Numerical Partial Differential Equations:

Basic Concepts

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An Overview

1. Why we need numerical methods?
   - It is a method for analyzing a problem in addition to theoretical and experiment approaches.
2. Why we need high-order methods?
   - For wave type problems it is an effective way to obtain numerical solutions with high accuracy. However, high-order computational schemes are very sensitive to the imposition of boundary conditions.
3. Does there exist a general methodology for constructing numerical schemes?
   - The answer is "Yes" to certain types of problems. General speaking we need to construct a well-posed analysis on the problem wherever possible. This analysis is our guideline for constructing numerical schemes.

Well-posedness of Initial Boundary Value Problem

Example (Model Wave Problem)

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad x \in [0,1], \quad t \geq 0,$$
$$u(x,0) = f(x), \quad x \in [0,1],$$
$$u(0,t) = g(t), \quad t \geq 0.$$

Smoothness condition : $f(0) = g(0)$

We say the problem is well-posed if

1. The solution exists.
2. The solution is unique.
3. The solution is stable.

Stable Solutions

- It is meaningful if there exists an unique solution to the problem.
- In physics we consider that a physical quantity is a finite number and can be measured by certain methods or devices. Moreover, we wish that the system of a physical problem is stable, in the sense that when a small perturbation is introduced into the system, the solution does not deviate away from the unperturbed one.

Well-posedness of the Initial Value Problem I

Example (2π-periodic scalar wave equation)

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad x \in [0, 2\pi], \quad t \geq 0, \tag{1}$$

$$u(x,t) = f(x), \quad \text{periodic}, \quad t \geq 0, \tag{2}$$

$$u^{(p)}(0,t) = u^{(p)}(2\pi,t), \quad u^{(p)} = \frac{\partial^{(p)} u}{\partial x^{(p)}}, \quad p = 0, 1, 2, \ldots \tag{3}$$

Does the solution exist ?

Well-posedness of the Initial Value Problem II

Assume

$$u(x,t) = \hat{u}_k(t)\, e^{ikx}, \quad k \in \mathbb{Z} \tag{4}$$

If (4) is a solution to (1) then

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \qquad \Rightarrow \qquad \frac{d\hat{u}_k(t)}{dt} \cdot e^{ikx} = (-ik)\, \hat{u}_k(t) \cdot e^{ikx}$$

$$\Rightarrow \quad \hat{u}_k(t) = \hat{u}_k(0) \cdot e^{-ikt} \qquad \Rightarrow \quad u(x,t) = \hat{u}_k(0) \cdot e^{-ikt} \cdot e^{ikx} = \hat{u}_k(0) \cdot e^{ik(x-t)}$$

Invoking linear superposition we have

$$u(x,t) = \sum_{k=-\infty}^{\infty} \hat{u}_k(0) e^{ik(x-t)}.$$

Take $t = 0$

$$u(x,0) = f(x) \quad \Rightarrow \sum_{k=-\infty}^{\infty} \hat{u}_k(0) e^{ikx} = f(x) \quad \Rightarrow \hat{u}_k(0) = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-ikx}\, dx$$

where $\hat{u}_k(0)$ is the fourier coefficients of the function f.

We have a solution to the problem.

Well-posedness of the Initial Value Problem III

Uniqueness: Is this the only one ?

Recall that u satisfies the initial value problem:

$$\frac{\partial u}{\partial t}+\frac{\partial u}{\partial x}=0, \quad u(x,0)=f(x), \quad u^{(p)}(0,t)=u^{(p)}(2\pi,t).$$

$$u(x,t)=\sum_{k=-\infty}^{\infty}\hat{u}_k(0)e^{ik(x-t)}, \quad \hat{u}_k(t)=\frac{1}{2\pi}\int_0^{2\pi}f(x)e^{ikx}dx$$

Assume that $v \neq u$ is also a solution to the problem, i.e.,

$$\frac{\partial v}{\partial t}+\frac{\partial v}{\partial x}=0, \quad v(x,0)=f(x), \quad v^{(p)}(0,t)=v^{(p)}(2\pi,t).$$

Let $w=u-v$ then

$$\frac{\partial w}{\partial t}+\frac{\partial w}{\partial x}=0, \quad w(x,0)=0, \quad w^{(p)}(0,t)=w^{(p)}(2\pi,t).$$

Hence

$$u(x,t)-v(x,t)=w(x,t)=\sum_{k=-\infty}^{\infty}\hat{w}_k(0)\,e^{ik(x-t)}=0 \implies u(x,t)=v(x,t)$$

$u(x,t)$ and $v(x,t)$ are identical.

Well-posedness of the Initial Value Problem IV

How do we know a solution is stable?

- In addition to the issues concerning the existence and uniqueness of the solution, we also need to know whether the solution is stable.

