The Pennsylvania State University
Department of Physics

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Summer Project: Introduction to Numerical Methods for Hyperbolic PDEs

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Task

Use numerical methods to integrate an initial value system of equations in *flux-conservative* form:

$$\boxed{\partial_t \mathbf{u} = -\nabla \cdot \mathbf{F}}$$

once an appropriate set of Initial Data is provided.

$$\left\{ \begin{array}{ll} \mathbf{u},\ \mathbf{F} & \text{vectors of arbitrary dimension} \\ \mathbf{u} \equiv \mathbf{u}(\mathbf{r}, t) & \\ \mathbf{F} \equiv \mathbf{F}(\mathbf{u}, \frac{\partial \mathbf{u}}{\partial \mathbf{r}}, \ldots) & (\textit{conserved flux}) \end{array} \right\}$$

Finite Difference Techniques

The space-time domain is discretized, i.e. the functions $\mathbf{u}(\mathbf{r}, t)$ are replaced by their values on a grid of points. Taylor-expanding $\mathbf{u}(\mathbf{r}, t)$ in terms of , and Space and time derivatives are expressed in terms of differences between grid points

This presentation:

- Either a single PDE or a system of two;
- A single space dimension:

$$\begin{aligned} x_j &= x_0 + j\,\Delta x \qquad j = 0, 1, \cdots \\ t_n &= t_0 + n\,\Delta t \qquad n = 0, 1, \cdots \end{aligned}$$

$$u(x, t) \rightarrow u_j^n$$

Equations

ADVECTION EQUATION: $\boxed{\partial_x u = -v \partial_t u}$

- Forward Time Centered Space (FTCS) scheme
- Lax-Friedrichs scheme
- Methods of Lines

WAVE EQUATION: $\boxed{\partial_{xx} u = v^2 \partial_{tt} u}$

- Leapfrog scheme
- Iterative Crank-Nicholson (ICN) scheme

Initial Data and Boundary Conditions

All algorithms were tested on two types of Initial Data:

A. Periodic Initial Data: $u_i(x) = \sin(kx)$;

B. Aperiodic Initial Data: $u_i(x) = \exp(-(x - x_0)^2/2\sigma^2)$.

Periodic boundary conditions were used in all cases.

Convergence tests

Richardson ansatz:

$u^h = u + h e_1 + \dots$	1st order convergence
$u^h = u + h^2 e_2 + \dots$	2nd order convergence
$u^h = u + h^4 e_4 + \dots$	4th order convergence

$$Q(t) = \frac{\|u^{4h} - u^{2h}\|}{\|u^{2h} - u^h\|} \quad \rightarrow \quad \begin{cases} 2 & \text{1st order convergence} \\ 4 & \text{2nd order convergence} \\ 16 & \text{4th order convergence} \end{cases}$$

FTCS

Second order in space, first order in time:

$$\partial_x u \;\rightarrow\; \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + \mathcal{O}(\Delta x^2)$$
$$\partial_t u \;\rightarrow\; \frac{u_j^{n+1} - u_j^n}{\Delta t} + \mathcal{O}(\Delta t)$$

$$\boxed{u_j^{n+1} = u_j^n - \tfrac{v\Delta t}{2\Delta x}(u_{j+1}^n - u_{j-1}^n)}$$

Numerical errors disrupt convergence!

Lax-Friedrichs scheme: the role of numerical dissipation and the CFL condition.

