

# Homework 5

## 2D Diffusion MPI

HPCSE I  
23.11.2022

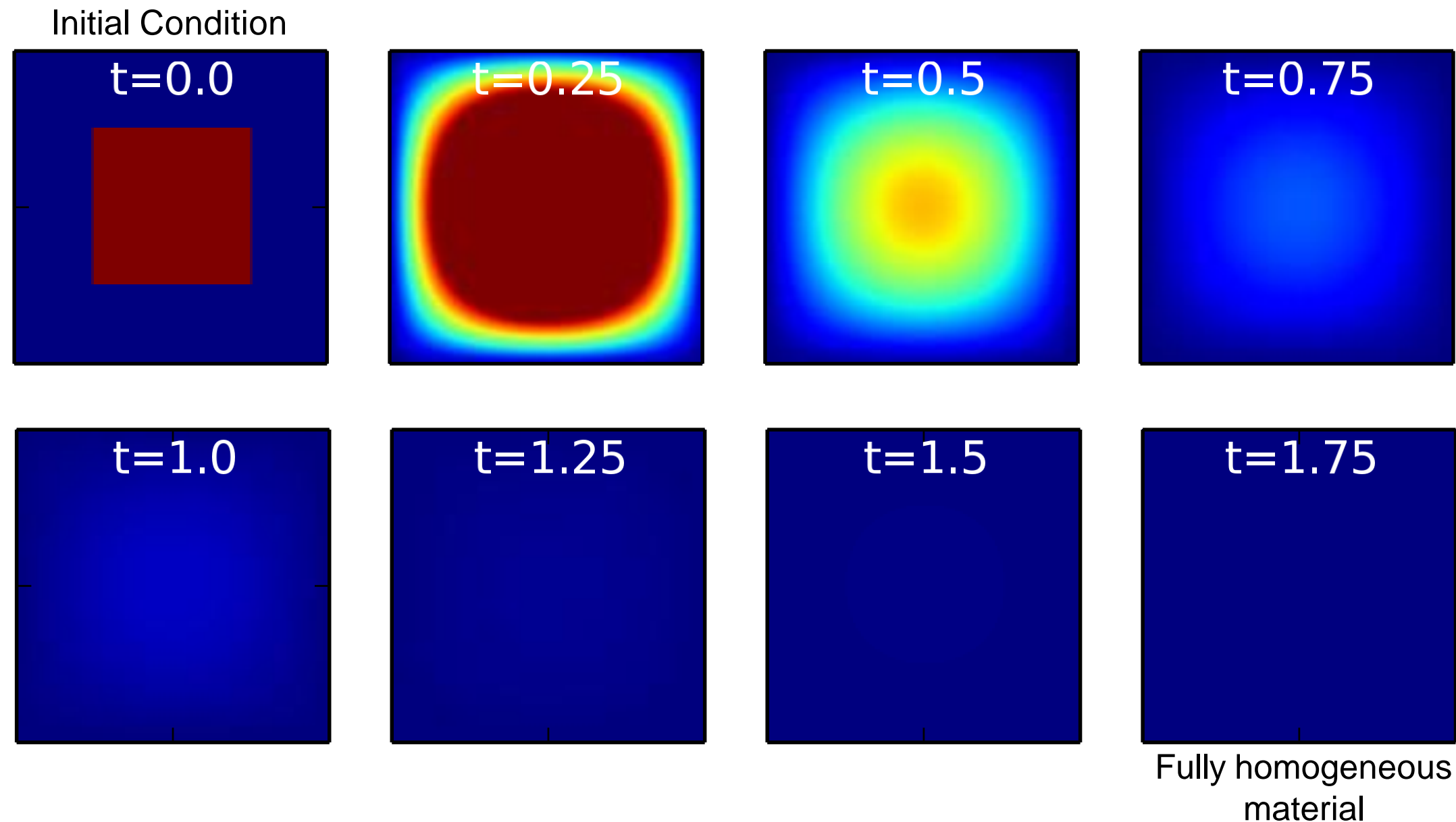
# Question 1: Diffusion

Given:

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

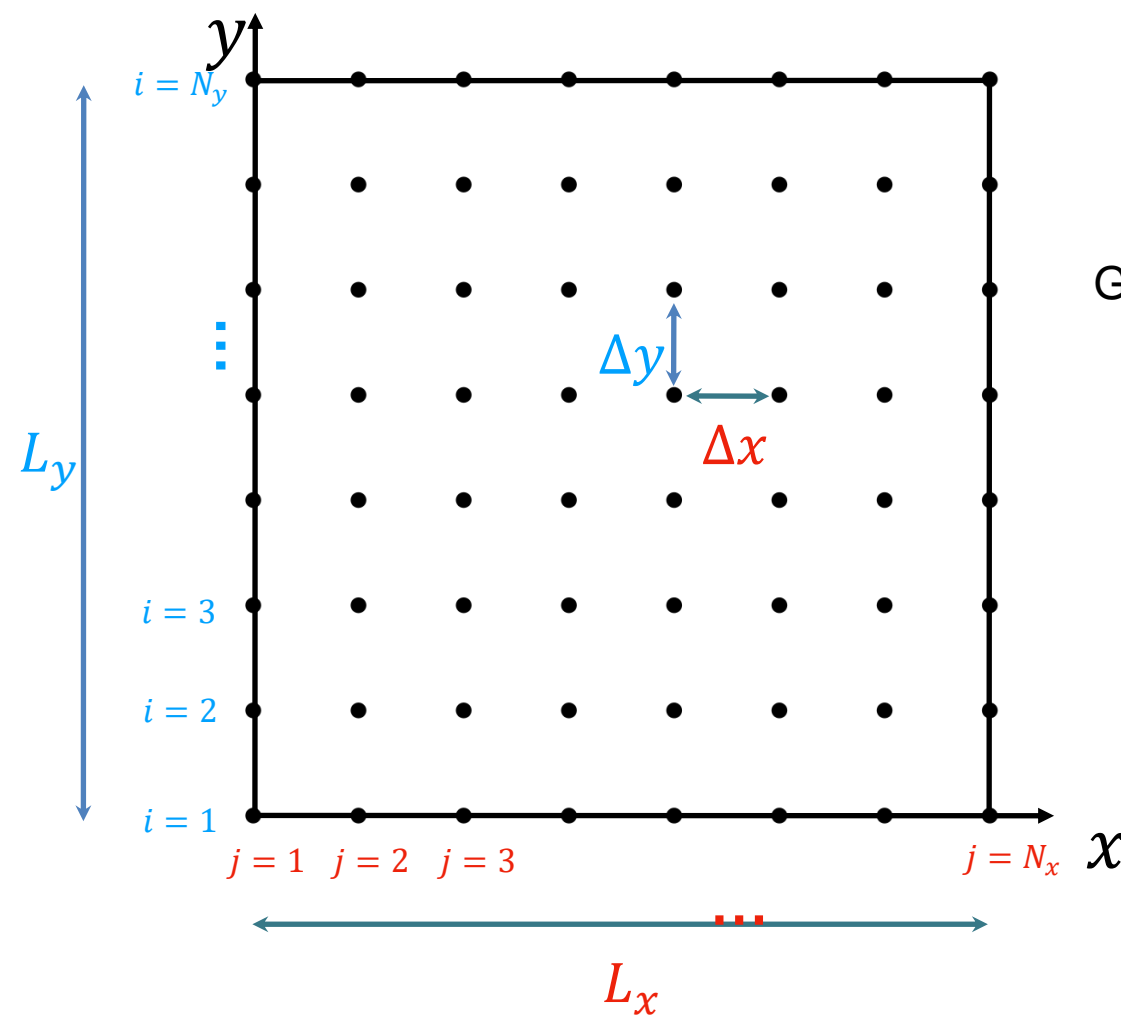
Find:

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



# Discretizing a 2D Space - Grids

## 1. Spatial discretization



Grid spacing:

