CS520: Variable coefficients and nonlinear problems (Ch. 5)

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Outline

- Freezing coefficients and dissipativity
- Schemes for hyperbolic systems in 1D
- Discontinuous solutions (Ch. 10)
- Semi-Lagrangian methods
- Nonlinear stability and energy method

Freezing coefficients

- Consider linear problems with variable coefficients, and nonlinear problems.
- Example: advection equations

$$u_t + a(x)u_x = 0, \quad \text{and } u_t + a(u)u_x = 0.$$

- To check stability, a common approach is to **freeze coefficients**: Check stability by Fourier analysis for a linearized version with constant coefficients. Based on this, choose a time step k (conservatively).

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Freezing coefficients cont.

- For the variable coefficients advection example, for a typical CFL condition, set
$$\hat{a} = \max_x |a(x)|$$
and require $\mu\hat{a} < 1$, i.e., $k < h\hat{a}$.
- For the nonlinear advection example, it's a bit trickier:
  - either use a known bound $\hat{a} \geq \max_{t,x} |a(u(t,x))|$,
  - or, at each time step n use $\hat{a} = \hat{a}_n = \max_j |a(v_j^n))|$. Then $k = k_n < h\hat{a}_n$.
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Example: Korteweg - de Vries (KdV)

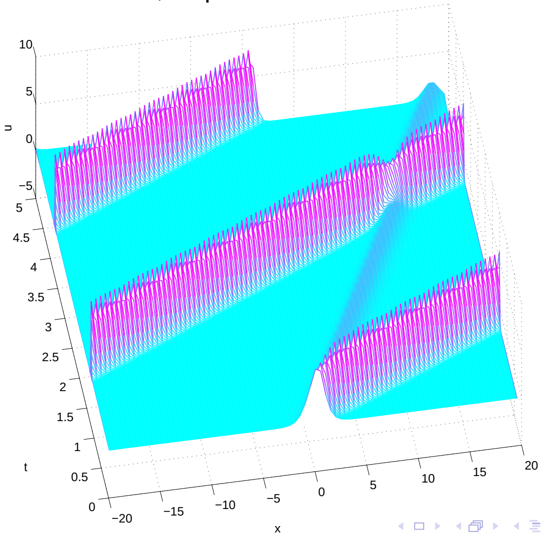
- A famous PDE: nonlinear, third derivative in x, admits soliton solutions:

$$\begin{aligned} u_t &= \alpha(u^2)_x + \rho u_x + \nu u_{xxx} \\ &= [V'(u)]_x + \nu u_{xxx}, \quad V(u) = \frac{\alpha}{3}u^3 + \frac{\rho}{2}u^2. \end{aligned}$$

- Initial conditions $u(0,x) = u_0(x)$
- Boundary conditions: periodic
- Set $\rho = 0$. Consider Eulerian finite volume/difference discretizations: on a fixed grid with step sizes k, h.

KdV soliton

Solution progress in time for a certain set of parameters displaying two solitons, using a conservative, implicit method:



Explicit numerical method

- [Zabusky & Kruskal ('65)]: use an extension of leap-frog – an explicit scheme.
- Their (good) variant reads

$$\begin{aligned} v_j^{n+1} &= v_j^{n-1} + \frac{2\alpha k}{3h}(v_{j-1}^n + v_j^n + v_{j+1}^n)(v_{j+1}^n - v_{j-1}^n) \\ &+ \frac{\nu k}{h^3}(v_{j+2}^n - 2v_{j+1}^n + 2v_{j-1}^n - v_{j-2}^n). \end{aligned}$$

- Constant coefficient stability analysis: restrict time step to

$$k < h / \left[\frac{|\nu|}{h^2} + 2|\alpha u_{\max}| \right]$$

Which can be very restrictive indeed, unless $\nu \ll 1$.

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Numerical example

- [Zhao & Qin ('00), Ascher & McLachlan ('04,'05)]: take

$$\nu = -0.022^2, \ \alpha = -0.5,$$
$$u_0(x) = \cos(\pi x), \quad \text{periodic on } [0, 2].$$

- Try various k, h satisfying linear stability bound.
- Obtain blowup for $t > 21/\pi$ (!)
  The instability takes time to develop, so results at $t = 1$ (say) do not indicate the trouble at a later time.

