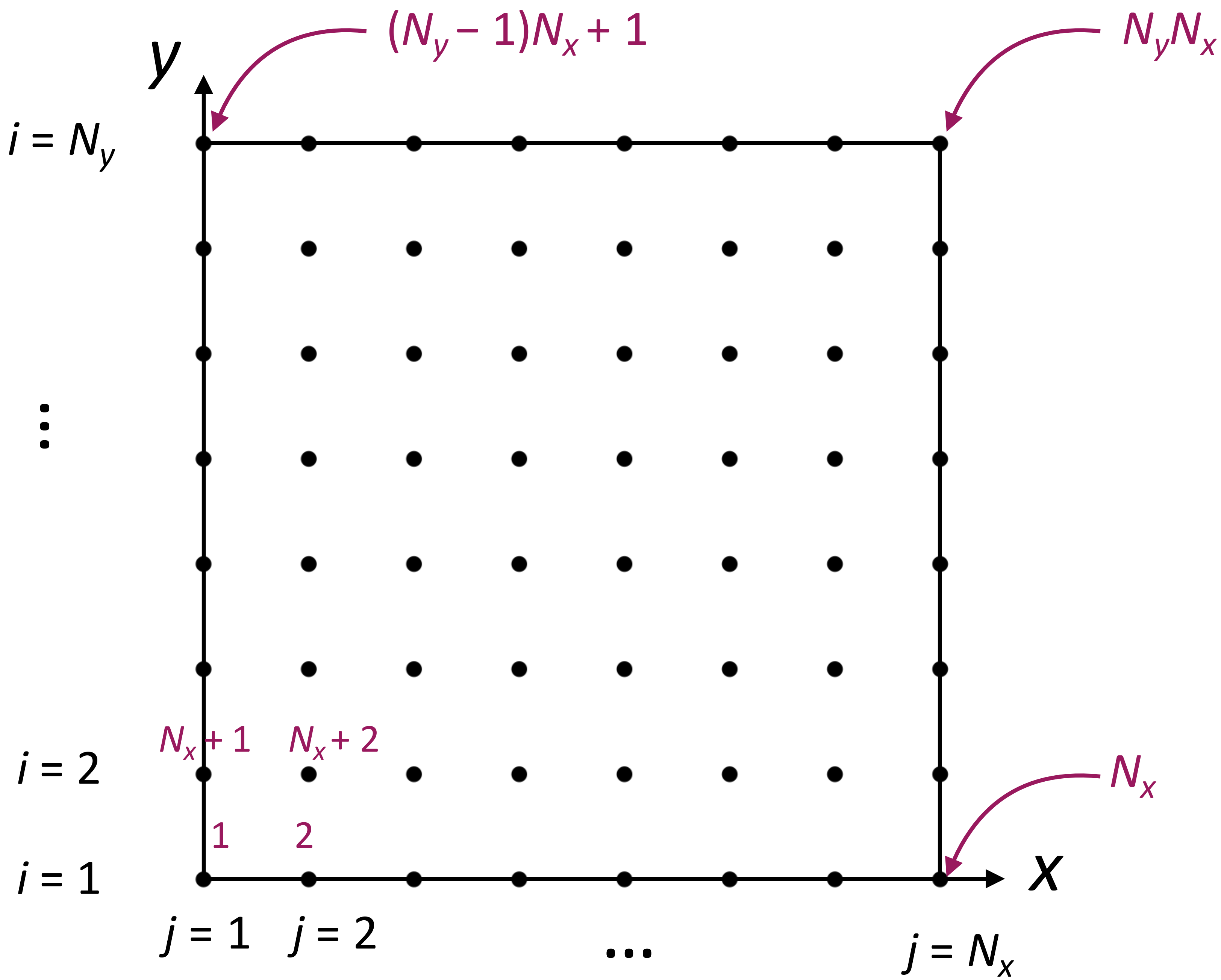


In the HW we will consider the following BC:

The concentration at all boundary grid-points is 0, i.e. $C(x_B, y_B, t) = 0$, where x_B, y_B denote the grid-points located on the domain boundary (perimeter).

