Third part: finite difference schemes and numerical dispersion

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BCAM and UPV/EHU courses 2011-2012:
Advanced aspects in applied mathematics
Topics on numerics for wave propagation

Linear transport equation

The simplest model for the wave propagation is the linear transport equation:

$$u_t + u_x = 0,\ x \in \mathbb{R}, t > 0, \quad u(x,0) = f(x). \tag{1}$$

$u = u(x,t)$ is a solution of (1) iff u is constant along the characteristic lines $x + t =$ constant.

The solution of (1) is $u(x,t) = f(x-t)$.

Semigroup theory for the transport equation (1). The Hilbert space $H := L^2(\mathbb{R})$, the operator $A := -\partial_x$ and its domain $D(A) := H^1(\mathbb{R})$.

- A is dissipative. $< Au, u >_{L^2(\mathbb{R})} = -\int_{\mathbb{R}} \partial_x u u \, dx = -\frac{1}{2} \int_{\mathbb{R}} \partial_x (u^2) \, dx = 0$.
- A is maximal. For any $f \in L^2(\mathbb{R})$, there exists an unique solution $u \in H^1(\mathbb{R})$ of the equation $u + \partial_x u = f$, which can be explicitly computed as

$$u(x) = \int_{-\infty}^{x} f(s) \exp(s-x) \, ds = \int_{-\infty}^{0} f(z+x) \exp(z) \, dz.$$

By the Minkowski inequality $\Rightarrow u \in L^2(\mathbb{R})$:

$$||u||_{L^2(\mathbb{R})} \leq \int_{-\infty}^{0} ||f||_{L^2(\mathbb{R})} \exp(z) \, dz = ||f||_{L^2(\mathbb{R})}.$$

$u_x = f - u \in L^2(\mathbb{R}) \Rightarrow u \in H^1(\mathbb{R})$.

Transport equation with reversed sign,

$$u_t - u_x = 0,\ x \in \mathbb{R}, t > 0, \quad u(x,0) = g(x). \tag{2}$$

The solution of (2) is $u(x,t) = g(x+t)$.

Three semi-discrete finite difference approximations of $u_t + u_x = 0$

$$\text{forward} \quad u_j'(t) + \frac{u_{j+1}(t) - u_j(t)}{h} = 0, \quad \text{centered} \quad u_j'(t) + \frac{u_{j+1}(t) - u_{j-1}(t)}{2h} = 0,$$
$$\text{backward} \quad u_j'(t) + \frac{u_j(t) - u_{j-1}(t)}{h} = 0. \tag{3}$$

Briefly, forward/centered/backward:

$$\mathbf{u}_h'(t) = A_h \mathbf{u}_h(t).$$

$$A_h = \begin{pmatrix} \ddots & \cdots & \cdots & \cdots & \cdots \\ 0 & 1/h & -1/h & 0 & \cdots \\ \ddots & \ddots & \ddots & \vdots & \vdots \\ \cdots & 0 & 0 & 1/h & -1/h \\ \cdots & \cdots & \cdots & \cdots & \ddots \end{pmatrix}$$

$$A_h = \begin{pmatrix} \ddots & \cdots & \cdots & \cdots & \cdots \\ -1/2h & 0 & 1/2h & 0 & \cdots \\ \ddots & \ddots & \ddots & \vdots & \vdots \\ \cdots & 0 & -1/2h & 0 & -1/2h \\ \cdots & \cdots & \cdots & \cdots & \ddots \end{pmatrix} \qquad A_h = \begin{pmatrix} \ddots & \cdots & \cdots & \cdots & \cdots \\ 1/h & -1/h & 0 & 0 & \cdots \\ \ddots & \ddots & \ddots & \vdots & \vdots \\ \cdots & 0 & 1/h & -1/h & 0 \\ \cdots & \cdots & \cdots & \cdots & \ddots \end{pmatrix}$$

Peter Lax convergence results

Peter Lax's equivalence theorem: CONVERGENCE⇔CONSISTENCY+STABILITY.

CONSISTENCY=insert a smooth solution of the continuous model in the discrete one + Taylor expansions.

STABILITY = von Neumann analysis.