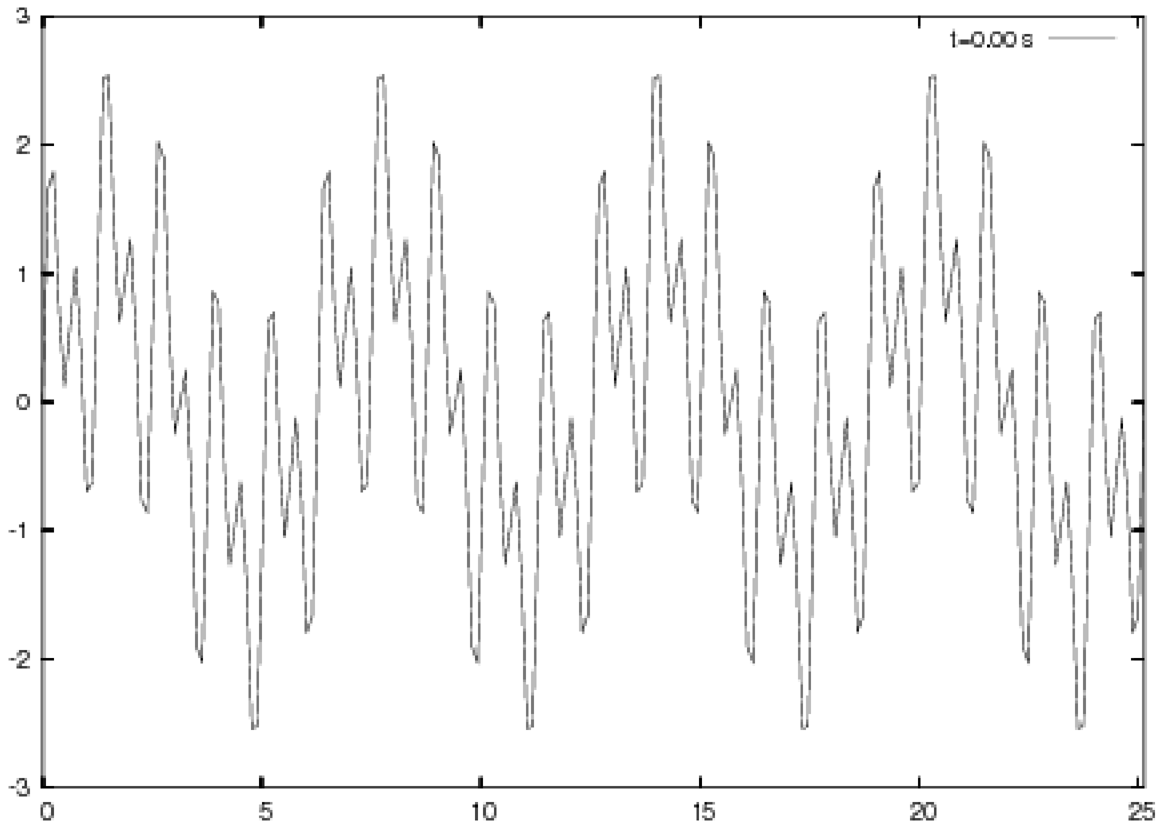
Exponentially growing modes in FTCS can be cured with the substitution:

$$u_j^n \rightarrow \frac{1}{2}(u_{j+1}^n + u_{j-1}^n)$$

Equivalent to an additional term:

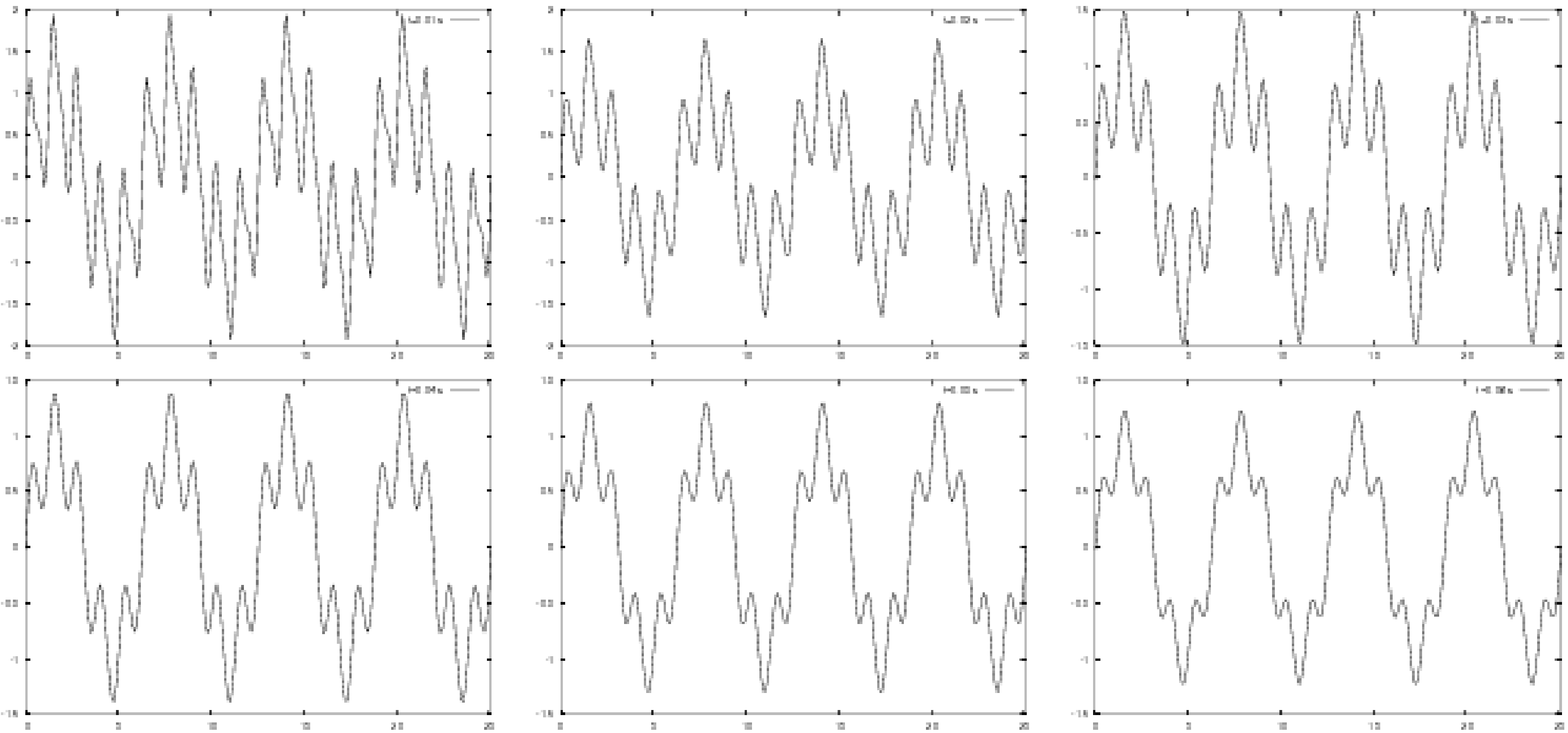
$$\partial_x u = -v\partial_t u + \sigma \partial_{xx} u$$

- **Numerical dissipation:** The dissipation coefficient $\sigma = \Delta x^2/2\Delta t$ affects high-frequency modes more than low-frequency ones.
- **Convergence:** The Courant-Friedrichs-Lewy (CFL) condition holds: the numerical domain must contain the causal one, or instabilities will arise.

