Steady-state Solution for the Continuity Equation

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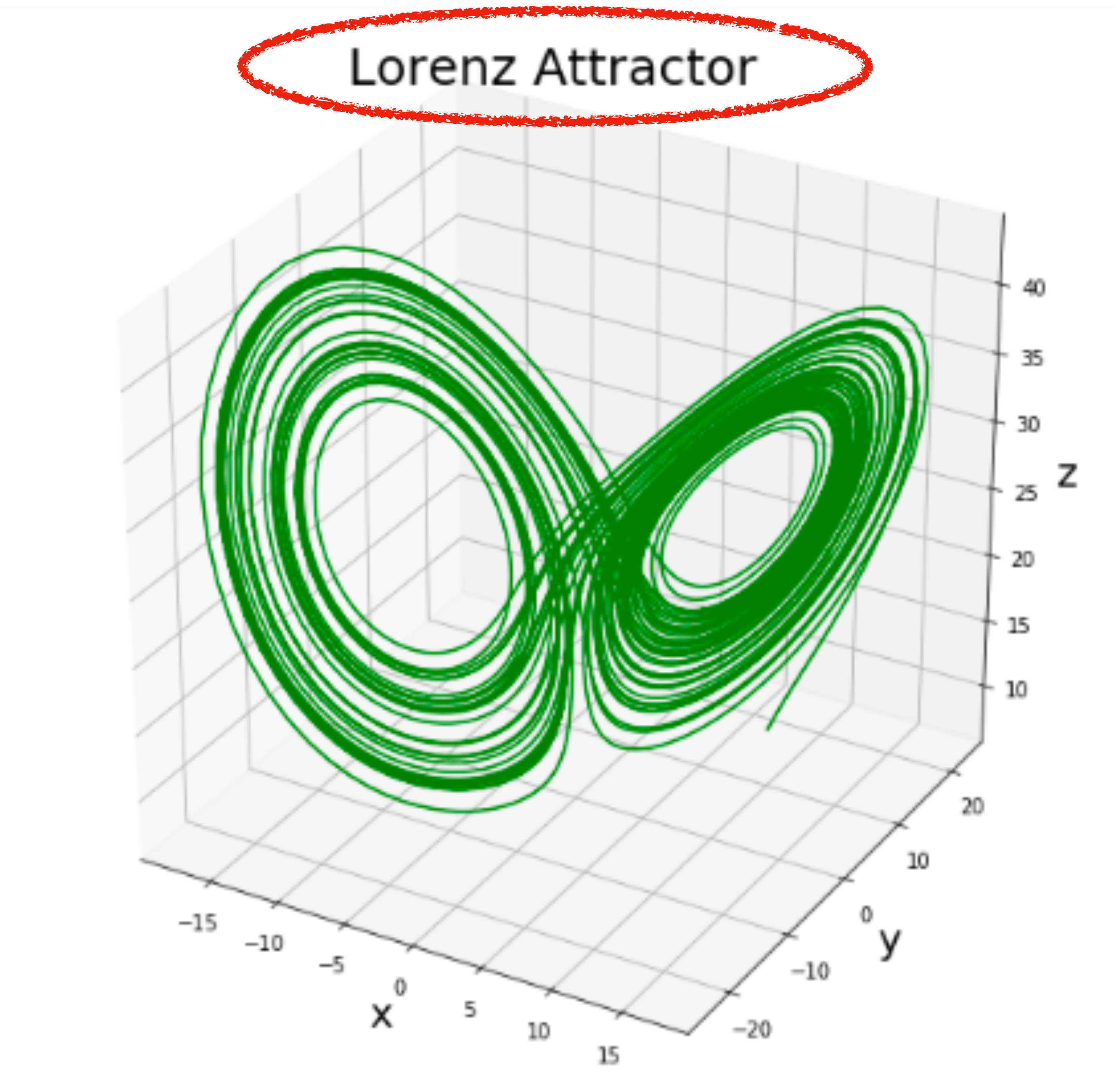
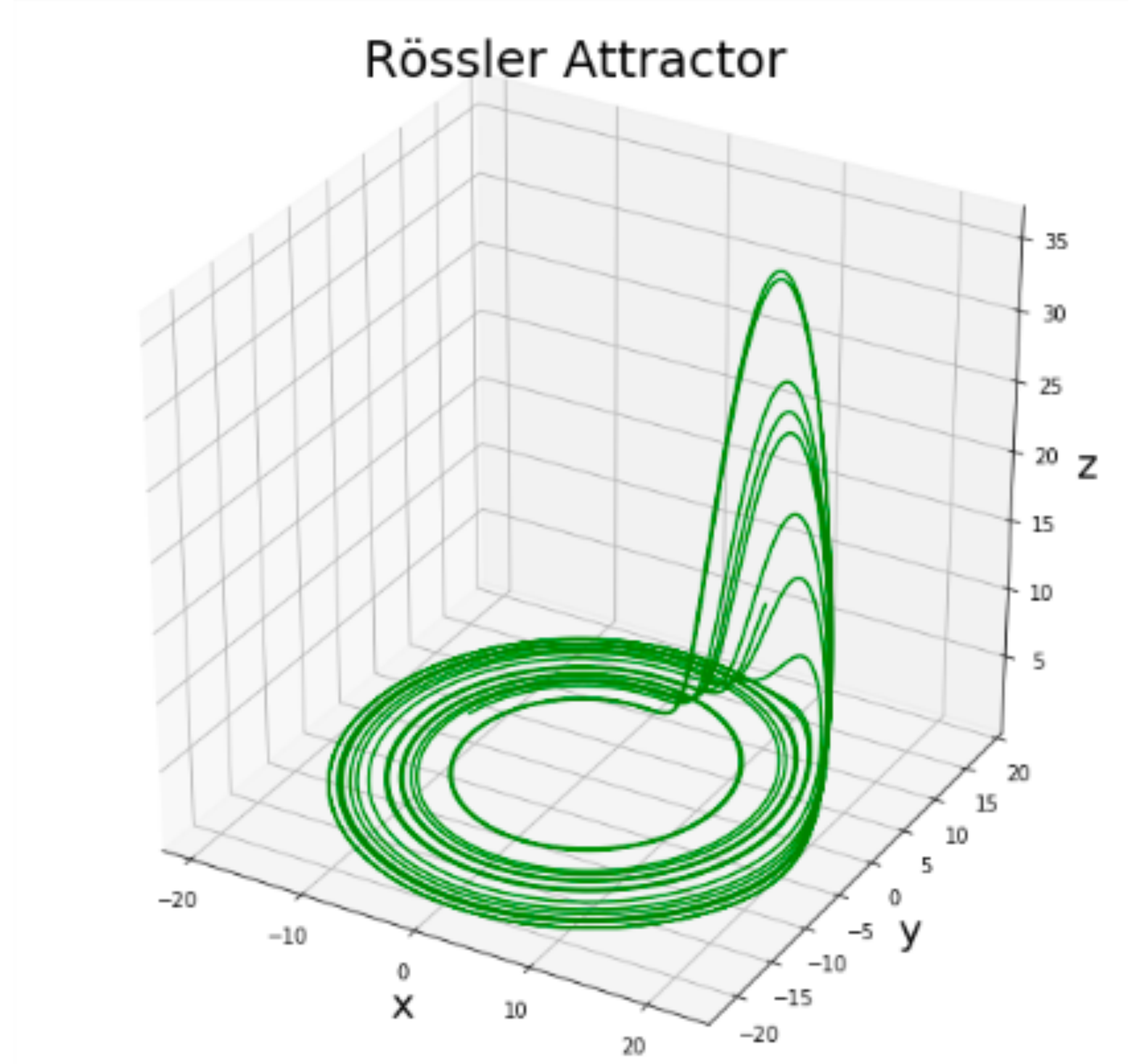
Background

