HPCSE I - Fall 2022

Tutorial: Diffusion

26 October 2022

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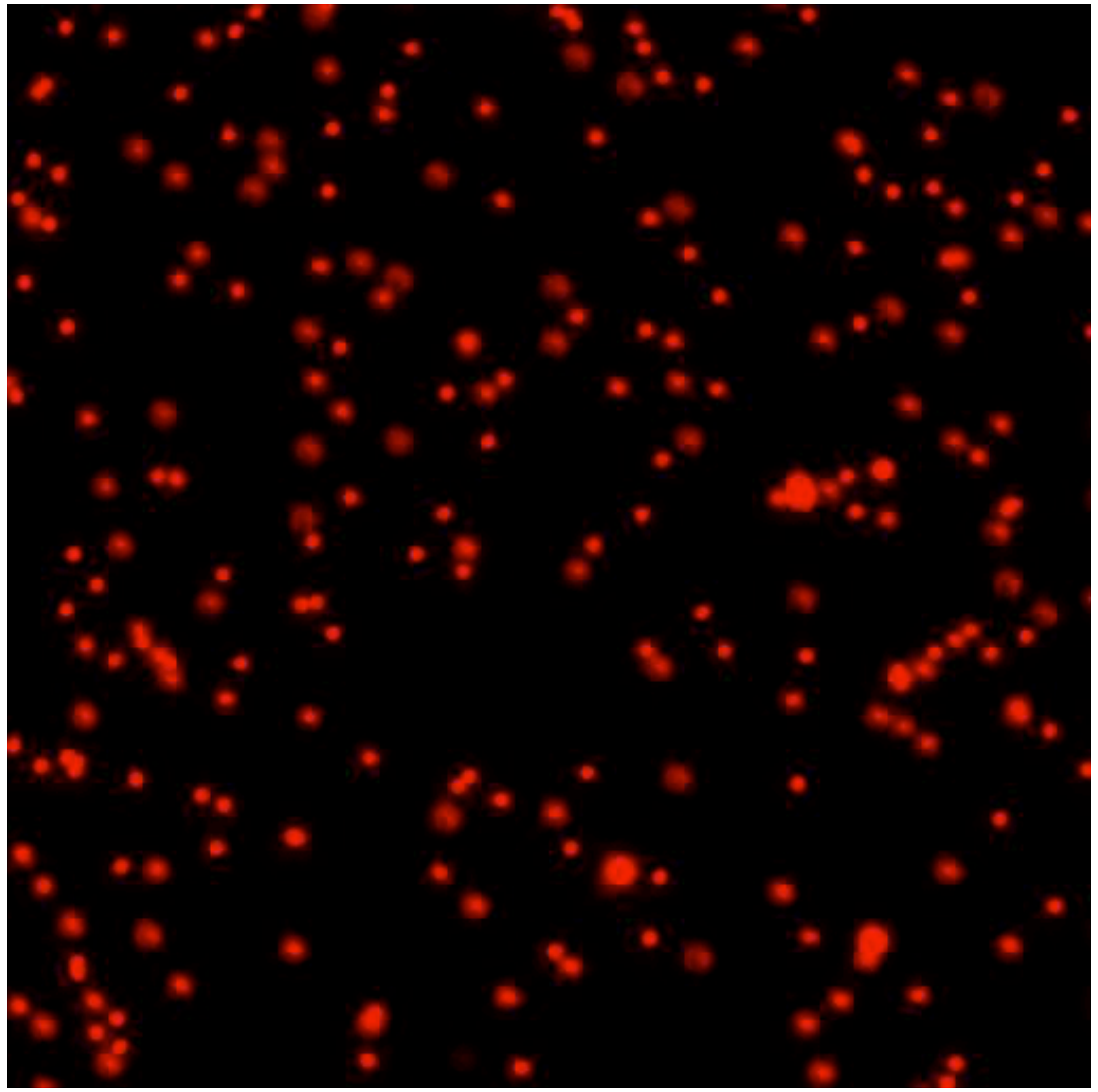
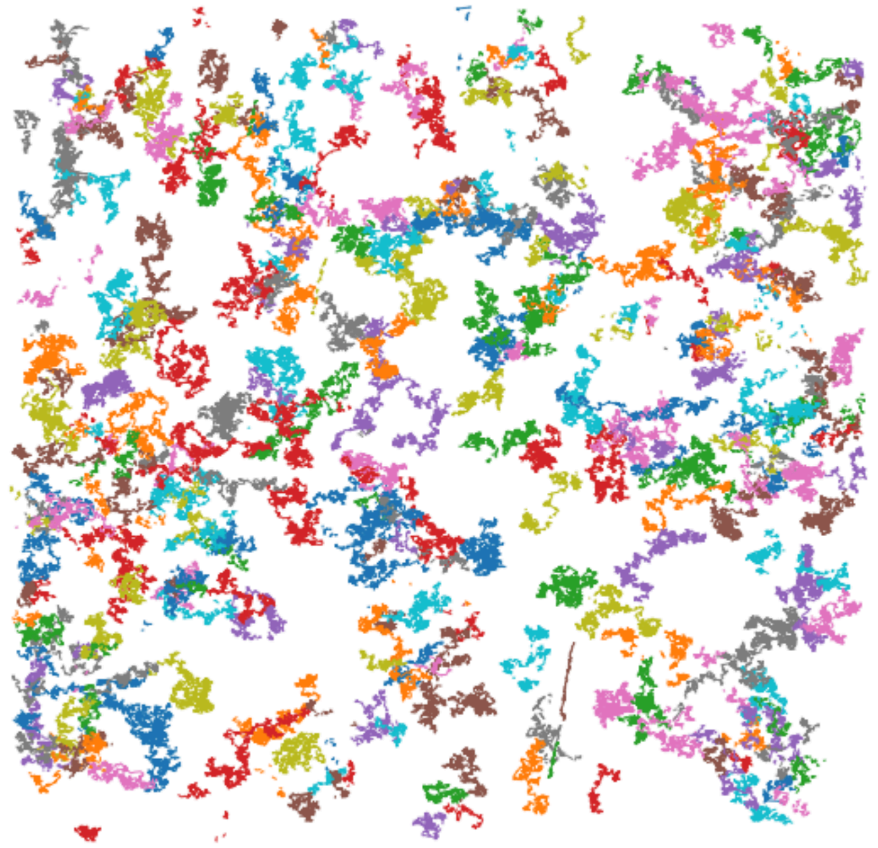
Computational **S**cience and **E**ngineering **Lab**
ETH Zürich

How to Quantify Diffusion?

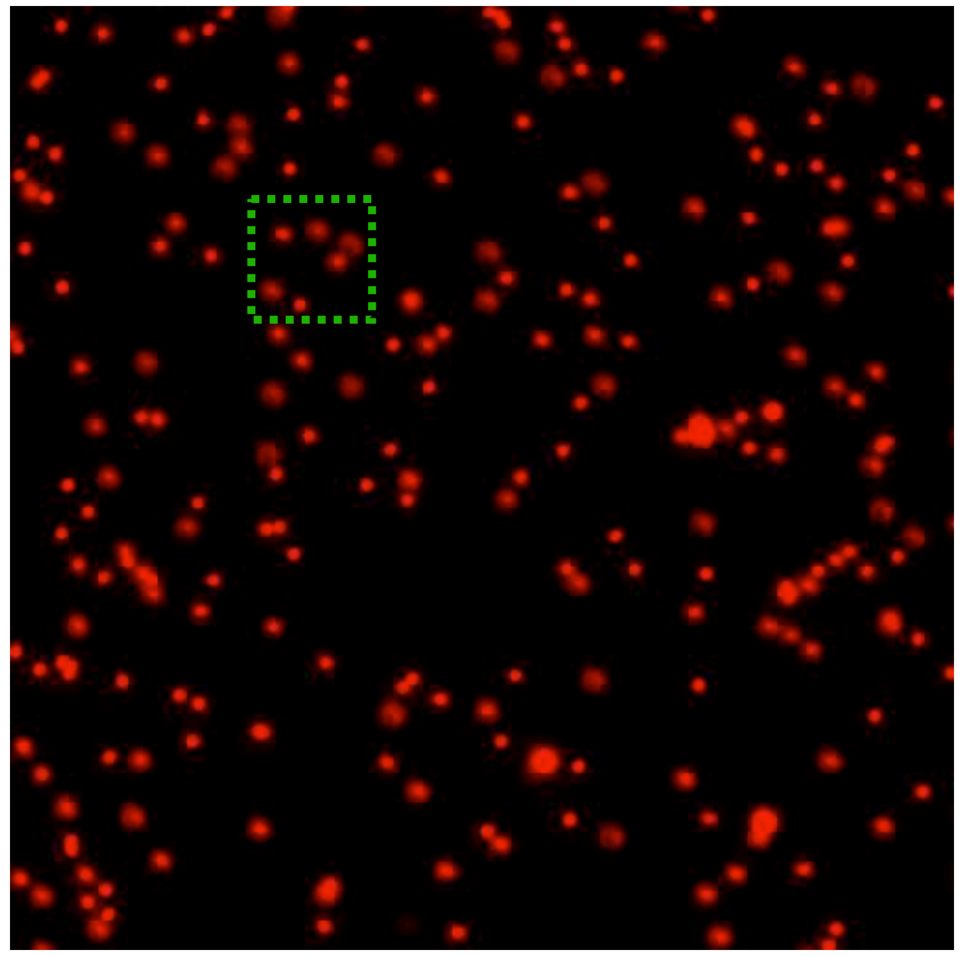
Brownian motion of particles



- ***Particle-level:*** Track individual **particle trajectory**, in time.
- *Outcome:* Estimation of diffusion coefficient, $D_{(2D)} = \frac{\langle x^2 \rangle}{4t}$



- ***Macroscale-level:*** Observe **concentration within a given volume**, in time.
- *Outcome:* Estimation of concentration field, $C(x, t)$, over time.