Consider the problem:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0,$$
$$u(x,0) = f(x),$$
$$u^{(p)}(0,t) = u^{(p)}(2\pi,t).$$

Energy of the system

Definition

$$E(t) = \int_0^{2\pi} u^2(x,t)\,dx$$

- We observe similar energy definitions for various types of physical systems, for example

1. in electromagnetism

$$\text{Energy} = \int_\Omega \frac{1}{2}\epsilon E^2 + \frac{1}{2}\mu H^2\,dx$$

2. in fluid dynamics

$$\text{Energy} = \int_\Omega \rho(V\cdot V)\,d\Omega$$

Energy Estimate

Consider the problem:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0,$$
$$u(x,0) = f(x),$$
$$u^{(p)}(0,t) = u^{(p)}(2\pi,t).$$

We have the energy rate equation

$$\frac{dE(t)}{dt} = \frac{d}{dt}\int_0^{2\pi} u^2(x,t)\,dx = \int_0^{2\pi} 2u\frac{\partial u(x,t)}{\partial t}\,dx$$
$$= \int_0^{2\pi} 2u\left(-\frac{\partial u}{\partial x}\right)\,dx = -\int_0^{2\pi}\frac{\partial u^2}{\partial x}\,dx = -u^2(x,t)\Big|_0^{2\pi} = 0$$

Hence,

$$E(t) = E(0) \Rightarrow \int_0^{2\pi} u^2(x,t)\,dx = \int_0^{2\pi} f^2(x)\,dx$$

Well-posedness of the Initial Value Problem V

Energy of a Perturbed System

Let us now consider the following problems.

Unperturbed Problem:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0$$
$$u(x,0) = f(x)$$
$$u^{(p)}(0,t) = u^{(p)}(2\pi,t)$$

Perturbed Problem:

$$\frac{\partial v}{\partial t} + \frac{\partial v}{\partial x} = 0$$
$$v(x,0) = f(x) + \epsilon(x), \ |\epsilon(x)| << 1$$
$$v^{(p)}(0,t) = v^{(p)}(2\pi,t)$$

Let $w = v - u$

$$\frac{\partial w}{\partial t} + \frac{\partial w}{\partial x} = 0, \quad w(x,0) = \epsilon(x), \quad w^{(p)}(0,t) = w^{(p)}(2\pi,t)$$

Then

$$\int_0^{2\pi} w^2(x,t)\,dx = \int_0^{2\pi} (v(x,t) - u(x,t))^2\,dx = \int_0^{2\pi} \epsilon^2(x)\,dx$$

The difference between u and v is bounded by the initial data.

Consistency

Define the grid points:

$$x_j = j \cdot h = j \cdot \frac{2\pi}{N+1}, \quad j = 0, 1, 2, \ldots, N$$

Let

$$u(x_j, t) = u_j(t)$$

Recall that $\dfrac{\partial u(x,t)}{\partial x}$ can be approximated by

- forward difference: $\dfrac{u_{j+1} - u_j}{h} + \mathcal{O}(h)$
- backward difference: $\dfrac{u_j - u_{j-1}}{h} + \mathcal{O}(h)$
- central difference: $\dfrac{u_{j+1} - u_{j-1}}{2h} + \mathcal{O}(h^2)$

Upwind Scheme: $\frac{dv_i}{dt} = -\frac{v_i - v_{i-1}}{h}$

Define the numerical solution as

$$v_i(t), \quad i = 0, 1, 2, \dots, N$$

satisfying the semi-discrete scheme

$$\frac{dv_i}{dt} + \frac{v_i - v_{i-1}}{h} = 0, \quad i = 0, 1, \dots, N$$
$$v_i(t) = f(x_i) = f_i, \quad v_{-1} = v_N.$$

Replacing $v_i(t)$ and $v_{i-1}(t)$ by $u(x_i, t)$ and $u(x_{i-1}, t)$ in the scheme, respectively, we get the truncation error (TE)

$$TE = \frac{\partial u(x_i, t)}{\partial t} + \frac{u(x_i, t) - u(x_{i-1}, t)}{h} = \frac{\partial u(x_i, t)}{\partial t} + \frac{\partial u(x_i, t)}{\partial x} + \mathcal{O}(h) = \mathcal{O}(h).$$

Observe that $TE \to 0$ as $h \to 0$. The scheme is consistent.

Upwind Scheme: $\frac{dv_i}{dt} = -\frac{v_i - v_{i-1}}{h}$ II

Energy Estimate

Define the discrete energy of the system as

$$E_D(t) = \sum_{i=0}^{N} v_i^2(t)h \quad \left(\text{mimicking } E(t) = \int_0^{2\pi} u^2(x,t)\,dx\right)$$

We have the discrete energy rate equation as

$$\begin{aligned}\frac{dE_D(t)}{dt} &= \sum_{i=0}^{N} 2v_i \frac{dv_i}{dt} h = -\sum_{i=0}^{N} 2v_i^2 + \sum_{i=0}^{N} 2v_i v_{i-1} - \sum_{i=0}^{N} v_{i-1}^2 + \sum_{i=0}^{N} v_{i-1}^2 \\ &= -\sum_{i=0}^{N} v_i^2 - \sum_{i=0}^{N} (v_i - v_{i-1})^2 + \sum_{i=0}^{N} v_i^2 \le 0\end{aligned}$$

implying

$$E_D(t) \le E_D(0) \implies \sum_{i=0}^{N} v_i^2 h \le \sum_{i=0}^{N} f_i^2 h \quad \left(\text{note } \int_0^{2\pi} u^2 dx = \int_0^{2\pi} f^2 dx\right).$$

The scheme has a bounded energy estimate for a given terminal time.