Semi-discrete Fourier transform at scale h: $\widehat{u}^h(\xi,t) = h\sum_{j\in\mathbb{Z}} u_j(t)\exp(-ix_j\xi), \quad \xi\in[-\pi/h,\pi/h].$

All the three schemes can be transformed into the first-order differential equation

$$\widehat{u}^h_t(\xi,t) = \widehat{p}^h(\xi)\widehat{u}^h(\xi,t), \quad \widehat{u}^h(\xi,0) = \widehat{u}^{h,0}(\xi)$$

whose solution is

$$\widehat{u}^h(\xi,t) = \widehat{u}^{h,0}(\xi)\exp(\widehat{p}^h(\xi)t).$$

Here, $$\widehat{p}^h(\xi) = \begin{cases} \frac{1-\exp(i\xi h)}{h}, & \text{forward scheme} \\ -\frac{i\sin(\xi h)}{h}, & \text{centered scheme} \\ \frac{\exp(-i\xi h)-1}{h}, & \text{backward scheme.} \end{cases}$$

Properties of the semi-discrete Fourier transform (SDFT)

Definition

Consider a sequence $\mathbf{f}^h := (f_j)_{j\in\mathbb{Z}} \in \ell^2_h$ related to a grid of size h (i.e. $f_j = f(x_j)$), its semi-discrete Fourier transform at scale h is $\widehat{f}^h(\xi) := h\sum_{j\in\mathbb{Z}} f_j \exp(-i\xi x_j)$, with $\xi \in [-\pi/h, \pi/h]$.

Inverse Fourier transform: $f_j = \frac{1}{2\pi}\int_{-\pi/h}^{\pi/h} \widehat{f}^h(\xi)\exp(i\xi x_j)\, d\xi$.

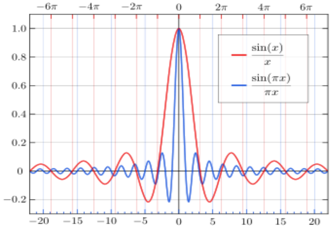
Remark

- Continuous Fourier transform: function $f(x)$, $x \in \mathbb{R}$, transformed into function $\widehat{f}(\xi)$, $\xi \in \mathbb{R}$.
- Semi-discrete Fourier transform: sequence $\mathbf{f}^h := (f_j)_{j\in\mathbb{Z}}$ transformed into function $\widehat{f}^h(\xi)$, $\xi \in [-\pi/h, \pi/h]$.

Parseval identity: $||\mathbf{f}^h||^2_{\ell^2_h} := h\sum_{j\in\mathbb{Z}} |f_j|^2 = \frac{1}{2\pi}||\widehat{f}^h||^2_{L^2(-\pi/h,\pi/h)} := \frac{1}{2\pi}\int_{-\pi/h}^{\pi/h} |\widehat{f}^h(\xi)|^2\, d\xi$.

Shannon sinc function: $\psi_0(x) = \frac{\sin(\pi x/h)}{\pi x/h}$, which is globally analytic and $\psi_0(0) = 1$.

Properties of the semi-discrete Fourier transform (SDFT)



The sinc function is a particular case of function f in the Paley-Wiener theorem:

Theorem (Paley-Wiener, see Rudin, Real and complex analysis)

If $A, C > 0$ and $f \in L^2(\mathbb{C})$ is an entire function s.t. $|f(z)| \leq C \exp(A|z|)$ (exponential growth at most A), for all $z \in \mathbb{C}$, then the Fourier transform $\widehat{f}$ of f has compact support in $[-A, A]$.

Exercise: $\psi_0 \in L^2(\mathbb{R})$ and $\widehat{\psi}_0(\xi) = h\chi_{(-\pi/h,\pi/h)}(\xi)$, with χ_S the characteristic function of set S.

Definition

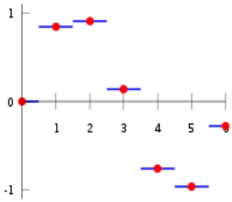
Set $\psi_j(x) = \psi_0(x - x_j)$ and the sequence $\mathbf{f}^h := (f_j)_{j\in\mathbb{Z}} \in \ell^2_h$. The continuous function $f^*(x) := \sum_{j\in\mathbb{Z}} f_j\psi_j(x)$ is called the sinc interpolation of $\mathbf{f}^h$.

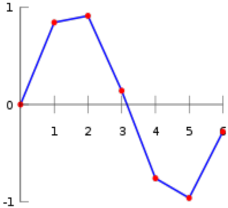
Important properties of the sinc interpolation (exercise): $\widehat{f^*}(\xi) = \widehat{f}^h(\xi)$ and $||f^*||_{L^2(\mathbb{R})} = ||\mathbf{f}||_{\ell^2_h}$.