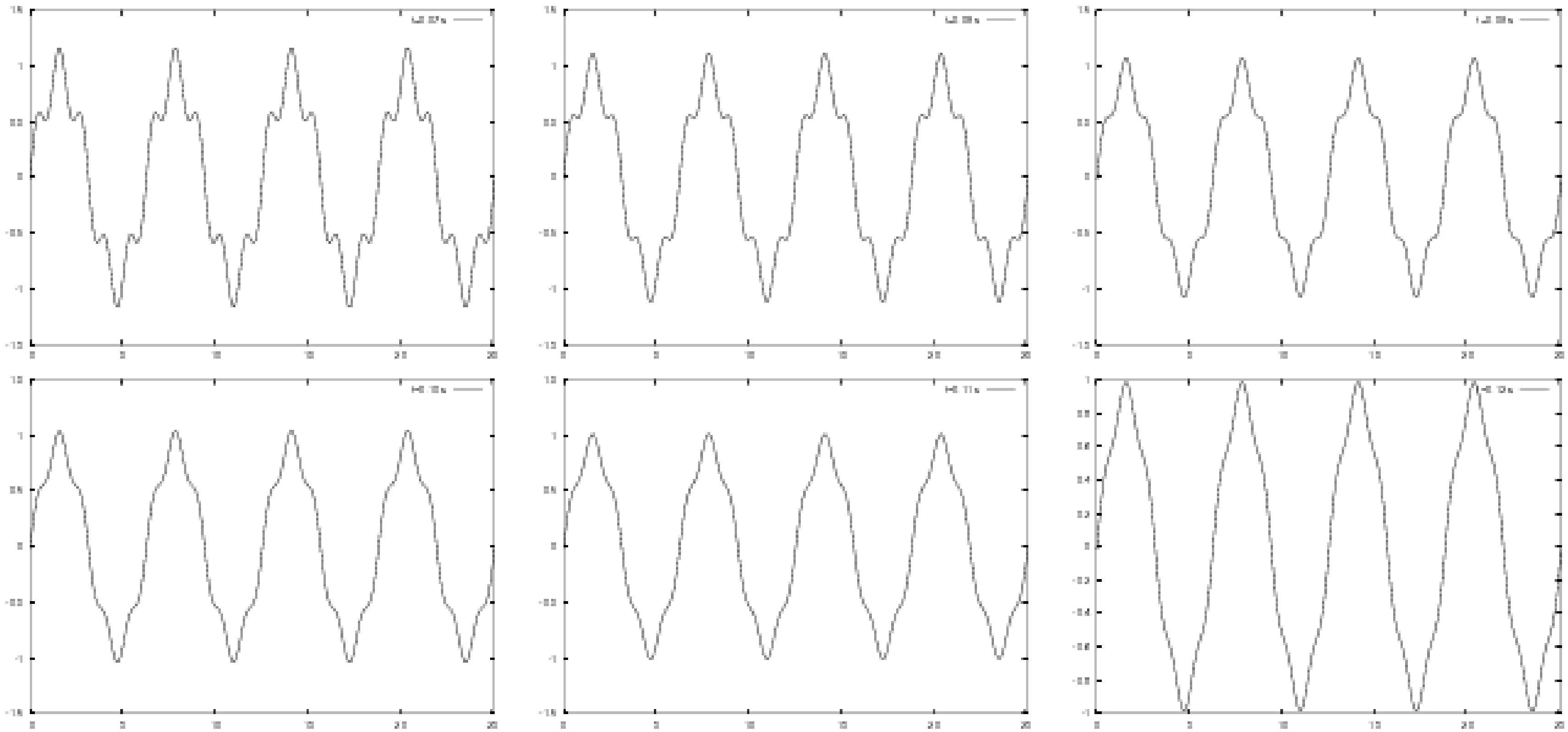


$$f(x) = \sin(\frac{2\pi}{5}x) + \sin(\frac{2\pi}{10}x) + \sin(\frac{2\pi}{50}x)$$