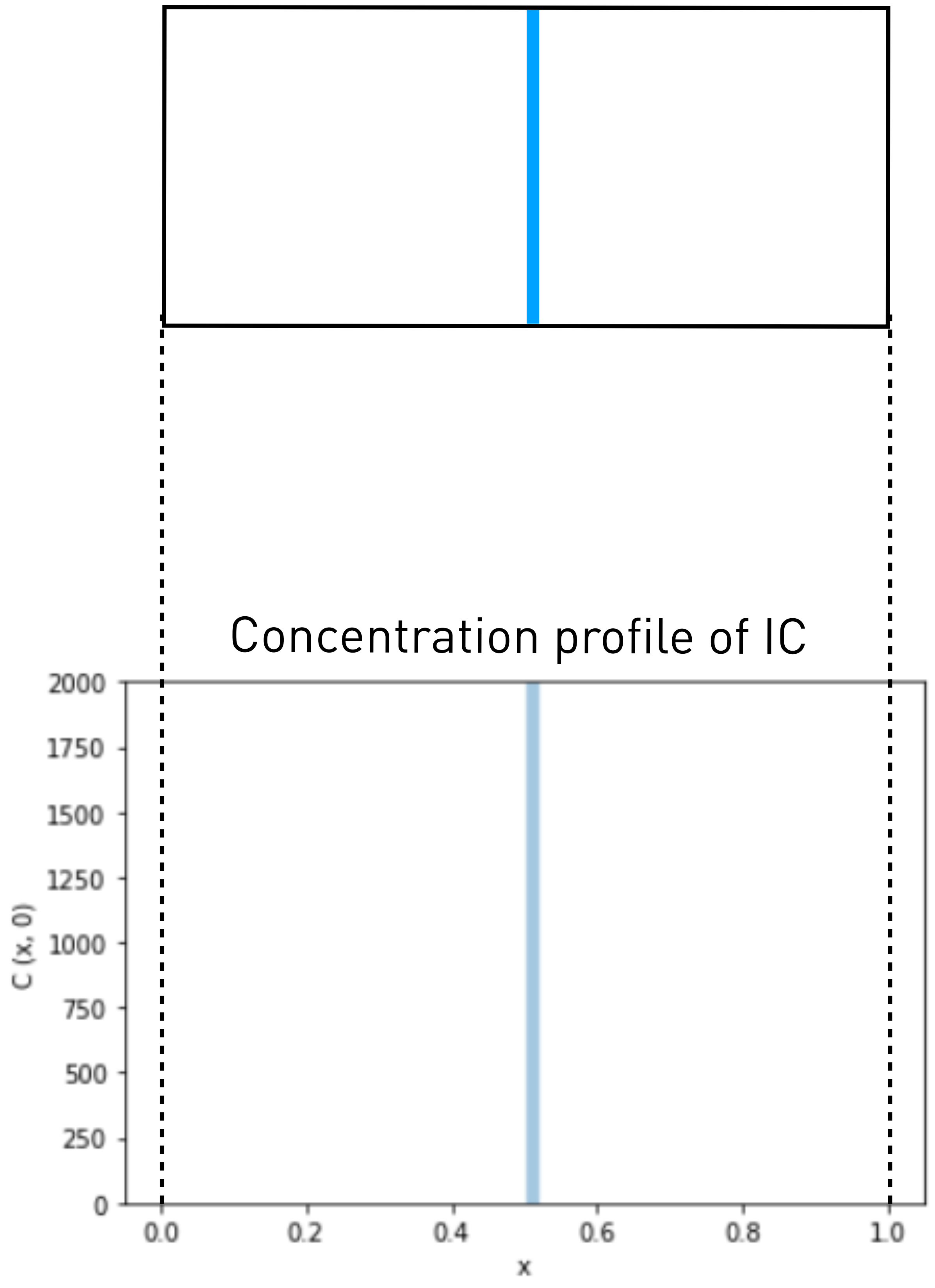


1D diffusion using Random Walks

Initial Condition (IC)

top-view of a plate with a dye placed on a line, at the middle of the plate

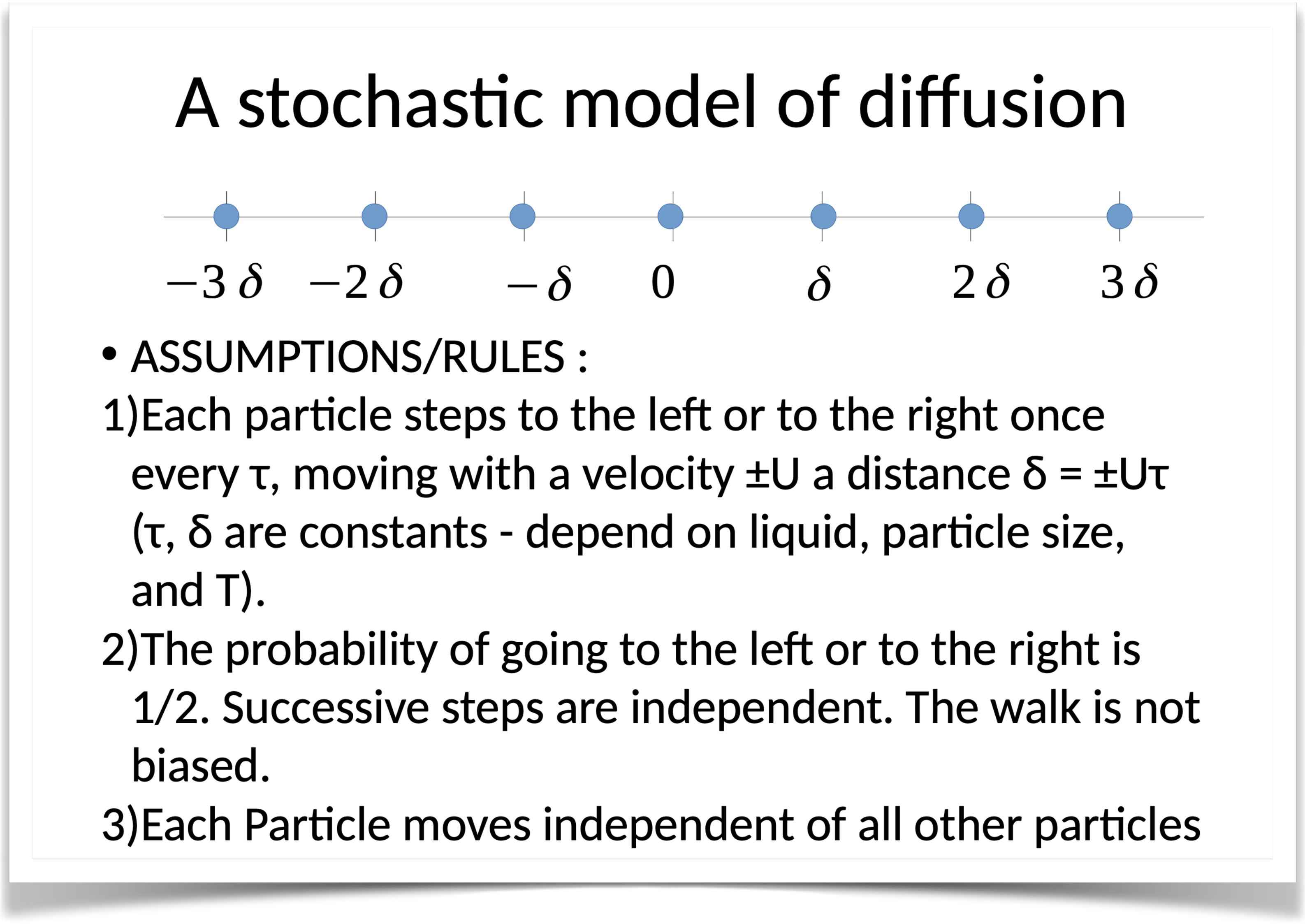
Concentration profile of IC



How would the dye "move" on the plate over time?

- How does the concentration profile of the dye change in time?

In the lecture:



A stochastic model of diffusion

$-3\,\delta$ $-2\,\delta$ $-\,\delta$ 0 δ $2\,\delta$ $3\,\delta$

- ASSUMPTIONS/RULES :

1)Each particle steps to the left or to the right once every τ, moving with a velocity ±U a distance δ = ±Uτ (τ, δ are constants - depend on liquid, particle size, and T).

2)The probability of going to the left or to the right is 1/2. Successive steps are independent. The walk is not biased.

3)Each Particle moves independent of all other particles

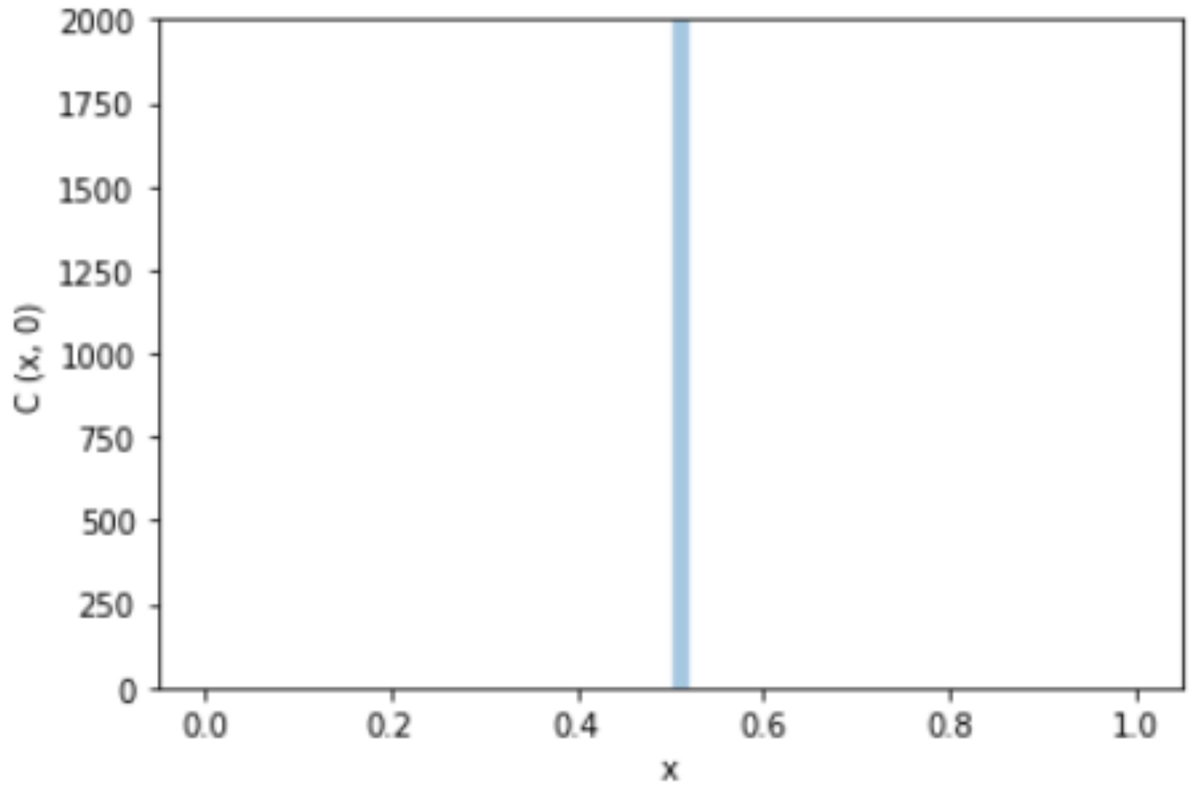
Let's simulate this!

- Simulate dye particles initially placed at the cyan line, in the middle of the plate.
- At each time-step: move each particle independently in space, with probability 0.5 to go left, and 0.5 to go right.
- Observe evolution of particles' position over time.
- Compute *concentration* of particles at each time step.