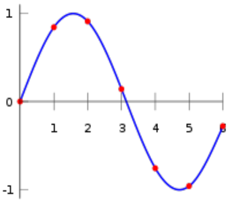
Other possible interpolations

- piecewise constant, using functions $\psi_j^0(x) := \chi_{[x_{j-1/2}, x_{j+1/2}]}$: $f^0(x) = \sum_{j\in\mathbb{Z}} f_j \psi_j^0(x)$.
- piecewise linear and continuous, using functions $\psi_j^1(x) := (\psi_j^0 * \psi_j^0)(x)$: $f^1(x) = \sum_{j\in\mathbb{Z}} f_j \psi_j^1(x)$.
- spline interpolation, using functions $\psi_j^m(x) = (\psi_j^0 * \cdots * \psi_j^0)(x)$ (m successive convolutions): $f^m(x) = \sum_{j\in\mathbb{Z}} f_j \psi_j^m(x)$.

$$||f^0||_{L^2(\mathbb{R})} = ||\mathbf{f}^h||_{\ell_h^2} \text{ and } \frac{1}{\sqrt{3}}||\mathbf{f}^h||_{\ell_h^2} \leq ||f^1||_{L^2(\mathbb{R})} \leq ||\mathbf{f}^h||_{\ell_h^2}.$$







Observation

- ψ_0^0 and ψ_0^1 have compact support, but their Fourier transforms $\widehat{\psi_0^0}(\xi) = h\mathrm{sinc}(\xi h/2)$ and $\widehat{\psi_0^1}(\xi) = (\widehat{\psi_0^0}(\xi))^2$ are spread.
- ψ_0 is spread, but its Fourier transform $\widehat{\psi_0}(\xi) = h\chi_{(-\pi/h,\pi/h)}(\xi)$ has compact support.

Cf. Heisenberg Uncertainty Principle, is not possible both f and its Fourier transform $\widehat{f}$ to have compact support:

Theorem (Heisenberg Uncertainty Principle, Stein & Shakarchi, Fourier analysis - an introduction)

Let $f \in \mathcal{S}(\mathbb{R})$, $||f||_{L^2(\mathbb{R})} = 1$. Then

$$\left(\int_{\mathbb{R}} |x|^2 |f(x)|^2\, dx\right)\left(\int_{\mathbb{R}} |\xi|^2 |\widehat{f}(\xi)|^2\, d\xi\right) \geq \frac{1}{16\pi^2},$$

with equality iff $f(x) = A\exp(-B|x|^2)$, $B > 0$ and $A^2 = \sqrt{2B/\pi}$. In fact, for all $x^0, \xi^0 \in \mathbb{R}$, $\Rightarrow$

$$\left(\int_{\mathbb{R}} |x - x^0|^2 |f(x)|^2\, dx\right)\left(\int_{\mathbb{R}} |\xi - \xi^0|^2 |\widehat{f}(\xi)|^2\, d\xi\right) \geq \frac{1}{16\pi^2}.$$

Interpretation in quantum mechanics. The more certain we are about the location of a particle, the less certain we can be about its momentum and vice versa.

Back to stabilization of numerical schemes...

Set $\widehat{p}^h_* = \max_{\xi \in [-\pi/h, \pi/h]} \mathrm{Re}(\widehat{p}^h(\xi))$. Using Parseval identity for the SDFT,

$$||\mathbf{u}^h(t)||^2_{\ell^2_h} = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} |\widehat{u}^{h,0}(\xi)|^2 \exp(2t\mathrm{Re}(\widehat{p}^h(\xi)))\, d\xi$$

$$\leq \exp(2t\widehat{p}^h_*) \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} |\widehat{u}^{h,0}(\xi)|^2\, d\xi = \exp(2t\widehat{p}^h_*) ||\mathbf{u}^{h,0}||^2_{\ell^2_h}.$$

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Numerical schemes (3) are stable iff $\widehat{p}^h_* \leq 0$. Otherwise $\widehat{p}^h_* \sim 1/h$ and $\exp(2t\widehat{p}^h_*) \to \infty$ as $h \to 0$.

- FORWARD: $\mathrm{Re}(\widehat{p}^h(\xi)) = 2\sin^2(\xi h/2)/h \geq 0$, $\forall \xi \in [-\pi/h, \pi/h]$, and $\widehat{p}^h_* = 2/h \Rightarrow$ UNSTABLE!!!.
- CENTERED: $\mathrm{Re}(\widehat{p}^h(\xi)) = 0$, $\forall \xi \in [-\pi/h, \pi/h]$, and $\widehat{p}^h_* = 0 \Rightarrow$ STABLE.
- BACKWARD: $\mathrm{Re}(\widehat{p}^h(\xi)) = -2\sin^2(\xi h/2)/h \leq 0$, $\forall \xi \in [-\pi/h, \pi/h]$, and $\widehat{p}^h_* = 0 \Rightarrow$ STABLE.