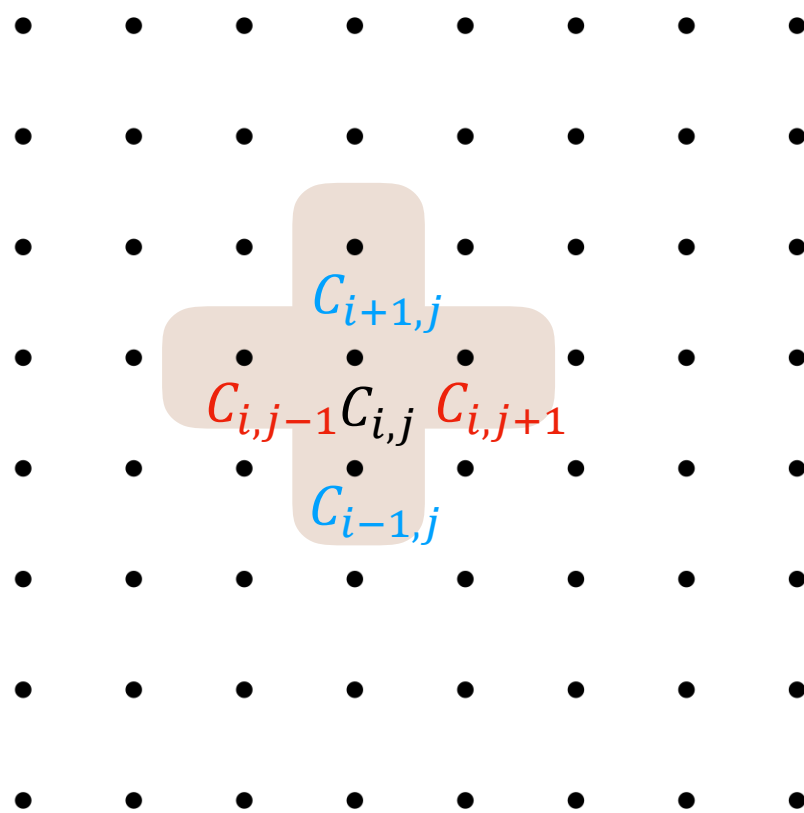
$$\Delta x = \frac{L_x}{N_x - 1}$$

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

# Spatial discretization: Central finite differences

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

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




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

# Time discretization: explicit Euler

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

$$\boxed{\frac{\partial C(x, y, t)}{\partial t}} = D \nabla^2 C(x, y, t)$$
$$\frac{\partial C(x, y, t)}{\partial t} \approx \frac{C^{n+1} - C^n}{\Delta t}$$

time index



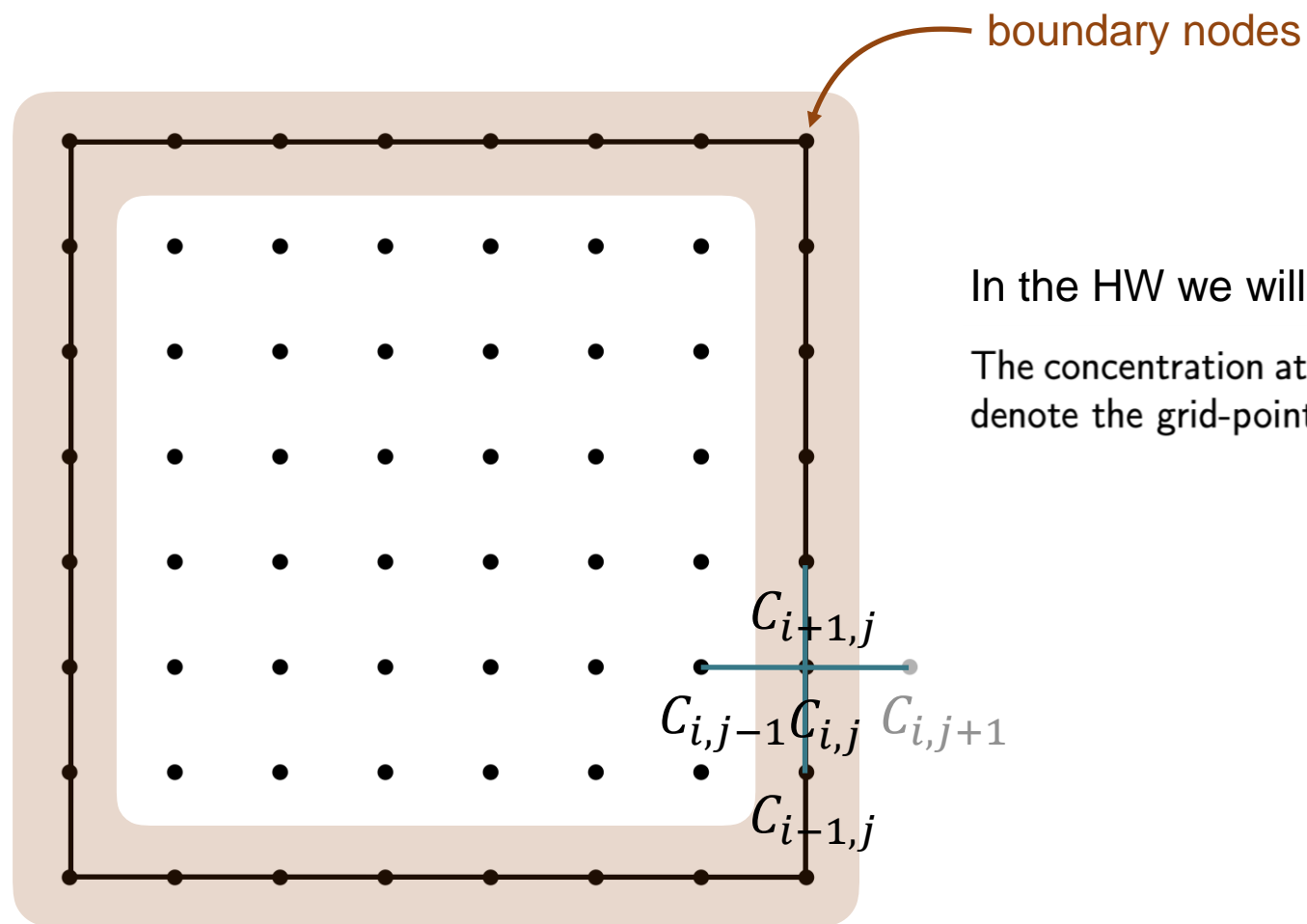
Combining all together:

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

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

# Boundary Condition

## 3. Boundary nodes: application of the Boundary Condition

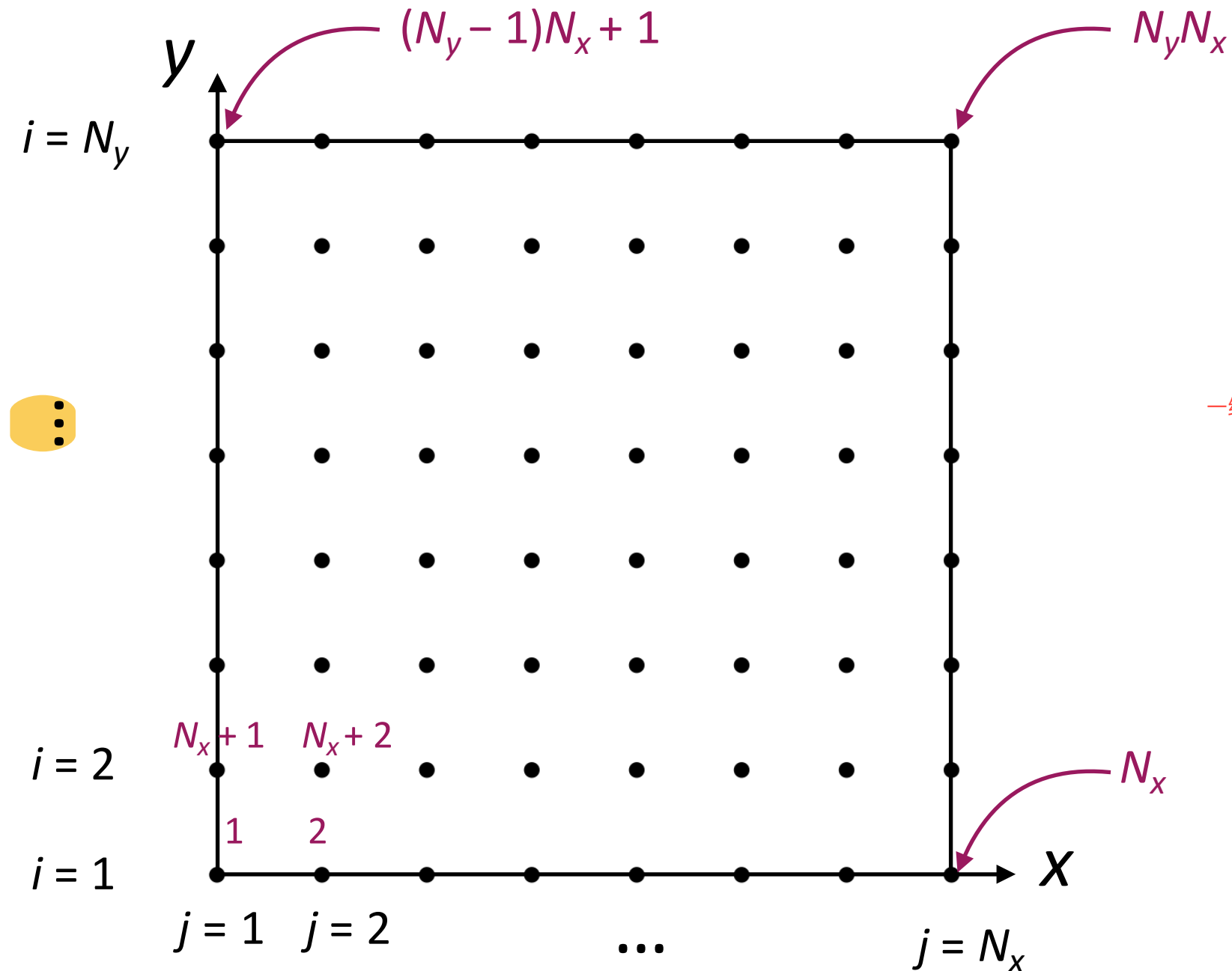


In the HW we will consider the following BC:

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



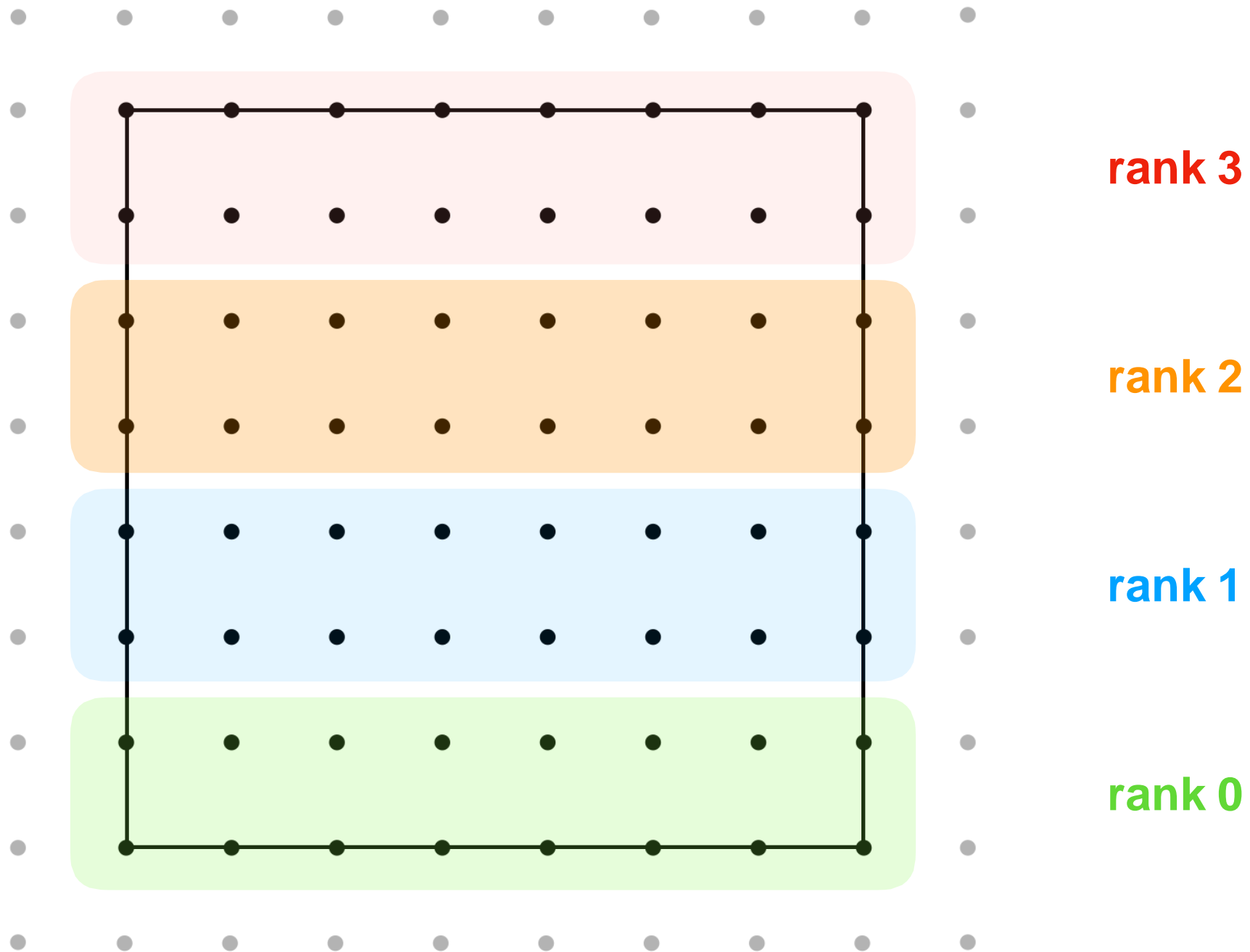
Global indexing:

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

一维的方式进行存储，所以需要进行global indexing的访问。

# Question 1: Diffusion

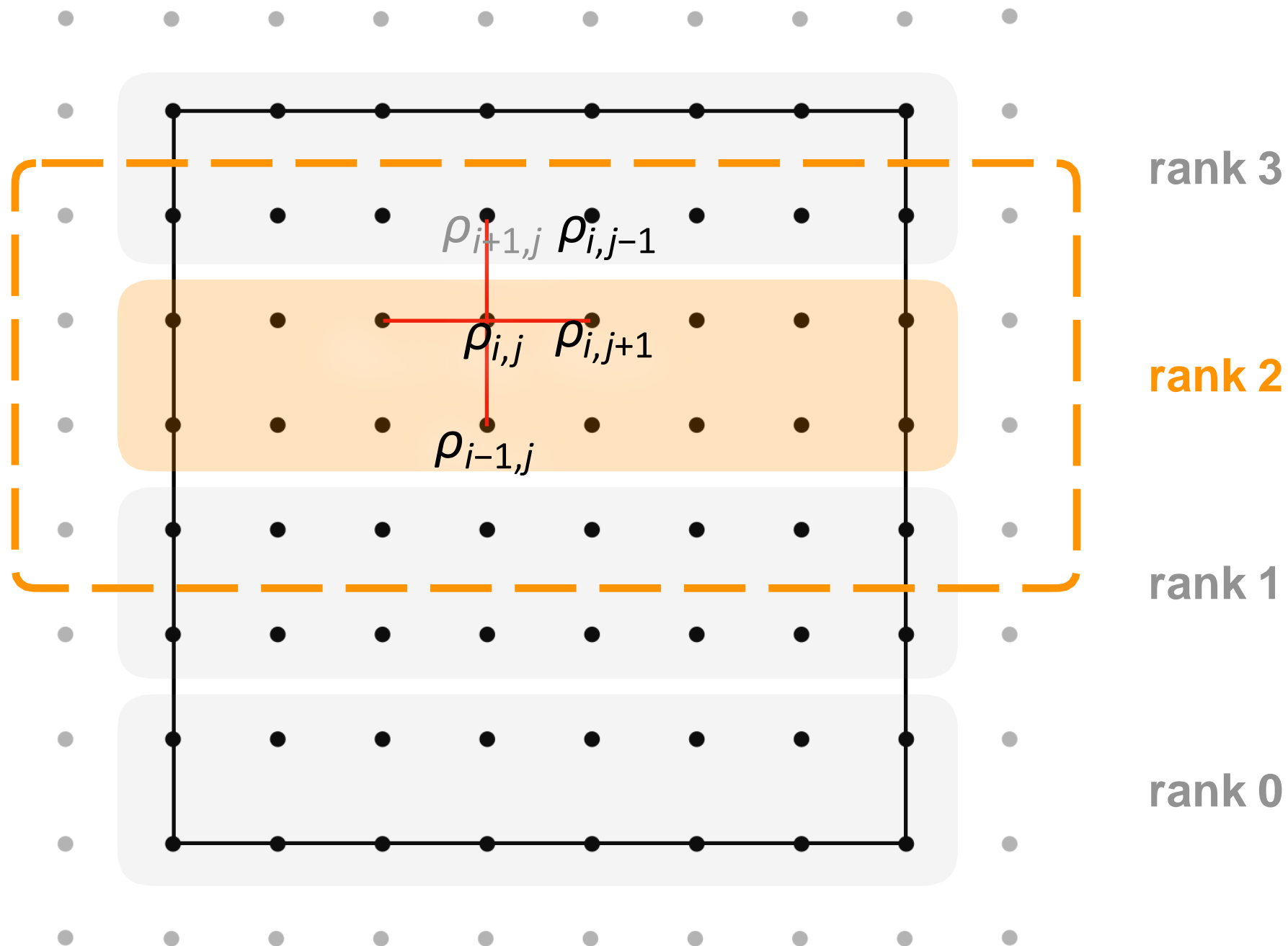
**HW:** Parallelization with MPI





# Question 1: Diffusion

**HW:** Parallelization with MPI



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