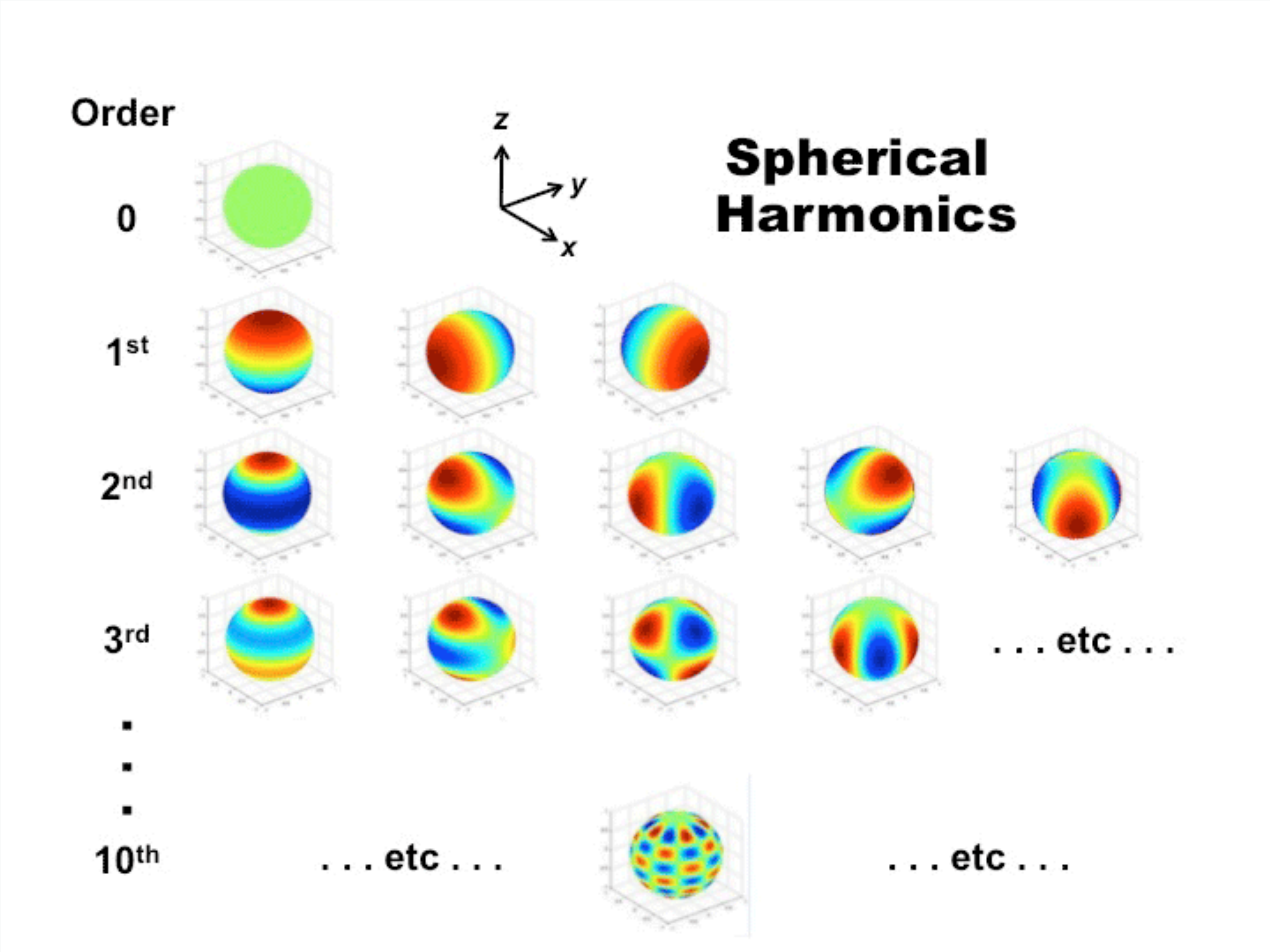
Introduction to the Discontinuous Galerkin method

김윤수 (Caltech)

Jul 28 2022,
@ NRGW Summer School, Busan

Motivation



https://mriquestions.com/uploads/3/4/5/7/34572113/_6902752_orig.gif

Motivation

e.g. Infinite square well (QM)

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}(x,t)\Psi(x,t), \qquad \Psi(0,t) = \Psi(L,t) = 0$$

introduce *basis* wave functions

$$\phi_k(x) = \sqrt{\frac{2}{L}}\sin\frac{k\pi x}{L} \qquad \langle\phi_i,\phi_j\rangle = \int_0^L \phi_i(x)\phi_j(x)dx = \delta_{ij}$$

then expand wavefunction: $\Psi(x,t) = \sum_{k=0}^{\infty} a_k\phi_k(x)$

Motivation

$$i\hbar \sum_{k=0}^{\infty} \frac{da_k}{dt} \phi_k = \sum_{k=0}^{\infty} a_k (\hat{H} \phi_k)$$

$$i\hbar \frac{da_i}{dt} = \sum_{k=0}^{\infty} \langle \phi_i, \hat{H} \phi_k \rangle a_k$$

Take product with a basis $\phi_i(x)$

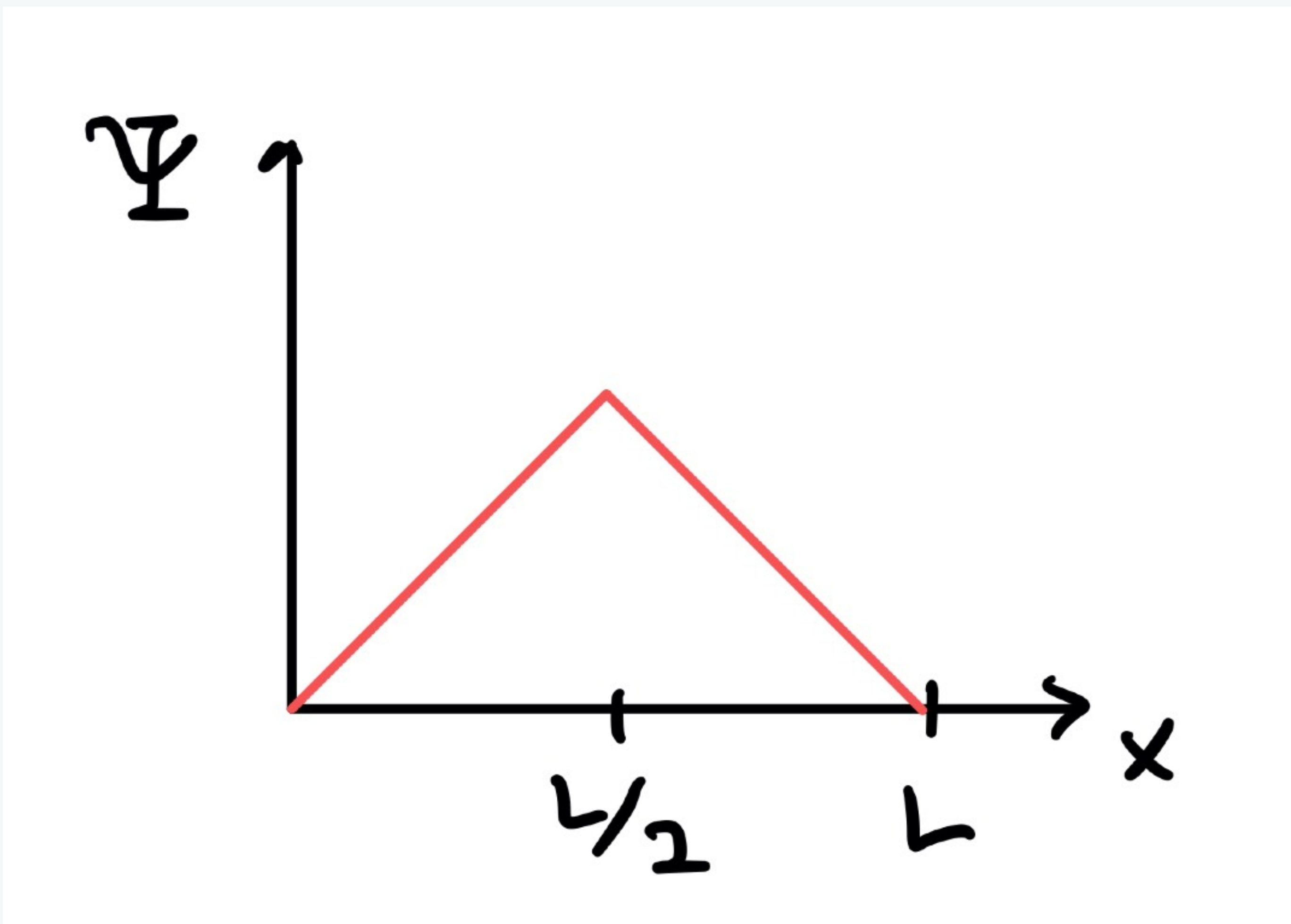
$$\frac{d}{dt} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix} = -\frac{i}{\hbar} \begin{bmatrix} H_{11} & H_{12} & \cdots \\ H_{21} & H_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix}$$

time evolution of expansion coefficients!

Motivation

In practice, series is truncated at finite k : $\Psi_N = \sum_{k=0}^{N} a_k \phi_k(x)$

How accurate is Ψ_N compared to Ψ ?



$$= \begin{cases} 0, & n \text{ even}, \\ (-1)^{(n-1)/2} \frac{4\sqrt{6}}{(n\pi)^2}, & n \text{ odd}. \end{cases}$$

Spectral method

- Finite difference : approximate the *equation*
  Spectral method : approximate the *solution*

- A truncated expansion with smooth basis functions $\phi_n(x)$

$$f(x) \rightarrow f_N(x) = \sum_{n=0}^{N} a_n \phi_n(x)$$

- Different choices of basis and methods of computing coefficients

Basis functions

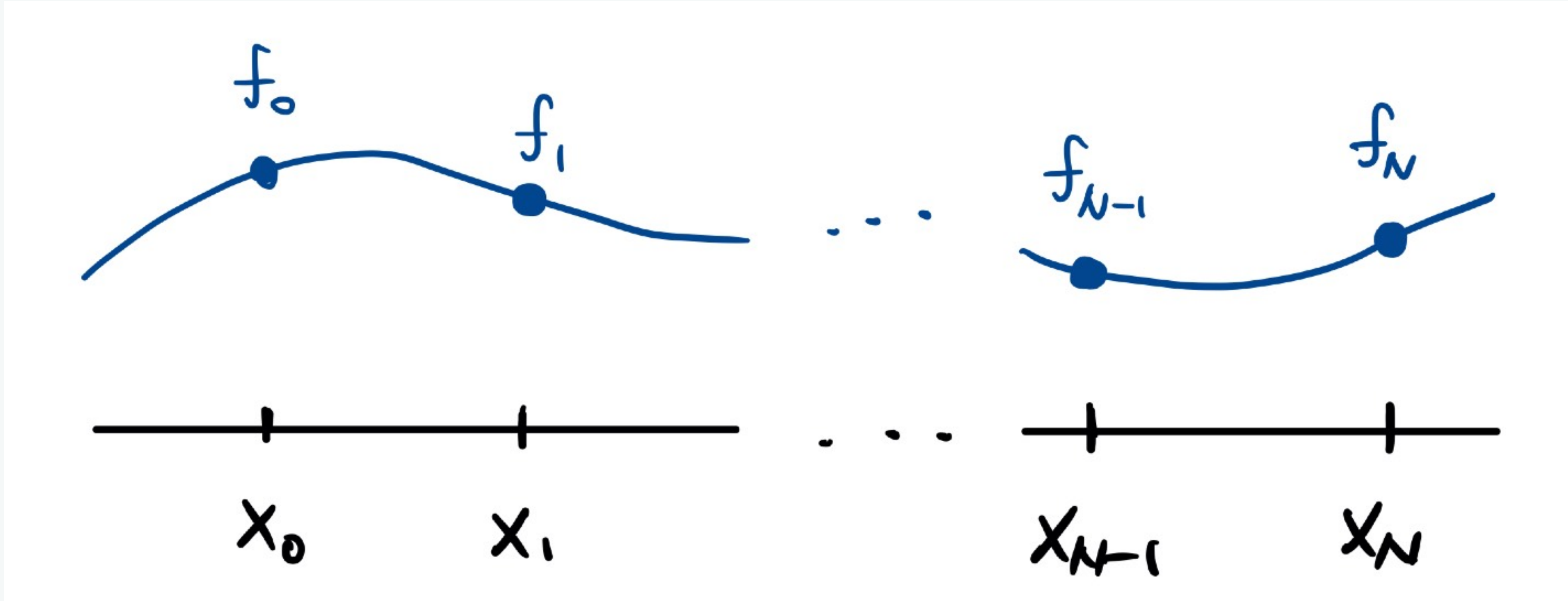
- Fourier basis
- Orthogonal polynomials (Chebyshev, Legendre)
- Nodal basis

How to compute a_n s?

- Tau method
- Galerkin method
- Collocation (or pseudospectral) method

Here we introduce collocation method with nodal approximation

Modal vs **Nodal**



modal representation

$$f_N(x) = \sum_{n=0}^{N} c_n P_n(x)$$

components of each modes
(spectral space)

nodal representation

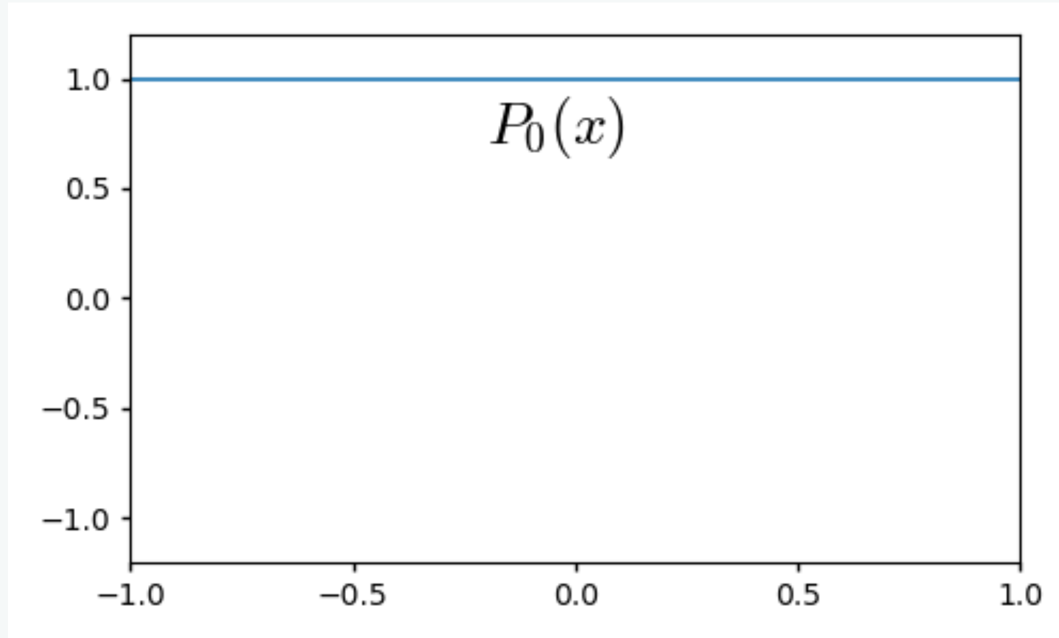
$$f_N(x) = \sum_{n=0}^{N} f_n l_n(x)$$

$$\begin{aligned} l_k(x) &= 1, \quad (x = x_k) \\ &= 0, \quad \text{otherwise} \end{aligned}$$