NECESSARY GEOMETRIC CONDITION FOR THE CONVERGENCE OF A NUMERICAL SCHEME: The domain of dependence of the numerical scheme MUST CONTAIN the domain of dependence of the continuous model.

Domains of dependence at a point (x_j, t):

- Continuous transport: the segment joining (x_j, t) with $(x_j - t, 0)$.
- Forward scheme: the semi-strip TO THE RIGHT of $x = x_j$ delimited by the times 0 and t.
- Centered scheme: the band delimited by the times 0 and t.
- Backward scheme: the semi-strip to the left of $x = x_j$ delimited by the times 0 and t.

Error estimates

Consistency errors: Consider u a smooth solution of the transport equation $u_t(x,t)+u_x(x,t)=0$, $u(x,0)=f(x)$, $x\in\mathbb{R}$. Then, by plugging u in the numerical scheme and using Taylor expansions, we obtain:

backward scheme:
$$u_t(x_j,t)+\frac{u(x_j,t)-u(x_{j-1},t)}{h}=\underbrace{u_t(x_j,t)+u_x(x_j,t)}_{=0,\ u \text{ solves } u_t+u_x=0}$$
$$-\frac{h}{2}u_{xx}(x'_{j-1/2},t):=O_j(t),\quad x'_{j-1/2}\in(x_{j-1},x$$

centered scheme:
$$u_t(x_j,t)+\frac{u(x_{j+1},t)-u(x_{j-1},t)}{2h}=\underbrace{u_t(x_j,t)+u_x(x_j,t)}_{=0,\ u \text{ solves } u_t+u_x=0}$$
$$+\frac{h^2}{12}(u_{xxx}(x'_{j-1/2},t)+u_{xxx}(x'_{j+1/2},t)),\quad x'_{j\pm1/2}\in(x_{j-1/2\pm1/2},x_{j+1/2\pm1/2}).$$

Set the error $\epsilon_j(t):=u_j(t)-u(x_j,t)$, where $u_j(t)$ is the solution of the backward scheme with data $u_j(0)=f(x_j)$. Then $\epsilon_j(t)$ solves the problem

$$\epsilon'_j(t)+\frac{\epsilon_j(t)-\epsilon_{j-1}(t)}{h}=-O_j(t),\quad \epsilon_j(0)=0. \tag{4}$$

Error estimates

ENERGY METHOD. Multiply (4) by $h\epsilon_j(t)$ and add in $j \in \mathbb{Z}$:

$$\frac{1}{2}\frac{d}{dt}\Big[h\sum_{j\in\mathbb{Z}}|\epsilon_j(t)|^2\Big] + \underbrace{\sum_{j\in\mathbb{Z}}(\epsilon_j^2(t) - \epsilon_j(t)\epsilon_{j-1}(t))}_{=\frac{1}{2}\sum_{j\in\mathbb{Z}}(\epsilon_j(t)-\epsilon_{j-1}(t))^2\geq 0} = h\sum_{j\in\mathbb{Z}} O_j(t)\epsilon_j(t). \tag{5}$$

$||\boldsymbol{\epsilon}^h(t)||^2_{\ell^2_h} := h\sum_{j\in\mathbb{Z}}|\epsilon_j(t)|^2$. By Cauchy-Schwarz inequality in (5) $\Rightarrow$ $\frac{1}{2}\frac{d}{dt}||\boldsymbol{\epsilon}^h(t)||^2_{\ell^2_h} \leq ||\mathbf{O}^h(t)||_{\ell^2_h}||\boldsymbol{\epsilon}^h(t)||_{\ell^2_h}$,

so that $\frac{d}{dt}||\boldsymbol{\epsilon}^h(t)||_{\ell^2_h} \leq ||\mathbf{O}^h(t)||_{\ell^2_h}$ and, since $||\boldsymbol{\epsilon}^h(0)||_{\ell^2_h} = 0$, $||\boldsymbol{\epsilon}^h(t)||_{\ell^2_h} \leq \int_0^t ||\mathbf{O}^h(s)||_{\ell^2_h}\, ds$.