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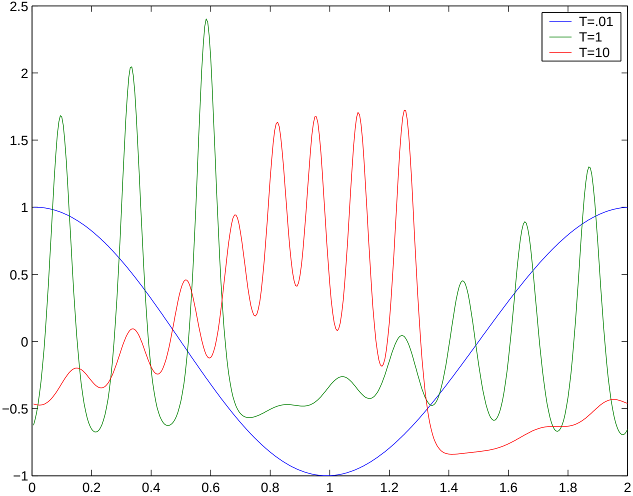
Solution for different times



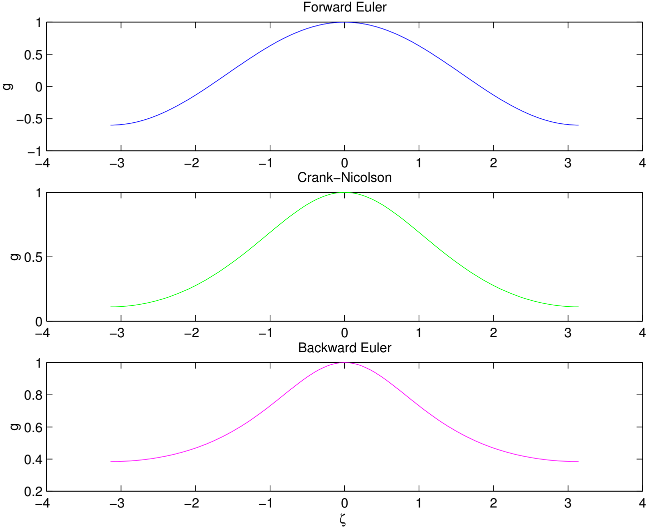
Dissipativity

- Observe that instability is caused by high wave numbers that do not necessarily contribute to accuracy.
- Hence, require damping of high wave number modes. The method has dissipativity of order $2r$ if

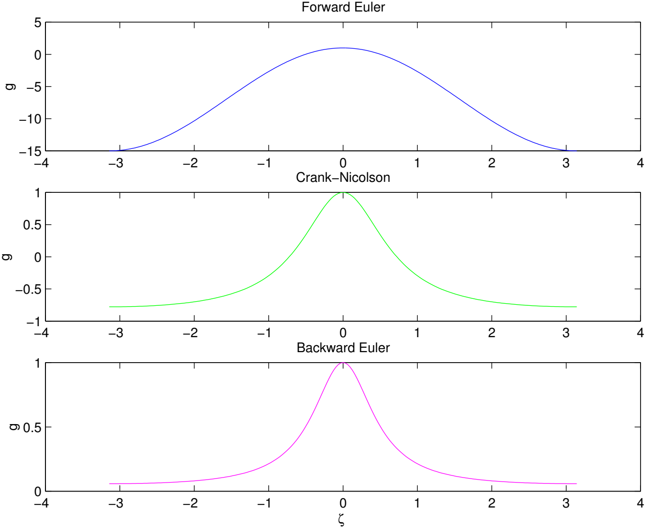
$$\rho(G(\zeta)) \le e^{\tilde{\alpha}k}(1 - \delta|\zeta|^{2r}), \quad \forall|\zeta| \le \pi.$$

- Kreiss (60's): This is sufficient for stability in many realistic situations for linear PDEs.
- Generally, dissipativity is natural for parabolic PDEs but not for hyperbolic PDEs.