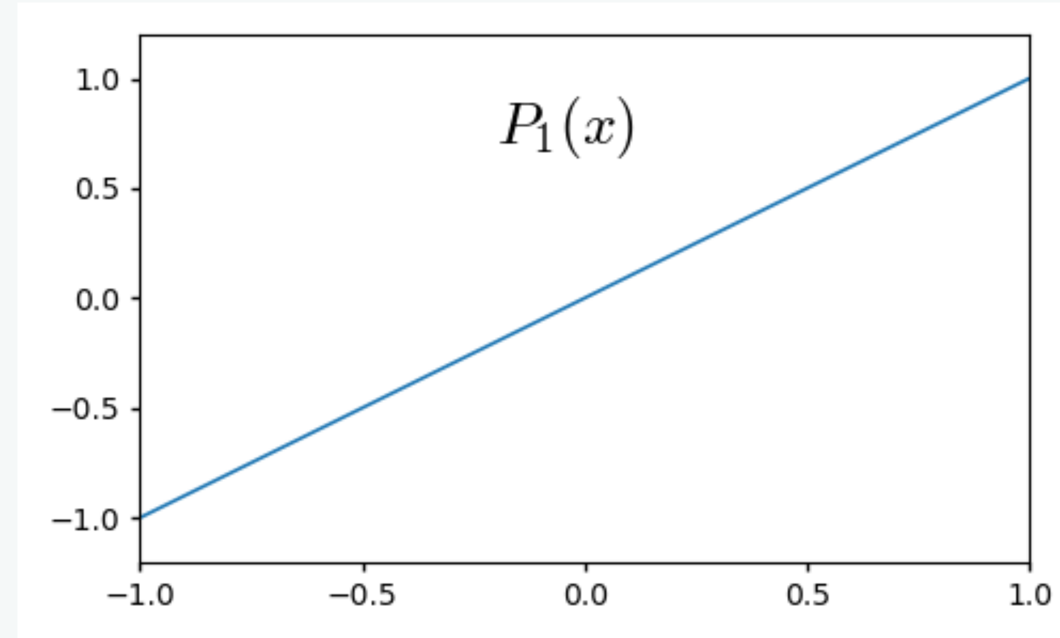
function values at each grid points
(physical space)