Assume $f \in C^2_c(\mathbb{R})$. Then $|O_j(t)| = h|f''(x'_{j-1/2} - t)|/2$ and

$$||\mathbf{O}^h(s)||^2_{\ell^2_h} = \frac{h^3}{4}\sum_{j\in\mathbb{Z}}|f''(x'_{j-1/2} - s)|^2 = \frac{h^3}{4}\sum_{j\in\mathbb{Z}\text{ s.t. } x'_{j-1/2}-s\in \mathrm{Supp} f''}|f''(x'_{j-1/2} - s)|^2$$

$$\leq \frac{h^3}{4}\frac{|\mathrm{Supp}(f'')|}{h}||f''||^2_{L^\infty(\mathbb{R})} = \frac{h^2}{4}|\mathrm{Supp}(f'')|||f''||^2_{L^\infty(\mathbb{R})}.$$

Theorem

For any initial data $f \in C^2_c(\mathbb{R})$ in the transport equation, the backward semi-discrete scheme with initial data $u_j(0) = f(x_j)$ is convergent of order h in ℓ^2_h and the error $\epsilon_j(t) = u_j(t) - u(x_j, t)$ satisfies the estimate

$$||\boldsymbol{\epsilon}^h(t)||_{\ell^2_h} \leq \frac{ht}{2}||f''||_{L^\infty(\mathbb{R})}\sqrt{|Supp(f'')|}, \quad \forall t \geq 0,\ \forall h > 0.$$

More about the energy method

The $||\cdot||_{L^2(\mathbb{R})}$-norm of the solution for the continuous transport equation $u_t + u_x = 0$ is conserved in time. Conservation law of the energy:

$$\frac{d}{dt}||u(\cdot,t)||^2_{L^2(\mathbb{R})} = 0.$$

The centered semi-discrete scheme is also conservative:

$$\frac{d}{dt}||\mathbf{u}^h(t)||^2_{\ell^2_h} = 0.$$

The backward semi-discrete scheme is dissipative since the energy decreases in time:

$$\frac{d}{dt}||\mathbf{u}^h(t)||^2_{\ell^2_h} + h||\partial^{h,-}\mathbf{u}^h(t)||^2_{\ell^2_h} = 0, \quad \text{where } \partial^{h,-}f_j := \frac{f_j - f_{j-1}}{h}.$$

The forward semi-discrete scheme is anti-dissipative since the energy increases in time:

$$\frac{d}{dt}||\mathbf{u}^h(t)||^2_{\ell^2_h} - h||\partial^{h,+}\mathbf{u}^h(t)||^2_{\ell^2_h} = 0, \quad \text{where } \partial^{h,+}f_j := \frac{f_{j+1} - f_j}{h}.$$

Fully discrete schemes for the transport equation

Leap-frog scheme: $$\frac{u_j^{k+1}-u_j^{k-1}}{2dt}+\frac{u_{j+1}^k-u_{j-1}^k}{2dx}=0.$$

Consistency $\Rightarrow$ exercise

Stability $\Rightarrow$ von Neumann method. Set $\widehat{u}^{h,k}(\xi)$ - the semi-discrete Fourier transform at scale h of the solution at time t^k, $(u_j^k)_j$ and $\mu := dt/dx$ - the Courant number. The sequence $(\widehat{u}^{h,k}(\xi))_k$ verifies the second-order recurrence:

$$\widehat{u}^{h,k+1}(\xi)+2i\mu\sin(\xi h)\widehat{u}^{h,k}(\xi)-\widehat{u}^{h,k-1}(\xi)=0.$$

The two roots of the characteristic polynomial are:

$$\lambda_\pm(\xi)=-i\mu\sin(\xi h)\pm\sqrt{1-\mu^2\sin^2(\xi h)}.$$

- When $\mu<1$, $1-\mu^2\sin^2(\xi h)>0$ for all ξ, so that $\lambda_\pm(\xi)\in\mathbb{C}$ of the same imaginary part and of opposite real parts. Also $|\lambda_\pm(\xi)|^2=\mu^2\sin^2(\xi h)+1-\mu^2\sin^2(\xi h)=1$. The stability is guaranteed by the fact that both roots $\lambda_\pm(\xi)$ are simple and of modulus 1, for any ξ.
- When $\mu=1$, $1-\mu^2\sin^2(\xi h)>0$, excepting the case $\xi h=\pi/2$ and $\xi h=3\pi/2$, for which there is a double root of unit modulus $\Rightarrow$ INSTABILITY.
- When $\mu>1$, there exists $\xi_\mu\in(0,2\pi/h)$ s.t. $1-\mu^2\sin^2(\xi h)>0$ for all $\xi\in(0,\xi_\mu)$ and $1-\mu^2\sin^2(\xi h)\le 0$ for all $\xi\in[\xi_\mu,2\pi)$. In this last case, the method is UNSTABLE:

$$\lambda_\pm(\xi)=-i(\mu\sin(\xi h)\mp\sqrt{\mu^2\sin^2(\xi h)-1})\text{ and }|\lambda_-(\xi)|=\mu\sin(\xi h)+\sqrt{\mu^2\sin^2(\xi h)-1}>1.$$