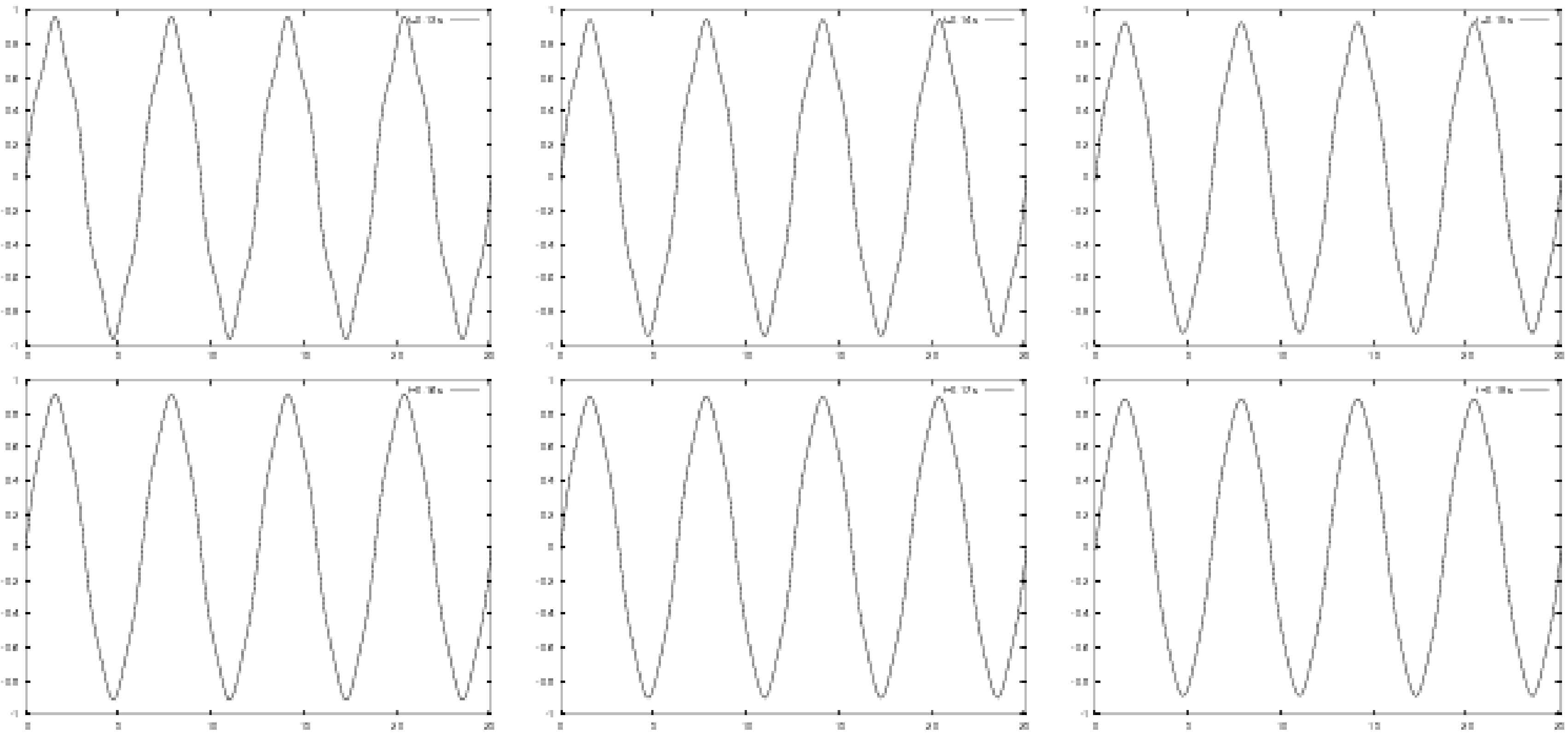
EXPERIMENTS: the Advection Equation

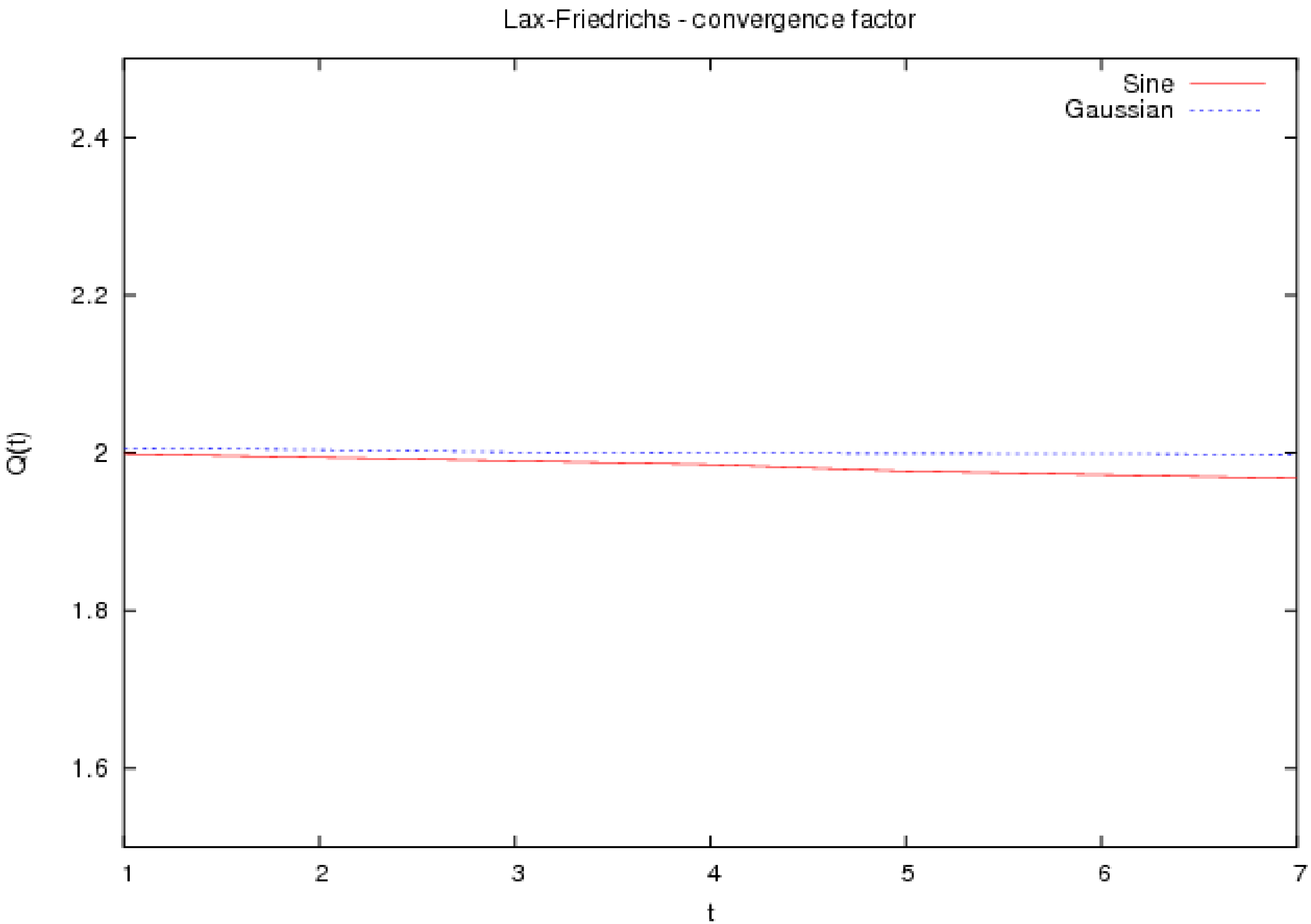


EXPERIMENTS: the Advection Equation



EXPERIMENTS: the Advection Equation




Lax-Friedrichs - convergence factor
Sine
Gaussian
Q(t)
2.4
2.2
2
1.8
1.6
1
2
3
4
5
6
7
t

Higher order schemes: the Method of Lines using RK4

First discretize spatial variables only:

$$\partial_{xx} = D_{xx} + \mathcal{O}(\Delta x^4) \rightarrow D_{xx} = \frac{-u_{j+2}(t) + 8(u_{j+1}(t) - u_{j-1}(t)) + u_{j-2}(t)}{12\Delta x}$$

The advection equation turns into a system of ODEs for the N functions $u_j(t)$.

$$\dot{u}_j(t) = \frac{-u_{j+2}(t) + 8(u_{j+1}(t) - u_{j-1}(t)) + u_{j-2}(t)}{12\Delta x}$$

The Runge-Kutta ODE solver can then integrate it to fourth order accuracy in time.

Staggered-Leapfrog scheme: half time steps and self-consistent initialization