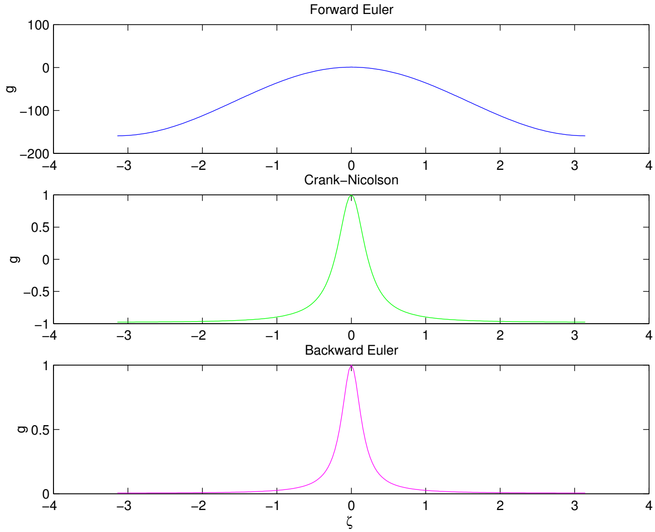
Dissipativity for heat equation, $\mu = k/h^2 = .4$



Dissipativity for heat equation, $\mu = k/h^2 = 4$



Dissipativity for heat equation, $\mu = k/h^2 = 40$



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Outline: schemes for hyperbolic systems

- Lax-Wendroff
- Conservation laws
- Leap-frog
- Lax-Friedrichs
- Upwind
- Modified PDE
- Box

Lax-Wendroff scheme

- For hyperbolic problems, "natural" discretizations do not automatically possess dissipativity. Nonetheless, the *Lax-Wendroff scheme* is dissipative!
- Derivation idea: Apply Taylor for $u(t+k,x)$, viz.

$$u(t+k,x) = u + ku_t + \frac{k^2}{2}u_{tt} + \cdots ,$$

and replace t-derivatives by x-derivatives using the PDE.

- For advection $u_t + au_x = 0$, we have $u_t = -au_x$ and $u_{tt} = (-au_x)_t = a^2 u_{xx}$. So, set $\mu = k/h$ and obtain

$$v_j^{n+1} = \left(I - \frac{\mu}{2} a D_0 + \frac{\mu^2}{2} a^2 D_+ D_- \right) v_j^n .$$

- This gives accuracy order $(2,2)$.

Lax-Wendroff scheme

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- Fourier analysis promises stability if CFL condition holds, i.e., $\mu|a| \leq 1$. But what about dissipativity?
- Calculating amplification factor, obtain

$$|g(\zeta)| \leq 1 - \delta |\zeta|^4$$

  if the CFL condition holds.
- Hence this scheme has dissipativity of order 4 and has guaranteed stability, under certain conditions, for variable coefficient problems.

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Conservation laws

- Many nonlinear hyperbolic systems can be written as

$$\mathbf{u}_t + \mathbf{f}(\mathbf{u})_x = \mathbf{0}.$$

- With Jacobian

$$A(\mathbf{u}) = \frac{\partial \mathbf{f}}{\partial \mathbf{u}}$$

can write conservation law in non-conservation form

$$\mathbf{u}_t + A(\mathbf{u})\mathbf{u}_x = \mathbf{0},$$

but the conservation form is often preferable.

- As usual, solution is constant along characteristics

$$\frac{dx}{dt} = a(u(t,x)).$$

So, the direction of the characteristic curves depends on the solution through initial values $u_0(x)$, but the characteristic curves are straight lines.

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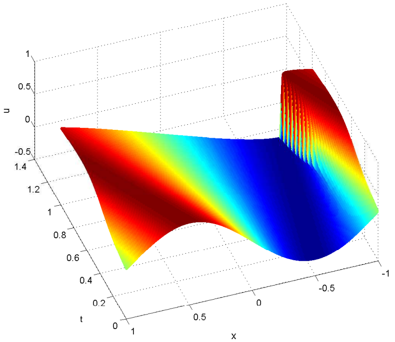
Example: the inviscid Burgers equation

$$
\begin{aligned}
u_t + \frac{1}{2}(u^2)_x &= 0 \quad \text{conservative} \\
u_t + u u_x &= 0 \quad \text{non} - \text{conservative.}
\end{aligned}
$$

Obtain shock when characteristic curves meet!