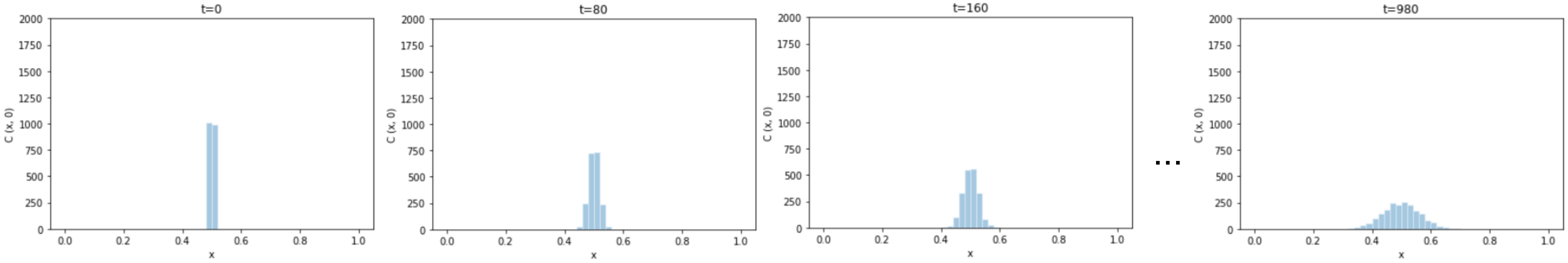
number of particles / volume of medium

1D diffusion using Random Walks

Initial Condition (IC)



Time evolution of particle concentration



... What happens at the Edge of the plate?? ⟶ Boundary Conditions (BC)

- Dye drops out of the plate (absorbing BC).
- Dye cannot leave the plate due to presence of walls (reflective BC).

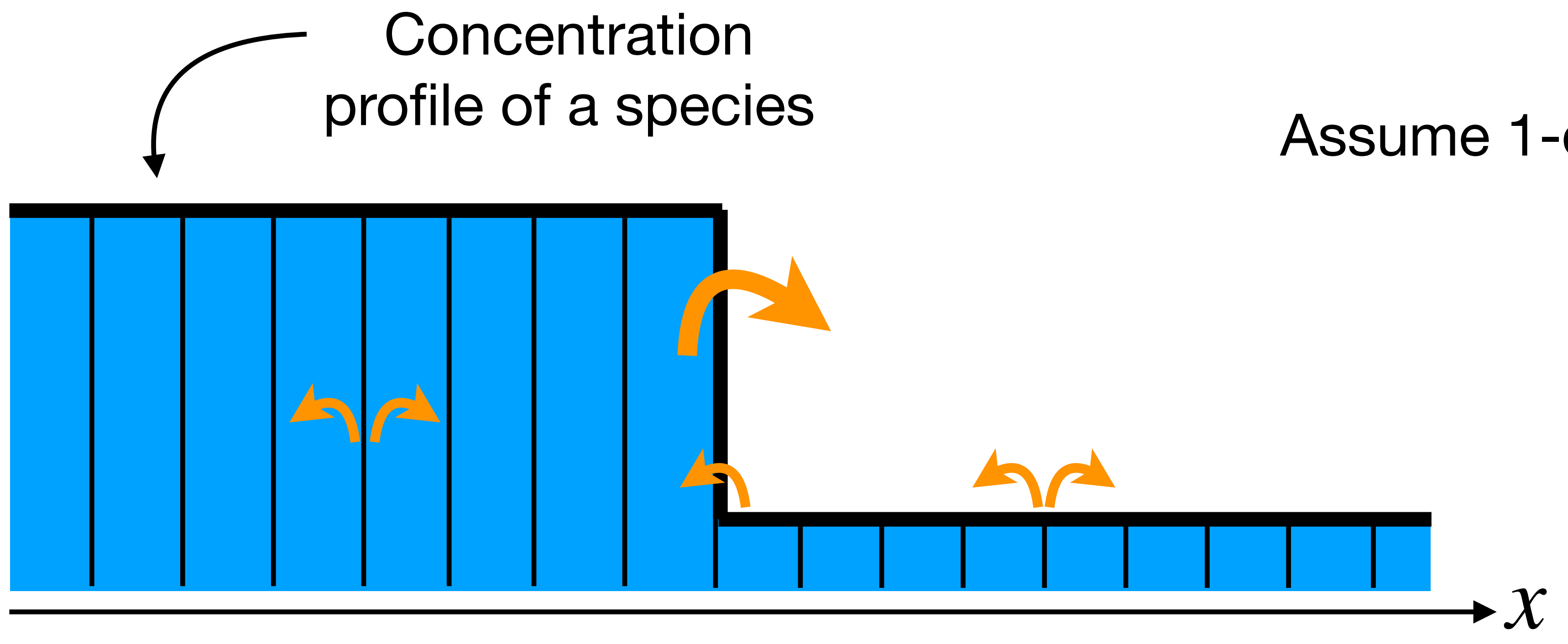
1D diffusion using Random Walks

According to our assumptions, the motion of **one particle** is fully time-reversible and **random**. Yet when **particles move together**, they move in a **particular direction**.

- *Why?*
- *... i.e. What determines the direction of the macroscopically observed motion?*

Particle-level picture:

Assume 1-d space



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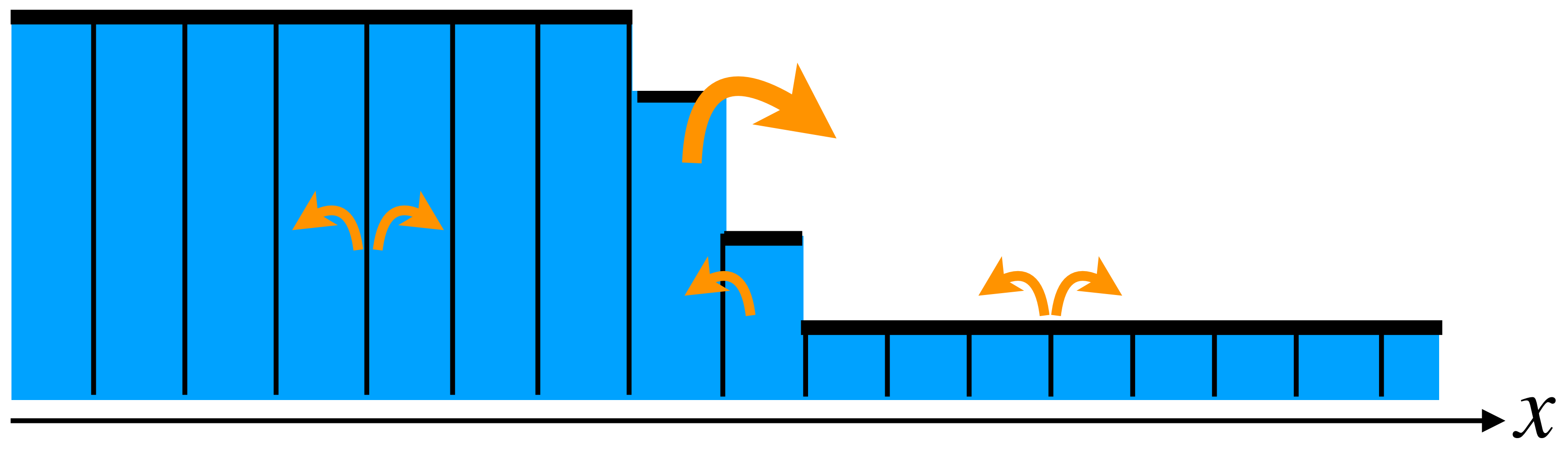
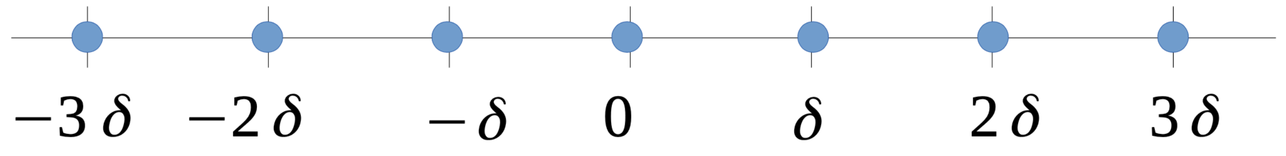


A stochastic model of diffusion



- ASSUMPTIONS/RULES :

1) Each particle steps to the left or to the right once every τ, moving with a velocity ±U a distance δ = ±Uτ (τ, δ are constants - depend on liquid, particle size, and T).
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3) Each Particle moves independent of all other particles

Fick's 2nd Law

$$\frac{\partial c}{\partial t} = -\frac{\partial J_x}{\partial x} = D\frac{\partial^2 c}{\partial x^2}$$

1D diffusion using Random Walks

Conclusion 1: Average particle position remains constant.

1D Random Walk

- According to rule 1: $x_i(n) = x_i(n-1) \pm \delta$
- Mean displacement of *N* particles after *n* steps:

$$< x_i(n) > = \frac{1}{N} \sum_{i=0}^{N} x_i(n)$$

$$< x_i(n) > = \frac{1}{N} \sum_{i=0}^{N} [x_i(n-1) \pm \delta]$$

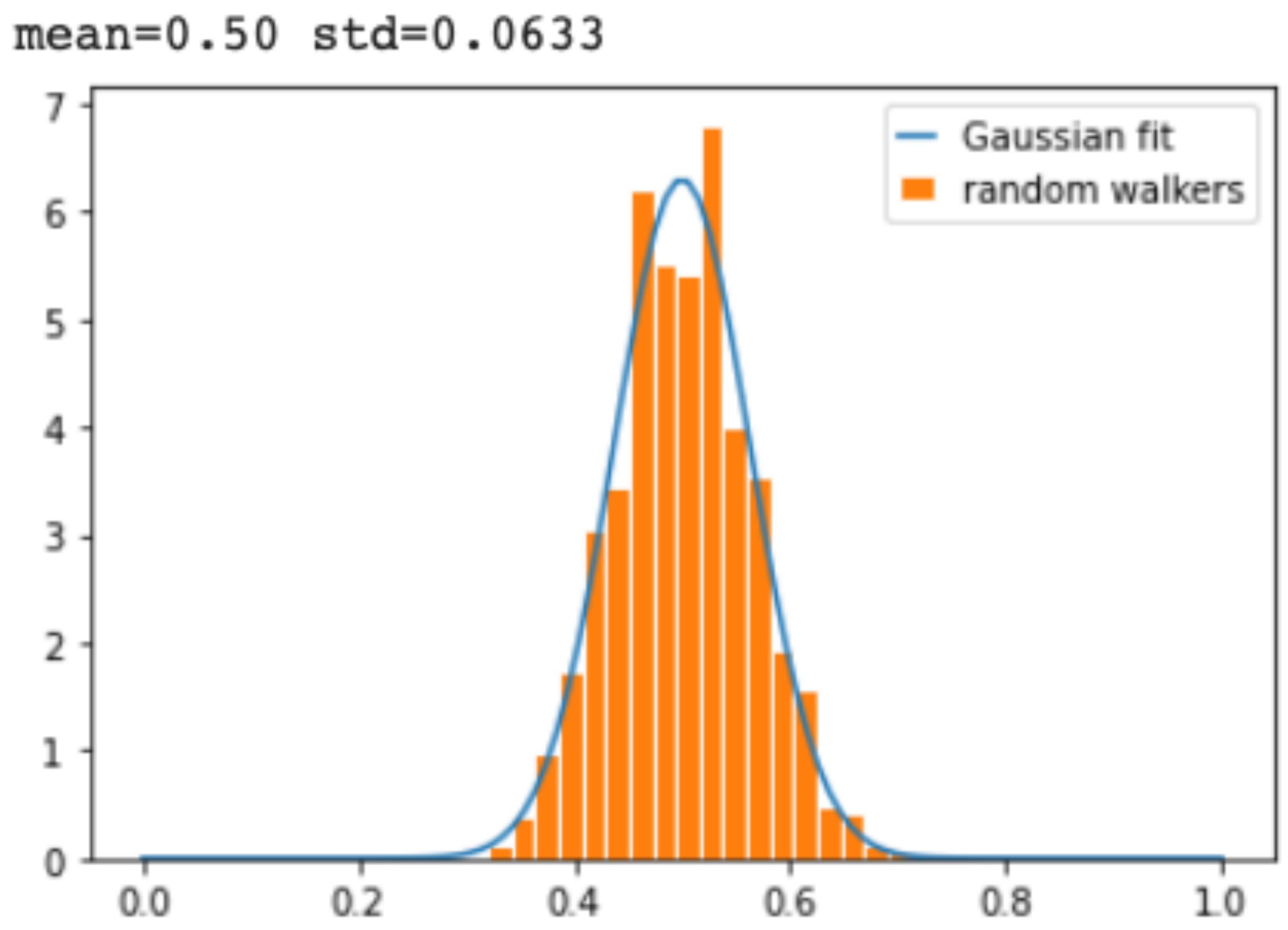
$$< x_i(n) > = \frac{1}{N} \sum_{i=0}^{N} [x_i(n-1)]$$

$$< x_i(n) > = < x_i(n-1) > = \ldots = < x_i(0) >$$

- **The average particle position remains constant.**

Let's verify this from our 1D particle simulation!

- We compare the distribution of the random walkers with the shape of a Gaussian probability density function (pdf).
- To do this, we use fit the x-positions of the random walkers at the final timestep, with a Gaussian pdf.
- We then plot together, the histogram of the x-positions of the random walkers, and the Gaussian pdf fit.



Computing the Diffusion coefficient

1D Random Walk (cont.)

- The particles spread:

$$<x_i^2(n)>=<x_i^2(0)>+n\delta^2$$

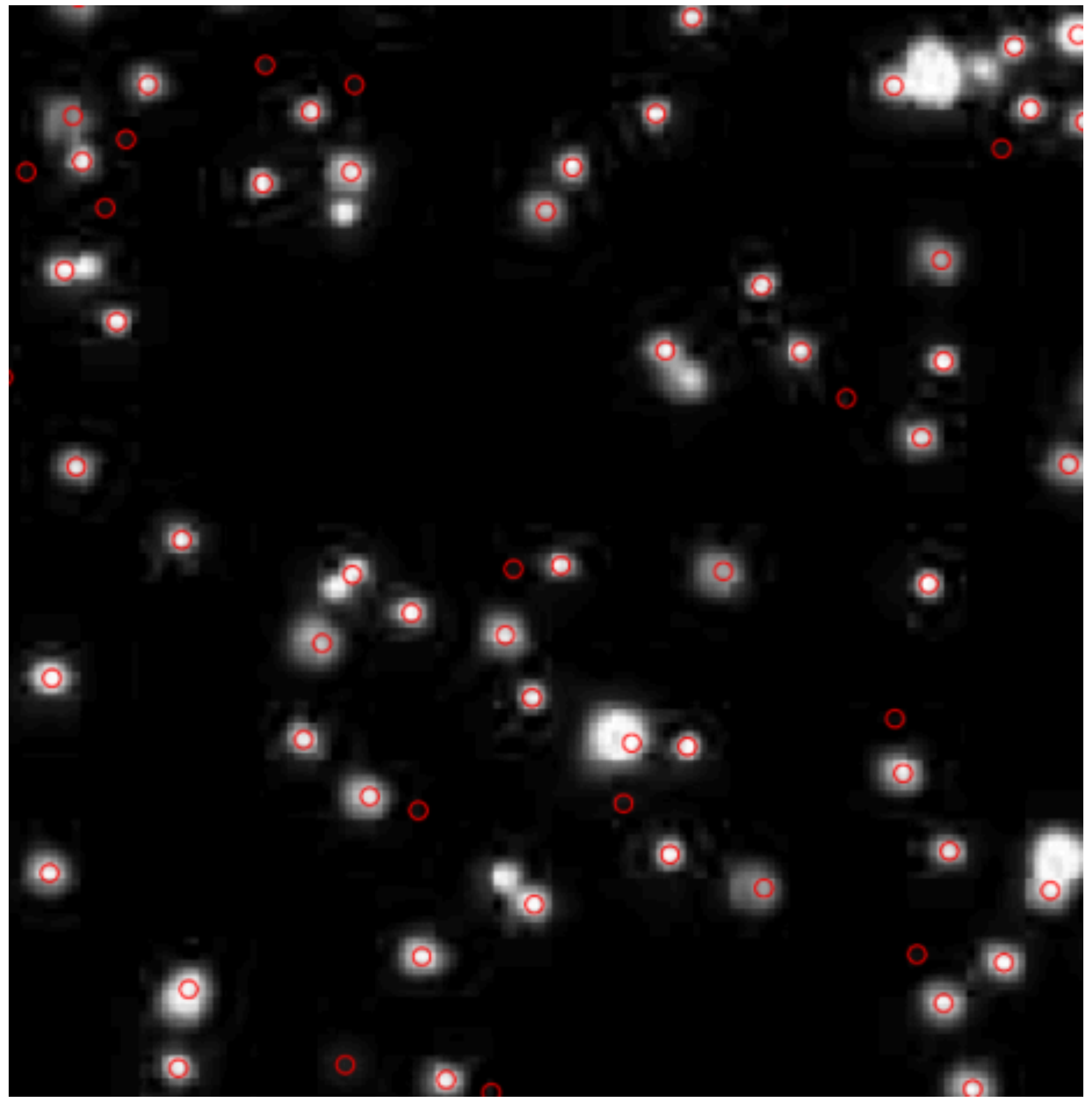
- The rate of the mean square displacement depends on the medium in which diffusion takes place and is linear in time:

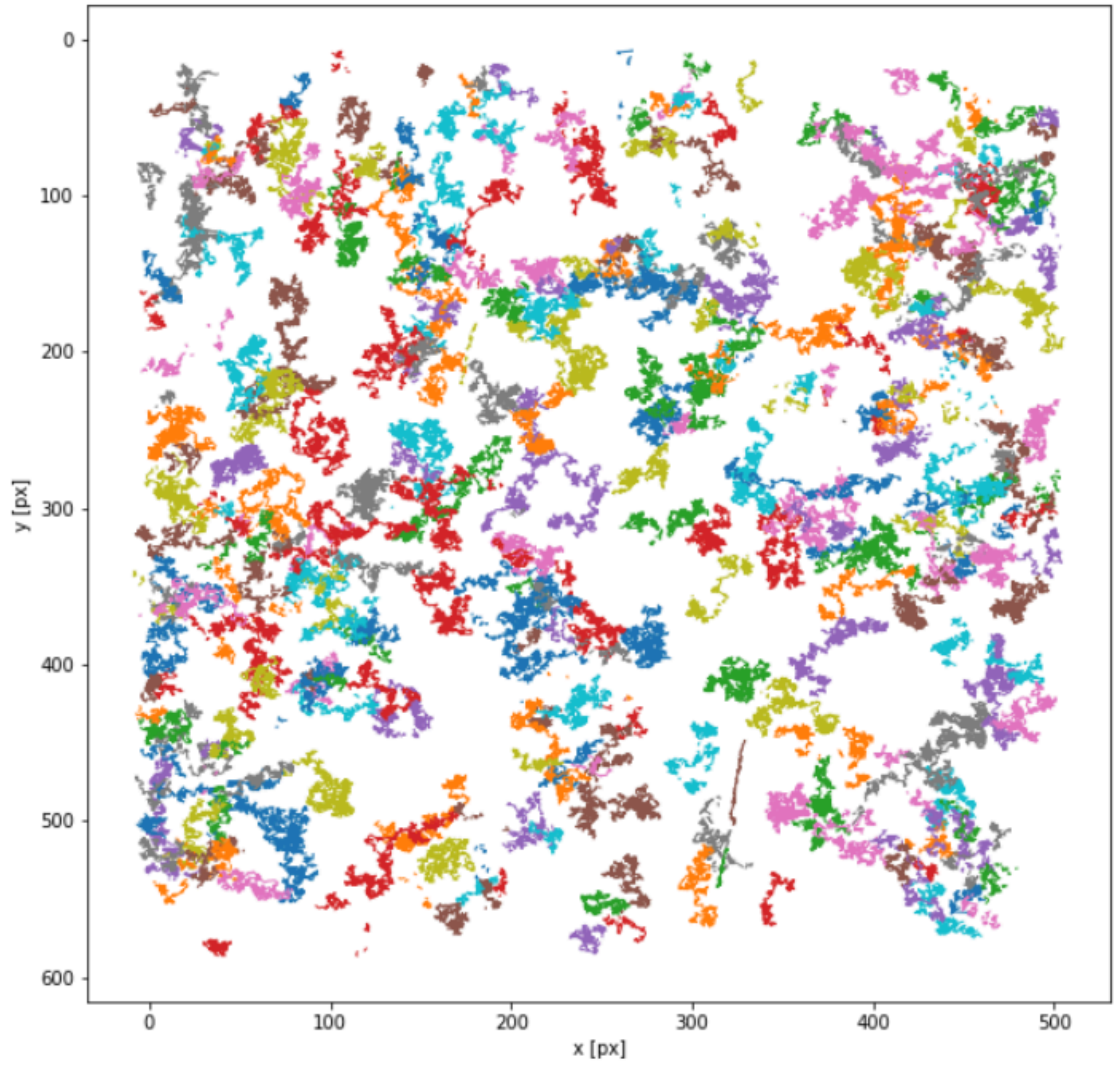
$$n\delta^2=\frac{t}{\tau}\delta^2=\frac{\delta^2}{\tau}t$$