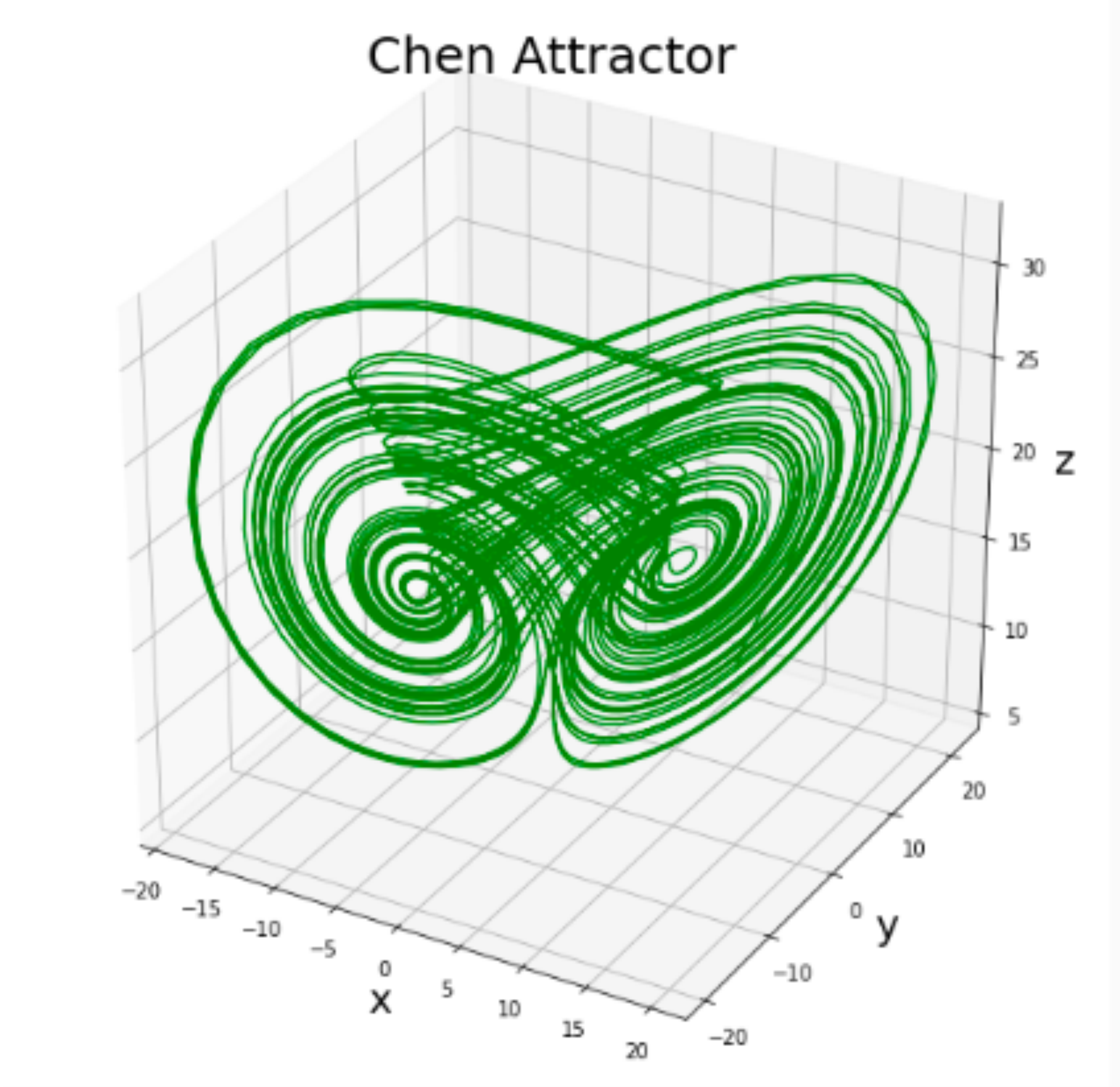
Parameter Identification [1]**:**

Given the **time** trajectories and **the dynamical system** → Adapt the parameters until the model is close to **experimental data**