Fully discrete schemes for the transport equation

backward Euler EXPLICIT: $$\frac{u_j^{k+1}-u_j^k}{dt}+\frac{u_j^k-u_{j-1}^k}{dx}=0.$$

Stability $\Rightarrow$ von Neumann method. The sequence $(\widehat{u}^{h,k}(\xi))_k$ verifies the first-order recurrence:

$$\widehat{u}^{h,k+1}(\xi)=[1+\mu(\exp(i\xi h)-1)]\widehat{u}^{h,k}(\xi).$$

For the stability is sufficient to guarantee that $|1+\mu(\exp(i\xi h)-1)|\leq 1$:

$$|1+\mu(\exp(i\xi h)-1)|^2=(1+\mu(\cos(\xi h)-1))^2+\mu^2\sin^2(\xi h)=1+2\mu(\mu-1)(1-\cos(\xi h))\leq 1 \text{ iff } \mu\leq 1.$$

backward Euler IMPLICIT: $$\frac{u_j^{k+1}-u_j^k}{dt}+\frac{u_j^{k+1}-u_{j-1}^{k+1}}{dx}=0.$$

Stability $\Rightarrow$ von Neumann method. The sequence $(\widehat{u}^{h,k}(\xi))_k$ verifies the first-order recurrence:

$$\widehat{u}^{h,k+1}(\xi)=\frac{1}{1+\mu(1-\exp(i\xi h))}\widehat{u}^{h,k}(\xi).$$

For the stability is sufficient to guarantee that $|1+\mu(1-\exp(i\xi h))|\geq 1$:

$$|1+\mu(1-\exp(i\xi h))|^2=(1+\mu(1-\cos(\xi h)))^2+\mu^2\sin^2(\xi h)=1+2\mu(\mu+1)(1-\cos(\xi h))\geq 1, \quad \forall\mu>0$$

UNCONDITIONAL STABILITY $\Leftrightarrow$ NO CONDITION on μ to guarantee stability.

Fully discrete schemes for the transport equation

Theorem

If $|\widehat{u}^{h,k+1}(\xi,t)| \leq |\widehat{u}^{h,k}(\xi)|$ *for all* $\xi \in [-\pi/h, \pi/h] \Rightarrow ||\mathbf{u}^{h,k+1}||_{\ell_h^2} \leq ||\mathbf{u}^{h,k}||_{\ell_h^2}$.

Proof: Parseval identity for the SDFT.

Other fully discrete schemes for the transport equation:

- Crank-Nicolson, inspired from the trapezoidal rule for solving ODEs, is unconditionally stable and of second-order in both time and space:

$$\frac{u_j^{k+1}-u_j^k}{dt}+\frac{1}{2}\Big[\frac{u_{j+1}^{k+1}-u_{j-1}^{k+1}}{2dx}+\frac{u_{j+1}^k-u_{j-1}^k}{2dx}\Big]=0.$$

- Lax-Wendroff, of second-order, conservative, stable iff $\mu \leq 1$ (exercise)

$$\frac{u_j^{k+1}-u_j^k}{dt}+\frac{u_{j+1}^k-u_{j-1}^k}{2dx}-\frac{dt}{2}\frac{u_{j+1}^k-2u_j^k+u_{j-1}^k}{dx^2}=0$$

- Lax-Friedrichs, of first-order, stable iff $\mu \leq 1$ (exercise)

$$\frac{u_j^{k+1}-\frac{1}{2}(u_{j+1}^k+u_{j-1}^k)}{dt}+\frac{u_{j+1}^k-u_{j-1}^k}{2dx}=0.$$

Definition (A-stability, cf. Iserles, A first course on numerical analysis of ODEs)

A numerical method is A-stable if it preserves the behaviour of the continuous solution as $t \to \infty$.