Upwind Scheme

Fully-discrete scheme

- Discretizing the dv_j/dt by forward difference we obtain

$$\frac{v_i^{n+1} - v_i^n}{\Delta t} + \frac{v_i^n - v_{i-1}^n}{\Delta x} = 0, \quad i = 0, 1, ..., N$$
$$v_i^0 = f(x_i), \quad v_{-1}^n = v_N^n$$

  where $v_j^n = v_j(t_n)$, $t_n = n\Delta t$ with Δt being the time step.

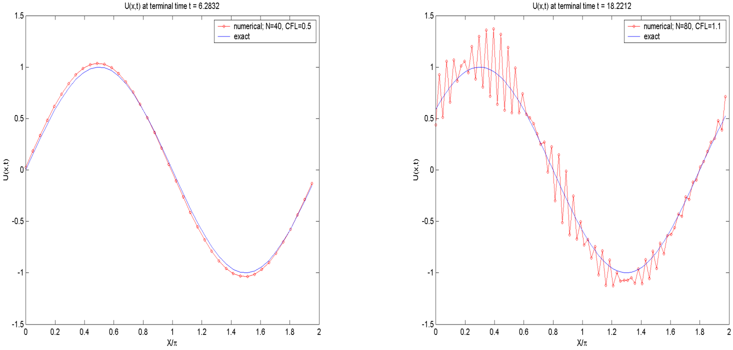
- Rewrite the scheme as follows

$$v_i^{n+1} = v_i^n + \lambda(v_i^n - v_{i-1}^n), \quad i = 0, 1, ..., N$$
$$v_i^0 = f(x_i), \quad v_{-1}^n = v_N^n$$

  where $\lambda = \Delta t/\Delta x$.

Example

- We solve the wave problem with $u(x,t) = \sin(x - t)$ as exact solution.
- Solutions are computed with $\lambda = 0.5$ (left) and 1.1 (right).



Convergence Study

l_∞ error, l_2 error, and convergence order:

$$||\varepsilon(N)||_\infty = \max_{i=0,\ldots,N} |u(x_i,t) - v_i(t)|, \quad ||\varepsilon(N)||_2 = \sqrt{\sum_{i=0}^{N} |u(x_i,t) - v_i(t)|\Delta x}$$

$$\alpha = \frac{\log\left(||\epsilon(N_2)||/||\epsilon(N_2)||\right)}{\log\left(N_1/N_2\right)}$$

Table: $t = 1$ period, $CFL = 0.9$. $\Delta t = CFL \cdot \Delta x$

N	$\|\epsilon(N)\|_\infty$	order	$\|\epsilon(N)\|_{l_2}$	order
20	9.6972E-02	-	6.8572E-02	-
40	4.9238E-02	0.98	3.4816E-02	0.98
80	2.4075E-02	1.03	1.7023E-02	1.03
160	1.2246E-02	0.98	8.6590E-03	0.98
320	6.1647E-03	0.99	4.3591E-03	0.99

The error decays as Δt and Δx both vanish

Convergence Study

Table: $t = 1$ period, CFL $= 1.1$

N	$\|\|\epsilon\|\|_\infty$	order	$\|\|\epsilon\|\|_{l_2}$	order
20	9.3013E-02	-	6.5886E-02	-
40	4.6286E-02	1.01	3.2743E-02	1.01
80	2.3795E-02	0.96	1.6827E-02	0.96
160	1.2118E-02	0.97	8.5694E-03	0.97
320	7.4377E+06	-29.19	2.6742E+06	-28.22

Truncation error $\to 0$ does not ensure the convergence of the numerical solution.

Consistency, Stability and Convergency I

- We have v_i^n satisfying the scheme

$$\frac{v_i^{n+1}-v_i^n}{\Delta t}+\frac{v_i^n-v_{i-1}^n}{\Delta x}=0, \quad i=0,1,...,N$$
$$v_i^{n+1}=(1-\lambda)v_i^n+\lambda v_{i-1}^n, \quad \lambda=\frac{\Delta t}{\Delta x}$$

- Note that $u(x_i,t^n)=u_i^n$ satisfy the following equation

$$\frac{u_i^{n+1}-u_i^n}{\Delta t}+\frac{u_i^n-u_{i-1}^n}{\Delta x}=r_i^n=\mathcal{O}(\Delta t,\Delta x)$$

- The error $e_i^n=u_i^n-v_i^n$ satisfies the equation

$$\frac{e_i^{n+1}-e_i^n}{\Delta t}+\frac{e_i^n-e_{i-1}^n}{\Delta x}=r_i^n$$
$$e_i^{n+1}=(1-\lambda)e_i^n+\lambda e_{i-1}^n+r_i^n\Delta t$$

Consistency, Stability and Convergency II

The scheme

$$e_i^{n+1} = (1-\lambda)e_i^n + \lambda e_{i-1}^n + r_i^n \Delta t, \quad \lambda = \frac{\Delta t}{\Delta x}$$

can be written in the following matrix-vector form

$$\boldsymbol{e}^{n+1} = \boldsymbol{Q}\boldsymbol{e}^n + \boldsymbol{r}^n \Delta t$$

where

$$\boldsymbol{e}^n = \begin{bmatrix} e_0^n \\ e_1^n \\ e_2^n \\ \vdots \\ e_N^n \end{bmatrix} \quad \boldsymbol{r}^n = \begin{bmatrix} r_0^n \\ r_1^n \\ r_2^n \\ \vdots \\ r_N^n \end{bmatrix} \quad \boldsymbol{Q} = \begin{bmatrix} 1-\lambda & 0 & \dots & 0 & \lambda \\ \lambda & 1-\lambda & \ddots & & 0 \\ 0 & \lambda & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \lambda & 1-\lambda \end{bmatrix}$$