Chaotic Dynamical System





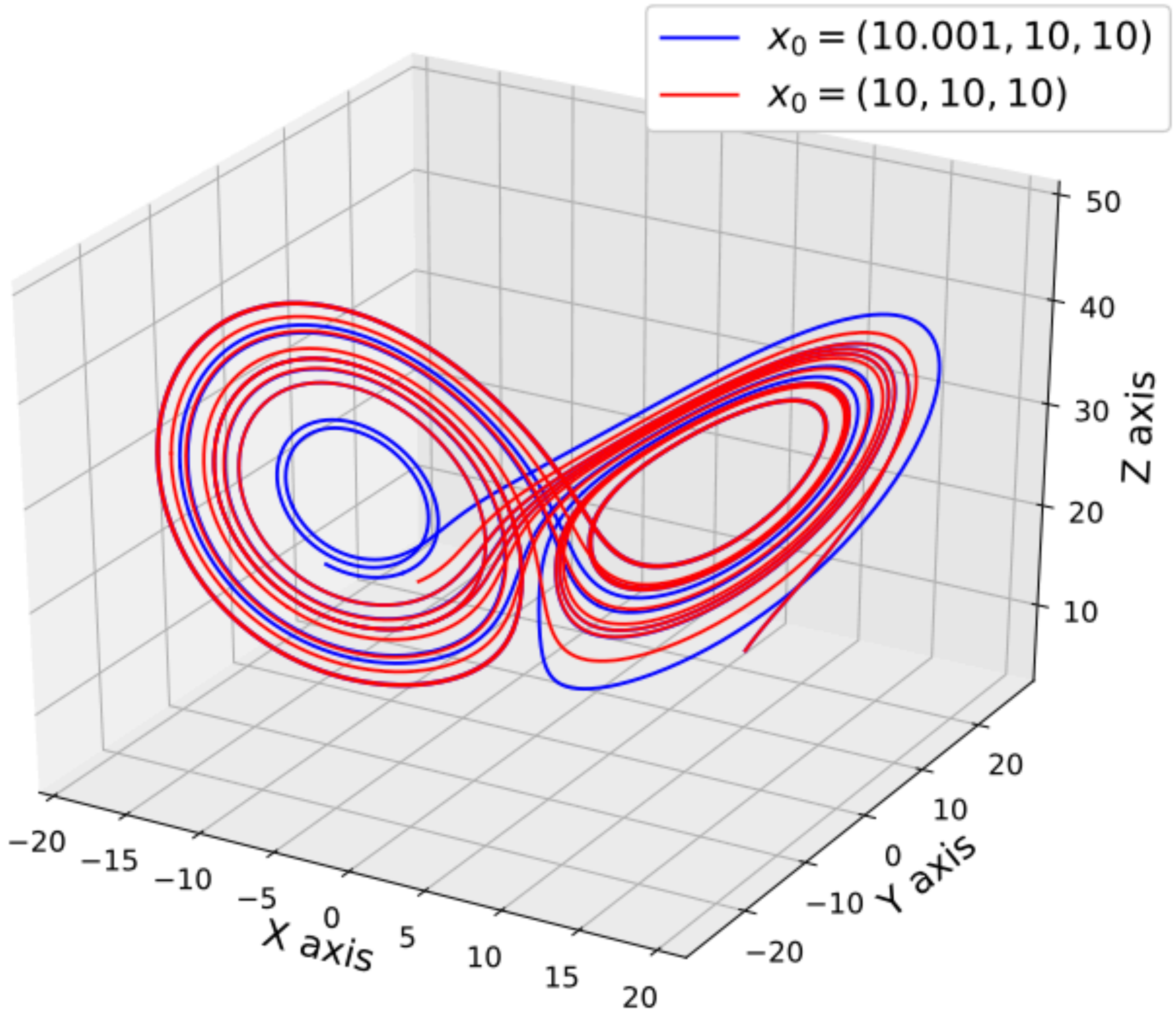


[1] Yang, Y., Nurbekyan, L., Negrini, E., Martin, R., & Pasha, M. (n.d.). Optimal Transport For Parameter Identification of Chaotic Dynamics via Invariant Measures.

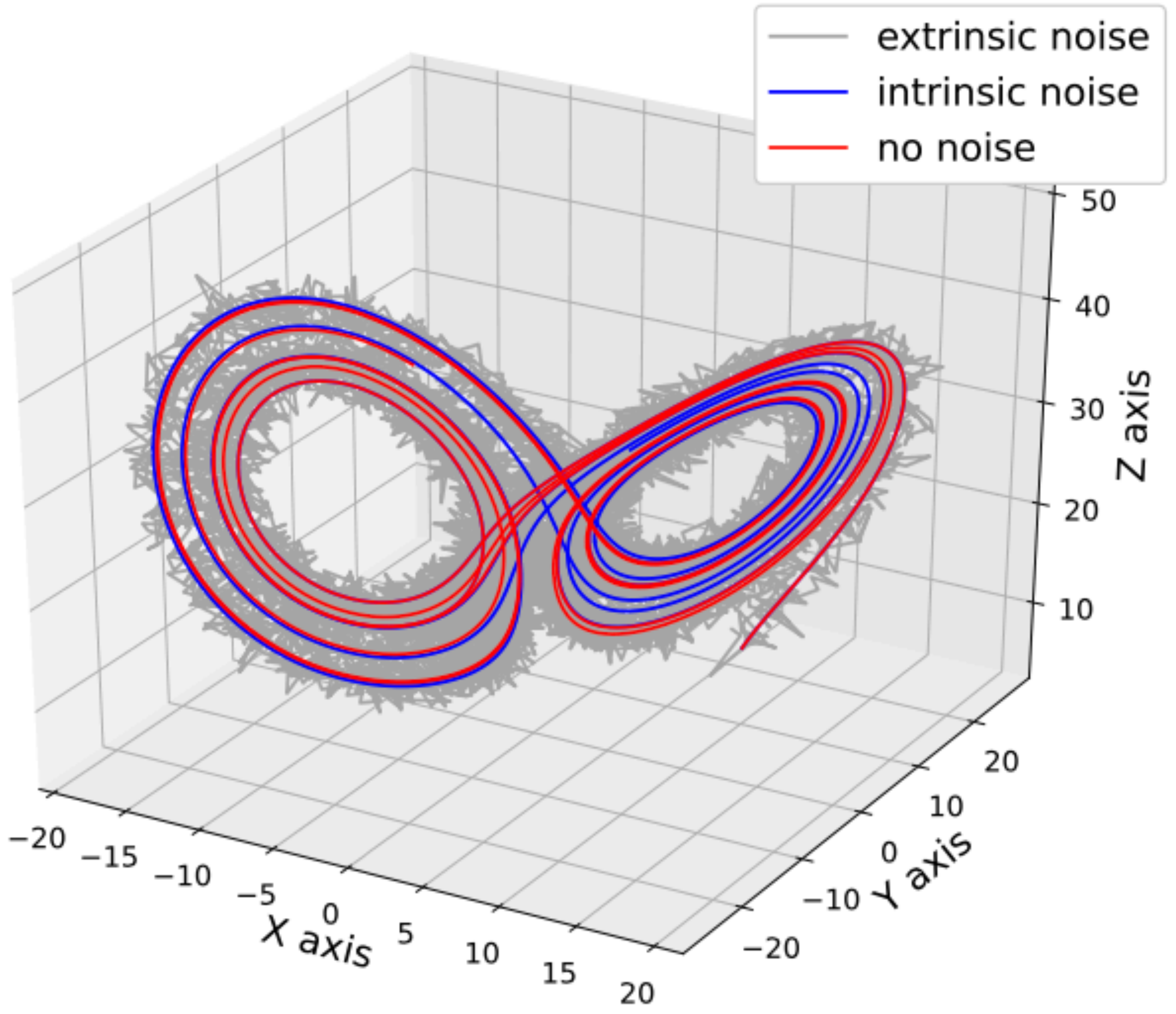
Background

- Challenges with Data-Driven Approaches:

1. Chaotic



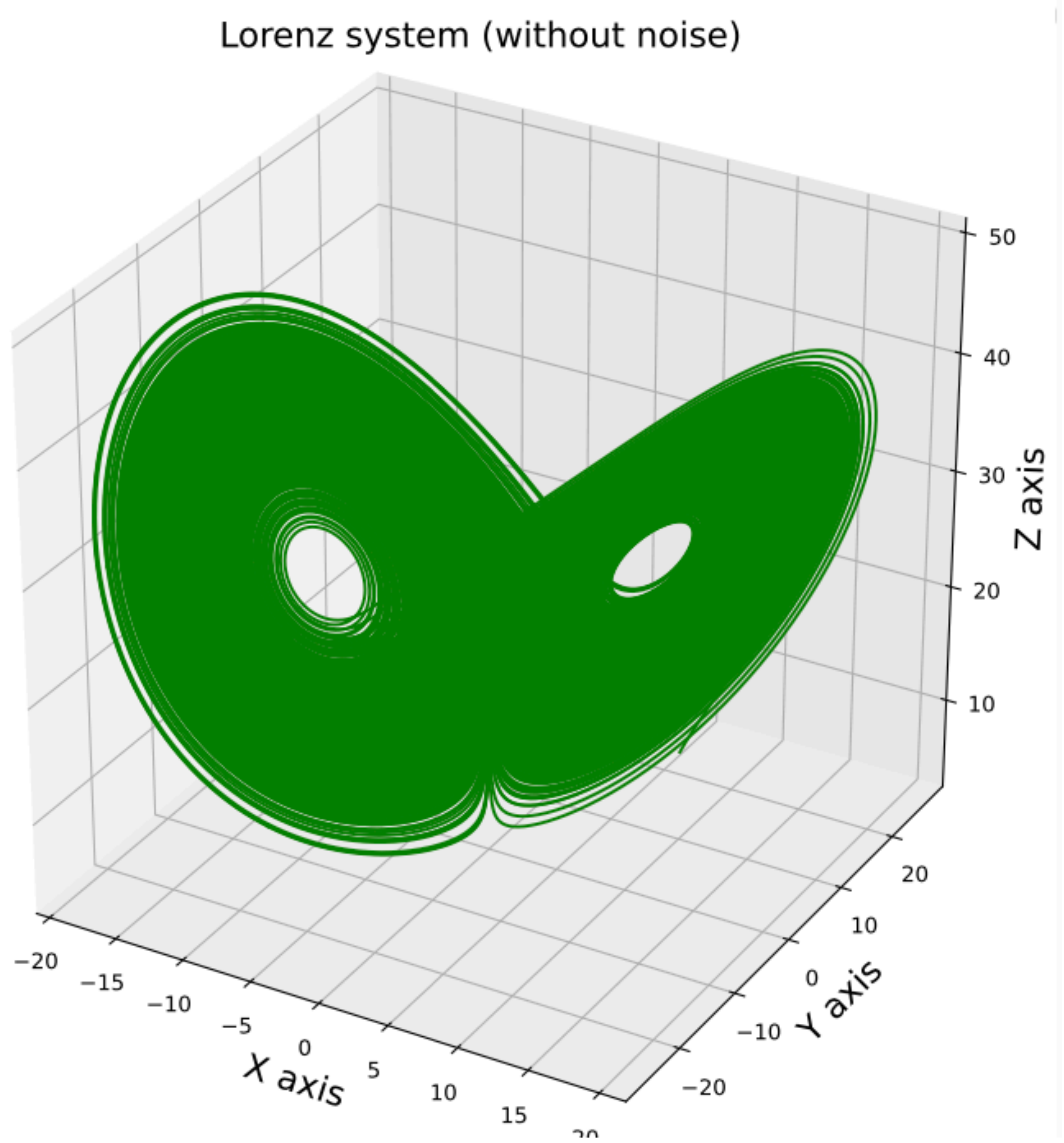
2. Noisy Measurements



[1] Yang, Y., Nurbekyan, L., Negrini, E., Martin, R., & Pasha, M. (n.d.). Optimal Transport For Parameter Identification of Chaotic Dynamics via Invariant Measures.

How to avoid these disturbances?

Background



Solution

1. Occupation Measure:
   Time trajectory with a large T
   -> Histogram
   -> Density

2. Sinai–Ruelle–Bowen (SRB)[2] measure:

$$\frac{\partial \rho}{\partial t} = -\nabla(v(x,\theta)\rho(x,t)) = 0$$

$\rho(x,t)$: probability density function of variable x in t

$v(x)$: the velocity of the flux at x

Past Challenges

→ Chaotic: invariant measure

→ Noisy Measurements:

→ Computation

Invariant Measure:
A measure μ is said to be invariant under the flow map f if, for every measurable set A in Σ,

$$\mu(f^{-1}(A)) = \mu(A)$$

Steady-State:

$$\frac{\partial \rho}{\partial t} = -\nabla(v(x,\theta)\rho(x,t)) = 0$$

[2] W. Cowieson and L.-S. Young, SRB measures as zero-noise limits, Ergodic Theory and Dynamical Systems, 25 (2005), p. 1115–1138
[3] Invariant measure. (2021, July 22). Wikipedia. https://en.wikipedia.org/wiki/Invariant_measure

Background

Original Problem (ODE)	Current Problem (PDE)
Given the **time trajectories** and the **dynamical system**, reconstruct the parameter.	Given the observed **invariant measure** and the **Continuity equation,** reconstruct the parameter.

"We treat the parameter identification problem for the dynamical system as a PDE-constrained optimization problem[1]: "

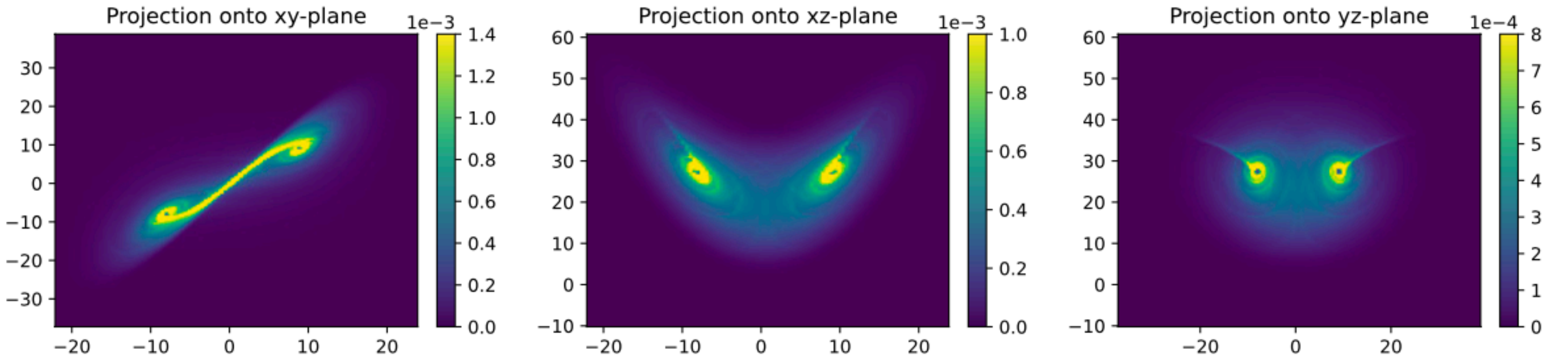
$$\theta = \underset{\theta}{\operatorname{argmin}}\, d(\rho^*, \rho(\theta)), \qquad \text{s.t. } \frac{\partial \rho}{\partial t} = -\nabla \cdot (v(x,\theta)\rho(x,t)) = 0$$

v(x): the velocity function of x

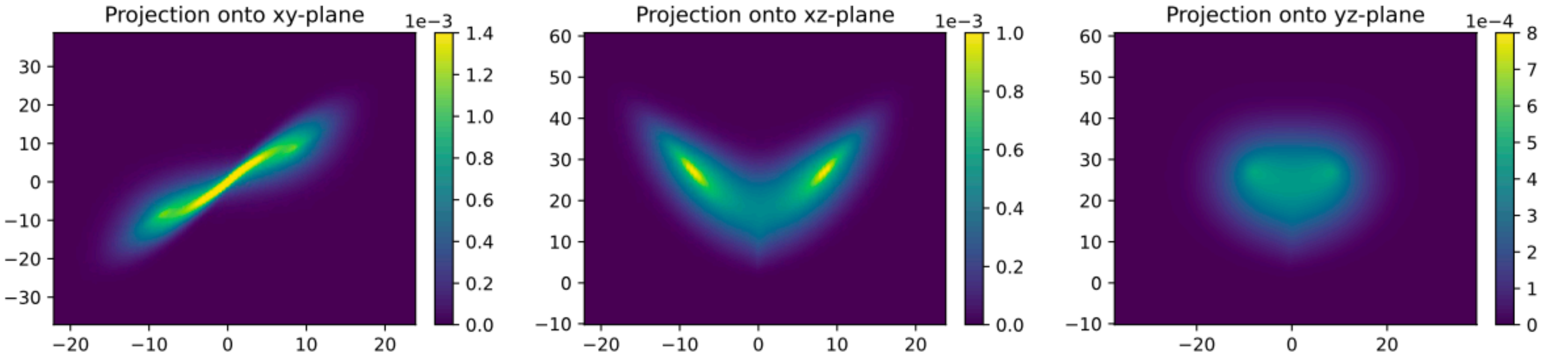
$\rho(\theta)$: the steady-state solution of the continuity equation ρ^* : the observed invariant measure converted from time trajectories