Numerical approximations for the wave equation

- The finite difference space semi-discretization: $u_j'' - \frac{u_{j+1}-2u_j+u_{j-1}}{h^2} = 0.$
- The explicit leapfrog fully discrete finite difference scheme is stable for $\mu = dt/dx \leq 1$:
$\frac{u_j^{k+1}-2u_j^k+u_j^{k-1}}{dt^2} - \frac{u_{j+1}^k-2u_j^k+u_{j-1}^k}{dx^2} = 0.$
- The implicit leapfrog fully discrete finite difference scheme is unconditionally stable:
$\frac{u_j^{k+1}-2u_j^k+u_j^{k-1}}{dt^2} - \frac{u_{j+1}^{k+1}-2u_j^{k+1}+u_{j-1}^{k+1}}{dx^2} = 0.$
- The implicit midpoint scheme is unconditionally stable:
$\frac{u_j^{k+1}-2u_j^k+u_j^{k-1}}{dt^2} - 0.5\frac{u_{j+1}^{k+1}-2u_j^{k+1}+u_{j-1}^{k+1}}{dx^2} - 0.5\frac{u_{j+1}^{k-1}-2u_j^{k-1}+u_{j-1}^{k-1}}{dx^2} = 0.$
- The finite element semi-discretization. Find
$u^h(x,t) = \sum_{j=1}^{N} u_j(t)\phi_j(x) \in V^h := \text{span}\{\phi_1, \cdots, \phi_N\}$ s.t.

  $$\frac{d^2}{dt^2}\int_0^1 u^h(x,t)\phi(x)\,dx + \int_0^1 u^h_x(x,t)\phi_x(x)\,dx = 0, \quad \forall \phi \in V^h.$$

  Here $\phi_j(x) = \begin{cases} \frac{x-x_{j-1}}{h}, & x \in (x_{j-1}, x_j) \\ \frac{x_{j+1}-x}{h}, & x \in (x_j, x_{j+1}), \\ 0, & \text{otherwise.} \end{cases}$, Then $(u_j(t))_j$ satisfies the system:

  $\frac{h}{6}u_{j+1}''(t) + \frac{2h}{3}u_j''(t) + \frac{h}{6}u_{j-1}''(t) - \frac{u_{j+1}(t)-2u_j(t)+u_{j-1}(t)}{h} = 0.$
- Finite difference semi-discretization of the $2-d$ wave equation:
$u_{j,k}''(t) - \frac{u_{j+1,k}(t)-2u_{j,k}(t)+u_{j-1,k}(t)}{h_x^2} - \frac{u_{j,k+1}(t)-2u_{j,k}(t)+u_{j,k-1}(t)}{h_y^2} = 0.$

Numerical dissipation and dispersion

Trefethen [6]: Finite difference approximations have more complicated physics than the equations they are designed to simulate. They are used not because the numbers they generate have simpler properties, but because those numbers are simpler to compute.

Plane wave solutions: $u(x,t) = \exp(i(\xi x + t\omega))$, where ξ is the wave number and ω is the frequency.

The PDE or the numerical scheme imposes a relationship between ω and ξ, $\omega = \omega(\xi)$, called dispersion relation.

Examples:

- Transport equation $u_t + u_x = 0 \Rightarrow \omega(\xi) = -\xi$
- Wave equation $u_{tt} - u_{xx} = 0 \Rightarrow \omega(\xi) = \pm\xi$
- Schrödinger equation $iu_t + u_{xx} = 0 \Rightarrow \omega(\xi) = -\xi^2$.
- Centered finite difference semi-discretization for the transport equation $u_j' + (u_{j+1} - u_{j-1})/2h = 0 \Rightarrow \omega_h(\xi) = -\sin(\xi h)/h$
- Finite difference semi-discretization of the wave equation $u_j'' - (u_{j+1} - 2u_j + u_{j-1})/h^2 = 0$ $\Rightarrow \omega_h(\xi) = \pm 2\sin(\xi h/2)/h$.
- Finite difference semi-discretization of the Schrödinger equation $iu_j' + (u_{j+1} - 2u_j + u_{j-1})/h^2 = 0 \Rightarrow \omega_h(\xi) = -4\sin^2(\xi h/2)/h^2$.

Dispersion relations for fully discrete schemes for the transport equation

- Leap-frog: $\sin(dt\omega_h(\xi)) + \mu \sin(dx\xi) = 0$, $\mu = dt/dx$, $h = dx$.
- Backward explicit Euler: $\exp(idt\omega_h(\xi)) - 1 + \mu(1 - \exp(-i\xi dx)) = 0$
- Backward implicit Euler: $1 - \exp(-idt\omega_h(\xi)) + \mu(1 - \exp(-i\xi dx)) = 0$
- Crank-Nicolson: $2\tan(dt\omega_h(\xi)/2) + \mu \sin(dx\xi) = 0$
- Lax-Wendroff: $\exp(idt\omega_h(\xi)) - 1 + i\mu \sin(dx\xi) + 2\mu^2 \sin^2(dx\xi/2) = 0$
- Lax-Friedrich: $\exp(idt\omega_h(\xi)) - \cos(dx\xi) + i\mu \sin(dx\xi) = 0$.