Consistency, Stability and Convergency III

Recursively applying the scheme we have

$$
\begin{aligned}
\boldsymbol{e}^{n+1} &= \boldsymbol{Q}\boldsymbol{e}^{n} + \boldsymbol{r}^{n}\Delta t = \boldsymbol{Q}(\boldsymbol{Q}\boldsymbol{e}^{n-1} + \boldsymbol{r}^{n-1}\Delta t) + \boldsymbol{r}^{n}\Delta t \\
&= \boldsymbol{Q}^{2}\boldsymbol{e}^{n-1} + \Delta t\sum_{k=0}^{1}\boldsymbol{Q}^{k}\boldsymbol{r}^{n-k} = \boldsymbol{Q}^{2}(\boldsymbol{Q}\boldsymbol{e}^{n-2} + \boldsymbol{r}^{n-2}\Delta t) + \Delta t\sum_{k=0}^{1}\boldsymbol{Q}^{k}\boldsymbol{r}^{n-k} \\
&= \boldsymbol{Q}^{3}\boldsymbol{e}^{n-2} + \Delta t\sum_{k=0}^{2}\boldsymbol{Q}^{k}\boldsymbol{r}^{n-k} = \boldsymbol{Q}^{3}(\boldsymbol{Q}\boldsymbol{e}^{n-3} + \boldsymbol{r}^{n-3}\Delta t) + \Delta t\sum_{k=0}^{2}\boldsymbol{Q}^{k}\boldsymbol{r}^{n-k} \\
&= \boldsymbol{Q}^{4}(\boldsymbol{e}^{n-3} + \boldsymbol{r}^{n-3}\Delta t) + \Delta t\sum_{k=0}^{3}\boldsymbol{Q}^{k}\boldsymbol{r}^{n-k} = \cdots = \boldsymbol{Q}^{n+1}\boldsymbol{e}^{0} + \Delta t\sum_{k=0}^{n}\boldsymbol{Q}^{k}\boldsymbol{r}^{n-k}
\end{aligned}
$$

leading to

$$
\boldsymbol{e}^{n} = \boldsymbol{Q}^{n}\boldsymbol{e}^{0} + \Delta t\sum_{k=0}^{n-1}\boldsymbol{Q}^{k}\boldsymbol{r}^{n-k-1} = \sum_{k=0}^{n-1}\boldsymbol{Q}^{k}\boldsymbol{r}^{n-k-1}
$$

Consistency, Stability and Convergency IV

We have

$$\boldsymbol{e}^n = \sum_{k=0}^{n-1} \boldsymbol{Q}^k(\lambda)\boldsymbol{r}^{n-k-1}, \quad \lambda = \Delta t/\Delta x$$

If $|\boldsymbol{Q}| \le 1$ as both $\Delta t \to 0$ and $\Delta x \to 0$, then

$$\begin{aligned} |\boldsymbol{e}^n| &= \left|\Delta t \sum_{k=0}^{n-1} \boldsymbol{Q}^k \boldsymbol{r}^{n-k-1}\right| \le \Delta t \sum_{k=0}^{n-1} |\boldsymbol{Q}|^k |\boldsymbol{r}^{n-k-1}| \\ &\le R\Delta t \sum_{k=0}^{n-1} 1^k, \quad R = \max_{0\le m\le n-1} |\boldsymbol{r}^m| = \mathcal{O}(\Delta t, \Delta x) \\ &= R(n\Delta t) \to 0 \end{aligned}$$

for a fixed terminal time $T = n\Delta t$, which implies the numerical solution converges to the exact one during mesh refinement provided that $|\boldsymbol{Q}|$ is bounded by unity.

Classical Theory on Convergency

Theorem (Lax-Richtmyer Equivalence Theorem)

A consistent approximation to a linear well-posed partial differential equation is convergent if and only if it is stable.

- From the example we have

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad \frac{v_i^{n+1} - v_i^n}{\Delta t} + \frac{v_j^n - v_{j-1}^n}{\Delta x} = 0 \quad \boldsymbol{e}^n = \Delta t \sum_{k=0}^{n-1} \boldsymbol{Q}^k \boldsymbol{r}^{n-k-1}$$

- Stability means

$$|\boldsymbol{Q}| \leq 1.$$

- Consistency means

$$R = \max_{0 \leq m \leq n-1} |\boldsymbol{r}^m| \to 0, \quad \text{as } \Delta t \to 0 \text{ and } \Delta x \to 0$$

while $\Delta t / \Delta x$ is fixed.