 [1] Yang, Y., Nurbekyan, L., Negrini, E., Martin, R., & Pasha, M. (n.d.). Optimal Transport For Parameter Identification of Chaotic Dynamics via Invariant Measures.

Motivation



Histogram accumulated from **Lorenz system** time trajectory



Steady-state solution

[1] Yang, Y., Nurbekyan, L., Negrini, E., Martin, R., & Pasha, M. (n.d.). Optimal Transport For Parameter Identification of Chaotic Dynamics via Invariant Measures.

Objective

Accuracy Improvement

1. Construct the solver with the **first-order finite volume split** discretization and the **Upwind Method** on a d-dimensional mesh in space and **time**.

2. **Improve the solver with corner transport.**

3. Derive the steady-state solution from the resulted matrix.

#1 First-Order Standard Upwind

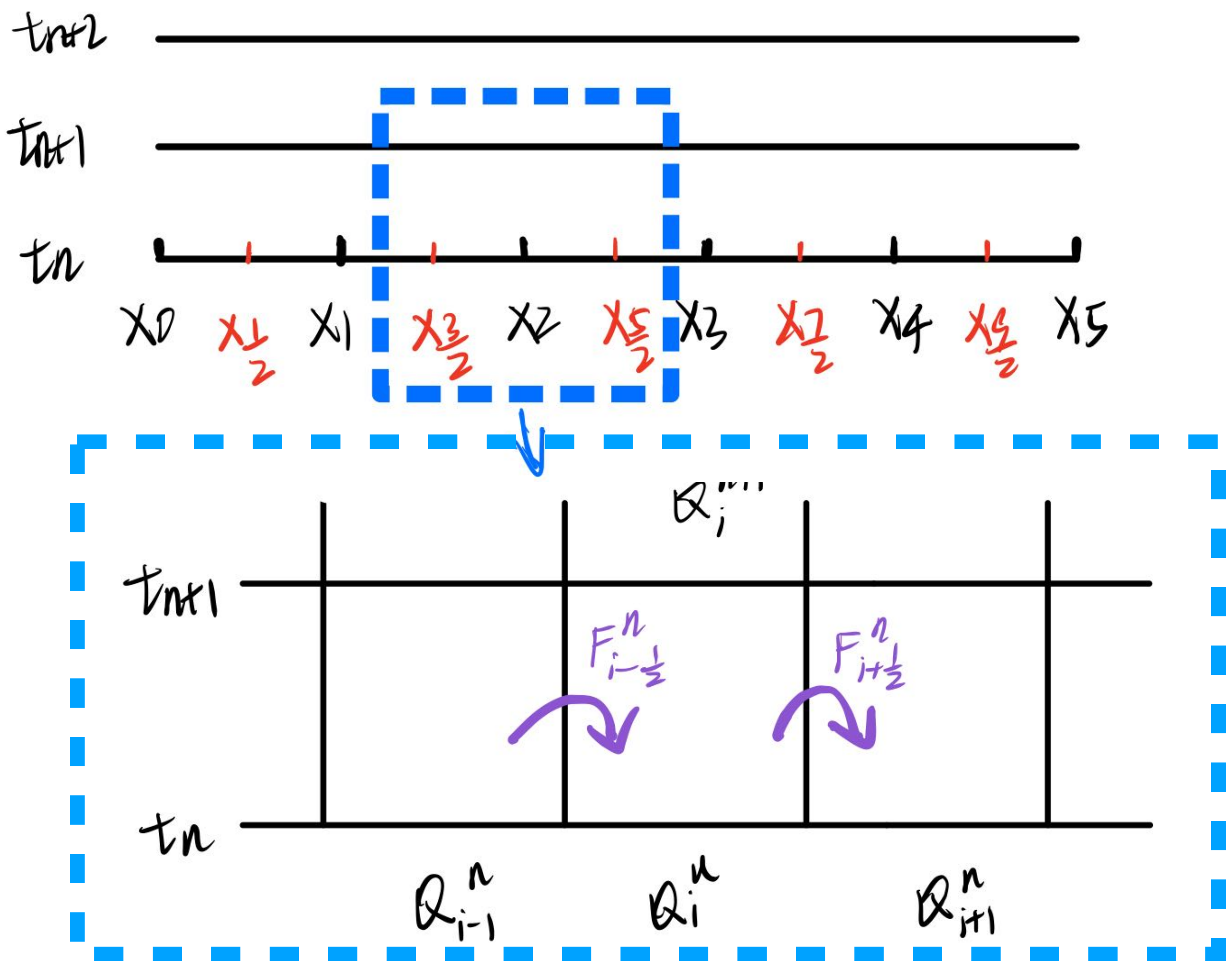
- Step 0: 1D

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(v(x)\rho(x,t)) = 0$$

- Step 1: Spatial Domain -> Intervals[4]

$$Q_i^n \approx \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+1/2}} \rho(x, t_n)\, dx$$

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}(F_{i+1/2}^n - F_{i-1/2}^n)$$



$v(x)$: the velocity of the flux at x

$\rho(x,t)$: probability density function of variable x

Q_i^n : the average value of ρ(x, tn) over the *i* th interval

$F_{i-1/2}^n$: the average flux along $x = x_{i-1/2}$

[4] LeVeque, R. J. (2002). *Finite volume methods for hyperbolic problems.* Cambridge University Press.