Define the diffusion constant (D):

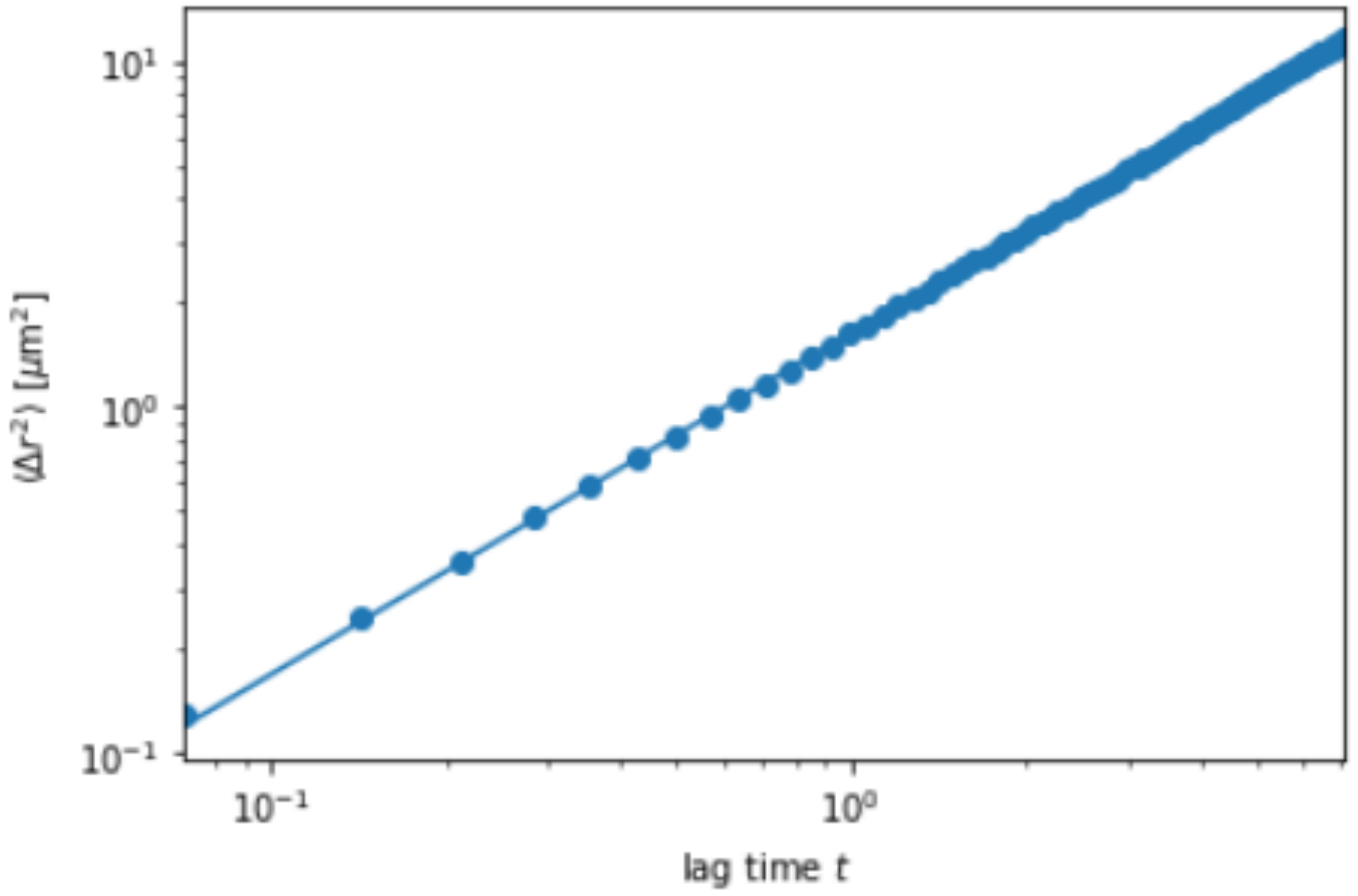
$$D=\frac{\delta^2}{2\tau}$$

Track each particle's position over time





Particle trajectories



Ensemble mean displacement over time

Macroscopic viewpoint: The Diffusion Equation

For the concentration $C(\boldsymbol{x}, t)$ we can describe the evolution in space $\boldsymbol{x} \in \Omega \subseteq \mathbb{R}^2$ and time $t \in [0,T]$ as

$$\underbrace{\boxed{\frac{\partial C(\mathbf{x}, t)}{\partial t}}}_{\text{first order time derivative}} = \underbrace{\boxed{D}}_{\text{diffusion coefficient}} \underbrace{\boxed{\nabla^2 C(\mathbf{x}, t)}}_{\text{second order spatial derivatives}}$$

where the diffusion constant D is a material property

Values of diffusion coefficients (gas)

Species pair (solute – solvent)	Temperature (°C)	*D* (cm^2/s)	Reference
Water (g) – air (g)	25	0.282	[3]
Oxygen (g) – air (g)	25	0.176	[3]

Values of diffusion coefficients (liquid)

Species pair (solute – solvent)	Temperature (°C)	*D* (cm^2/s)	Reference
Acetone (dis) – water (l)	25	1.16×10^{-5}	[3]
Air (dis) – water (l)	25	2.00×10^{-5}	[3]
Ammonia (dis) – water (l)	25	1.64×10^{-5}	[3]

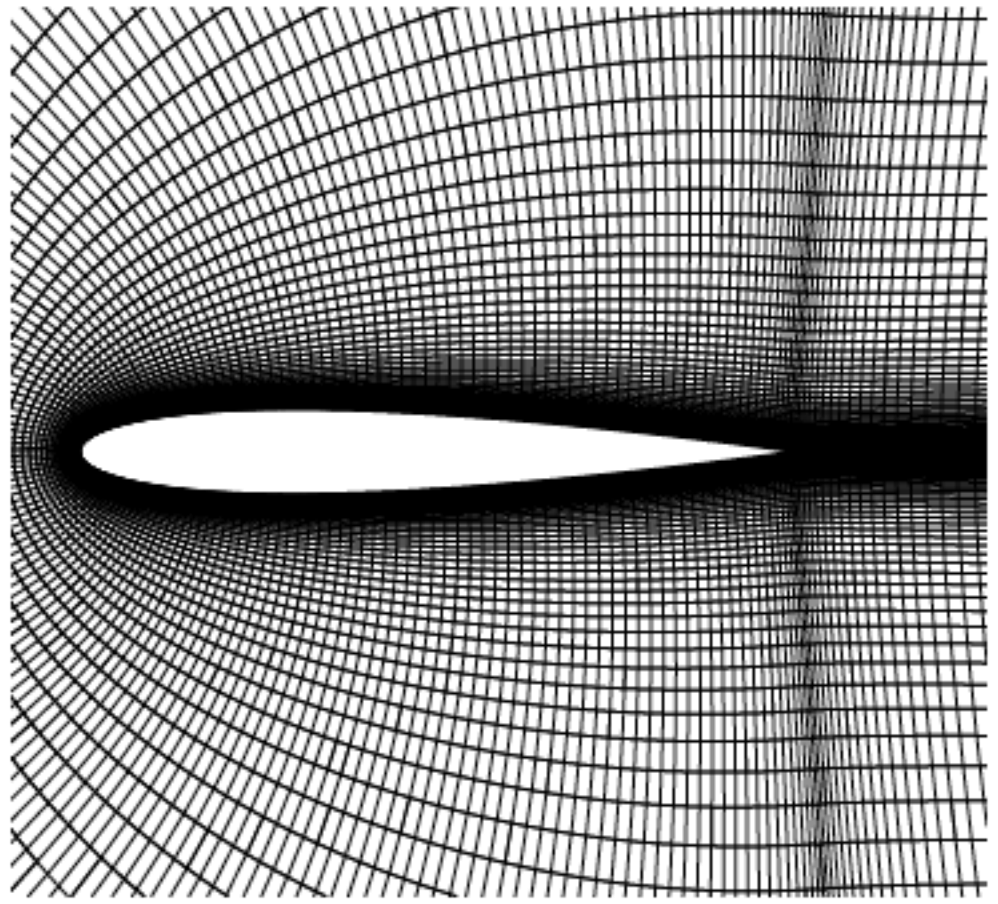
Values of diffusion coefficients (solid)

Species pair (solute – solvent)	Temperature (°C)	*D* (cm^2/s)	Reference
Hydrogen – iron (s)	10	1.66×10^{-9}	[3]
Hydrogen – iron (s)	100	124×10^{-9}	[3]
Aluminium – copper (s)	20	1.3×10^{-30}	[3]