Example: Incompressible Navier-Stokes

- Models incompressible fluid flow. In two space dimensions, (u, v)–velocity, p–pressure, ν–viscosity constant.

$$\begin{aligned} u_t + uu_x + vu_y + p_x &= \nu \Delta u, \\ v_t + uv_x + vv_y + p_y &= \nu \Delta v, \\ u_x + v_y &= 0. \end{aligned}$$

- Use incompressibility to write material derivatives in conservation form: add $u(u_x + v_y)$ to first eqn, $v(u_x + v_y)$ to second, obtaining

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Lax-Wendroff for conservation laws

- Replacing 2nd time derivatives with spatial ones is trickier.
- Want to avoid the Jacobian matrix $A(\mathbf{u})$ if possible.
- One popular variant:

$$
\begin{aligned}
\bar{\mathbf{v}}_j &= \frac{1}{2}(\mathbf{v}_j^n + \mathbf{v}_{j+1}^n) - \frac{1}{2}\mu(\mathbf{f}_{j+1}^n - \mathbf{f}_j^n) \\
\mathbf{v}_j^{n+1} &= \mathbf{v}_j^n - \mu(\mathbf{f}(\bar{\mathbf{v}}_j) - \mathbf{f}(\bar{\mathbf{v}}_{j-1}))
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Leap-frog

- Recall the scheme of accuracy order (2,2):

$$\mathbf{v}_j^{n+1} = \mathbf{v}_j^{n-1} - \mu A_j^n(\mathbf{v}_{j+1}^n - \mathbf{v}_{j-1}^n).$$

- This extends to conservation laws in an obvious way,

$$\mathbf{v}_j^{n+1} = \mathbf{v}_j^{n-1} - \mu(\mathbf{f}_{j+1}^n - \mathbf{f}_{j-1}^n).$$

- This method is **conservative and non-dissipative**.
- Can introduce dissipativity artificially:

$$\mathbf{v}_j^{n+1} = \left(I - \frac{\varepsilon}{16} D_+^2 D_-^2\right) \mathbf{v}_j^{n-1} - \mu A_j^n D_0 \mathbf{v}_j^n.$$

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Lax-Friedrichs

- Recall the method for the advection equation

$$v_j^{n+1} = \frac{1}{2}(v_{j+1}^n + v_{j-1}^n) - \frac{k}{2h}a(v_{j+1}^n - v_{j-1}^n)$$

 satisfies the strong stability bound $\|v^{n+1}\|_\infty \le \|v^n\|_\infty$ provided CFL holds.

- Write it for a linear hyperbolic system as

$$\mathbf{v}_j^{n+1} = \mathbf{v}_j^n + \frac{1}{2}(\mathbf{v}_{j-1}^n - 2\mathbf{v}_j^n + \mathbf{v}_{j+1}^n) - \frac{\mu}{2}A_j^n(\mathbf{v}_{j+1}^n - \mathbf{v}_{j-1}^n),$$

 highlighting the extra diffusion term in the modified PDE.

- Method has accuracy order $(1,1)$ provided $\mu = k/h$ is fixed.

Modified PDE

- A method constructed for a given (usually hyperbolic) PDE can often be seen as approximating another, *modified PDE*, to a higher accuracy order.
- The properties of such a modified PDE may then shed light on the numerical method's properties.
- **Example**: Lax-Friedrichs for advection approximates the PDE

$$u_t + au_x = \nu u_{xx}$$

with $\nu = \frac{h}{2\mu}(1 - \mu^2 a^2)$ to accuracy order $(2, 2)$.
- The ν-term suggests artificial viscosity (or artificial diffusion). The larger it is, the more smoothing (and smearing) of the solution.
- Note if $k = h^2$ then $\nu \approx 1/2$. Hence error for advection equation no longer decreases as $h \to 0$: must have μ fixed in mesh refinement process.

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Modified PDE for upwind and Lax-Wendroff schemes

- Recall the upwind (one-sided) scheme for advection:

$$v_j^{n+1} = v_j^n - \mu a \begin{cases} \left(v_{j+1}^n - v_j^n\right), & a < 0 \\ \left(v_j^n - v_{j-1}^n\right), & a > 0 \end{cases}.$$

  This approximates the PDE $u_t + au_x = \nu u_{xx}$ with $\nu = \frac{h}{2\mu}\left(\mu|a| - \mu^2 a^2\right)$ to accuracy order $(2, 2)$.

- So, both of these monotone 1st order schemes (i.e., upwind and L-F) have artificial viscosity, though upwind has less if $\mu|a| < 1$.
- The Lax-Wendroff scheme for advection has the modified PDE

$$u_t + au_x = -\frac{ah^2}{6}\left(1 - \mu^2 a^2\right) u_{xxx}.$$

  Note the 3rd rather than 2nd derivative in the added term!