#1 First-Order Standard Upwind

- Step 3:

Upwind Method:

Define $v_i = v(x_i)$, then $F^n_{i-1/2} = v^+_{i-1/2}Q^n_{i-1} + v^-_{i-1/2}Q^n_i$

$F^n_{i+1/2} = v^+_{i+1/2}Q^n_{i-1} + v^-_{i+1/2}Q^n_i$

$$Q^{n+1}_i = Q^n_i - \frac{\Delta t}{\Delta x}(F^n_{i+1/2} - F^n_{i-1/2})$$

=> $$Q^{n+1}_i = Q^n_i - \frac{\Delta t}{\Delta x}(v^+_{i-1/2}Q^n_{i-1} + (v^-_{i-1/2} - v^+_{i+1/2})Q^n_i - v^-_{i+1/2}Q^n_{i+1})$$

=> $$\begin{bmatrix} Q^{n+1}_0 \\ Q^{n+1}_1 \\ \vdots \\ Q^{n+1}_N \end{bmatrix} = \begin{bmatrix} Q^n_0 \\ Q^n_1 \\ \vdots \\ Q^n_N \end{bmatrix} - \frac{\Delta t}{\Delta x} \underbrace{\begin{bmatrix} -v^+_{1/2,0} & -v^-_{1/2,0} & 0 & \dots & 0 \\ v^+_{1/2,0} & v^-_{1/2,0} - v^+_{3/2,0} & -v^-_{3/2,0} & \dots & 0 \\ 0 & v^+_{3/2,0} & v^-_{3/2,0} - v^+_{5/2,0} & -v^-_{5/2,0} & \dots \\ \dots & & & & \end{bmatrix}}_{K} \begin{bmatrix} Q^n_0 \\ Q^n_1 \\ \vdots \\ Q^n_N \end{bmatrix}$$

$v(x)$: the velocity of the flux at x

$v^+ = max(v(x),0)$

$v^- = min(v(x),0)$

Q^n_i : the average value of ρ(x, tn) over the i th interval

$F^n_{i-1/2}$: the average flux along $x = x_{i-1/2}$

#1+#3 First-Order Standard Upwind

- 1D $Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x}(F_{i+1/2}^n - F_{i-1/2}^n)$
- 2D $Q_{ij}^{n+1} = Q_{ij}^n - \frac{\Delta t}{\Delta x}(F_{i+1/2,j}^n - F_{i-1/2,j}^n) - \frac{\Delta t}{\Delta y}(G_{i,j+1/2}^n - G_{i,j-1/2}^n)$
- 3D $Q_{ijk}^{n+1} = Q_{ijk}^n - \frac{\Delta t}{\Delta x}(F_{i+1/2,j,k}^n - F_{i-1/2,j,k}^n) - \frac{\Delta t}{\Delta y}(G_{i,j+1/2,k}^n - G_{i,j-1/2,k}^n) - \frac{\Delta t}{\Delta z}(H_{i,j,k+1/2}^n - H_{i,j,k-1/2}^n)$

$$=> \begin{bmatrix} Q_0^{n+1} \\ Q_1^{n+1} \\ \vdots \\ Q_N^{n+1} \end{bmatrix} = \begin{bmatrix} Q_0^{n} \\ Q_1^{n} \\ \vdots \\ Q_N^{n} \end{bmatrix} - \left(\frac{\Delta t}{\Delta x}T_1 + \frac{\Delta t}{\Delta y}T_2 + \frac{\Delta t}{\Delta z}T_3\right)\begin{bmatrix} Q_0^{n} \\ Q_1^{n} \\ \vdots \\ Q_N^{n} \end{bmatrix}$$

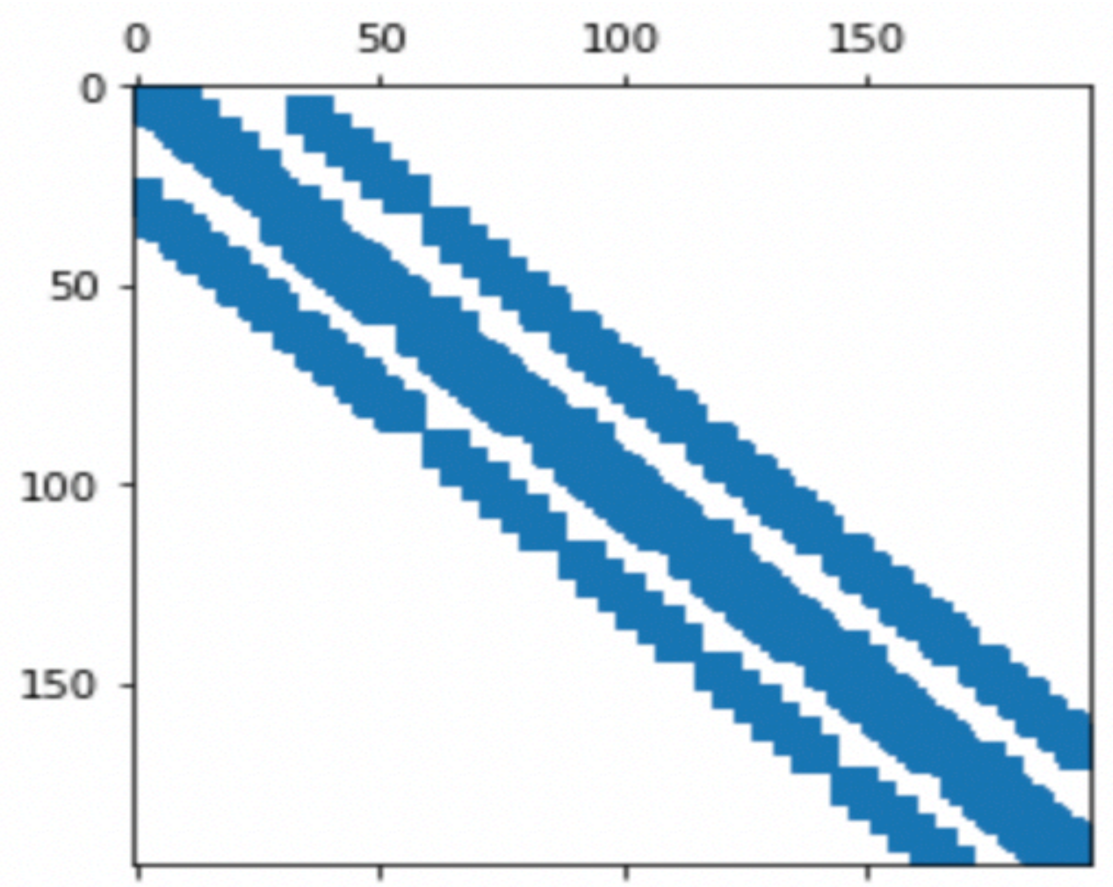
$$K = \frac{\Delta t}{\Delta x}T_1 + \frac{\Delta t}{\Delta y}T_2 + \frac{\Delta t}{\Delta z}T_3$$