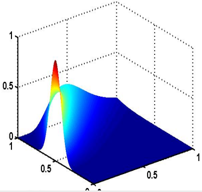
Definition

A finite difference scheme is dissipative of order $2r$ if the dispersion relation satisfies $\mathrm{Im}(\omega_h(\xi)dt) \geq \gamma|\xi dx|^{2r}$, for all $\xi \in [-\pi/dx, \pi/dx]$, $\gamma > 0$. A finite difference scheme is non-dissipative if $\mathrm{Im}(\omega_h(\xi)) = 0$.

Example non-dissipative schemes: leap-frog, Crank-Nicolson

Example dissipative schemes: Lax-Wendroff, backward explicit Euler, Lax-Friedrich (in figure)...

Effect of dissipation: The amplitude of the numerical solution decays in time.



Group velocity, phase velocity

Wave packet:

$$u(x,t) = \int_{\mathbb{R}} \widehat{\phi}(\xi) \exp(it\omega(\xi) + i\xi x)\, d\xi.$$

Data concentrated around $x = 0$ and oscillating at frequency ξ^0: $\phi(x) = \psi(x)\exp(i\xi^0 x)$.

Example - finite difference semi-discretization:
$\omega = \omega_h(\xi) = 2\sin(\xi h/2)/h \sim \omega_h(\xi^0) + (\xi - \xi^0)\omega_h'(\xi^0) \Rightarrow$

$$u(x,t) \sim \exp(i\xi^0(x + t\omega_h(\xi^0)/\xi^0))\psi(x + t\omega_h'(\xi^0)).$$

- Phase velocity: $\omega_h(\xi^0)/\xi^0$ - the velocity of propagation for the oscillation
- Group velocity: $\omega_h'(\xi^0)$ - the velocity of propagation for the envelope ψ.

Geometric Optics

Light has a dual nature: is particle (photon) and is wave (and oscillates at a certain wavelength).

Geometric Optics (GO) studies the propagation of light particles along trajectories called rays.

Hamilton principle states that the trajectory of a particle between times t_1 and t_2 minimizes the action $\int_{t_1}^{t_2} L(q, q', t)\, dt$, where $L = T - V$ is the difference between kinetic and potential energies, q is the vector of generalized coordinates and $q' = \partial_t q$.

Hamiltonian system associated to $H = H(p, q)$: $p'(s) = \nabla_q H(p(s), q(s))$,
$q'(s) = -\nabla_p H(p(s), q(s))$.

For the continuous wave equation, $H = H(x, t, \xi, \tau) = \tau^2 - |\xi|^2$ and the rays of GO verify the Hamiltonian system:
$x'(s) = \nabla_\xi H(x(s), t(s), \xi(s), \tau(s)) = -2\xi(s)$, $t'(s) = \partial_\tau H(x(s), t(s), \xi(s), \tau(s)) = 2\tau(s)$
$\xi'(s) = -\nabla_x H(x(s), t(s), \xi(s), \tau(s)) = 0 \Rightarrow \xi(s) = \xi^0$, $\tau'(s) = -\nabla_t H(x(s), t(s), \xi(s), \tau(s)) = 0$
$\Rightarrow \tau(s) = \tau^0$.

Null-bi-characteristics. $H(x(0), t(0), \xi(0), \tau(0)) = 0$. Then $H(x(s), t(s), \xi(s), \tau(s)) = 0\ \forall s > 0$.

Characteristics. Replace s by t in the Hamiltonian system. Since $H(x(0), 0, \xi(0), \tau(0)) = 0$ has two roots as equation in τ^0, $\tau^0 = \pm|\xi^0|$, then $x'(t) = \pm\xi^0/|\xi^0| \Rightarrow$ two characteristics:
$x(t) = x^0 \pm t\xi^0/|\xi^0|$. They propagate at unit velocity.

For the finite difference semi-discretization of the wave equation, the Hamiltonian is
$H(x, t, \xi, \tau) = \tau^2 - 4\sin^2(\xi h)/h^2$ and the characteristics propagate with the group velocity, i.e.
$x(t) = x^0 \pm t\cos(\xi^0 h/2)$ (exercise).

Some related bibliography

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