- Then for any fix terminal time $T = n\Delta t$ we have the convergence

$$|\boldsymbol{e}^n| \leq R(n\Delta t) \to 0$$

von Neumann Analysis I

- For stable computation we need to ensure $|Q(\lambda)| \leq 1$ by properly choosing λ.
- The numerical solution v_j^n satisfies the scheme

$$\frac{v_i^{n+1} - v_i^n}{\Delta t} + \frac{v_j^n - v_{j-1}^n}{\Delta x} = 0$$

- Assume $v_j^n = \hat{v}_k^n e^{ikx_j}$ for $-N/2 \leq k \leq N/2$. Then

$$\begin{aligned}
&\frac{\hat{v}_k^{n+1} - \hat{v}_k^n}{\Delta t} \cdot e^{ikx_j} + \frac{\hat{v}_k^n e^{ikx_j} - \hat{v}_k^n e^{ikx_{j-1}}}{\Delta x} = 0, \quad (x_{j-1} = x_j - \Delta x) \\
\Rightarrow \quad & \hat{v}_k^{n+1} - \hat{v}_k^n = -\lambda \left(\hat{v}_k^n\right)\left(1 - e^{-ik\Delta x}\right) \\
\Rightarrow \quad & \hat{v}_k^{n+1} = \left(1 - \lambda(1 - e^{-ik\Delta x})\right) \hat{v}_k^n \\
\Rightarrow \quad & \hat{v}_k^{n+1} = \left(1 - \lambda(1 - e^{-ik\Delta x})\right)^{n+1} \hat{v}_k^0 = \hat{Q}_k^{n+1}(\lambda)\hat{v}_k^0.
\end{aligned}$$

- $\hat{Q}_k = 1 - \lambda(1 - e^{-ik\Delta x})$ is called the amplification factor.

von Neumann Analysis II

- We have

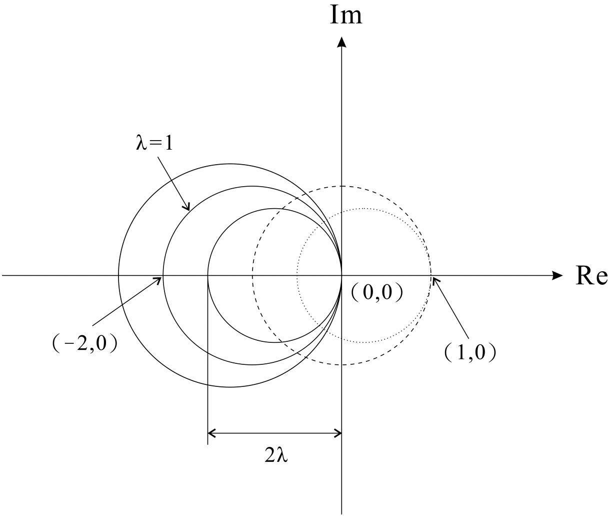
$$\hat{v}_k^n = \hat{Q}_k^n \hat{v}_k^0, \quad |k| \le N/2$$
$$\hat{Q}_k(\lambda) = 1 + \lambda(e^{-ik\Delta x} - 1).$$

- If $|\hat{Q}_k(\lambda)| \le 1$ then

$$|\hat{v}_k^n| = |\hat{Q}_k^n||\hat{v}_k^0| = |\hat{Q}_k|^n|\hat{v}_k^0| \le |\hat{v}_k^0|$$

  implying stability.
- For $|\hat{Q}_k| \le 1$ we need

$$\lambda = \frac{\Delta t}{\Delta x} \le 1$$



von Neumann Analysis III

- suitable for period problems described by linear and constant coefficient equations.
- only need to investigate the bound of $\hat{Q}_k$ resulting from each mode solution $\hat{v}^n e^{ikx_j}$ individually, instead of analyzing the norm of the matrix $\boldsymbol{Q}$.
- For problems involving boundary conditions we need to use GKS theory (normal mode analysis) to analyze the stability of numerical boundary conditions.

Phase Error Analysis I

Consider $u = u(x,t)$ satisfying the linear wave problem (2π-periodic)

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}, \qquad u(x,0) = e^{ikx} \qquad 0 \le x \le 2\pi,$$

The solution to the problem is a traveling wave

$$u(x,t) = e^{ik(x-ct)} \quad c\text{: phase speed.}$$

Introduce the grid points as

$$x_j = j\,\Delta x = \frac{2\pi j}{N+1}, \quad j \in [0,\ldots,N].$$

Consider the semi-discrete approximations for the problem

2nd-order: $$\frac{dv_j(t)}{dt} = -c\frac{v_{j+1} - v_{j-1}}{2\Delta x}, \qquad v_j(0) = e^{ikx}$$

4th-order: $$\frac{dv_j(t)}{dt} = -c\frac{-v_{j+2} + 8v_{j+1} - 8v_{j-1} + v_{j-2}}{12\Delta x}, \quad v_j(0) = e^{ikx}$$

where $v_j(t)$ are the numerical values approximating $u(x_j,t)$.