Q_i^n : the average value of $\rho(x, t_n)$ over the i th interval

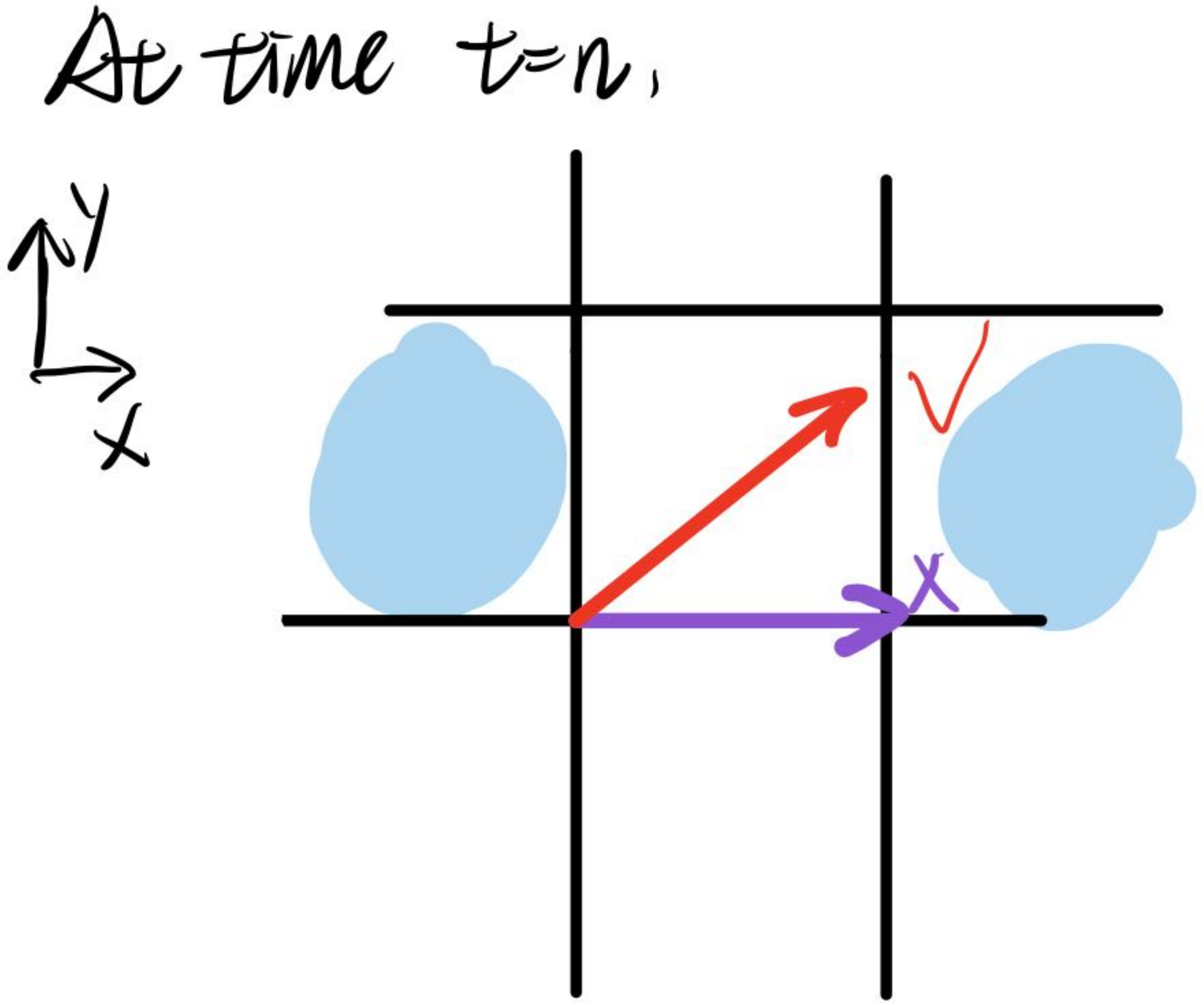
$F_{i-1/2}^n$: the average flux along $x = x_{i-1/2}$

$G_{i-1/2}^n$: the average flux along $y = y_{i-1/2}$

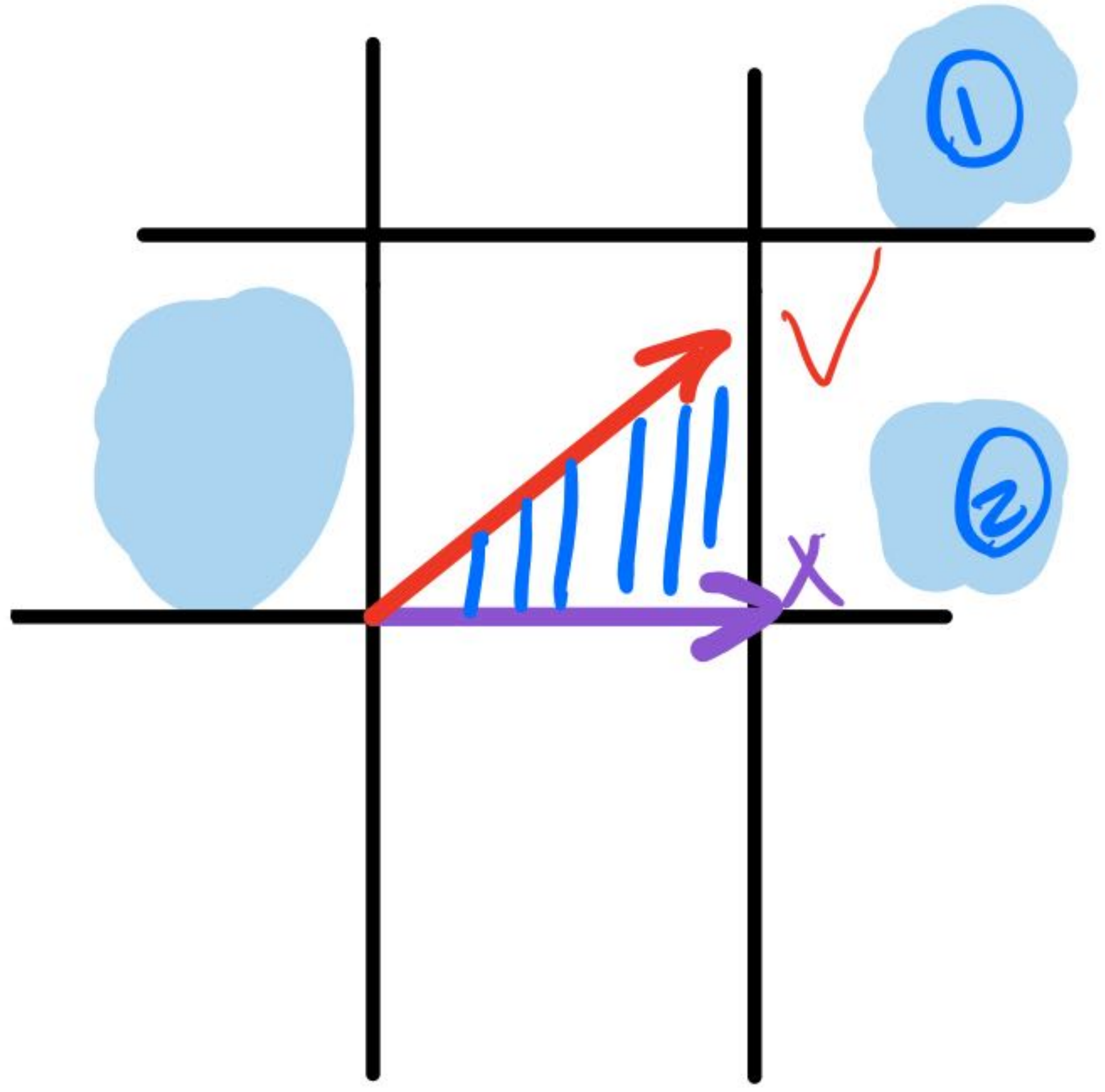
$H_{i-1/2}^n$: the average flux along $z = z_{i-1/2}$