Modal representation

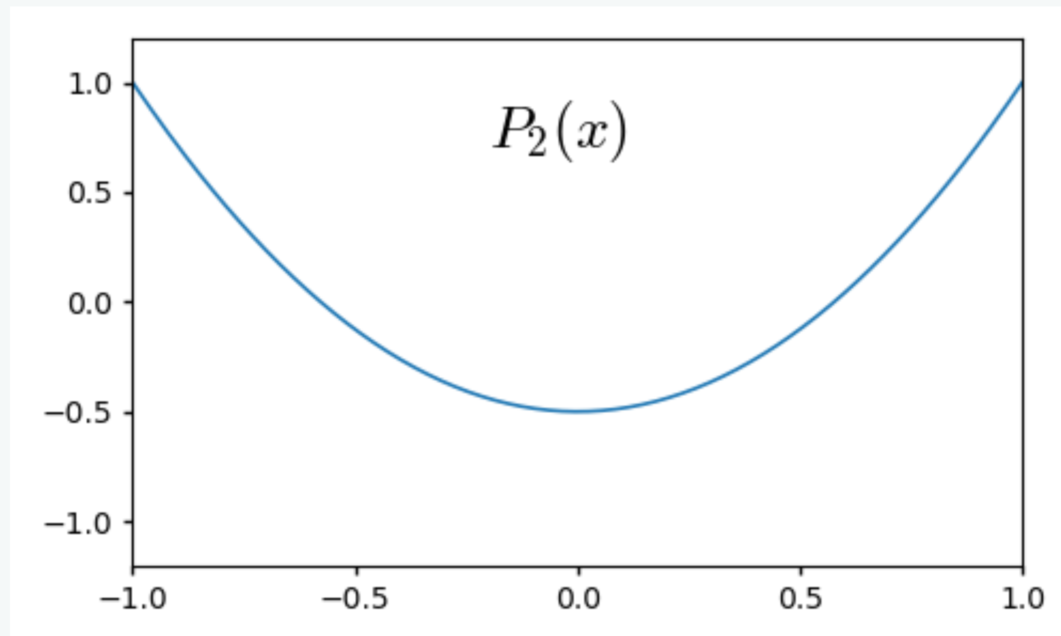
$y_N(x) = c_0$



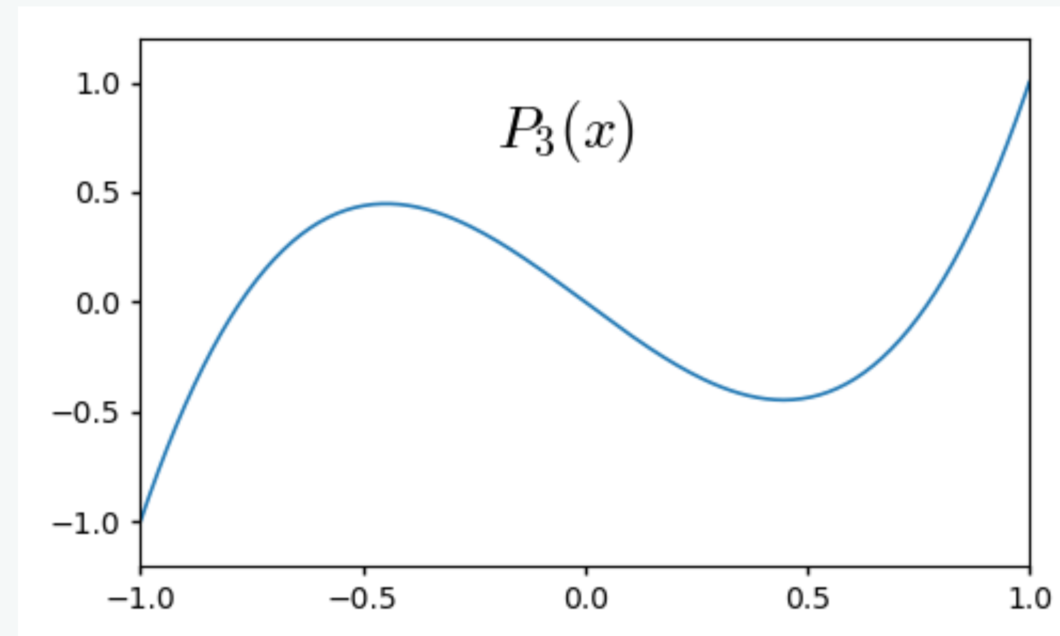
$+ \; c_1$



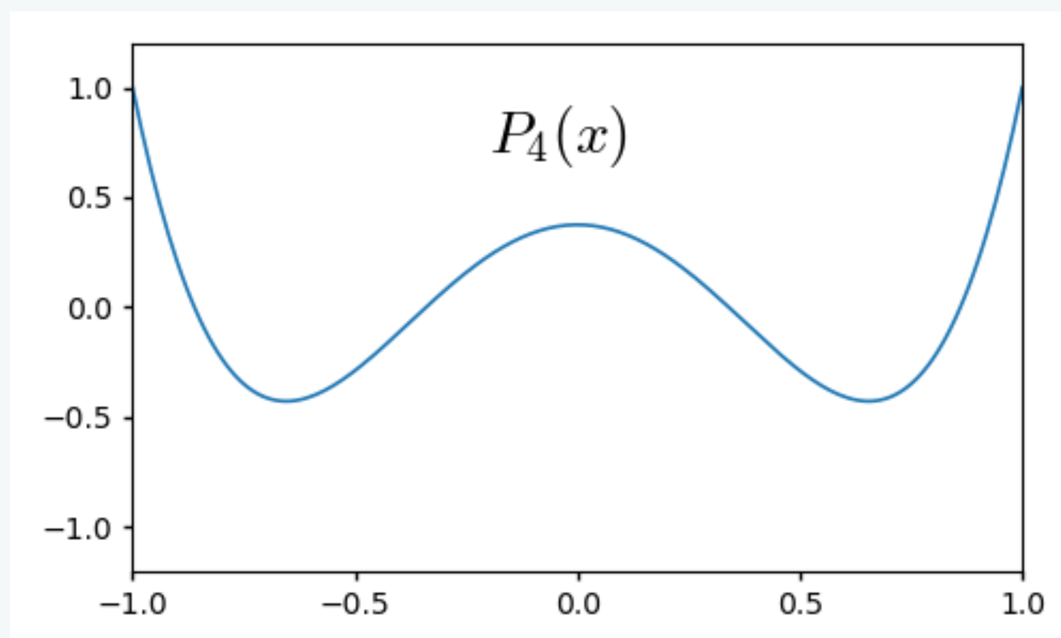
$+ \; c_2$



$+ \; c_3$



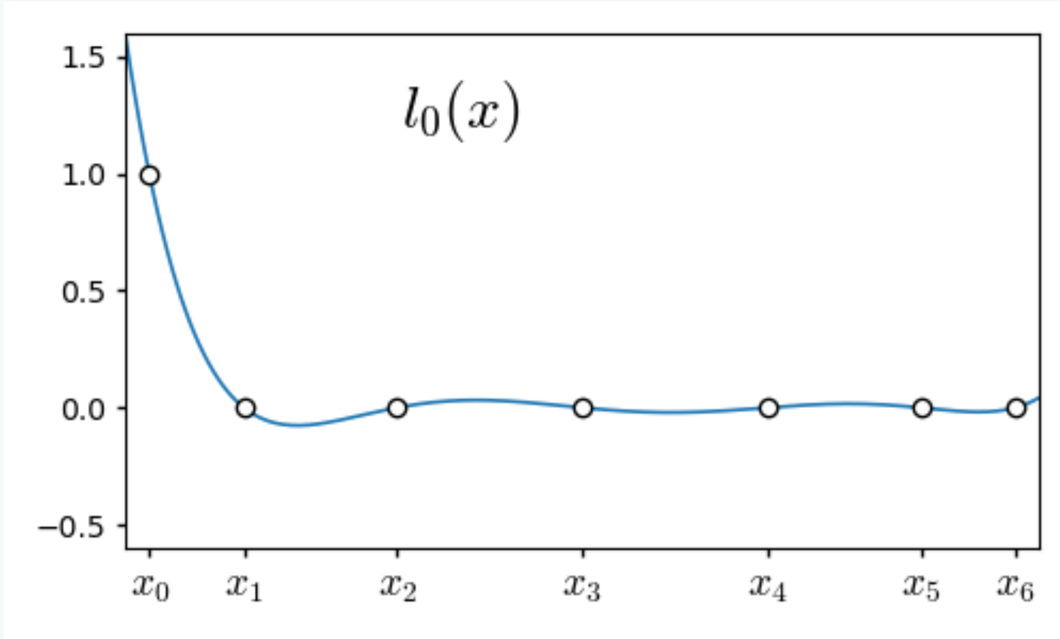
$+ \; c_4$



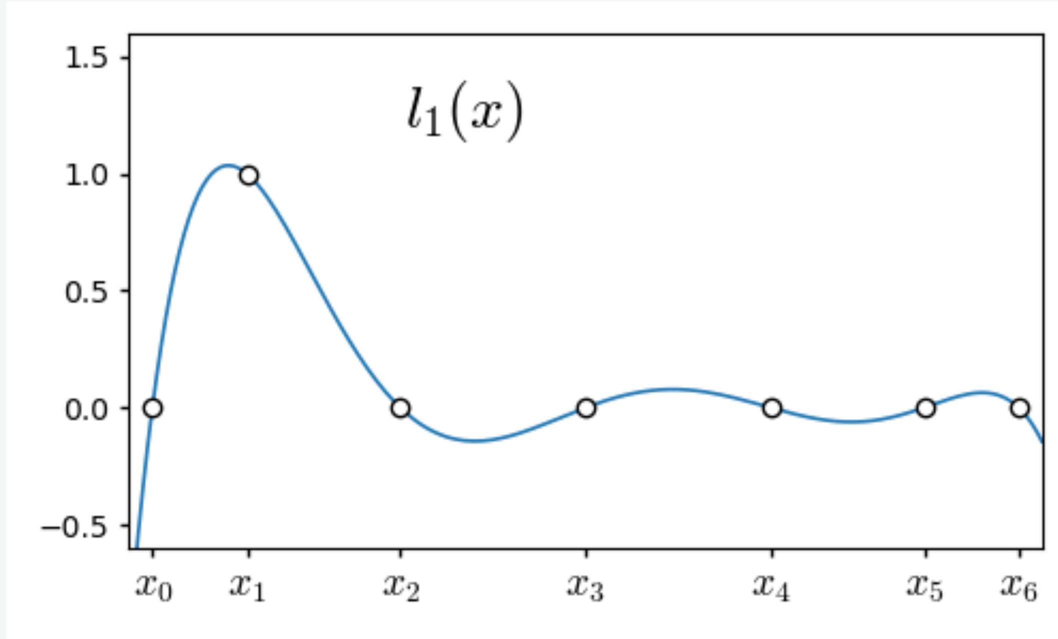
$+ \; \cdots$

Nodal representation

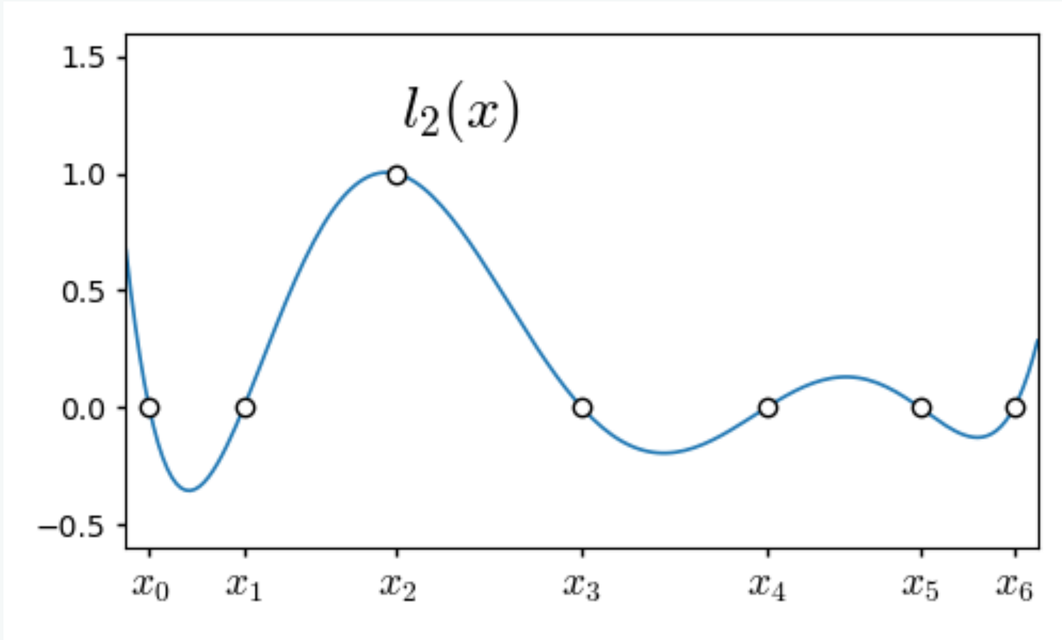
$y_N(x) = y_0$



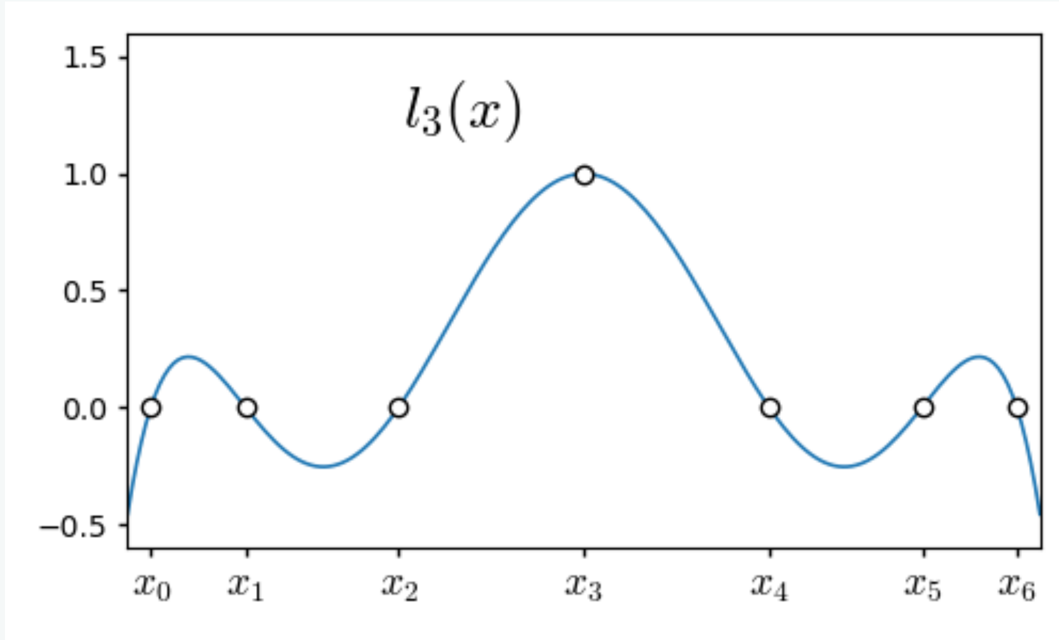
$+ \; y_1$



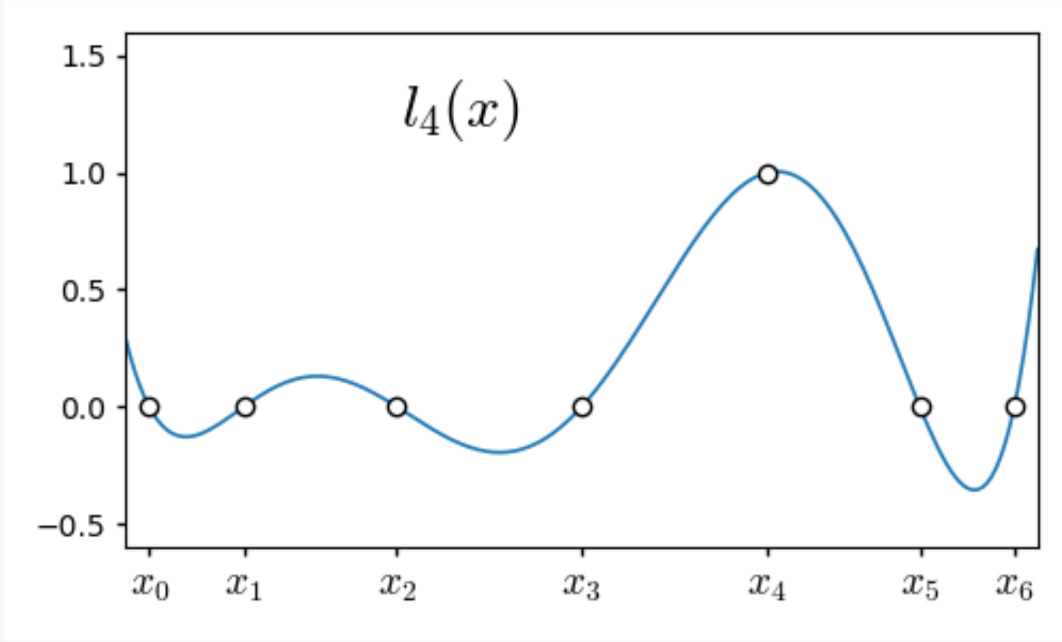
$+ \; y_2$



$+ \; y_3$

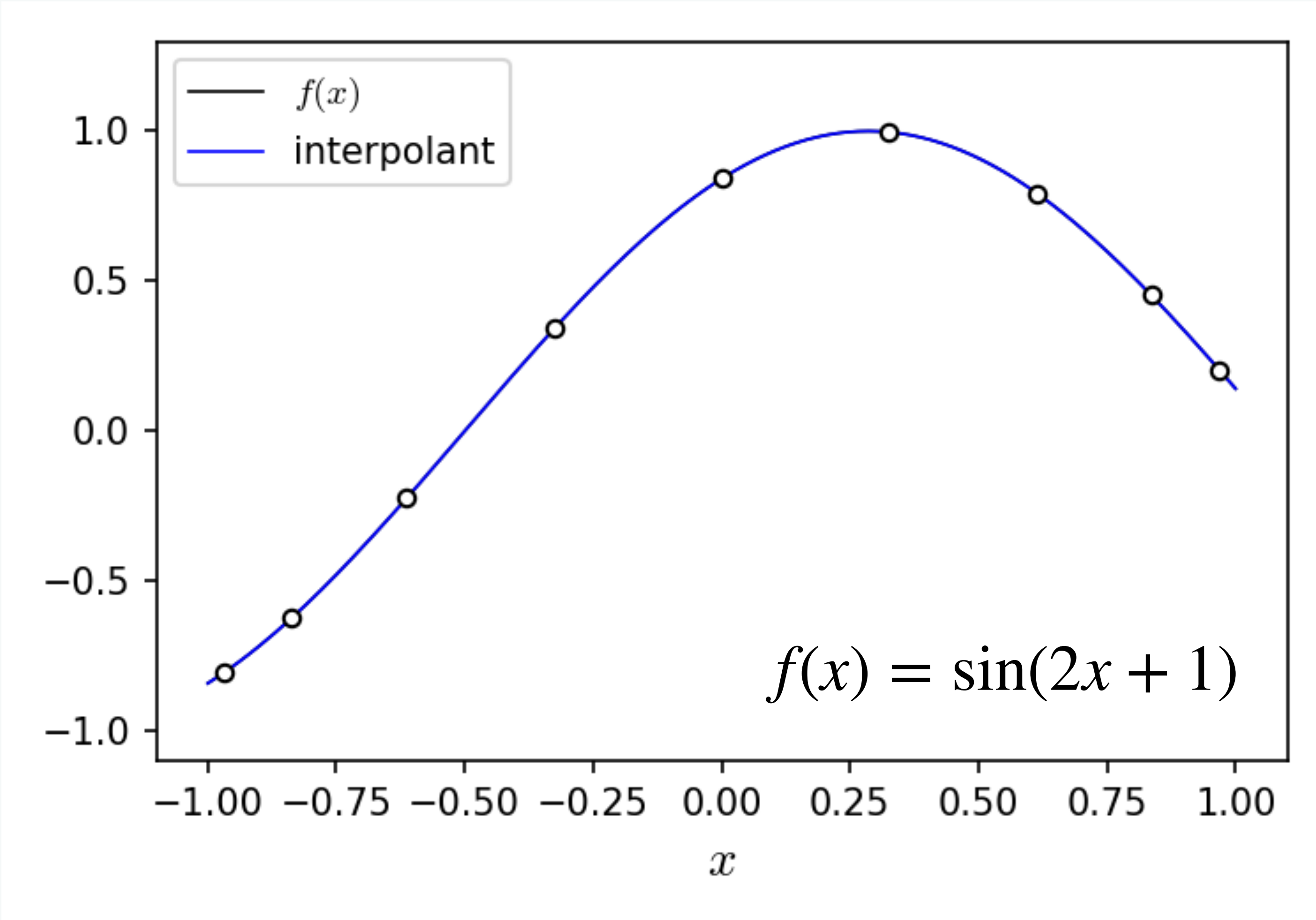


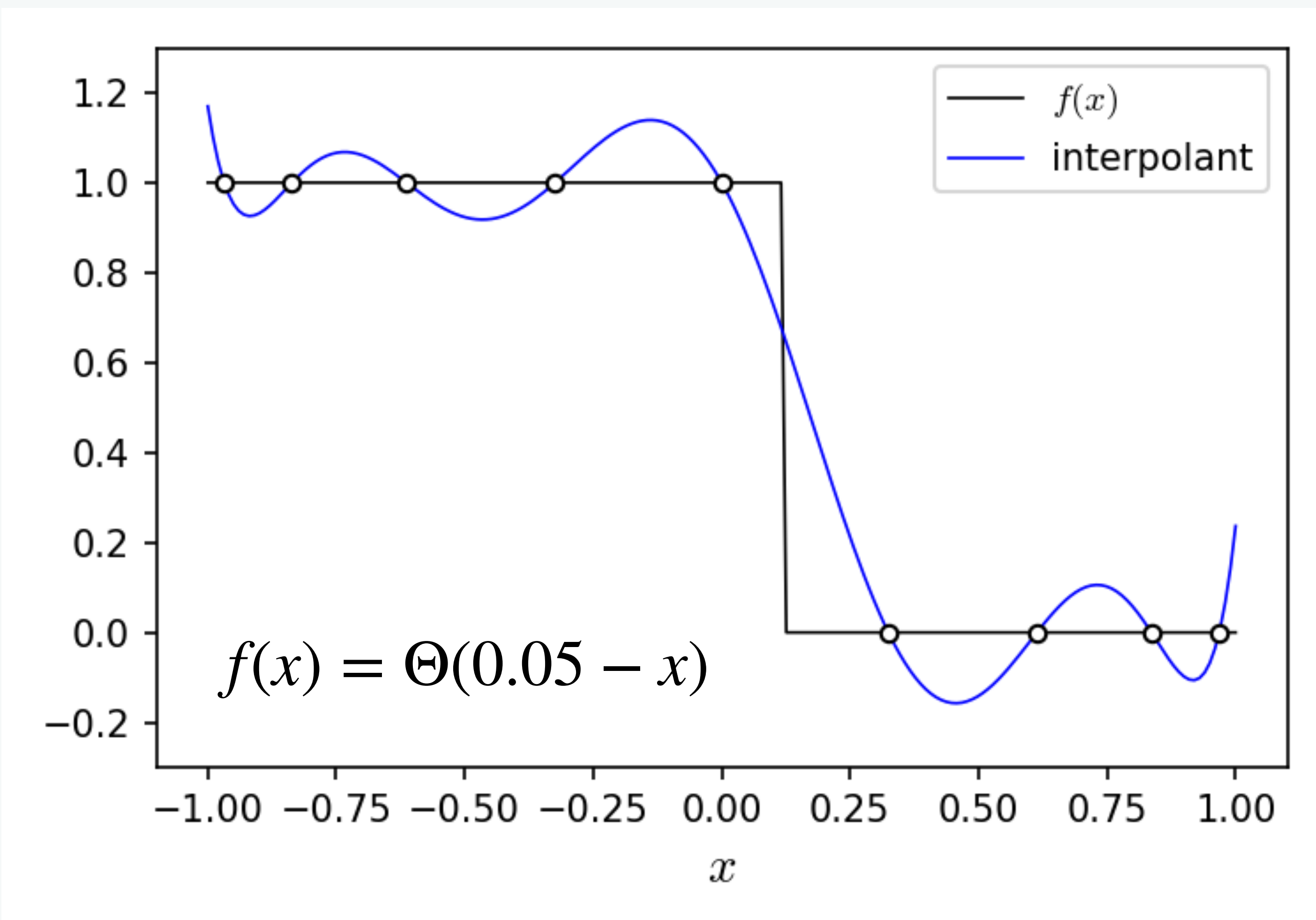
$+ \; y_4$

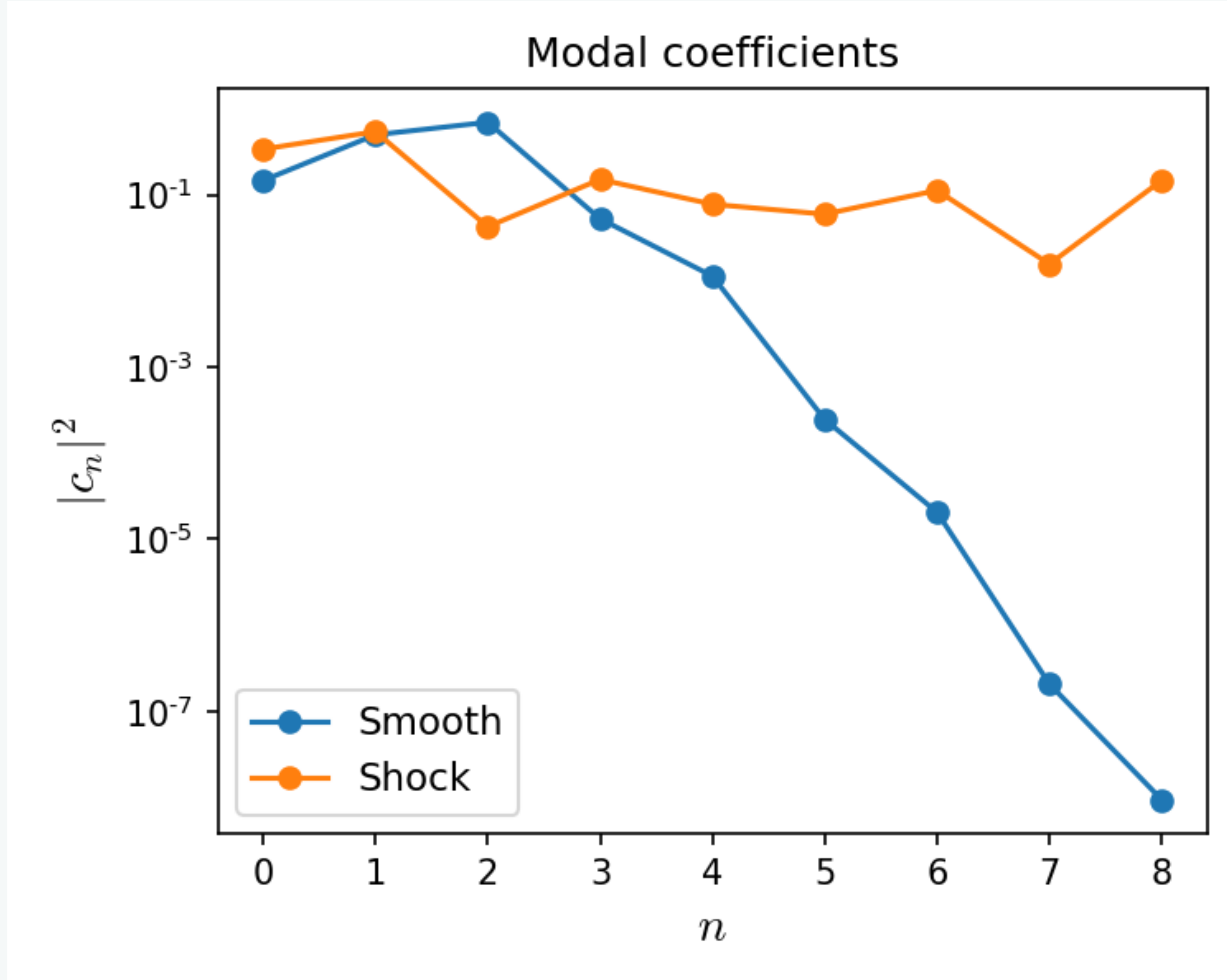


$+ \; \cdots$

fall-off rate of modal coefficients shows how well the approximation is working

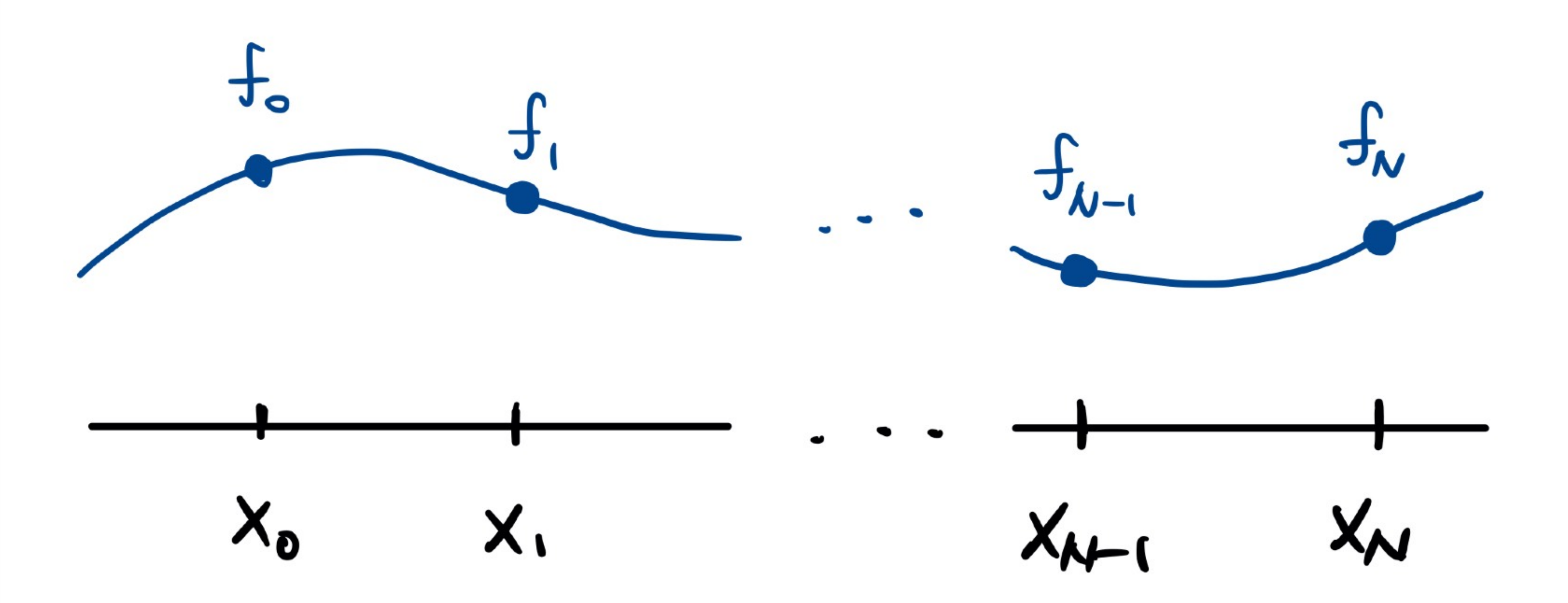






Collocation method

- Let $x \in [-1, 1]$
- How to choose collocation points $\{x_i\}$?