Phase Error Analysis II

Consider the 2nd order accurate semi-discrete approximation

2nd-order: $$\frac{dv_j(t)}{dt} = -c\frac{v_{j+1} - v_{j-1}}{2\Delta x} \qquad v_j(0) = e^{ikx}$$

Assume that $v_j(t) = \hat{v}_k(t)e^{ikx_j}$. Then

$$\frac{d\hat{v}_k(t)}{dt} = -c\left(\frac{e^{ik\Delta x} - e^{-ik\Delta x}}{2\Delta x}\right)\hat{v}_k(t) = -ikc_2\hat{v}_k(t),$$
$$c_2(k) = c\left(\frac{\sin(k\Delta x)}{k\Delta x}\right), \quad |k| \leq N/2$$

leading to

$$\hat{v}_k(t) = \hat{v}_k(0)e^{-ikc_2t} \implies v_j(t) = \hat{v}_k(0)e^{ik(x-c_2(k)t)}.$$

Applying the initial condition we have $\hat{v}(0) = 1$. Thus,

$$v_j(t) = e^{ik(x-c_2(k)t)}$$

Phase Error Analysis III

We have the problem and difference approximation as

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}, \qquad u(x,0) = e^{ikx}, \qquad u(x,t) = e^{ik(x-ct)}$$

$$\frac{dv_j(t)}{dt} = -c\frac{v_{j+1} - v_{j-1}}{2\Delta x}, \qquad v_j(0) = e^{ikx}, \qquad v_j(t) = e^{ik(x-c_2(k)t)}$$

- $c_2(k) = c\left(\frac{\sin(k\Delta x)}{k\Delta x}\right)$ is the numerical wave speed resulting from the 2nd-order accurate central difference approximation, and

$$c_2 = c\left(1 - \frac{(k\Delta x)^2}{6} + \mathcal{O}((k\Delta x)^4)\right) \implies |c - c_2| = c\frac{(k\Delta x)^2}{6} + \mathcal{O}((k\Delta x)^4)$$

- The dependence of c_2 on k is known as the dispersion relation.

Phase error $e_2(k)$: leading term in the relative error between $u(x_j, t)$ and $v_j(t)$:

$$\left|\frac{u(x,t) - v(x,t)}{u(x,t)}\right| = \left|1 - e^{ik(c-c_2(k))t}\right| \approx |k(c - c_2(k))t| = e_2(k).$$

Phase Error Analysis IV

We have the phase error $e_2(k,t)$ as

$$e_2(k,t) = |k(c - c_2(k))t| = kct\left|1 - \frac{\sin(k\Delta x)}{k\Delta x}\right|$$

Introduce

$$N_{ppw} = \frac{N+1}{k} = \frac{2\pi}{k\Delta x} \quad \text{(number of points per wavelength)}$$

$$p = \frac{kct}{2\pi} \quad \text{(number of periods in time)}$$

We have the phase error in term of N_{ppw} and p as follows,

$$e_2(N_{ppw}, p) = 2\pi p\left|1 - \frac{\sin(2\pi N_{ppw}^{-1})}{2\pi N_{ppw}^{-1}}\right| \approx \frac{\pi p}{3}\left(\frac{2\pi}{N_{ppw}}\right)^2.$$

Phase Error Analysis V

Consider the 4th-order approximation for the problem:

$$\frac{dv_j(t)}{dt} = -c\frac{-v_{j+2} + 8v_{j+1} - 8v_{j-1} + v_{j-2}}{12\Delta x}, \quad v_j(0) = e^{ikx}$$

Following a similar approach we obtain the corresponding numerical wave speed as

$$c_4(k) = c\left(\frac{8\sin(k\Delta x) - \sin(2k\Delta x)}{6k\Delta x}\right) = c\left(1 - \frac{(k\Delta x)^4}{30} + \mathcal{O}\left((k\Delta x)^6\right)\right)$$

and the phase error as

$$e_4(k,t) = kct\left|1 - \frac{8\sin(k\Delta x) - \sin(2k\Delta x)}{6k\Delta x}\right| \approx \frac{\pi p}{15}\left(\frac{2\pi}{N_{ppw}}\right)^4$$

Phase Error Analysis VI

The leading order approximations of e_2 and e_4 are

$$e_2(N_{ppw},p) \approx \frac{\pi p}{3}\left(\frac{2\pi}{N_{ppw}}\right)^2, \quad e_4(N_{ppw},p) \approx \frac{\pi p}{15}\left(\frac{2\pi}{N_{ppw}}\right)^4$$

- The phase errors are proportional to the number of periods p.

To ensure a phase error, $e_p \leq \epsilon$, after p periods. Then, we obtain

$$\text{2nd-order: } N_{ppw} \geq 2\pi\sqrt{\frac{p\pi}{3\epsilon}}, \quad \text{4th-order: } N_{ppw} \geq 2\pi\sqrt[4]{\frac{p\pi}{15\epsilon}}$$

ϵ	2nd order	4th-order	6th-order
$10^{-1}(10\%)$	$N_{ppw} \geq 20\sqrt{p}$	$N_{ppw} \geq 7\sqrt[4]{p}$	$N_{ppw} \geq 6\sqrt[6]{p}$
$10^{-2}(1\%)$	$N_{ppw} \geq 64\sqrt{p}$	$N_{ppw} \geq 13\sqrt[4]{p}$	$N_{ppw} \geq 8\sqrt[6]{p}$
$10^{-5}(.001\%)$	$N_{ppw} \geq 643\sqrt{p}$	$N_{ppw} \geq 43\sqrt[4]{p}$	$N_{ppw} \geq 26\sqrt[6]{p}$

Long-Time Computations by High-Order Methods

Test problem:

$$\frac{\partial u(x,t)}{\partial t} + \frac{\partial u(x,t)}{\partial x} = 0,$$
$$u(x,0) = e^{\cos x}$$

Problem solved by Fourier, 4-th order, and 6-th order methods, in space, and 4-th order Runge-Kutta method in time.