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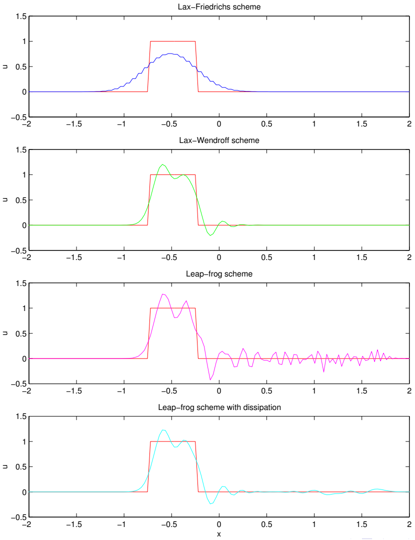
Error comparison for a smooth problem

$u_t = u_x,\ u_0(x) = \sin(\eta x),\ \mu = k/h.$

η	h	μ	Lax-Wendroff	Lax-Friedrichs	Box
1	$.01\pi$	0.5	1.2e-4	2.3e-2	6.1e-5
	$.001\pi$	0.5	1.2e-6	2.4e-3	6.2e-7
	$.001\pi$	5.0	*	*	2.0e-5
10	$.01\pi$	0.5	1.2e-1	9.0e-1	6.1e-2
	$.001\pi$	0.5	1.2e-3	2.1e-1	6.2e-4
	$.0005\pi$	0.5	3.1e-4	1.1e-1	1.5e-4

Error comparison for square wave $\mu = .5$, $h = .01\pi$



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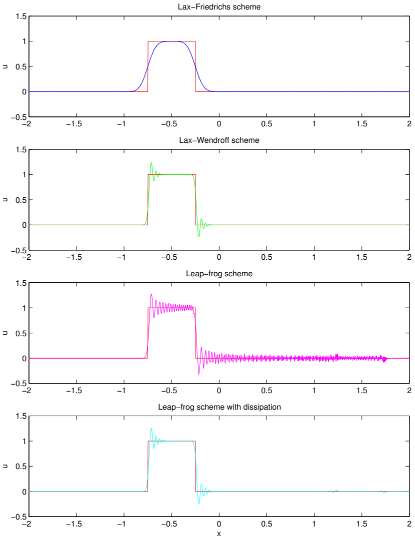

Box

- Finite volume: Integrate conservation law $\mathbf{u}_t + \mathbf{f}(\mathbf{u})_x = \mathbf{0}$ over "box"

$$V = [x_j, x_{j+1}] \times [t_n, t_{n+1}].$$

- Obtain

$$\mathbf{u}^{n+1}_{j+1/2} - \mathbf{u}^{n}_{j+1/2} + \mathbf{f}^{n+1/2}_{j+1} - \mathbf{f}^{n+1/2}_{j} = \mathbf{0}$$

where quantities are line integrals.

- Discretize by trapezoidal rule:

$$\begin{aligned} & \mathbf{v}^{n+1}_{j+1} + \mathbf{v}^{n+1}_{j} - \mathbf{v}^{n}_{j+1} - \mathbf{v}^{n}_{j} \\ + \quad & \mu(\mathbf{f}^{n+1}_{j+1} + \mathbf{f}^{n}_{j+1} - \mathbf{f}^{n+1}_{j} - \mathbf{f}^{n}_{j}) = \mathbf{0}. \end{aligned}$$

- The method is **compact, conservative, implicit, unconditionally stable**, and has accuracy order $(2, 2)$.

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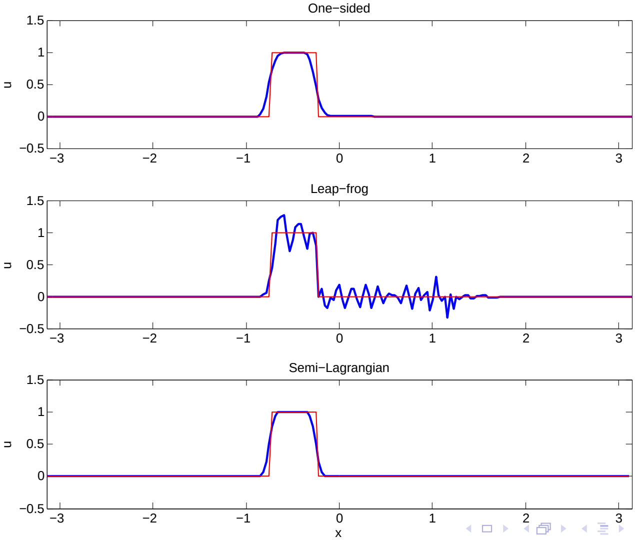
Semi-Lagrangian (SL) method for advection