recall — in FD method, we used uniform (equidistance) grid

Answer : they need to be more clustered near endpoints

Runge phenomenon

- Interpolation of

$$f(x) = \frac{1}{1 + 25x^2}$$

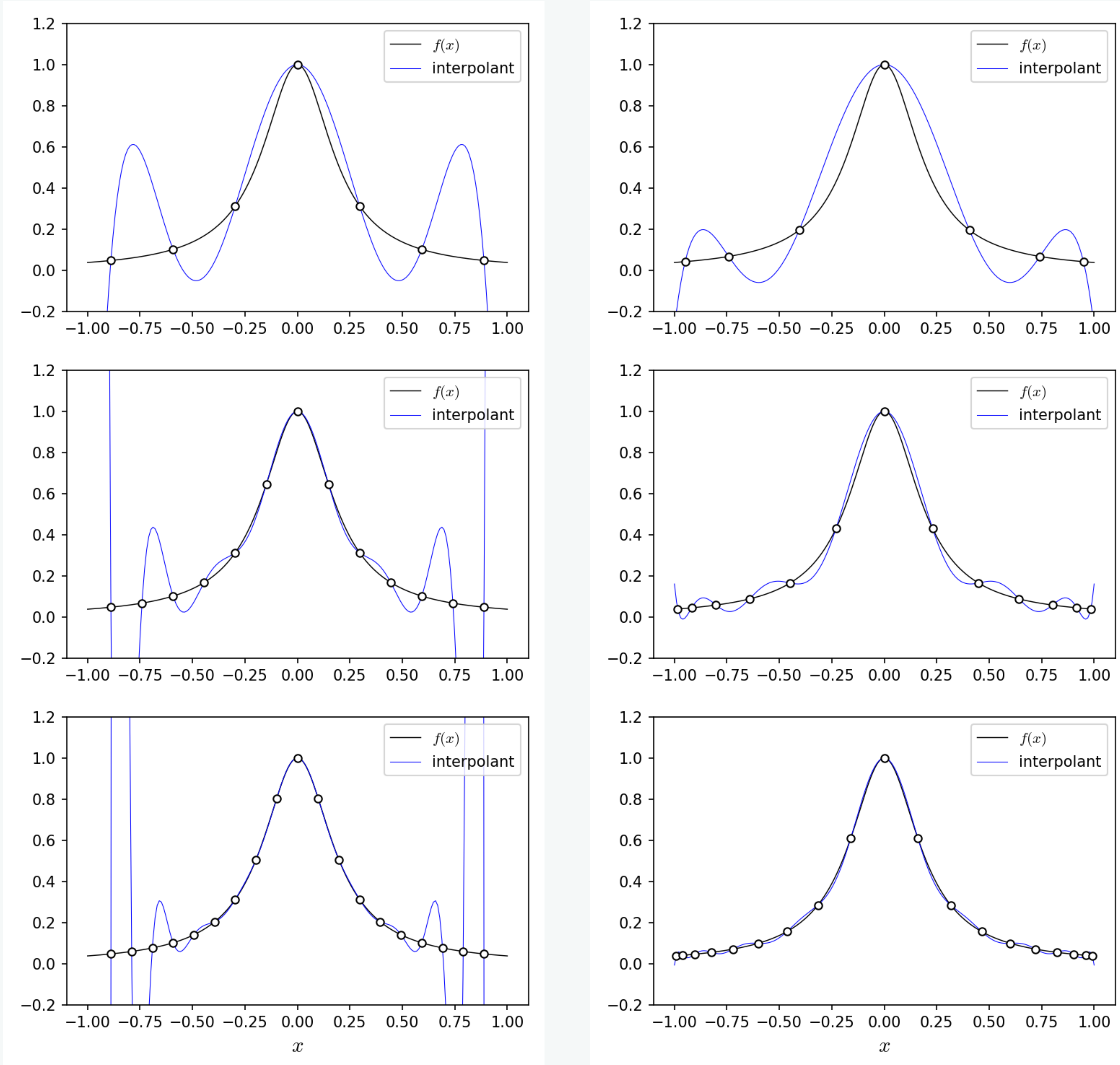
Uniformly spaced grids

Gauss-Legendre points

$N = 7$

$N = 13$

$N = 19$

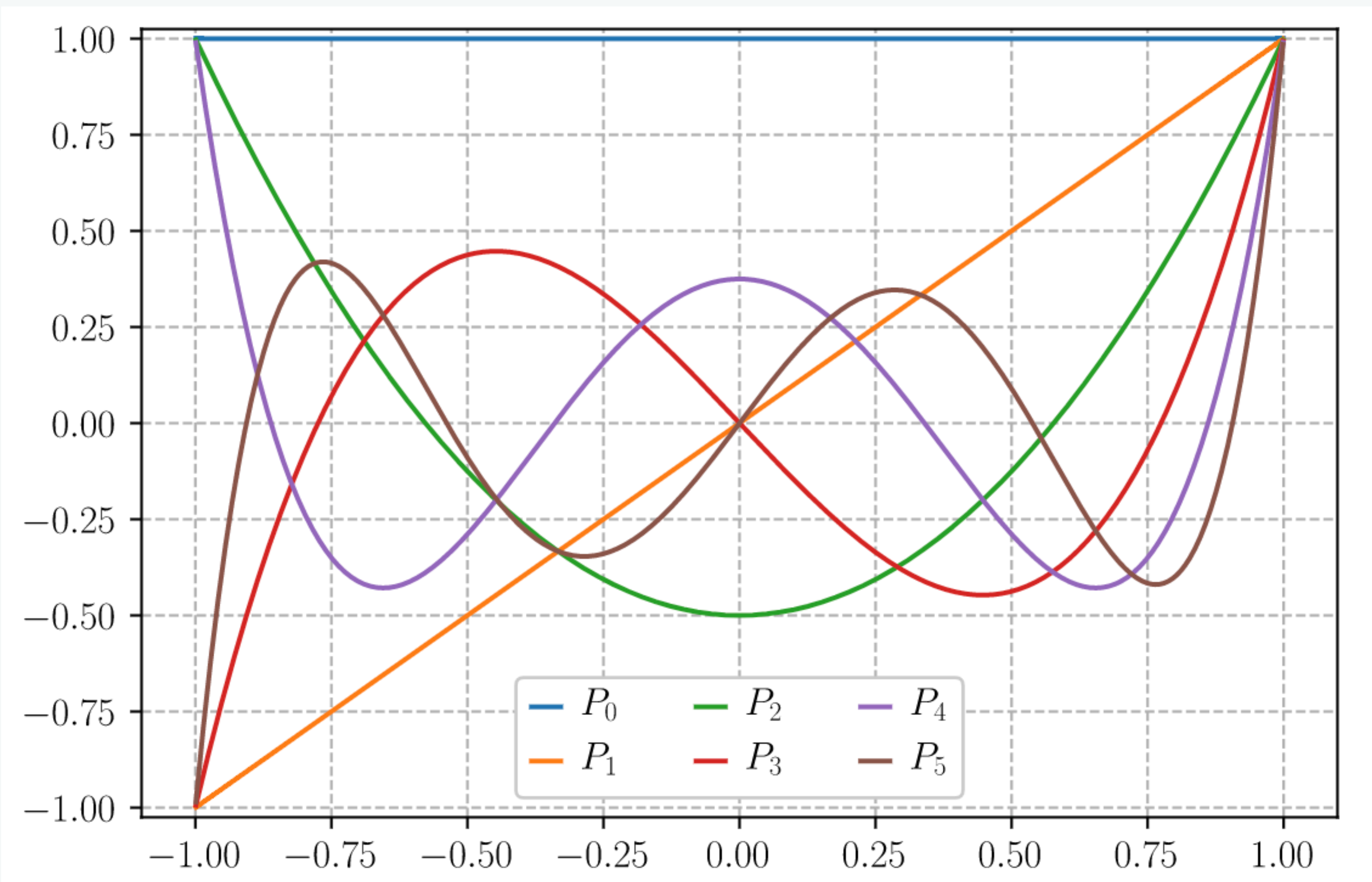


Collocation points

- For practical applications we use special classes of points

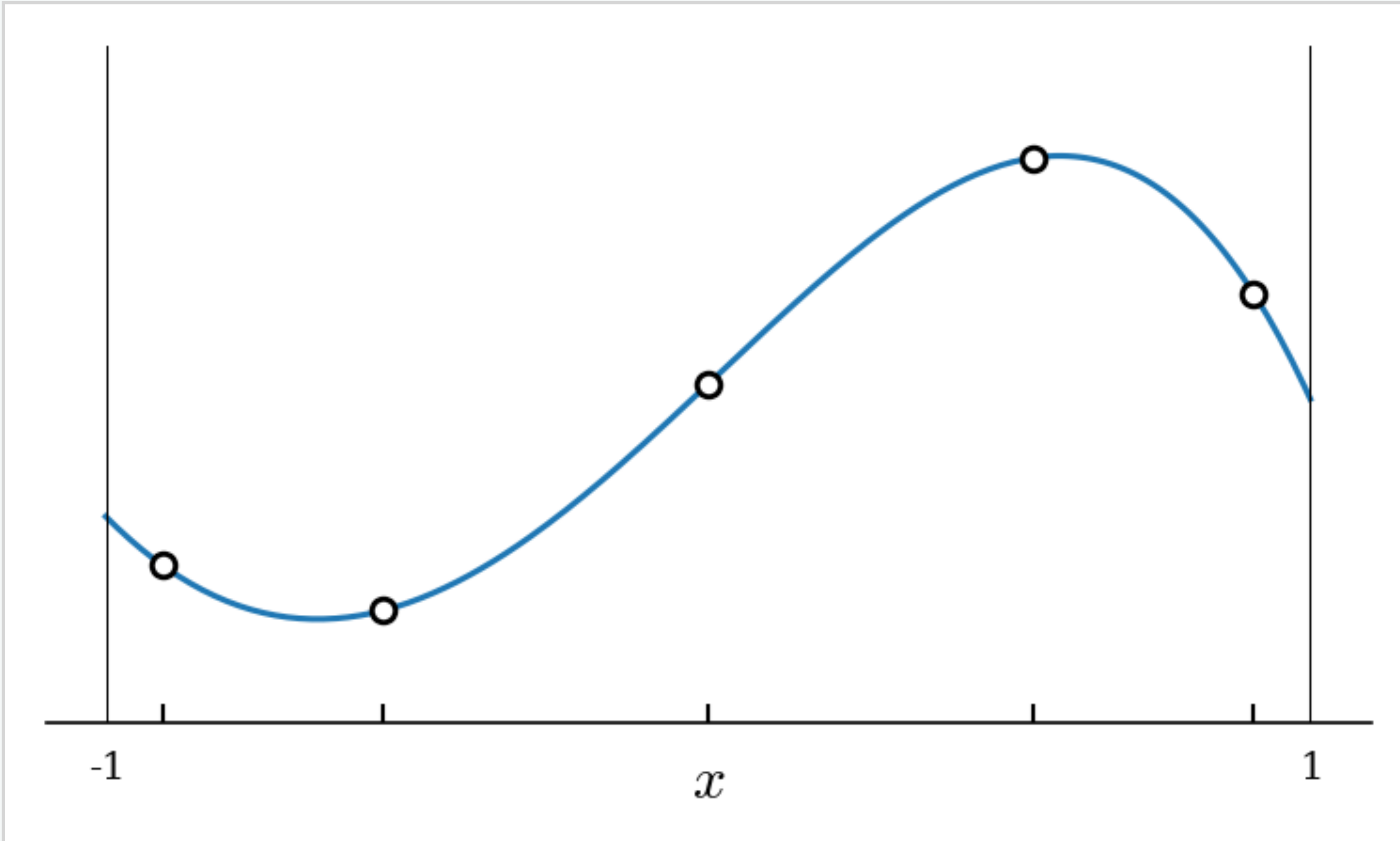
  e.g. Gauss-Legendre points

  x_i are i-th root of a Legendre polynomial $P_N(x)$



Number of points, n	Points, x_i	
1	0	
2	$\pm\frac{1}{\sqrt{3}}$	±0.57735···
3	0	
	$\pm\sqrt{\frac{3}{5}}$	±0.774597···
4	$\pm\sqrt{\frac{3}{7}-\frac{2}{7}\sqrt{\frac{6}{5}}}$	±0.339981···
	$\pm\sqrt{\frac{3}{7}+\frac{2}{7}\sqrt{\frac{6}{5}}}$	±0.861136···
5	0	
	$\pm\frac{1}{3}\sqrt{5-2\sqrt{\frac{10}{7}}}$	±0.538469···
	$\pm\frac{1}{3}\sqrt{5+2\sqrt{\frac{10}{7}}}$	±0.90618···