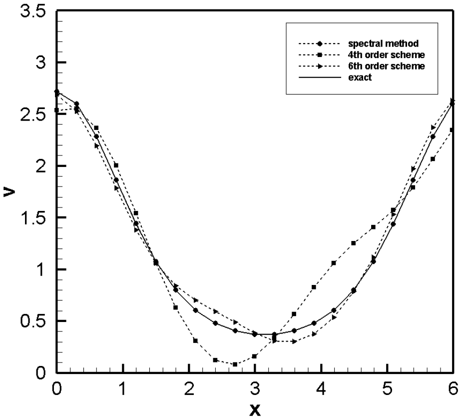


Figure: Numerical results obtained by different high-order methods after 100 periods, $N = 20$

Legendre Pseudospectral Method I

Concepts and Notations

- $P_N(x)$: Legendre polynomial of degree N.
- Legendre-Gauss-Lobatto (LGL) grid points x_i

$$-1 = x_0 < x_1 < x_2 < \cdots < x_{N-1} < x_N = 1, \quad \text{roots of } (1-x^2)P_N'(x)$$

- Lagrange interpolation polynomials:

$$l_j(x) = \frac{-(1-x^2)P_N'(x)}{N(N+1)(x-x_j)P_N(x_j)}, \quad l_j(x_i) = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

- Approximation of $u(x)$ defined on $[-1,1]$ and its derivative u':

$$u(x) \approx \mathcal{I}_N u(x) = \sum_{j=0}^{N} l_j(x) u(x_j), \quad u'(x) \approx \frac{d}{dx}\mathcal{I}_N u(x) = \sum_{j=0}^{N} l_j'(x) u(x_j)$$

- LGL quadrature integration rule:

$$\int_{-1}^{1} f(x)\,dx = \sum_{i=0}^{N} \omega_i f(x_i), \quad \omega_i\text{: quadrature weights}$$

provided that $f(x)$ is a polynomial of degree at most $2N-1$.

Legendre Pseudospectral Method II

Exponential Convergency

- Numerical derivatives at the LGL points:

$$u'(x_i) \approx \frac{d}{dx}\mathcal{I}_N u(x_i) = \sum_{j=0}^{N} l_j'(x_i)u(x_j)$$

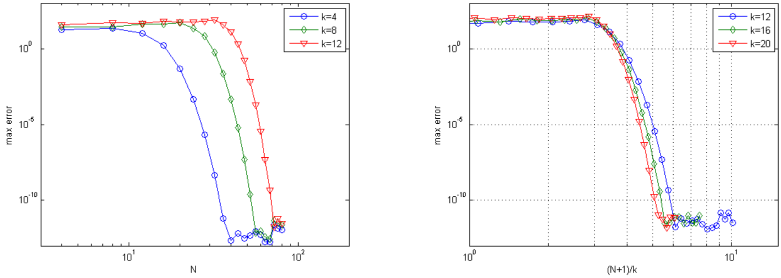


Figure: Errors of the numerical differentiation $u'(x_i) - \frac{d}{dx}\mathcal{I}_N u(x_i)$ for $u = \sin(k\pi x)$ for various values of k.

Model Wave Problem

Consider $u(x,t)$ satisfying the problem:

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} &= 0 \quad x \in [-1,1] \quad t \geq 0 \\ u(x,0) &= f(x) \quad x \in [-1,1] \quad t = 0 \\ u(-1,t) &= g(t) \quad x = -1 \quad t \geq 0. \end{aligned}$$

Define the energy-norm for u as

$$E(t) = \int_{-1}^{1} u^2(x,t)\, dx$$

Then we have

$$\begin{aligned} \frac{dE(t)}{dt} &= \frac{d}{dt}\int_{-1}^{1} u^2 dx = \int_{-1}^{1} 2u\frac{\partial u}{\partial t}\, dx = -\int_{-1}^{1} 2u\frac{\partial u}{\partial x}\, dx = -\int_{-1}^{1} \frac{\partial u^2}{\partial x}\, dx \\ &= -\, u^2\Big|_{-1}^{1} = u^2(-1,t) - u^2(1,t) = g^2(t) - u^2(1,t) \leq g^2(t) \end{aligned}$$

implying that

$$E(t) \leq E(0) + \int_0^t g^2(\xi)\, d\xi \leq E(0) + t \cdot G, \quad G = \max_{\xi \in [0,t]} g^2(\xi)$$

$$\Rightarrow \int_{-1}^{1} u^2(x,t) dx \leq \int_{-1}^{1} f^2(x) dx + t \cdot G$$

Legendre Pseudospectral Method III

Consider the problem:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \quad x \in [-1,1],\ t \geq 0$$
$$u(x,0) = f(x) \quad x \in [-1,1]$$
$$u(-1,t) = g(t) \quad t \geq 0$$

satisfying the energy estimate

$$\int_{-1}^{1} u^2(x,t)dx \leq \int_{-1}^{1} f^2(x)dx + t \cdot G$$

$$G = \max_{\xi \in [0,t]} g^2(\xi)$$

We seek a numerical solution of the form

$$v(x,t) = \sum_{j=0}^{N} l_j(x) v_j(t)$$

satisfying the equation

$$\frac{\partial v(x,t)}{\partial t} + \frac{\partial v(x,t)}{\partial x} = -\tau \cdot l_0(x) \cdot (v_0(t) - g(t)), \quad v(x_j,0) = f(x_j)$$

where the boundary condition is imposed weakly and τ is a parameter.