$$\partial_{tt}u = v^2\partial_{xx}u \qquad \Longleftrightarrow \qquad \begin{cases} \partial_t r = v\partial_x s \\ \partial_t s = v\partial_x r \end{cases} \quad \text{where} \quad \begin{cases} r \equiv v\partial_x u \\ s \equiv \partial_t u \end{cases}$$

$$r^n_{j+1/2} = v\frac{u^n_{j+1} - u^n_j}{\Delta x}$$

$$s^{n+1/2}_j = \frac{u^{n+1}_j - u^n_j}{\Delta t}$$

$$\boxed{u^{n+1}_j = \lambda^2(u^n_{j+1} + u^n_{j-1} + 2(1-\lambda^2)u^n_j - u^{n-1}_j}$$

$$\{\lambda \equiv v\Delta t/\Delta x\}$$

Initialization!

ICN: implicit to explicit through iteration

$$\partial_{tt}u = v^2\partial_{xx}u \qquad \Longleftrightarrow \qquad \begin{cases} \partial_t u = p \\ \partial_t p = v^2\partial_{xx}u \end{cases}$$

First iteration:

$$\begin{cases} {}^{(1)}u_j^n = u_j^n + \Delta t \cdot p_j^n \\ {}^{(1)}p_j^n = p_j^n + \Delta t \cdot \delta^2 u_j^n \end{cases}$$

Second iteration:

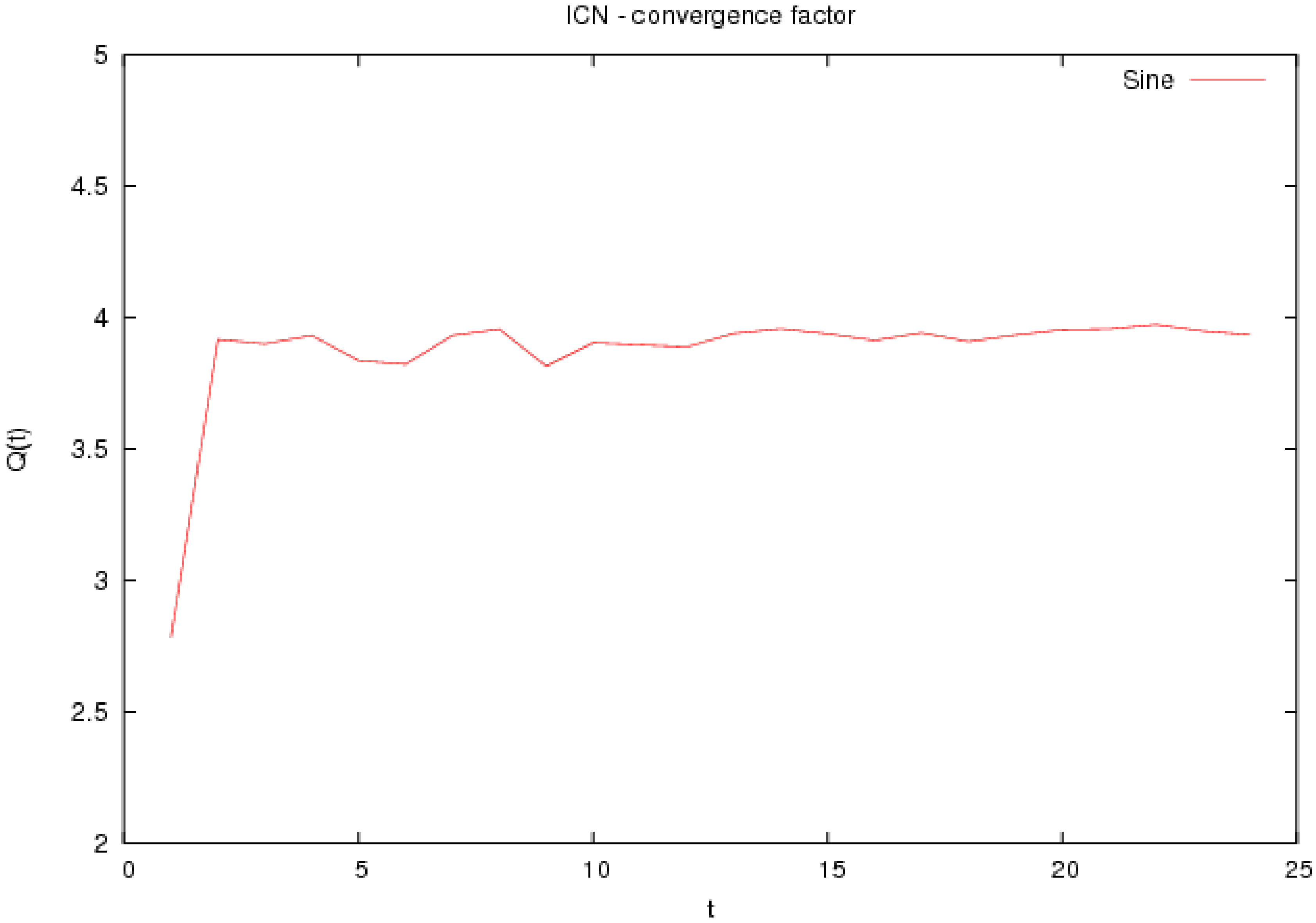
$$\begin{cases} {}^{(2)}u_j^n = u_j^n + \frac{\Delta t}{2}\left({}^{(1)}p_j^n + p_j^n\right) \\ {}^{(2)}p_j^n = p_j^n + \frac{\Delta t}{2\Delta x^2}\,\delta^2\left({}^{(1)}u_j^n + u_j^n\right) \end{cases}$$

Third iteration:

$$\begin{cases} {}^{(3)}u_j^n = u_j^n + \frac{\Delta t}{2}\left({}^{(2)}p_j^n + p_j^n\right) \\ {}^{(3)}p_j^n = p_j^n + \frac{\Delta t}{2\Delta x^2}\,\delta^2\left({}^{(2)}u_j^n + u_j^n\right) \end{cases}$$

Finally:

$$\begin{cases} u_j^{n+1} = {}^{(3)}u_j^n \\ p_j^{n+1} = {}^{(3)}p_j^n \end{cases}$$


ICN - convergence factor
Sine
Q(t)
t
5
4.5
4
3.5
3
2.5
2
0
5
10
15
20
25

Summary

- One first-order and one second-order PDE discretized; solutions evolved, starting from both periodic and aperiodic initial data;
- FTCS, Lax-Friedrichs, Leapfrog, ICN and MOL used;
- First, second (and fourth?) order convergence attained.