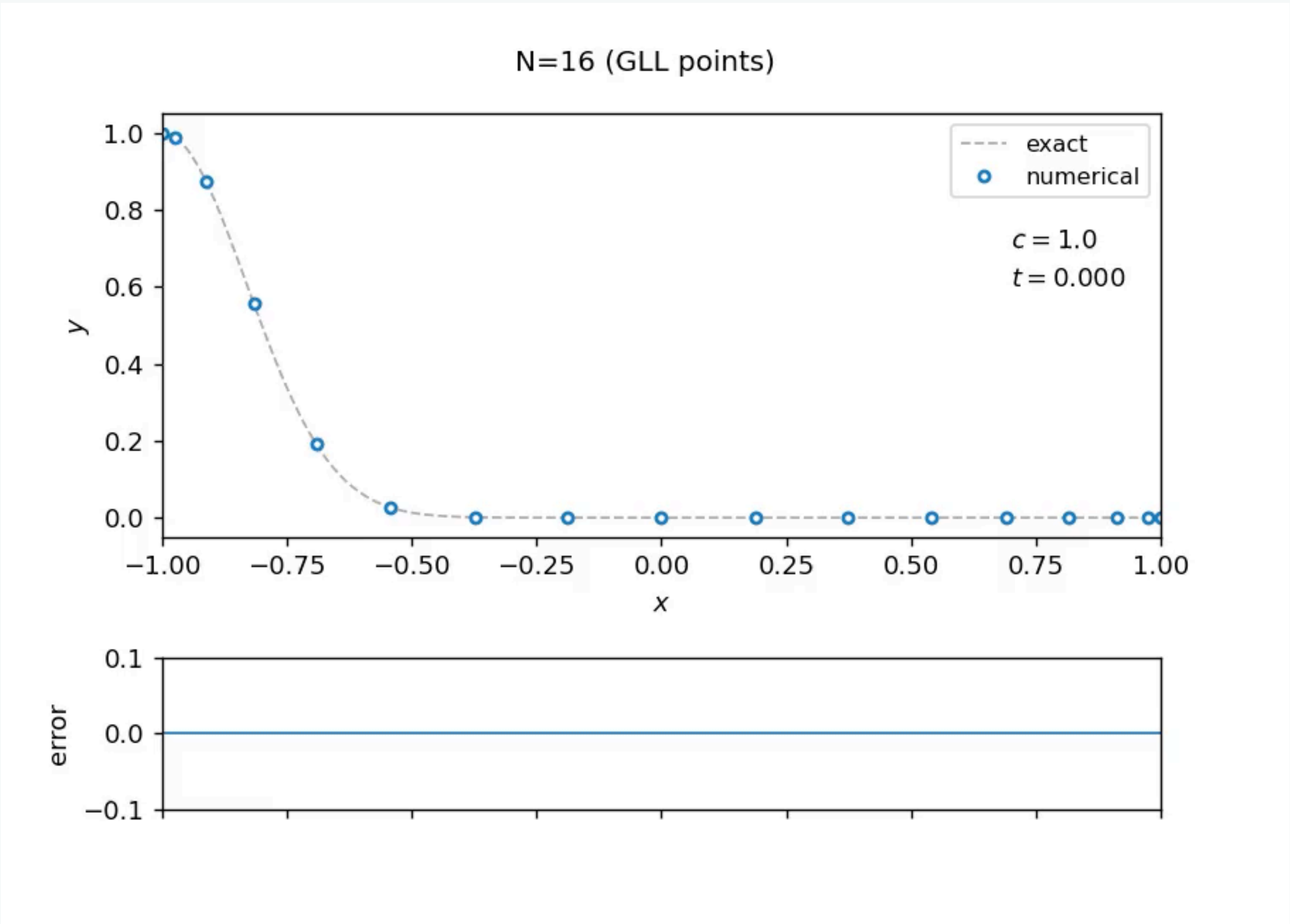
Image and table credit : https://en.wikipedia.org/wiki/Gauss%E2%80%93Legendre_quadrature



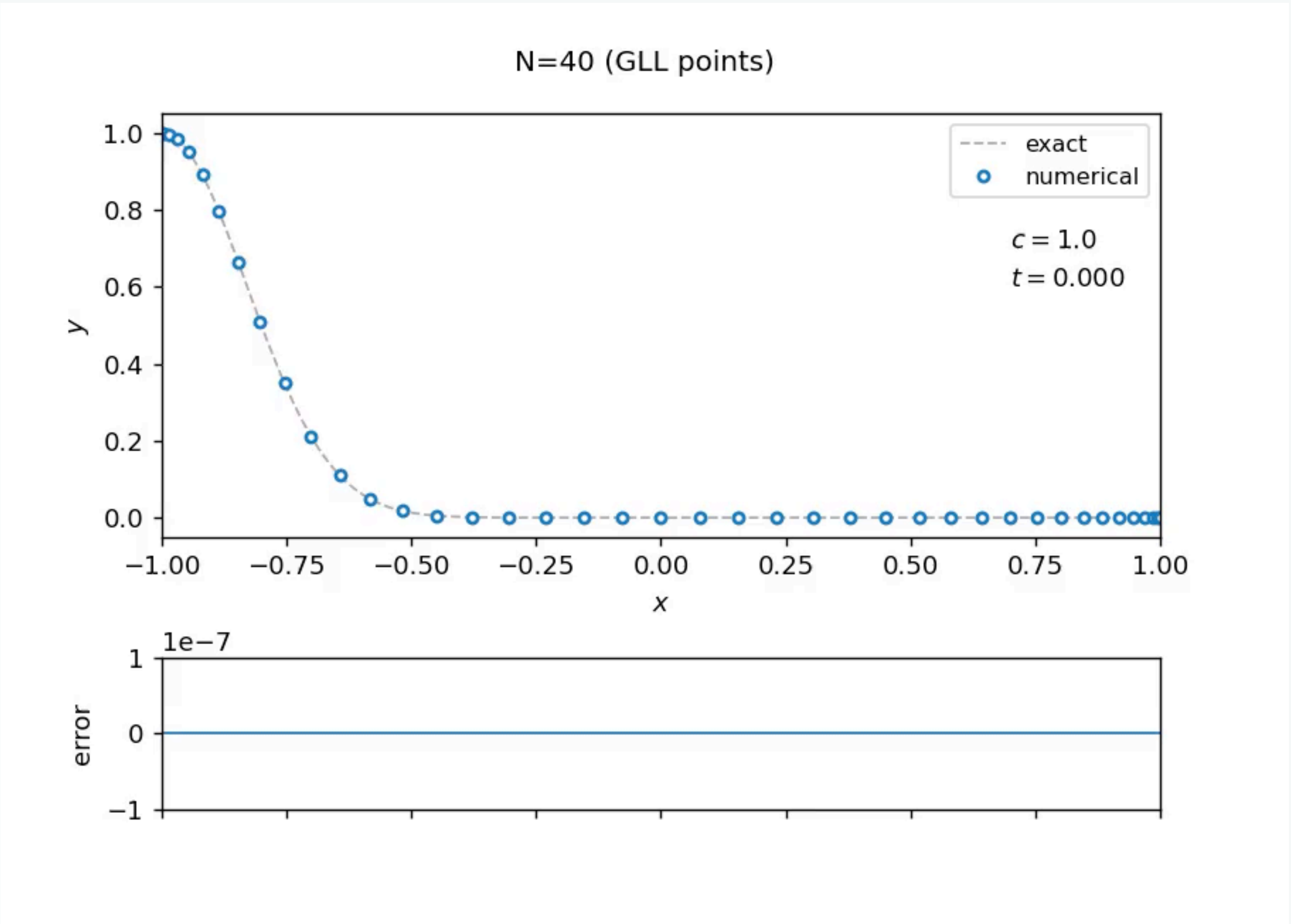
Number of grid points = 5

Collocation method

- Example : scalar advection system $$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0$$

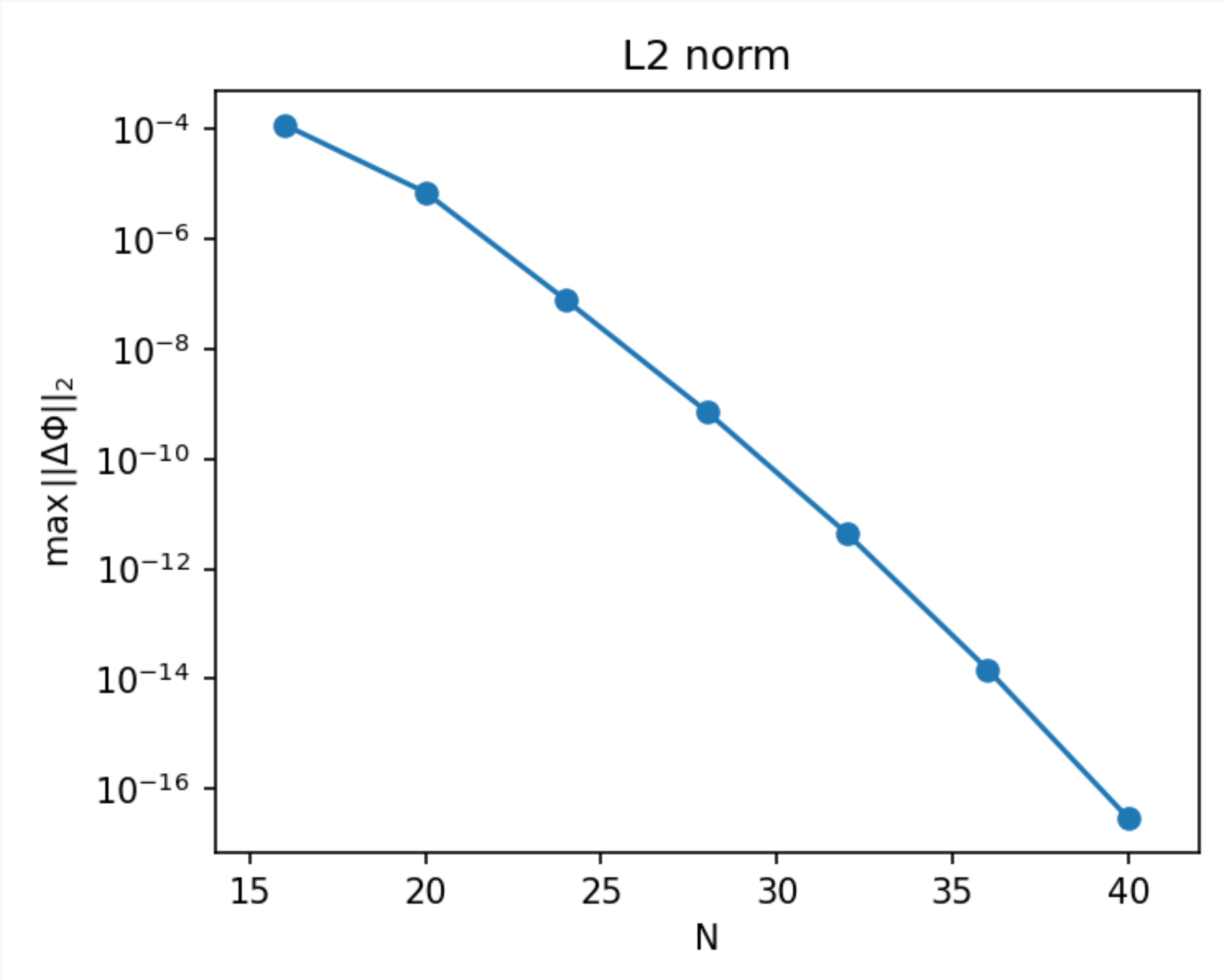


N=16



N=40

- **Error goes ~ exp(-N)** recall) error goes $\sim 1/N^k$ for k-th order finite difference method



Pros

Exponential accuracy
(Error goes $\sim e^{-N}$)

Cons

Spectral methods work well for smooth solutions.
Discontinuities like shocks are bad — don't even try spectral methods

- Numerical Recipes

recall) Gibbs phenomena

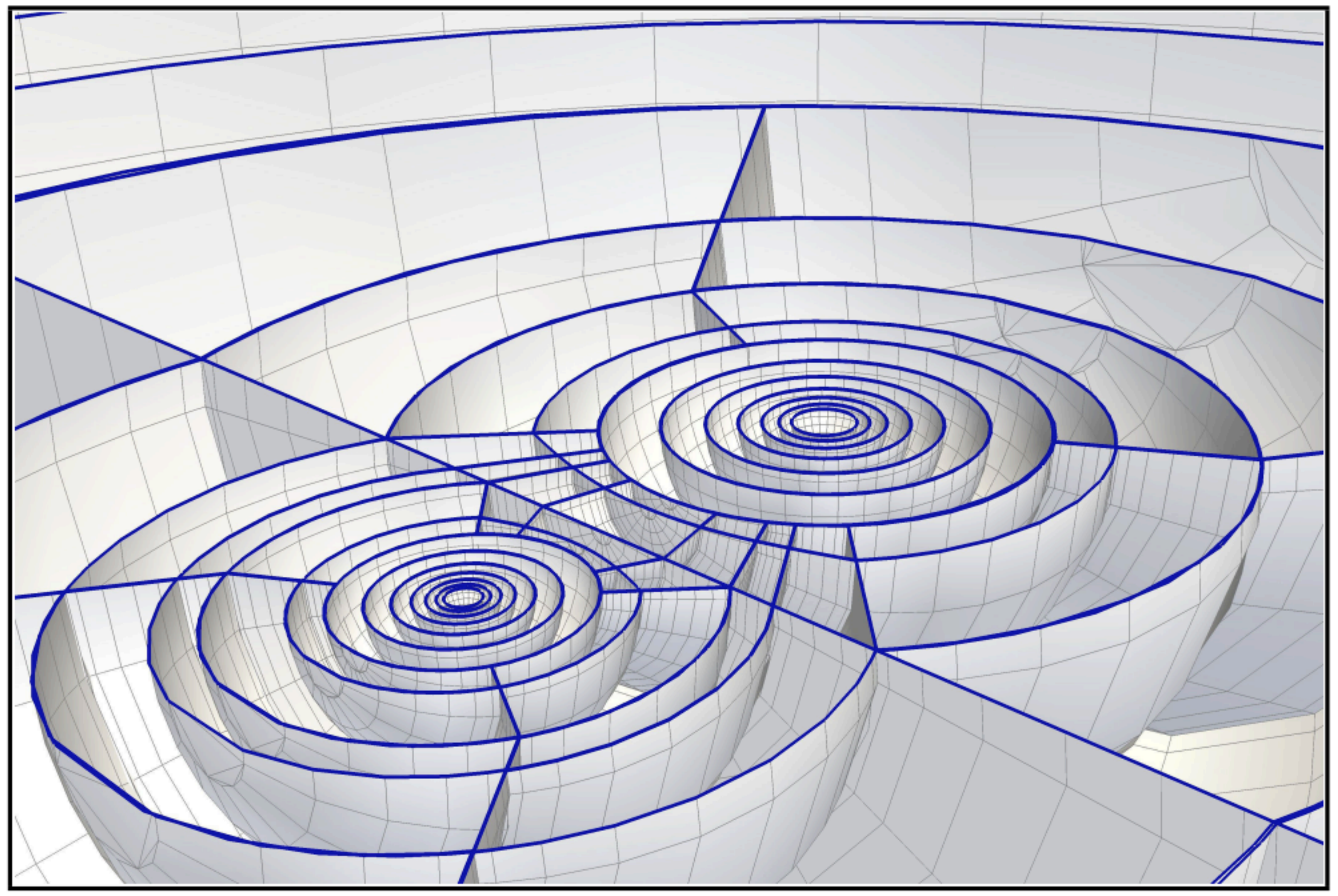
in numerical relativity

For vacuum spactime, solutions are always smooth

e.g. Spectral Einstein Code (SpEC)

For hydro simulations, we want…

- spectral accuracy where solution is smooth
- ability to handle shocks and surfaces.



Buchman+2012

Discontinuous Galerkin method

We cover nodal discontinuous Galerkin method

- *nodal* — working in physical space
- *Galerkin* — weak form
- *discontinuous* — ?