- For the advection equation $u_t + au_x = 0$, extend the interpretation of the one-sided scheme as tracing the characteristic, by tracing the characteristic curve further back!
- Imagine the one-sided scheme on a coarse grid with widths $\tilde{k} = lk$ and $\tilde{h} = lh$ for some $l \geq 1$, but instead of interpolating between x_j and $\tilde{x}_{j+1} = x_j + \tilde{h}$, find ν such that $x_{j+\nu} \leq x_* \leq x_{j+\nu+1}$ and interpolate $v^{\tilde{n}}_{j+\nu}$ and $v^{\tilde{n}}_{j+\nu+1}$ linearly for v_*. Then set this value to be $v^{\tilde{n}+1}_j$ as before. The new time step is therefore l times larger, with the same spatial mesh as before.
- Explicit stability restriction is no longer binding because can increase l arbitrarily for the $(\tilde{k}, h)$ mesh, so, for a fixed h can take $\tilde{k}$ arbitrarily large without stability concerns in this way!

Example: $u_t = u_x$ with u_0 a square wave

u_0 square wave on $[.25, .75]$, $k = .9h$, **five** times larger for SL, $h = .01\pi$



EXAMPLE: $u_t = u_x$ WITH u_0 A SQUARE WAVE

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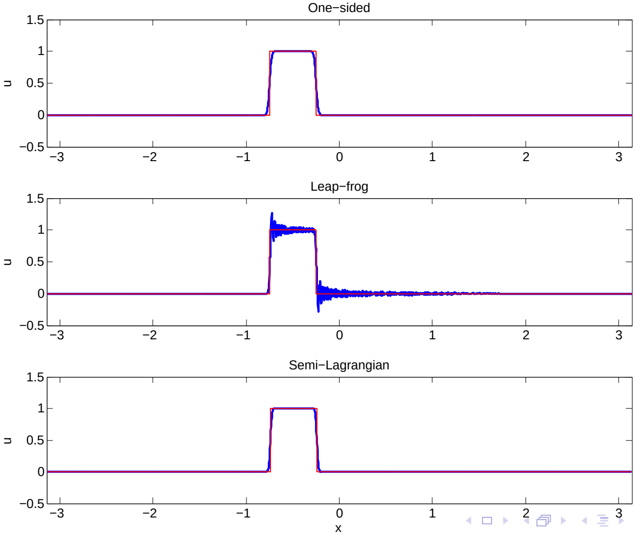

Second order semi-Lagrangian method: constant coefficients

- The foot of the characteristic is at

$$x_* = x_j + \tilde{k}a = x_{j+\nu} + h_*, \quad \nu = \mathtt{fix}\big((-a)\tilde{k}/h\big), \; h_* = wh.$$

- The method we have seen is given by linear interpolation

$$v_j^{n+1} = v_{*L} = w * v_{j+\nu+1}^n + (1-w) * v_{j+\nu}^n,$$

  so it's 1st order accurate.

- To obtain 2nd order, can interpolate using also $v_{j+\nu+2}$, i.e., quadratic interpolation:

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SL early assessment

- For constant-coefficient advection the SL method looks "too good to be true"!
- Indeed, it makes heavy use of particular knowledge regarding a test equation, for which the exact solution is known.
- Still, there are many fluid problems where non-constant advection equations arise. Then, using a large time step, we are trading accuracy for stability.
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SL for variable coefficient advection

- Consider next
$$u_t + a(t,x)u_x = 0.$$
- The characteristic curve passing through (t_{n+1}, x_j) and (t_n, x_*) is not necessarily a straight line (even if $a = a(x)$ is independent of time). In any case, where is x_*?
- Integrate $\frac{dx}{dt} = a(t,x)$ approximately using trapezoidal rule:
$$x_j - x_* = \frac{k}{2}\left(a(t_{n+1}, x_j) + a(t_n, x_*)\right).$$
  This is a nonlinear equation for x_*. Solve using either
  I fixed point iteration (provided $.5k|a_x| < 1$), or
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- Initial guess: $x_*^0 = x_j - k * a(t_{n+1}, x_j)$.