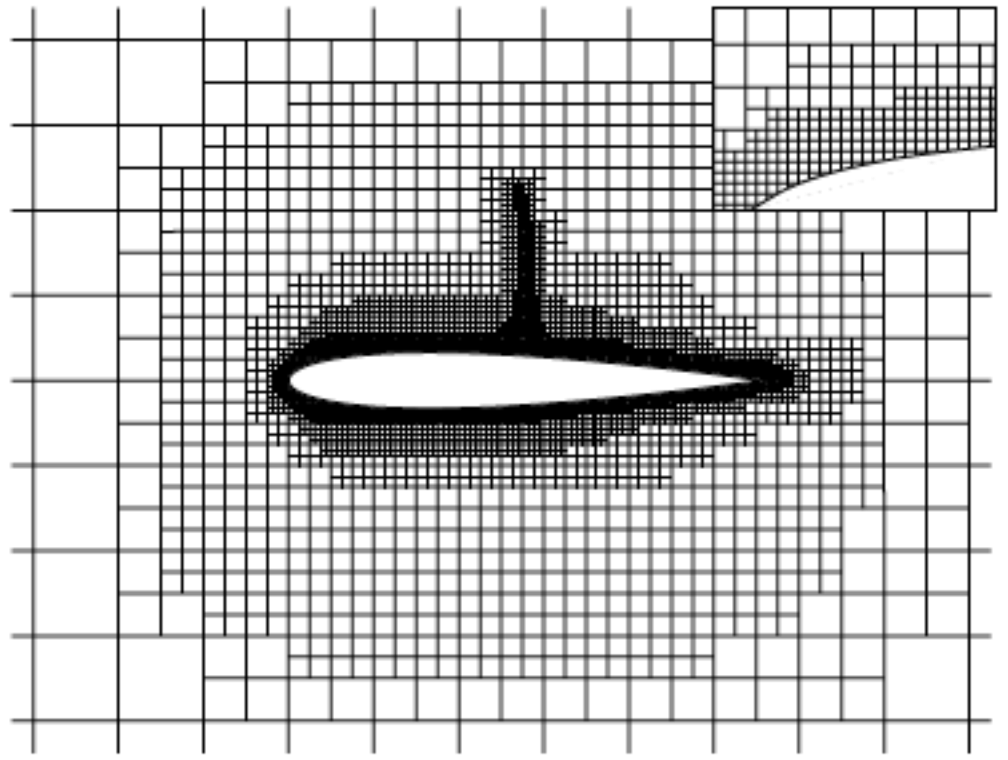
Discretizing Space - Grids

In order to solve the equations numerically we discretize them on a **grid**

structured

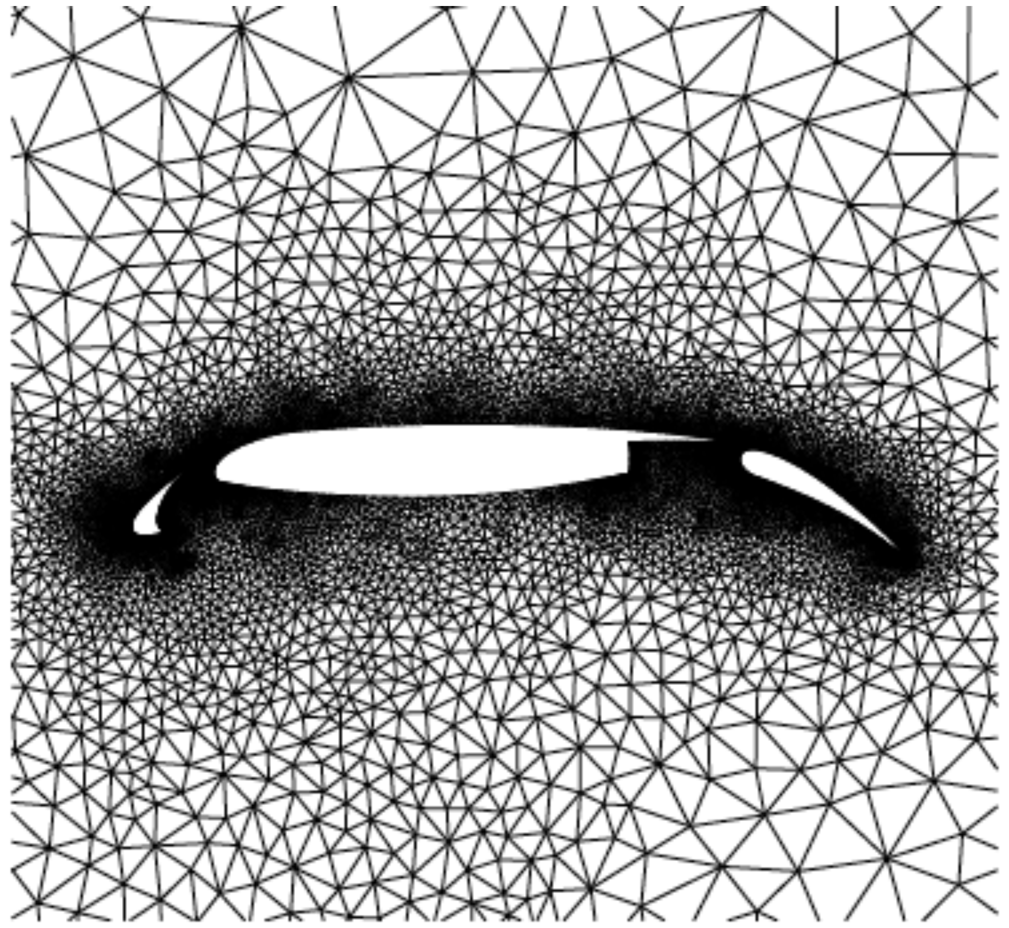


body-fitted



cartesian

unstructured



triangular

On the grid, the field $C(\boldsymbol{x}, t)$ takes discrete values $C_{i,j}^{n} \equiv C(x_i, y_j, t_n)$

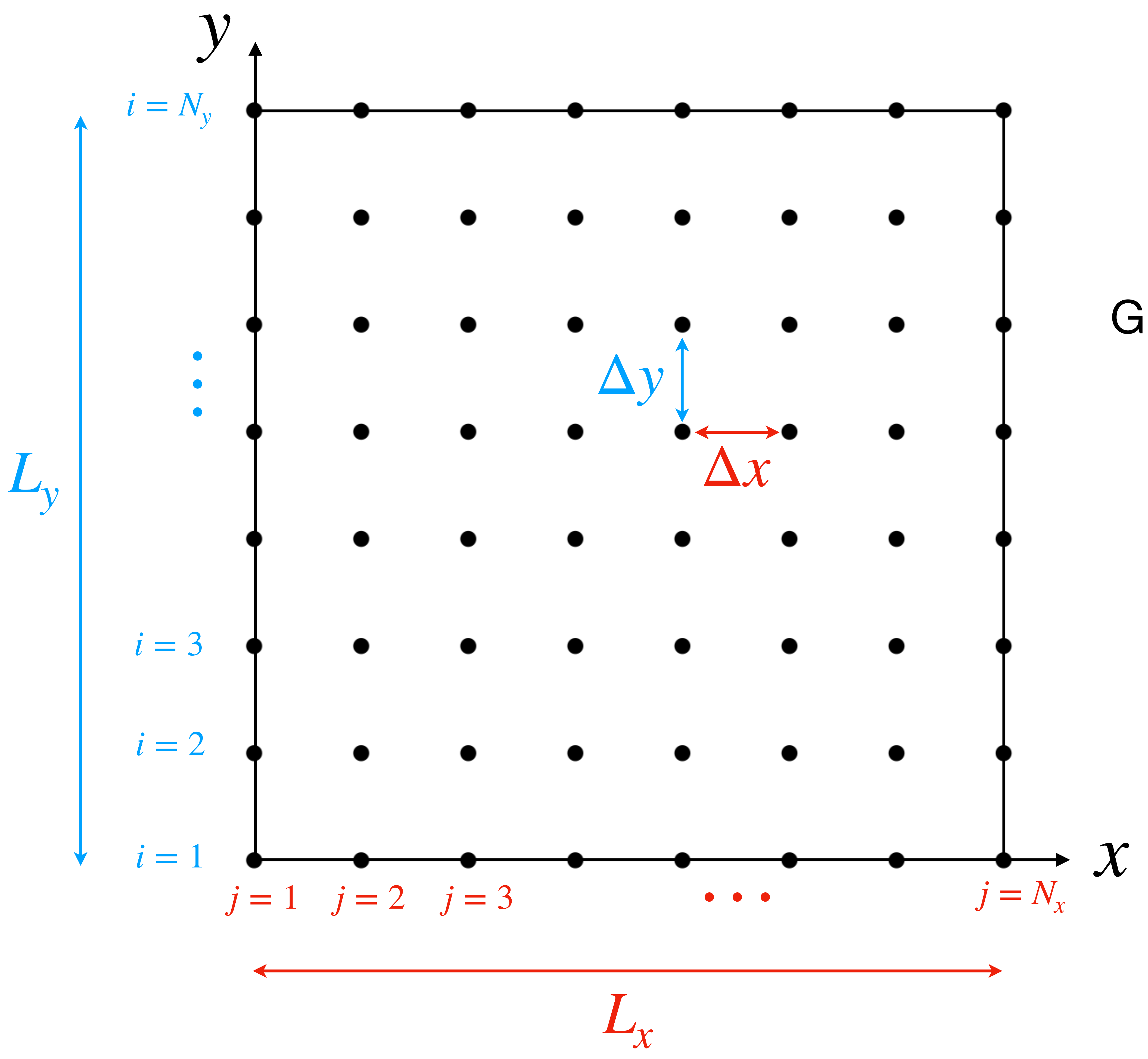
Example:

- (uniform) Cartesian Grid $x_i = x_0 + i\Delta x$, $y_i = y_0 + j\Delta y$ and $t_n = t_0 + n\Delta t$

Inspired from «Fundamentals of CFD Methods» course by A. Haselbacher

Discretizing a 2D Space - Grids

1. Spatial discretization



Grid spacing:

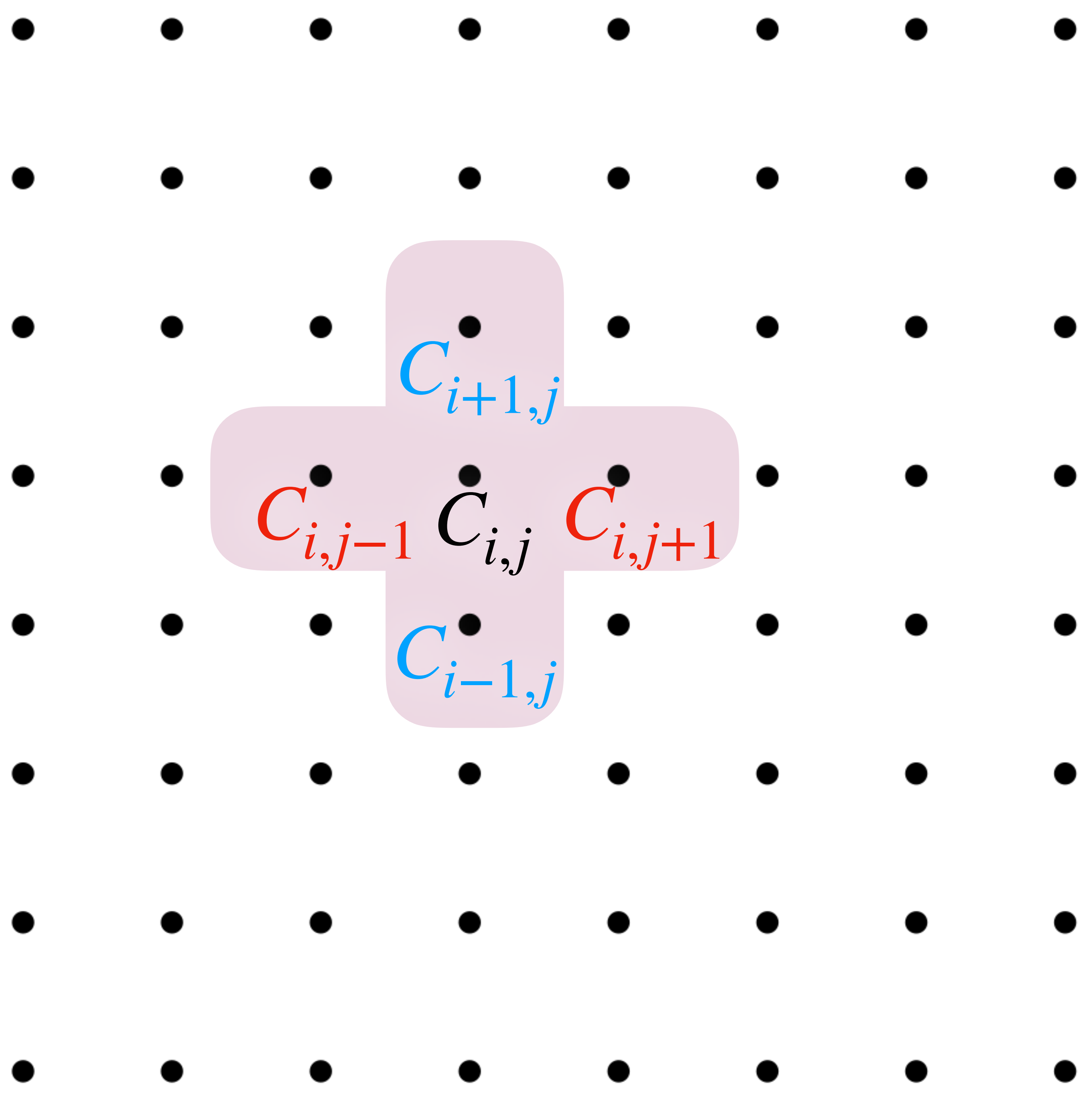
$$\Delta x = \frac{L_x}{N_x - 1}$$

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

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:

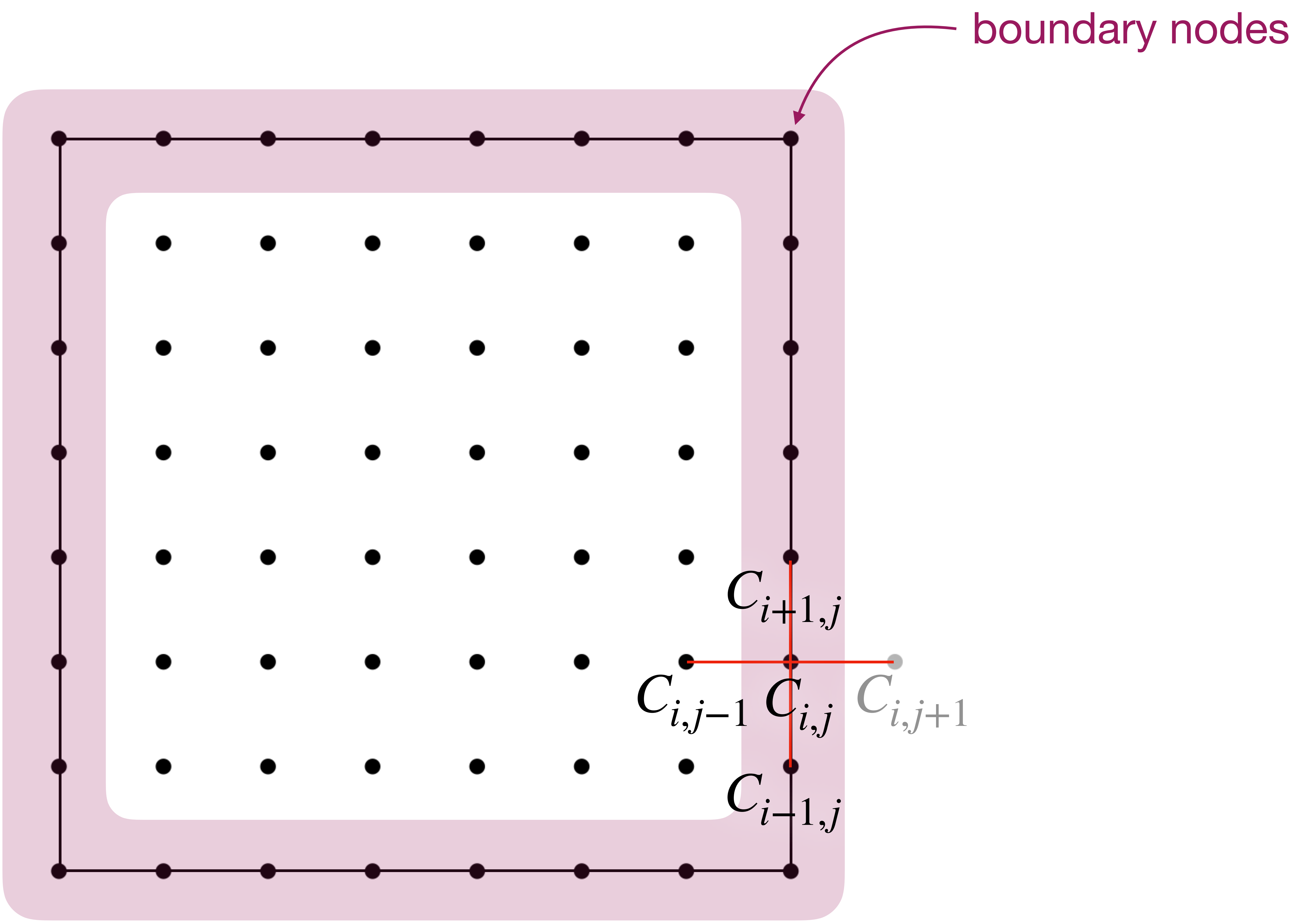
$$\frac{C^{n+1}_{i,j} - C^{n}_{i,j}}{\Delta t} = D\left(\frac{C^{n}_{i,j-1} - 2C^{n}_{i,j} + C^{n}_{i,j+1}}{\Delta x^2} + \frac{C^{n}_{i-1,j} - 2C^{n}_{i,j} + C^{n}_{i+1,j}}{\Delta y^2}\right)$$