- **Consider a conservation law :** $$\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = S$$

take product with a basis l_j : $$\int_{-1}^{1} \left[\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} - S \right] l_j(x)\, dx = 0$$ weak formulation

integration by parts $$\int (\partial_x F) l_j \rightarrow F l_j \Big|_{-1}^{+1} - \int F l_j'$$

Apply nodal approximation :

$$u \approx \sum_{k=0}^{N} u_k l_k(x) \qquad F \approx \sum_{k=0}^{N} F_k l_k(x) \qquad S \approx \sum_{k=0}^{N} S_k l_k(x)$$

....

....

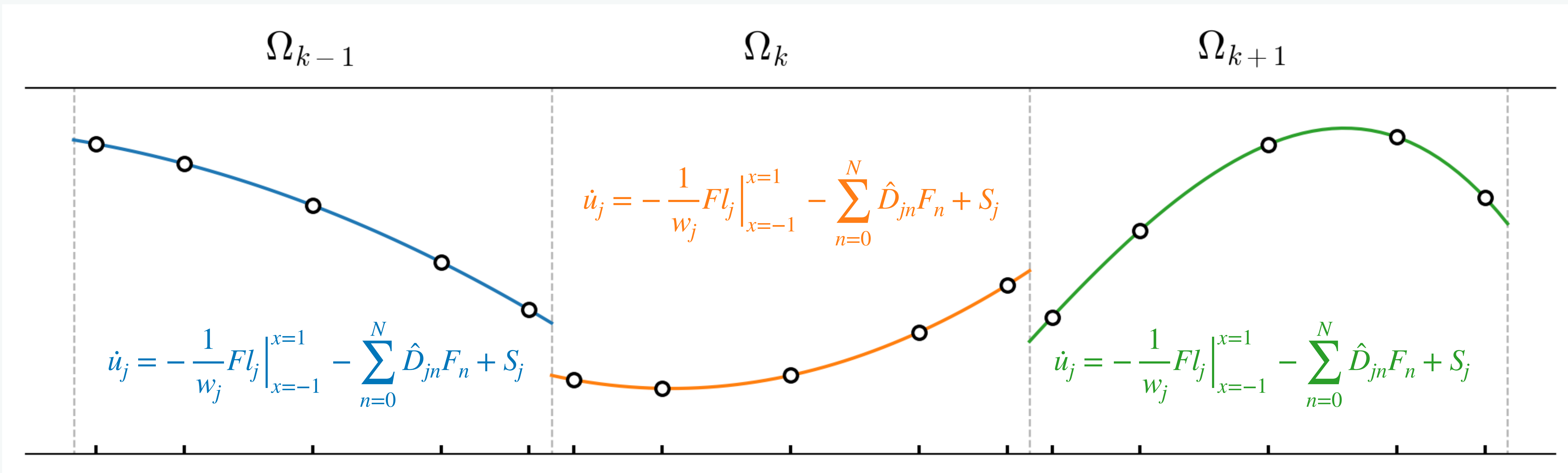
(left as an exercise for the reader)

Computed time derivative :

$$\dot{u}_j = -\frac{1}{w_j} F l_j \Big|_{x=-1}^{x=1} - \sum_{n=0}^{N} \hat{D}_{jn} F_n + S_j$$

- $\hat{D}, w_j$ are pre-computed quantities
- note the "boundary" flux term $F(+1)$ and $F(-1)$

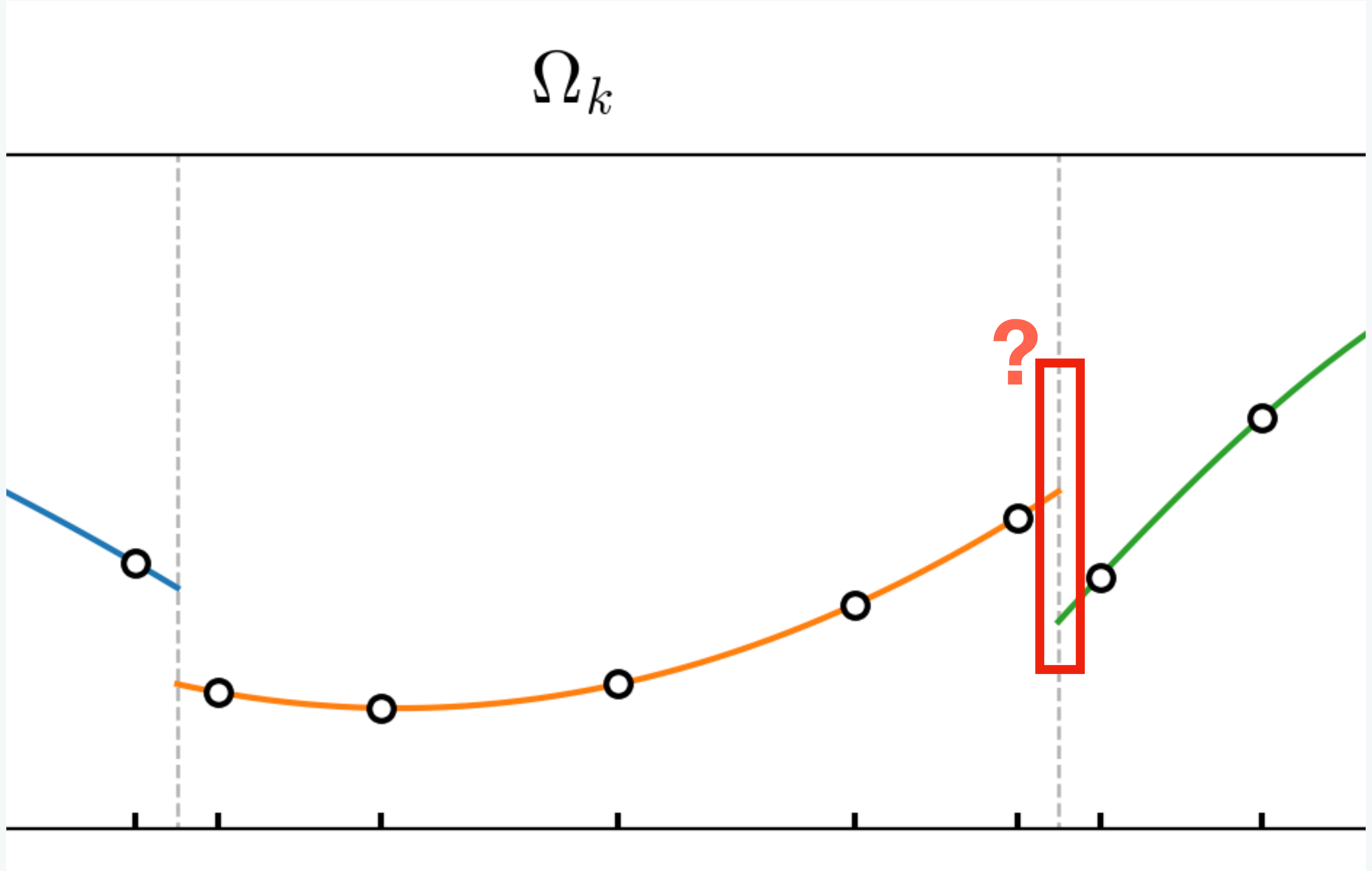
Discontinuous Galerkin method



- Divide computational domain into cells
- perform spectral expansion in each cells

Question: which value of F should we use at the boundary — from left? right?

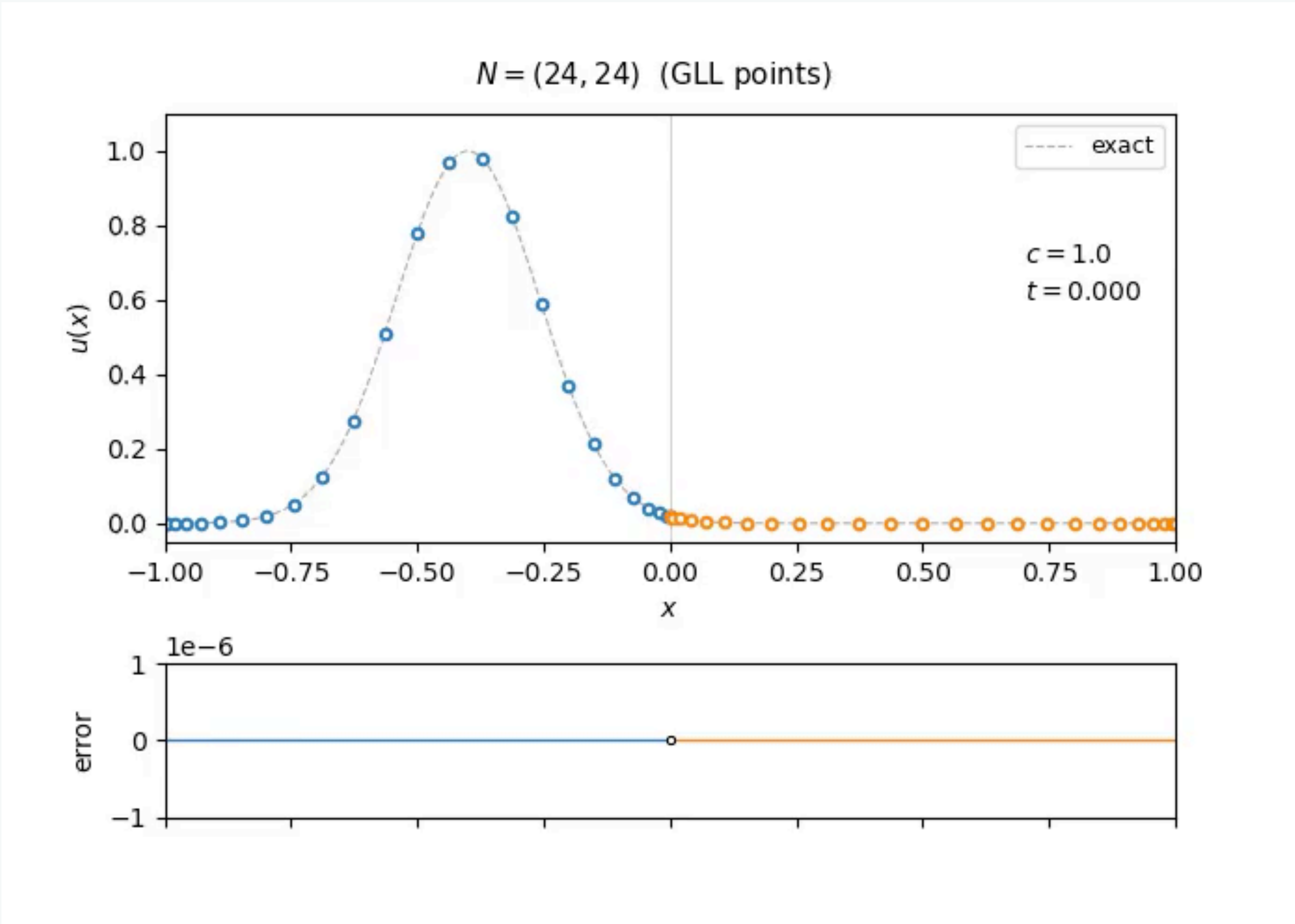
$$\dot{u}_j = -\frac{1}{w_j} \boxed{F l_j \Big|_{x=-1}^{x=1}} - \sum_{n=0}^{N} \hat{D}_{jn} F_n + S_j$$



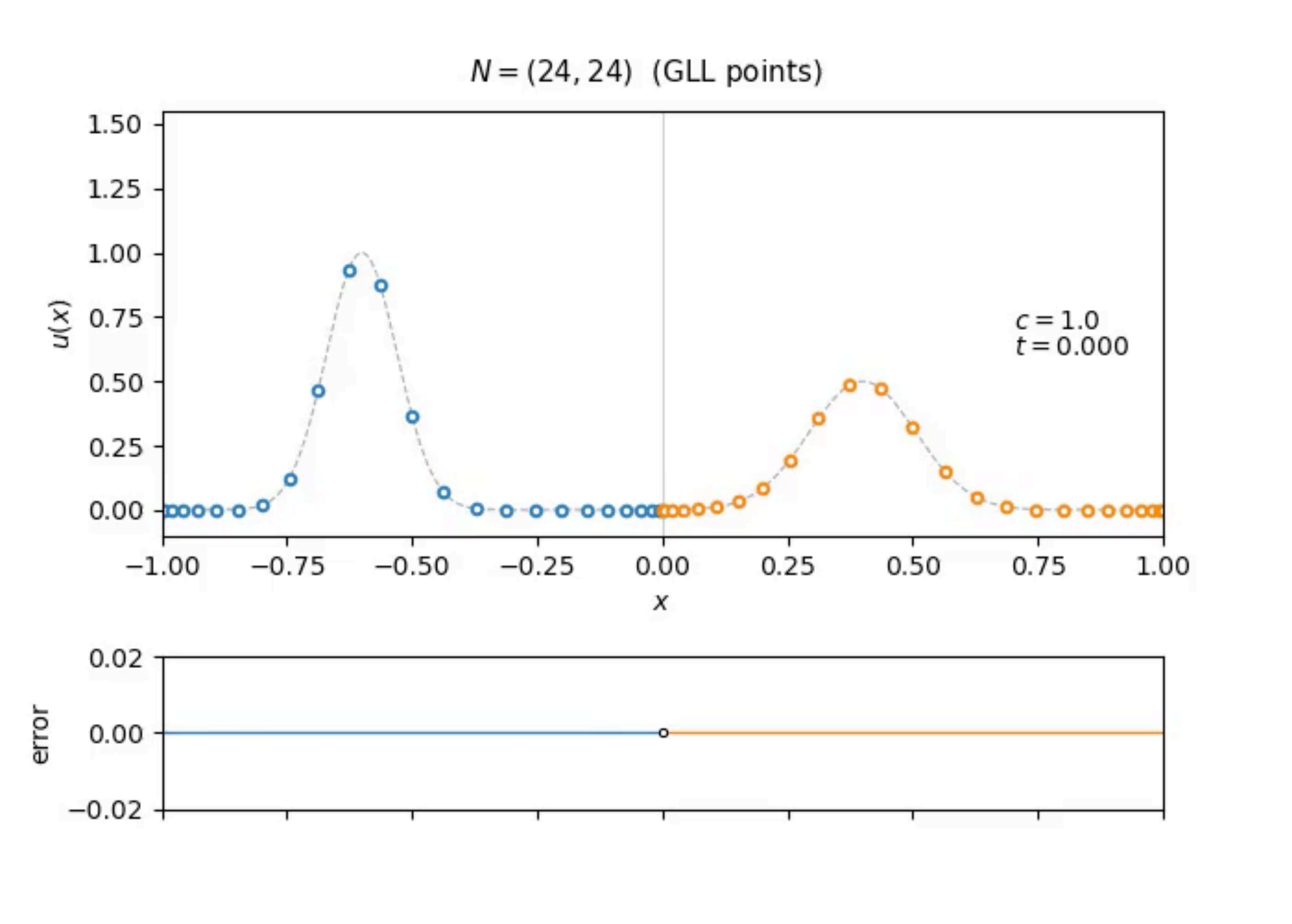
Riemann solver gives an appropriate value $F^*(U_L, U_R)$ **numerical flux**