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SL for variable coefficient advection cont.

$$u_t + a(t,x)u_x = 0.$$

- So, for each j
  - I compute x_* satisfying

$$x_* + \frac{k}{2}a(t_n, x_*) = x_j - \frac{k}{2}a(t_{n+1}, x_j).$$

  - II Calculate v_*^n using either linear or quadratic interpolation as for the constant coefficient case.
  - III Set $v_j^{n+1} = v_*^n$.
- For the more general PDE

$$u_t + a(t,x)u_x + b(t,x)u = q(t,x),$$

use in place of step (iii) the equation

$$\left(1 + \frac{k}{2}b_j^{n+1}\right)v_j^{n+1} = \left(1 - \frac{k}{2}b_*^n\right)v_*^n + \frac{k}{2}\left(q_*^n + q_j^{n+1}\right).$$

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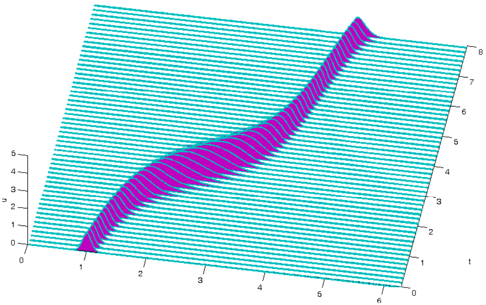
$u_0(x) = \exp(-100(x-1)^2)$; $J = 256$, $h = 2\pi/J$, $k = h/4$

4th order centred in space, leap-frog in time



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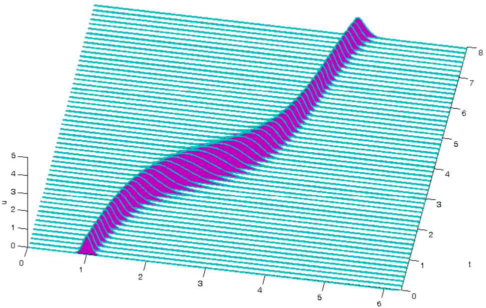

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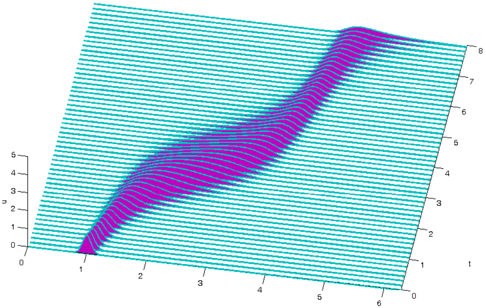
Semi-Lagrangian, linear interpolation at characteristic root



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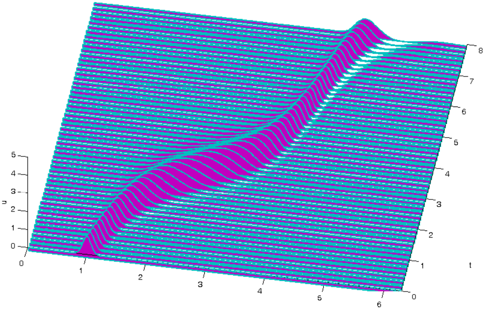

Outline

- Freezing coefficients and dissipativity
- Schemes for hyperbolic systems in 1D
- Discontinuous solutions (Ch. 10)
- Semi-Lagrangian methods
- Nonlinear stability and energy method

Stability for nonlinear problems

- We have seen in the KdV example that nonlinear stability can be tricky: a Fourier stability analysis for the frozen coefficient problem gives (usually) necessary but not sufficient conditions: **no guarantee**.
- Other examples exist: certainly for problems with discontinuous solutions, but also splitting methods for the nonlinear Schrödinger equation, etc.
- So instead try to bound

$$\|v(nk,\cdot)\| \le \|v(0,\cdot)\|$$

in the ℓ_2 norm, if a corresponding bound for the exact solution holds.