#2 Improvement



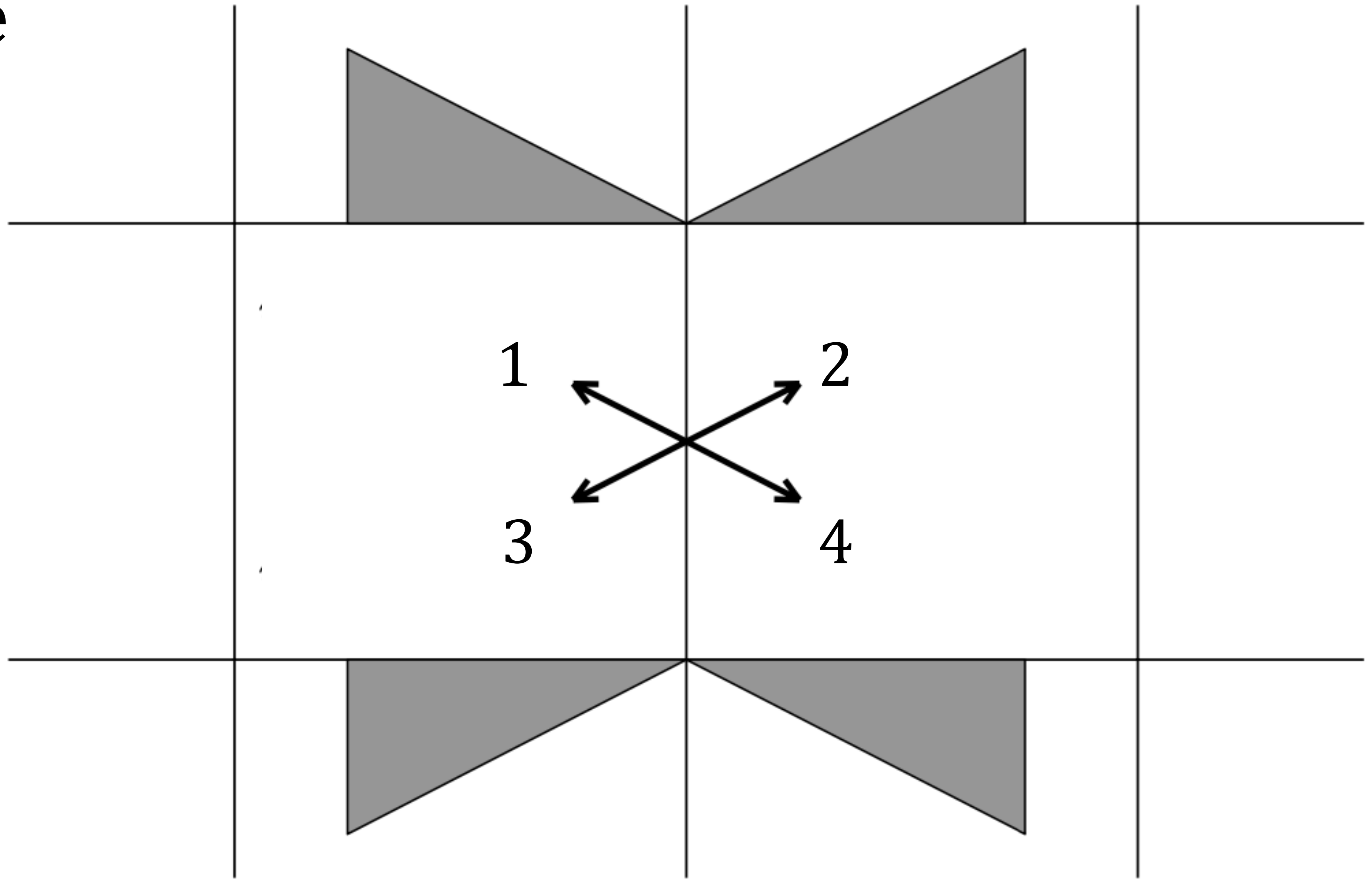
(1)



(2)

#2 Improvement—Corner transport[4]

- 2D (8): X-Y Plane



- 3D (24): X-Y Plane
  Y-Z Plane
  X-Z Plane

$$\tilde{F}_{i+1/2,j-1} = -\frac{1}{2}\frac{\Delta t}{\Delta y}u^{+}_{i+1/2,j-1}v^{-}_{i,j-1/2}(Q_{i,j} - Q_{i,j-1}) \qquad \tilde{F}_{i-1/2,j-1} = -\frac{1}{2}\frac{\Delta t}{\Delta y}u^{-}_{i-1/2,j-1}v^{-}_{i,j-1/2}(Q_{i,j} - Q_{i,j-1})$$

$$\tilde{F}_{i-1/2,j} = -\frac{1}{2}\frac{\Delta t}{\Delta y}u^{-}_{i-1/2,j}v^{+}_{i,j-1/2}(Q_{i,j} - Q_{i,j-1}) \qquad \tilde{F}_{i+1/2,j} = -\frac{1}{2}\frac{\Delta t}{\Delta y}u^{+}_{i+1/2,j}v^{+}_{i,j-1/2}(Q_{i,j} - Q_{i,j-1})$$

[4] LeVeque, R. J. (2002). *Finite volume methods for hyperbolic problems.* Cambridge University Press.

#3 Steady-state solution

1. Derive the matrix K from the linear system with finite volume split discretization and the Upwind Method:

$$\begin{bmatrix} Q_0^{n+1} \\ Q_1^{n+1} \\ \vdots \\ Q_N^{n+1} \end{bmatrix} = \begin{bmatrix} Q_0^{n} \\ Q_1^{n} \\ \vdots \\ Q_N^{n} \end{bmatrix} - \left(\frac{\Delta t}{\Delta x}T_1 + \frac{\Delta t}{\Delta y}T_2 + \frac{\Delta t}{\Delta z}T_3\right)\begin{bmatrix} Q_0^{n} \\ Q_1^{n} \\ \vdots \\ Q_N^{n} \end{bmatrix} \rightarrow K = \frac{\Delta t}{\Delta x}T_1 + \frac{\Delta t}{\Delta y}T_2 + \frac{\Delta t}{\Delta z}T_3$$

2. Modify the solver with corner transport, where $\tilde{K}$ **is multi-diagonal with columns summing to 0:**

$$\begin{aligned} Q^{n+1} &= Q^n - K * Q^n + CornerTransport * Q^n \\ &= Q^n - \tilde{K} * Q^n \end{aligned}$$

$\rightarrow$ $\tilde{M} = I + s\ \tilde{K}$ with a sufficiently small s

<u>The Markov Matrix $\tilde{M}$ preserves the property of the probability density:</u>

— Columns sum to 1

— Mass Conservation

#3 Steady-state solution

Markov Matrix

Imply the steady-state solution:

— ρ is the dominant eigenvector of M:

$$M\rho = \rho$$

$$\rho^{n+1} = (I + sK)\rho^n = M\rho^n$$

$$M\rho_{steady} = \rho_{steady}$$

— Tools:

(1) Power Method
(2) Sparse Direct Solve
(3) Richardson Iteration
...

Questions

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Thank you for listening