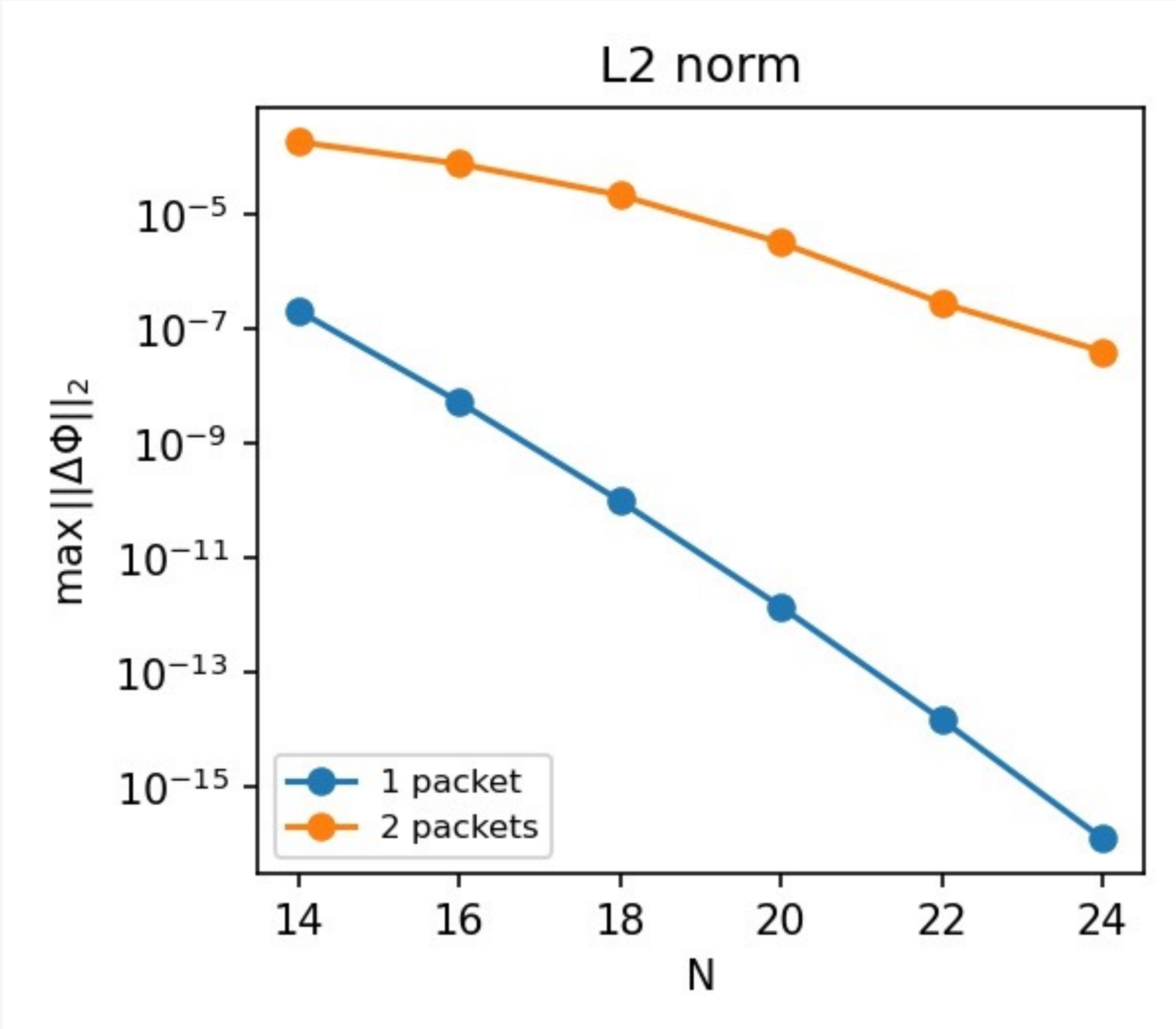
Each cell "communicates" with neighbors with the numerical flux

- Example : 1D scalar wave $\dfrac{\partial^2 u}{\partial t^2} = \dfrac{\partial^2 u}{\partial x^2}$



- Example : 1D scalar wave $\dfrac{\partial^2 u}{\partial t^2} = \dfrac{\partial^2 u}{\partial x^2}$



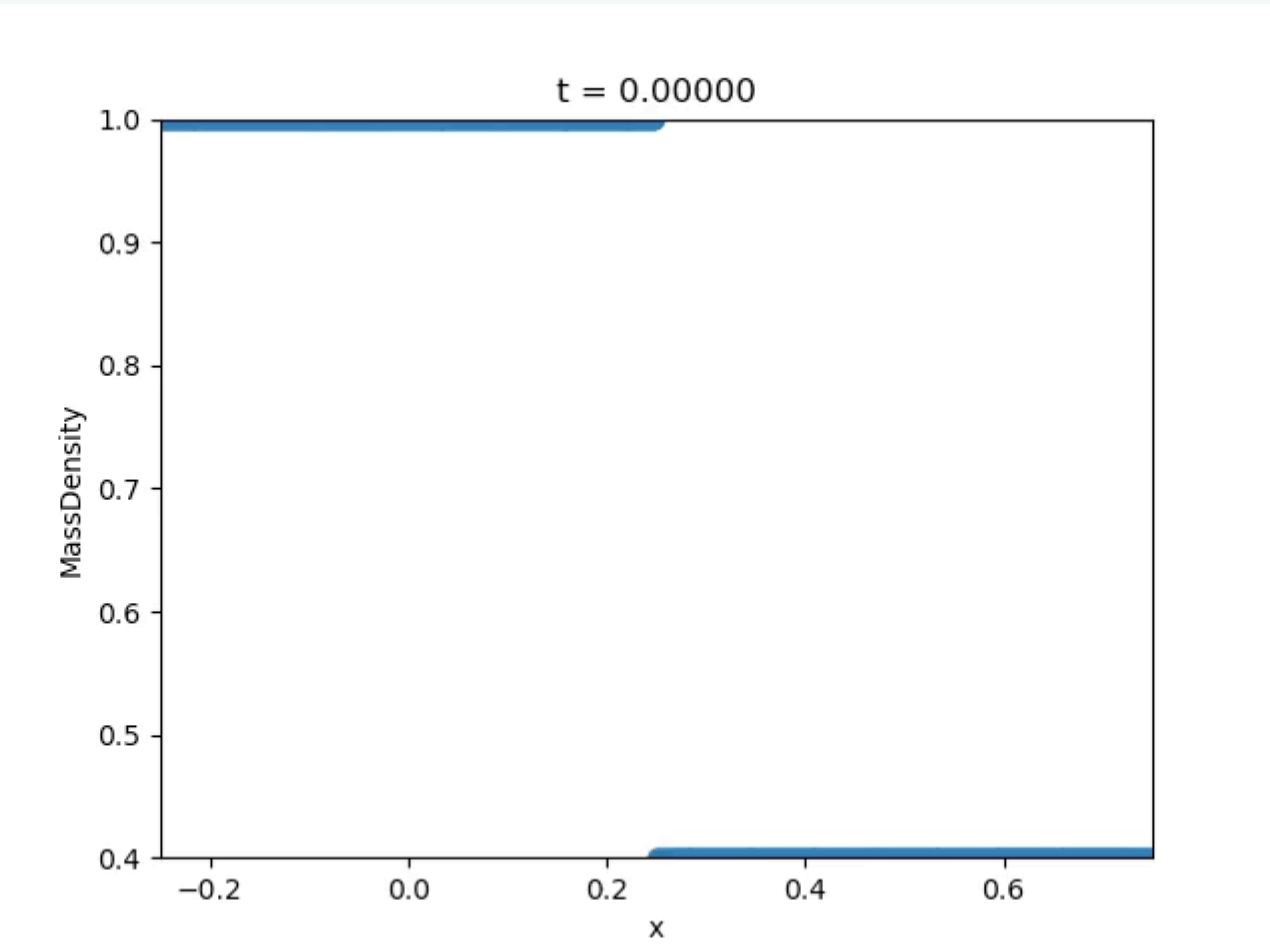


L2 norm
$\max ||\Delta\Phi||_2$
10^{-5}
10^{-7}
10^{-9}
10^{-11}
10^{-13}
10^{-15}
14
16
18
20
22
24
N
1 packet
2 packets

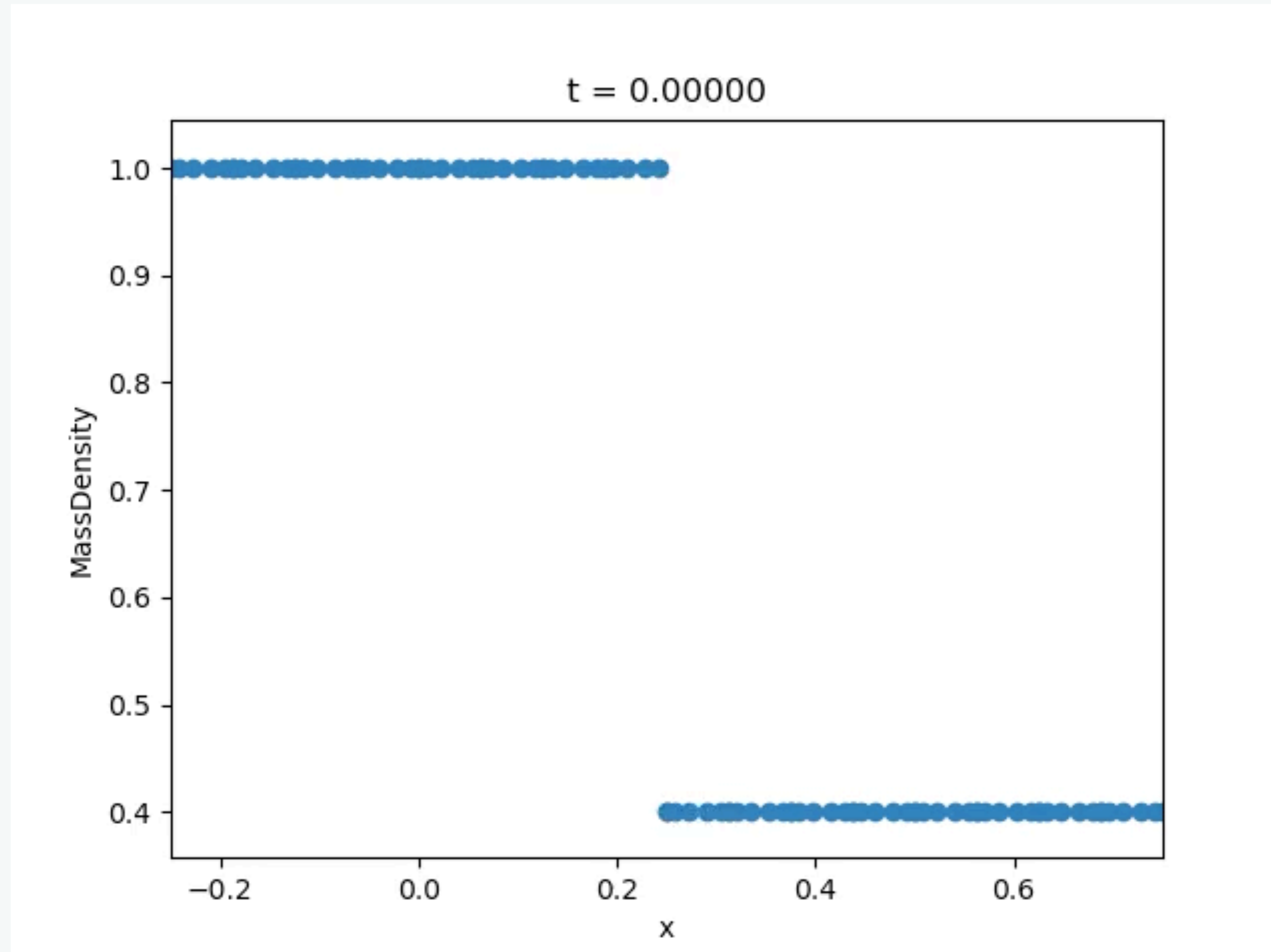
Shock capturing for DG

- Resolving sub-cell scale shock is still difficult

e.g. Sod problem (Newtonian hydrodynamics)