Legendre Pseudospectral Method IV

At the LGL grid points we have

$$\frac{\partial v(x_i,t)}{\partial t} + \frac{\partial v(x_i,t)}{\partial x} = -\tau\,\delta_{0i}\,(v_0 - g(t)), \quad \forall i = 0,1,2,\ldots,N$$

Observe that

1. as $\tau \to 0$

$$\frac{\partial v(x_0,t)}{\partial t} + \frac{\partial v(x_0,t)}{\partial x} = -\tau\,(v_0 - g(t)) \to 0 \quad \text{(mimicking PDE)}$$

2. as $\tau \to \infty$

$$v_0 - g(t) = \frac{-1}{\tau}\left(\frac{\partial v(x_0,t)}{\partial t} + \frac{\partial v(x_0,t)}{\partial x}\right) \to 0 \quad \text{(mimicking BC)}$$

Legendre Pseudospectral Method IV

Energy Estimate for Non-homogeneous Boundary Condition

We have the scheme:

$$\frac{\partial v(x_i,t)}{\partial t} + \frac{\partial v(x_i,t)}{\partial x} = -\tau\,\delta_{0i}\,(v_0 - g(t)), \quad \forall i = 0,1,2,\ldots,N$$

Define the discrete energy-norm as

$$E_D(t) = \sum_{i=0}^{N} v_j^2(t)\omega_i$$

We have the energy rate equation as

$$\begin{aligned}\frac{dE_D(t)}{dt} &= \sum_{i=0}^{N} 2v_i \frac{dv_i}{dt}\omega_i = -\sum_{i=0}^{N} 2v(x_i,t)\frac{\partial v(x_i,t)}{\partial x}\,\omega_i - \sum_{i=0}^{N} 2\tau\,\delta_{0i}\,\omega_i\,v_i\,(v_0 - g(t)) \\ &= \int_{-1}^{1} 2v(x,t)\frac{\partial v(x_i,t)}{\partial x}\,dx - 2\tau\omega_0 v_0(v_0 - g(t)) \\ &= -v(x,t)|_{-1}^{1} - 2\tau\omega_0 v_0(v_0 - g(t)) = -v_N^2 + v_0^2 - 2\tau\omega_0 v_0(v_0 - g(t))\end{aligned}$$

Legendre Pseudospectral Method IV

Energy Estimate for Non-homogeneous Boundary Condition

We obtain the energy rate equation as

$$\frac{dE_D(t)}{dt} = -v_N^2 + v_0^2 - 2\tau\omega_0 v_0(v_0 - g(t))$$

Taking $\tau = 1/\omega_0$ we obtain

$$\begin{aligned}\frac{dE_D(t)}{dt} &= -v_N^2 + v_0^2 - 2v_0^2 - 2v_0 g(t) - g^2(t) + g^2(t)\\ &= -v_N^2 - (v_0 - g(t))^2 + g^2(t) \leq g^2(t)\end{aligned}$$

implying

$$E_D(t) \leq E_D(0) + \int_0^t g^2(\xi)\, d\xi \leq E_D(0) + t\,G, \quad G = \max_{\xi\in[0,t]} g^2(\xi)$$

or equivalently,

$$\sum_{i=0}^{N} v_j^2(t)\omega_i \leq \sum_{i=0}^{N} f_j^2\omega_i + t\,G \quad \text{mimicking} \quad \int_{-1}^{1} u^2(x,t)dx \leq \int_{-1}^{1} f^2(x)dx + t\cdot G.$$

Convergence Test

Test example:
$u(x,t) = \sin(\pi(x-t))$
Legendre method in space
Runge-Kutta 4th order in time

N	Error	Order
8	5.3860e-03	7.37
12	7.7090e-06	16.15
16	2.4318e-06	4.01
20	9.9604e-07	4.00
24	4.8032e-07	4.00

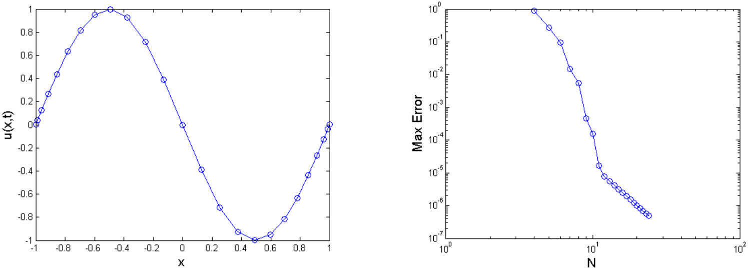


Figure: Left: Computed wave profile at time = 1.00. Right: Maximum errors $|u(x,t) - v_j(t)|$ for different values of N at time = 1.00.

References

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