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

$$C^{n+1}_{i,j} = \ldots (TODO)$$

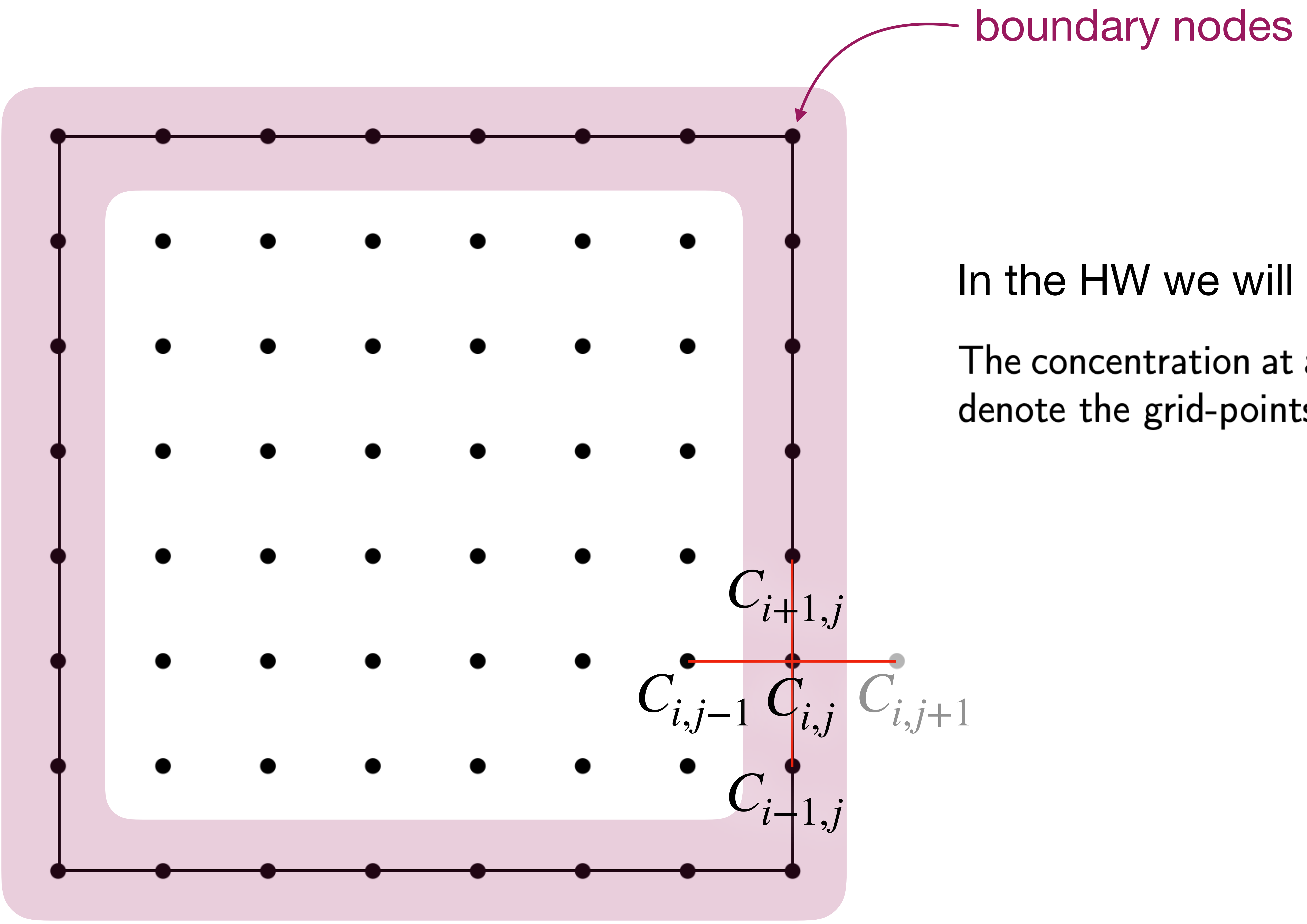
HW#4: **Q3**: Diffusion

3. Boundary nodes: application of the Boundary Condition



HW#4: **Q3**: Diffusion

3. Boundary nodes: application of the Boundary Condition

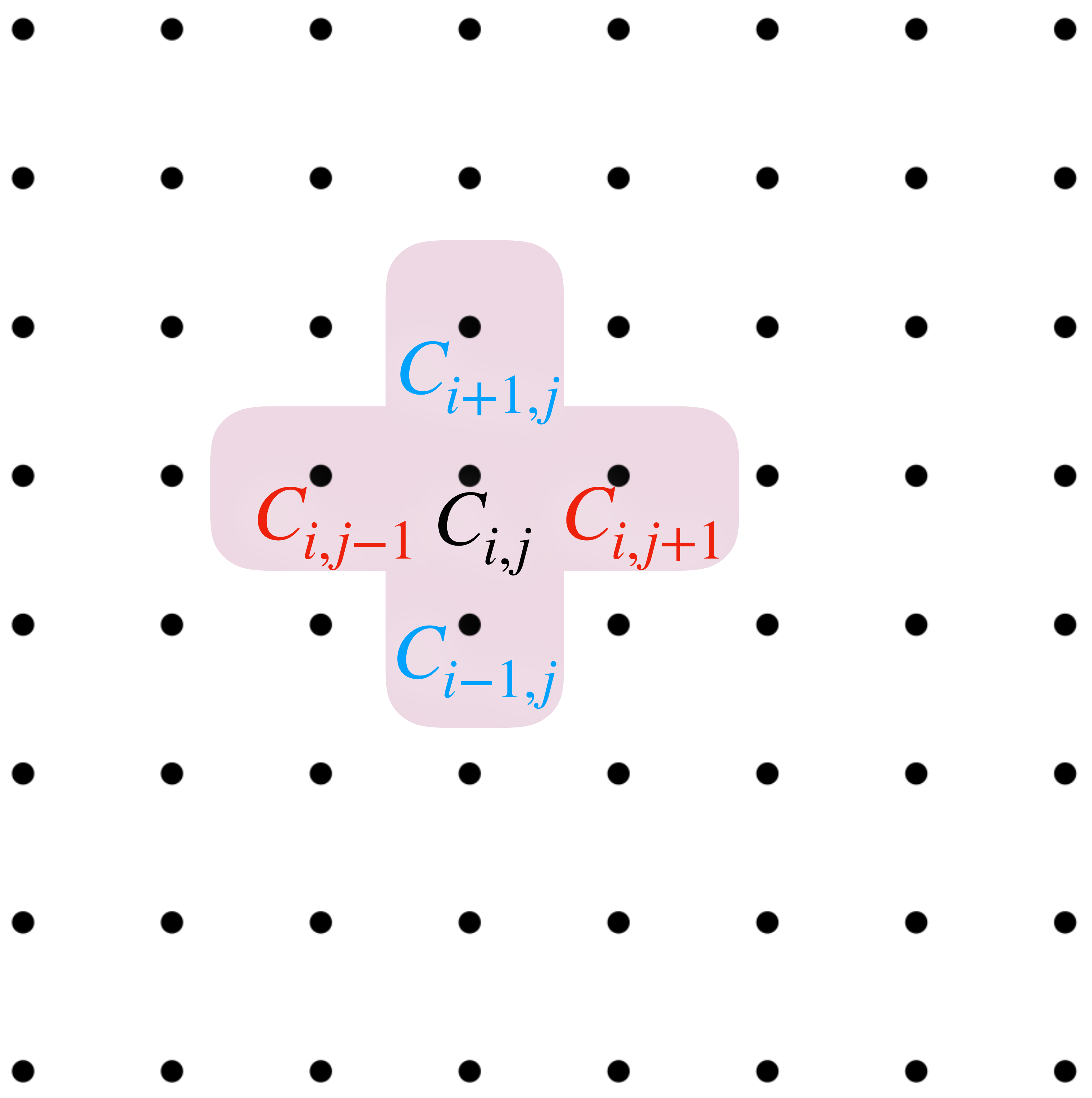


In the HW we will consider the following BC:

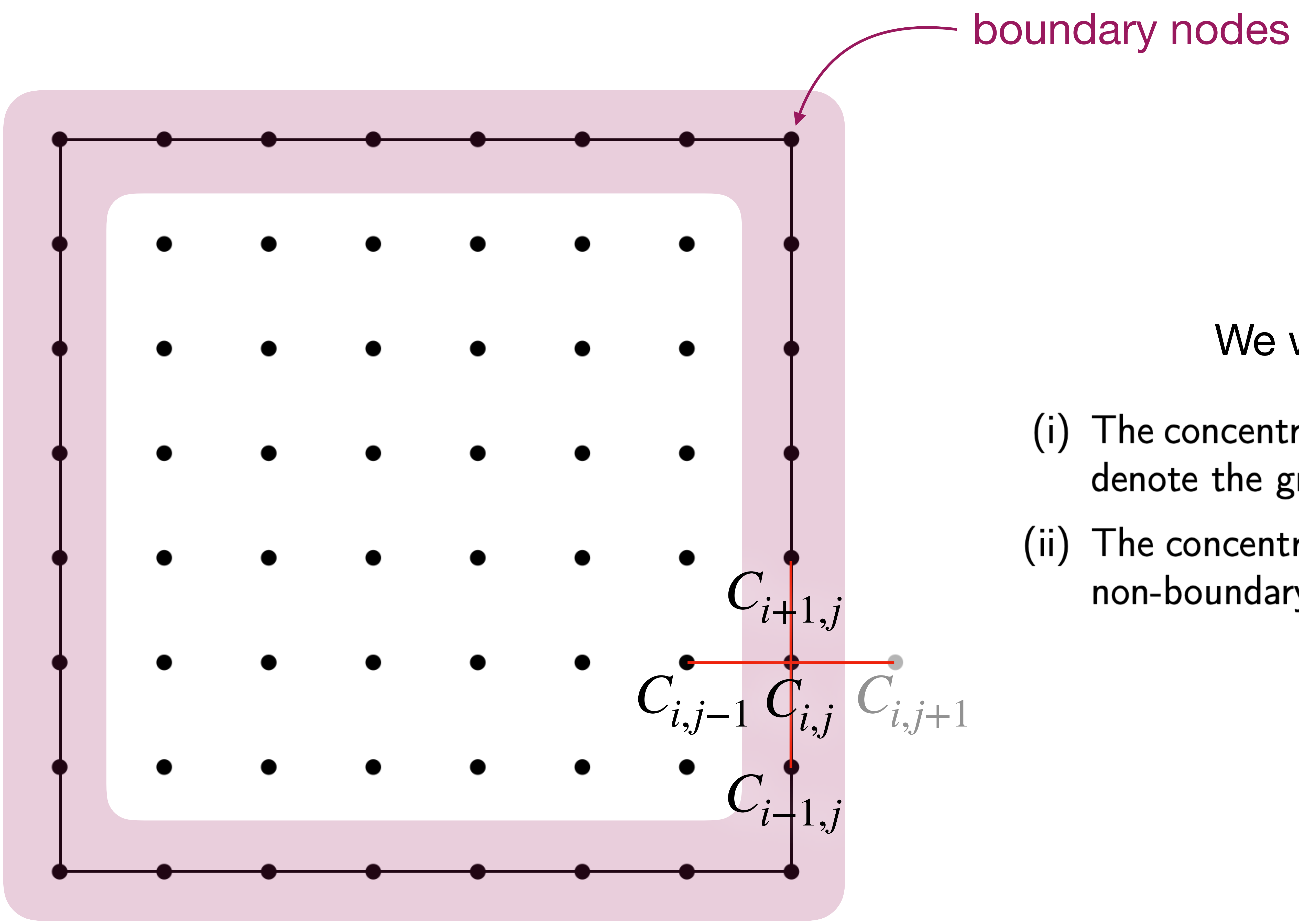
The concentration at all boundary grid-points is 0, i.e. $C(x_B, y_B, t) = 0$, where x_B, y_B denote the grid-points located on the domain boundary (perimeter).

Discretizing Derivatives - Finite Differences

$$\nabla^2 C(x, y, t) = \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \approx \frac{C_{i,j-1} - 2C_{i,j} + C_{i,j+1}}{\Delta x^2} + \frac{C_{i-1,j} - 2C_{i,j} + C_{i+1,j}}{\Delta y^2}$$



Discretizing Derivatives - Finite Differences



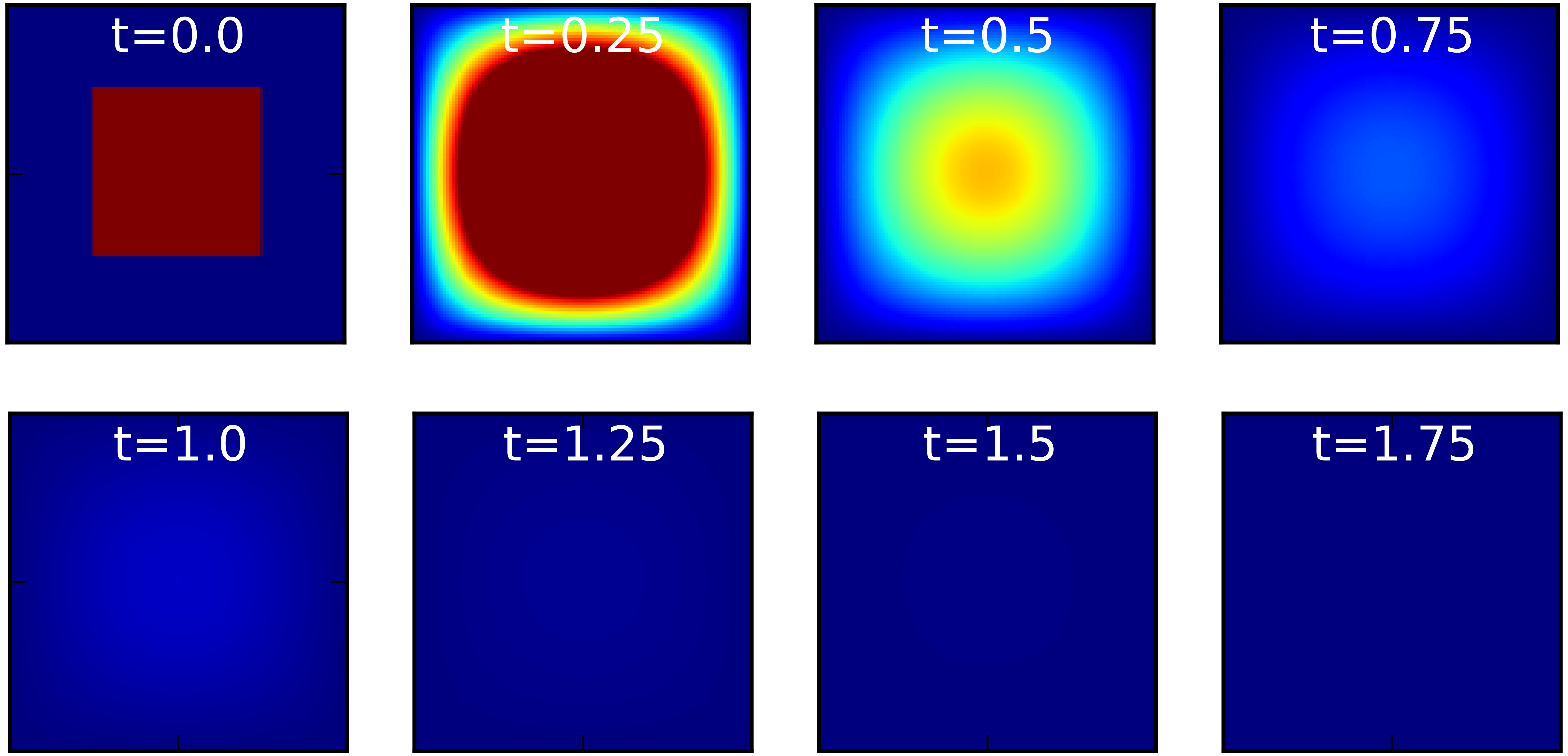
We will consider 2 cases, with 2 Boundary Conditions:

(i) 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).

(ii) The concentration of a boundary grid-point is equal to the concentration of its closest non-boundary grid-point.

Diffusion with a square as Initial Condition

Initial Condition



Using absorbing BCs !!

Fully homogeneous material