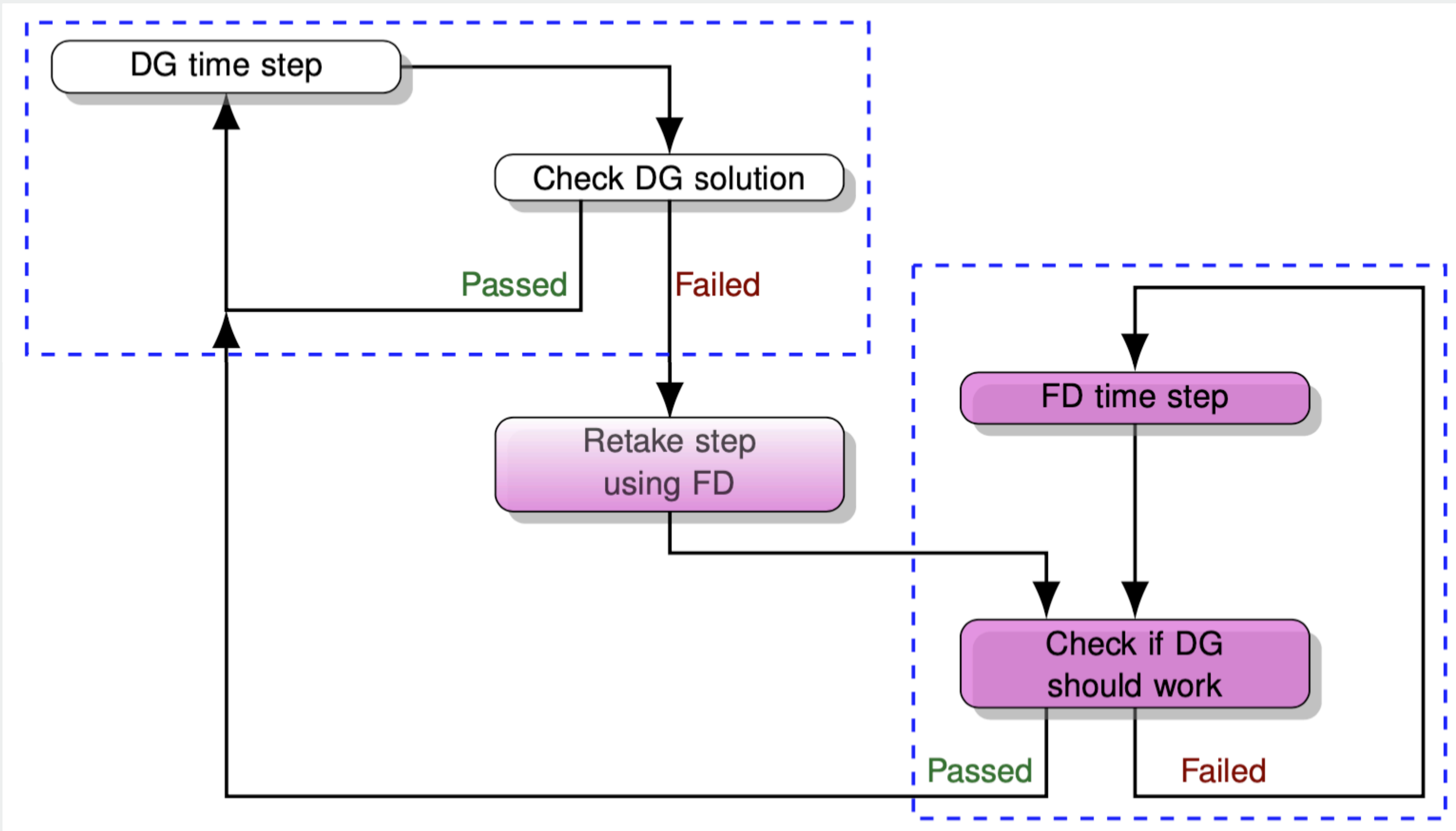


High resolution finite difference



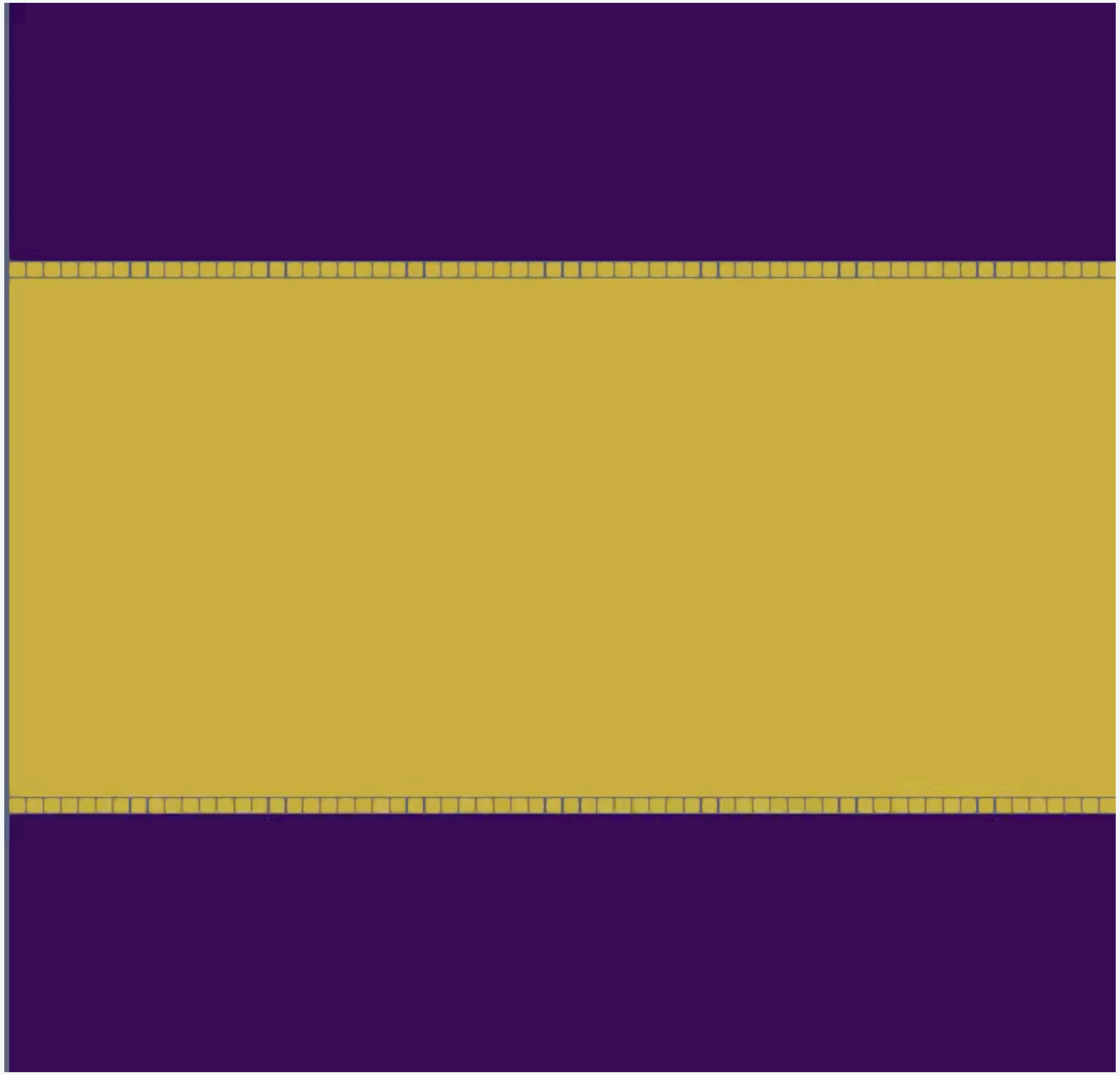
DG evolution

Shock capturing for DG

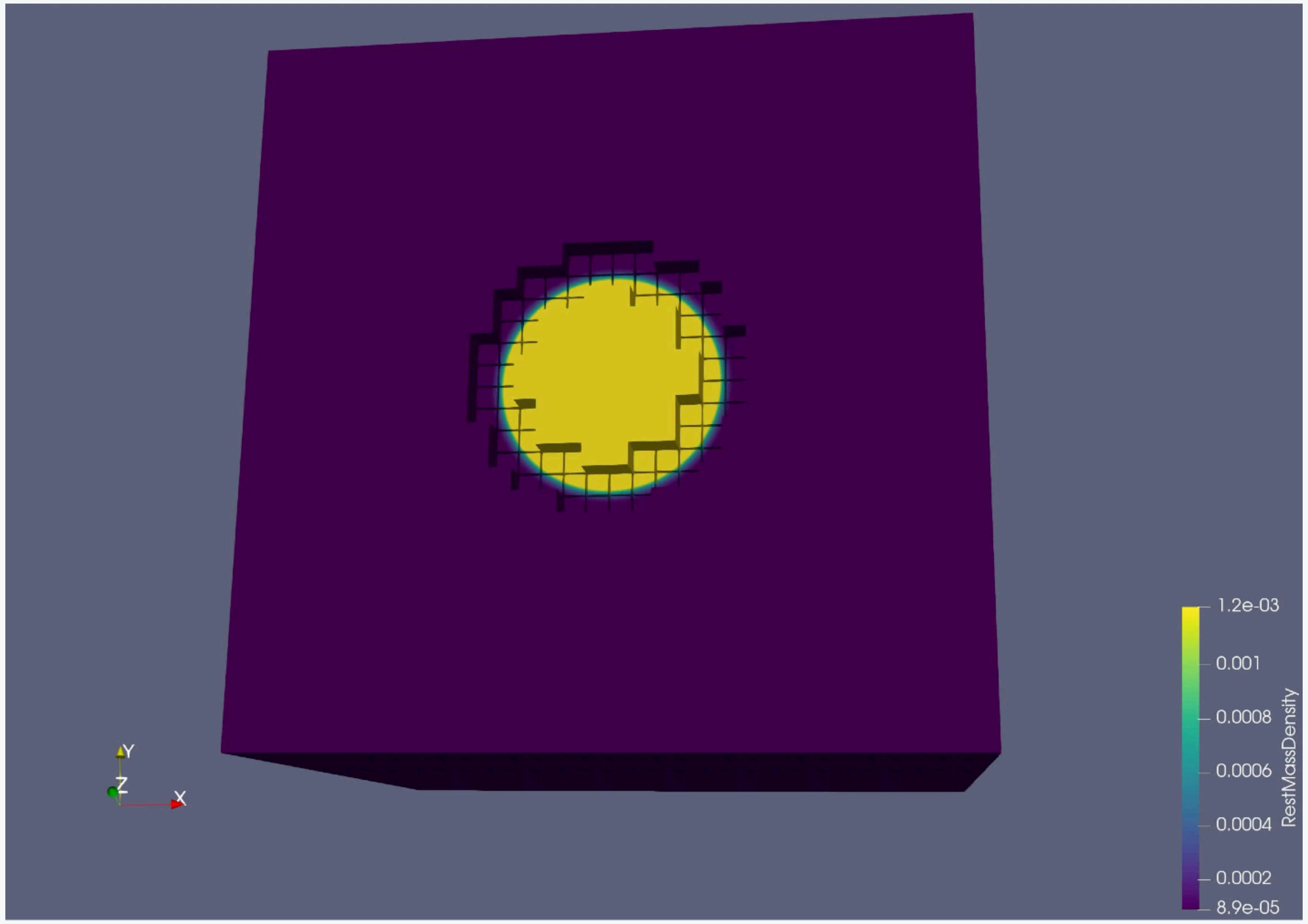


Deppe+ 2109.12033; 2109.11645

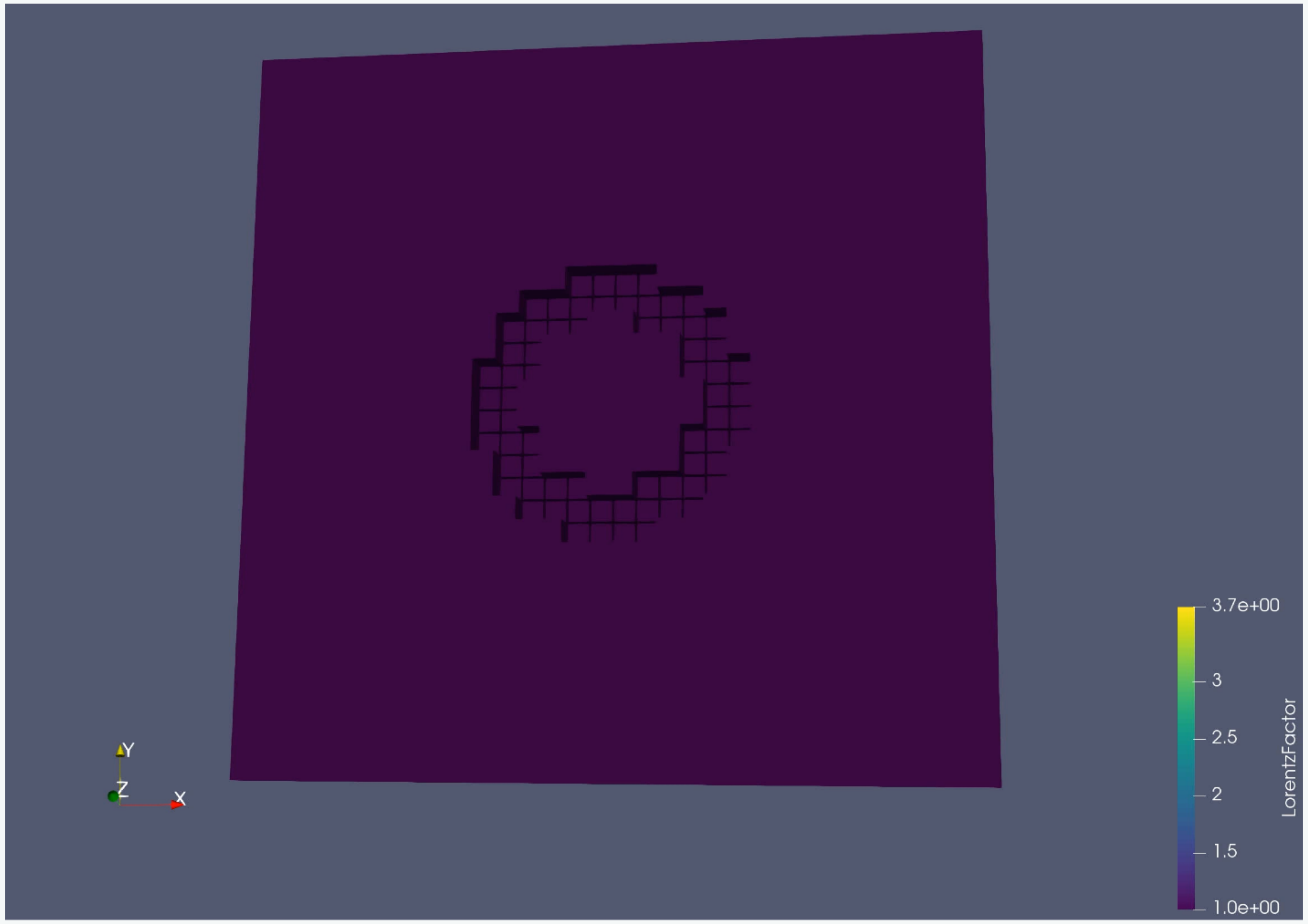
Example) **Kelvin-Helmholtz instability**



Example) **GRMHD blast wave**



Mass density



Lorentz factor

Discontinuous Galerkin method

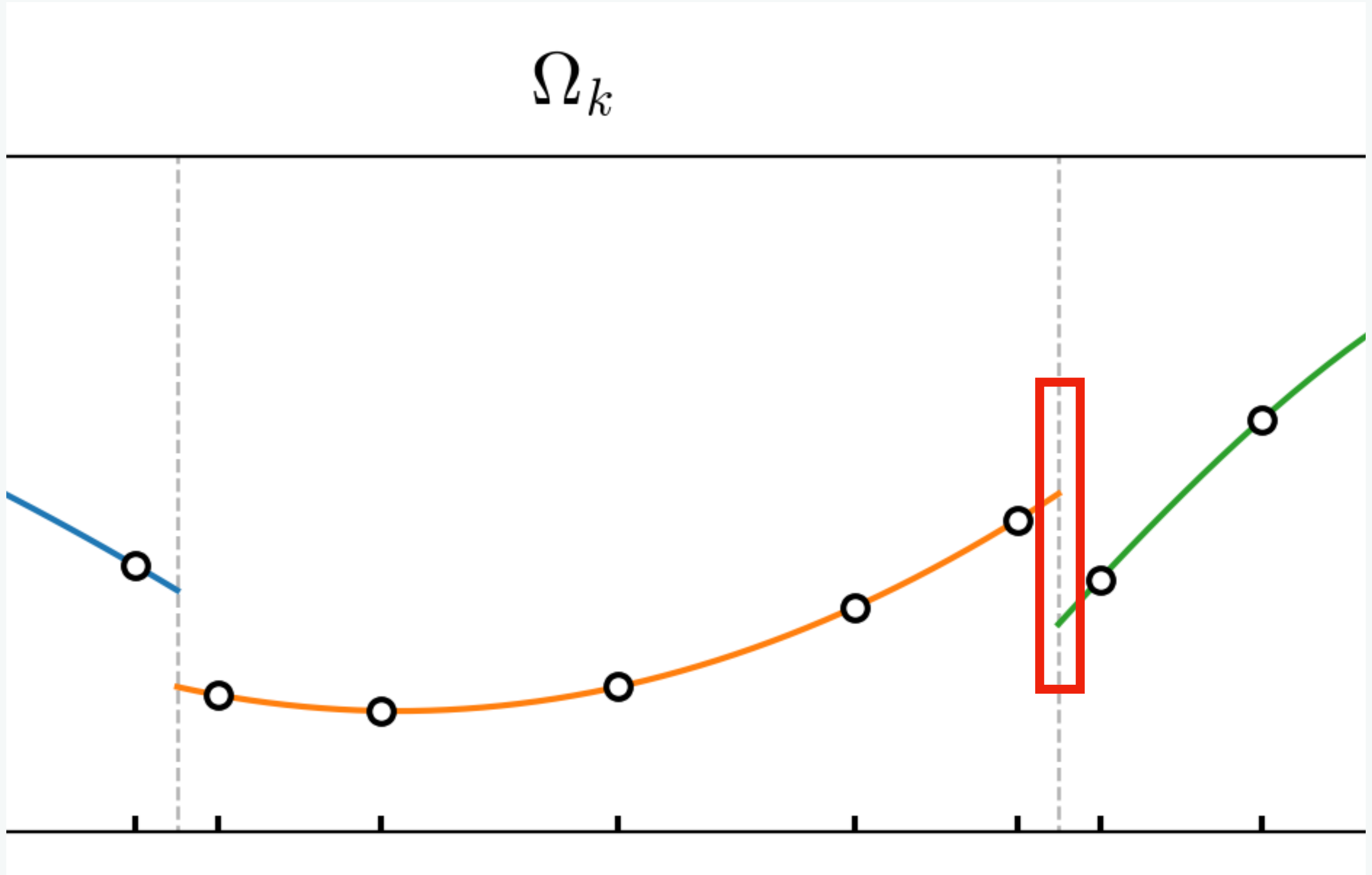
- Spectral accuracy for each cells

- Discontinuities are resolved at cell interfaces

- Smaller (tighter) CFL limit than finite difference

$$\Delta t \leq \frac{c}{d(2N+1)} \frac{\Delta x}{\lambda_{\max}}$$

- Suited for parallelization
  - nearest-neighbor communication



SpECTRE **code**

https://github.com/sxs-collaboration/spectre

- Evolves first-order hyperbolic systems using DG method
- Open source
- Task-based parallelism: `Charm++` (https://charm.cs.illinois.edu/)
- Elliptic solver (Vu+2022)
- Generalized Harmonic (GR) + Valencia (GRMHD) formulation