Energy method: PDE problem

- Observe

$$\int_{-\infty}^{\infty} 2uu_t dx = \frac{\partial}{\partial t} \int_{-\infty}^{\infty} u^2(t,x)dx.$$

- So, for pure IVP (Cauchy) PDE

$$u_t = f(t, x, u_x, u_{xx}, u_{xxx}, \ldots),$$

if

$$\int_{-\infty}^{\infty} uf(t, x, u_x, u_{xx}, u_{xxx}, \ldots)dx \leq 0$$

then $\|u(t)\| \leq \|u(0)\|$, $\forall t \geq 0$, yielding L_2-stability.

Energy method: PDE problem

- Important tool: integration by parts. If f and g are periodic on $[a, b]$ then

$$0 = f(b)g(b) - f(a)g(a) = \int_a^b (fg)' dx = \int_a^b f' g dx + \int_a^b fg' dx.$$

- Example: Cauchy problem for heat equation, or periodic BC for

$$u_t = u_{xx}.$$

Then $\int u \cdot u_{xx} dx = - \int \left(u_x(t,x)\right)^2 dx \leq 0.$
So, $\|u(t)\|^2 \leq \|u(0)\|^2$.

Energy method: discretized problem

- For an infinite, uniform mesh, define

$$(v, w) = h \sum_{j=-\infty}^{\infty} v_j \bar{w}_j, \qquad \|v\|^2 = (v, v).$$

- Identities:

$$\frac{\partial}{\partial t}(\|v\|^2) = 2\Re\,(v, v_t)$$
$$(v, D_0 w) = -(D_0 v, w), \qquad \text{hence } \Re\,(v, D_0 v) = 0$$
$$(v, D_+ w) = -(D_- v, w)$$
$$\Re\,(v, Rv) = 0 \quad \Leftrightarrow \quad \Re\,(v, Rw) = -\Re\,(Rw, v), \forall v, w \in \ell_2$$

Example: the Burgers equation

- Obviously, for the pure initial value PDE

$$u_t + \frac{1}{2}\left(u^2\right)_x = 0,$$

so long as the solution is smooth,

$$\|u(t)\| = \|u(0)\| \;\; \forall t.$$

- So does the KdV equation for all times.
- Consider the discretizations $D_0\left(v^2\right)$ for $\left(u^2\right)_x$ and $2vD_0v$ for $2uu_x$.
- Obtain $(v, D_0v^2) = -(D_0v, v^2)$, which is **different from** $2(v, vD_0v) = 2(v^2, D_0v) = 2(D_0v, v^2)$.
- Write Burgers as

$$u_t + \frac{\theta}{2}\left(u^2\right)_x + (1-\theta)uu_x = 0,$$

and discretize.

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$$v_t + \frac{1}{2h}\left[\frac{\theta}{2}D_0 v^2 + (1-\theta)vD_0 v\right] = 0.$$

- Multiply by v and sum up:

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- Choose $\theta = 2/3$. Then $\theta/2 = 1-\theta$, so $\left(\|v\|^2\right)_t = 0$, hence

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Obtain stability of semi-discretization so long as solution is smooth!

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Example: the Burgers equation cont.

- In the presence of shocks want to discretize the conservation form $\theta = 1$.
- But if solution is smooth, use $\theta = 2/3$ for a stable semi-discretization.
- Discretize in time: leap-frog may generate difficulties (recall KdV example).
- Using instead implicit midpoint, obtain method

$$v_j^{n+1} - v_j^n + \frac{k}{6h}\left(v_{j+1}^{n+1/2} + v_j^{n+1/2} + v_{j-1}^{n+1/2}\right) D_0 v_j^{n+1/2} = 0.$$

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RK FOR SKEW-SYMMETRIC SEMI-DISCRETIZATION

- Consider a large constant-coefficient ODE system

$$\mathbf{v}_t = L\mathbf{v},$$

where L is $J \times J$ skew-symmetric: $L^T = -L$.

- Obtain such L e.g. from symmetric (centred) semi-discretization of a constant-coefficient hyperbolic PDE.
- Note all eigenvalues of L are imaginary; and $\|\mathbf{v}(t)\| = \|\mathbf{v}(0)\|, \ \forall t$.
- Implicit midpoint in time stable for all k and conserves the invariant

$$\|\mathbf{v}^n\| = \|\mathbf{v}^0\|, \ \forall n.$$

- If $k \le \frac{2\sqrt{2}}{\rho(L)}$ then the classical explicit RK4 satisfies

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See Example 5.12 (pp. 175–177) in the text.

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