Question 1: Diffusion

Note: global and local indexing

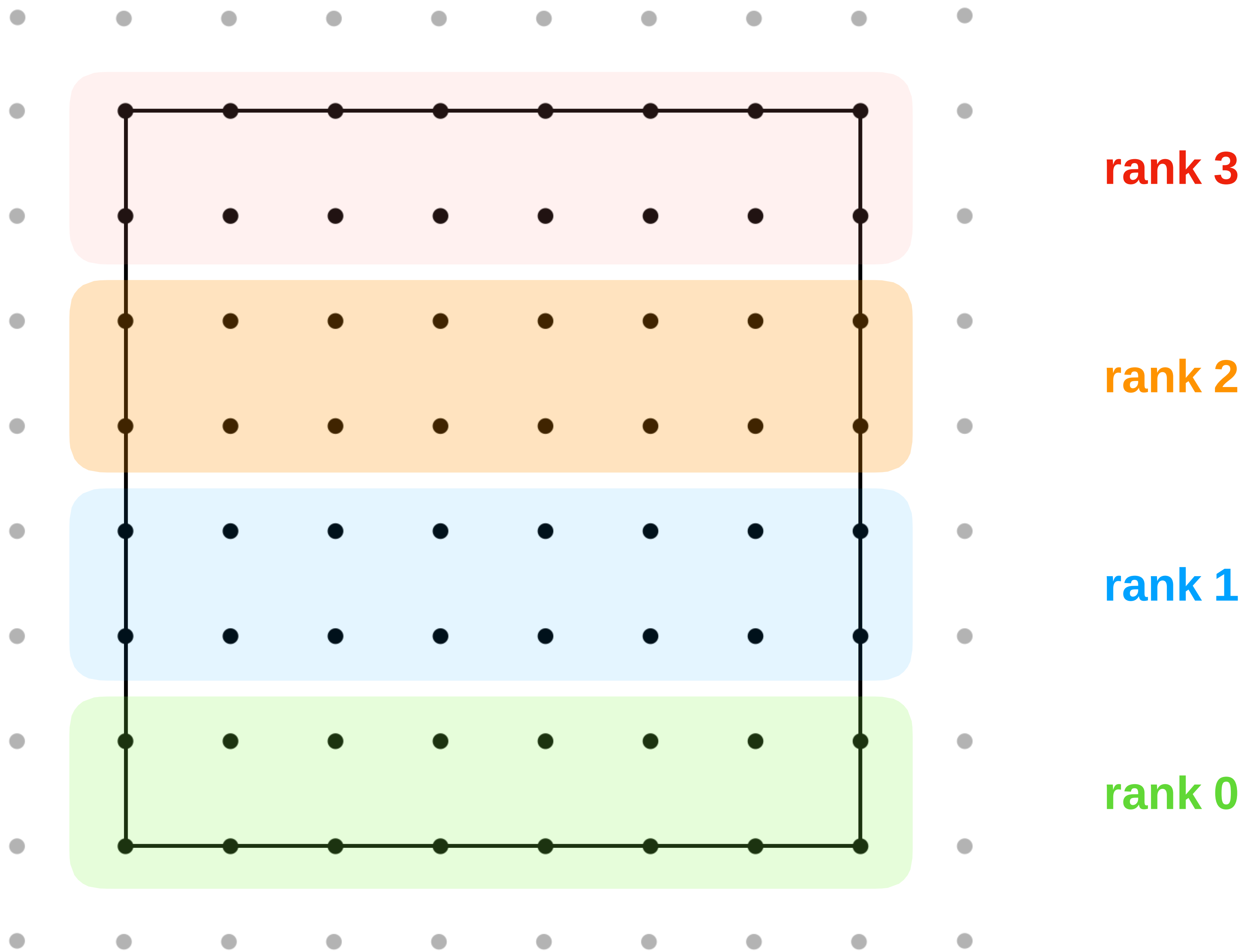


Global indexing:

$g = (i - 1)N_x + j$

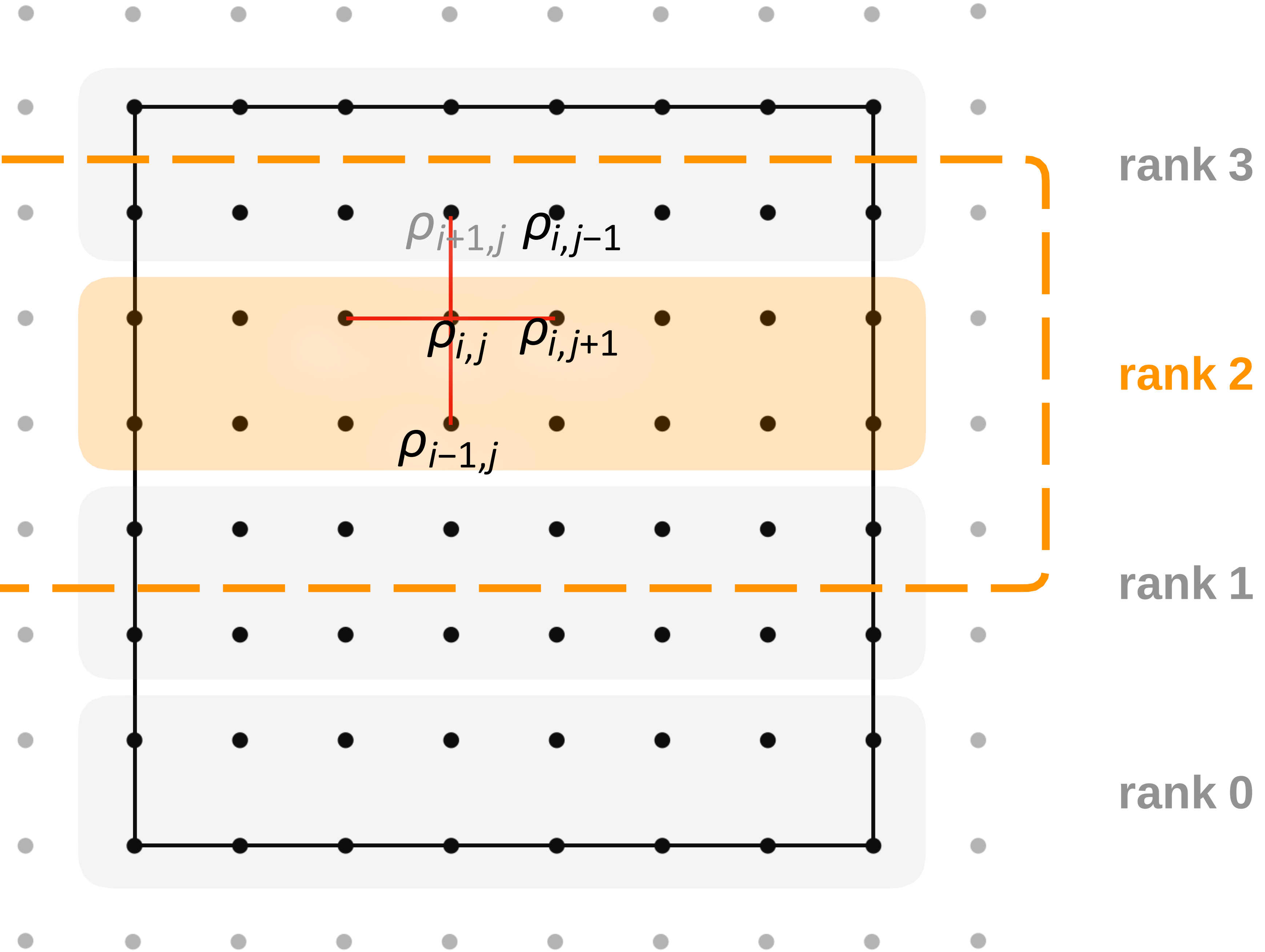
Question 1: Diffusion

HW: Parallelization with MPI



Question 1: Diffusion

HW: Parallelization with MPI



Now let's have a look at the skeleton code ...