Numerical Solutions to PDEs

Lecture Notes #7

— Stability for Multistep Schemes —

Leapfrog Scheme; General Multistep Schemes

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Outline

Last Time

We checked the stability of the Lax-Wendroff and Crank-Nicolson schemes, and came up with the following:

	Lax-Wendroff	**Crank-Nicolson**
Mode	Explicit	Implicit
Order of Accuracy	(2,2)	(2,2)
Stability Criterion	$\|a\lambda\| \le 1$ (CFL)	Unconditionally Stable

Difference Notation $\left\{\delta_+,\, \delta_-,\, \delta_0,\, \delta^2\right\}$ and the Difference Calculus, was introduced as a convenient tool to derive higher order schemes.

The main course on the menu was the discussion on **boundary conditions**. For finite difference schemes we must both respect **physical boundary conditions** as well as (sometimes) introduce additional **numerical boundary conditions**. The implementation of these boundary conditions affect both the **order of accuracy**, and **stability** of the scheme.

Stability for Multistep Schemes: Introduction

We have seen the necessary and sufficient conditions for the stability of one-step schemes:

Theorem (The CFL Condition)

For an explicit scheme for the hyperbolic equation

$$u_t + a u_x = 0,$$

of the form

$$v_m^{n+1} = \alpha v_{m+1}^n + \beta v_m^n + \gamma v_{m-1}^n,$$

with $\lambda = k/h$ held constant, a **necessary condition** *for stability is the* **Courant-Friedrichs-Lewy (CFL) condition**,

$$|a\lambda| \le 1.$$

For systems of equations for which $\bar{\mathbf{v}}$ is a vector and α, β, and γ are matrices, we must have $|a_i\lambda| \le 1$ for all eigenvalues a_i of the matrix A.

Stability for Multistep Schemes: Introduction

Theorem (Von Neumann Stability)

A one-step finite difference scheme (with constant coefficients) is stable in a stability region Λ if and only if there is a constant K (independent of θ, k, and h) such that

$$|g(\theta, k, h)| \leq 1 + Kk,$$

with $(k, h) \in \Lambda$. If $g(\theta, k, h)$ is independent on h and k, the stability condition can be replaced with the restricted stability condition

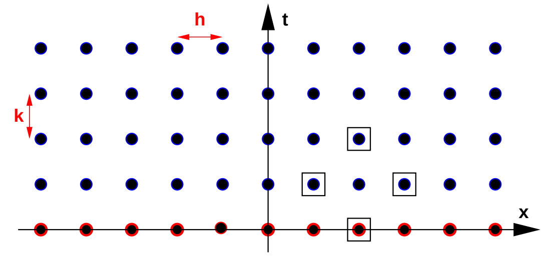
$$|g(\theta)| \leq 1.$$

Now, we **extend this analysis to multi-step schemes.** Starting with the leap-frog scheme, moving to general multi-step schemes. Additional theoretical tools: — the Schur, and von Neumann polynomials which will help us determine stability criteria for multi-step methods.

Stability for the Leapfrog Scheme

The leapfrog (central-time-central-space) scheme for the homogeneous one-way wave equation is given by

$$\frac{v_m^{n+1} - v_m^{n-1}}{2k} + a\frac{v_{m+1}^n - v_{m-1}^n}{2h} = 0.$$



As usual we set $v_m^n \rightsquigarrow g^n e^{imh\xi}$ (from application of the Fourier inversion formula), and eliminate common factors (here $g^{n-1}e^{imh\xi}$).

Stability for the Leapfrog Scheme

We get — ($h\xi \equiv \theta$, throughout this lecture) —

$$\begin{aligned}
\frac{v_m^{n+1} - v_m^{n-1}}{2k} + a\frac{v_{m+1}^n - v_{m-1}^n}{2h} &= 0 \\
\frac{g^2 - 1}{2k} + a\frac{g(e^{i\theta} - e^{-i\theta})}{2h} &= 0 \\
\mathbf{g^2 - 1 + 2ia}\lambda \sin(\theta)\mathbf{g} &= \mathbf{0}
\end{aligned}$$

Hence,

$$g_\pm(\theta) = -ia\lambda \sin(\theta) \pm \sqrt{1 - (a\lambda)^2 \sin^2(\theta)}. \qquad (1)$$

I. When $\mathbf{g_+ \neq g_-}$, the solution is given by

$$\hat{v}^n(\xi) = A_+(\xi)g_+(h\xi)^n + A_-(\xi)g_-(h\xi)^n, \qquad (2)$$

and $A_\pm(\xi)$ are determined by initial conditions.

Stability for the Leapfrog Scheme

Sometimes it is useful to rewrite (2) in the form

$$\hat{v}^n(\xi) = A(\xi)g_+(h\xi)^n + B(\xi)\left[\frac{g_-(h\xi)^n - g_+(h\xi)^n}{g_-(h\xi) - g_+(h\xi)}\right], \qquad (3)$$

where $A(\xi)$ and $B(\xi)$ are determined by initial conditions.

II. When $\mathbf{g_+ = g_-} = g$, the solution is given by

$$\hat{v}^n(\xi) = A(\xi)g(h\xi)^n + n \cdot B(\xi)g(h\xi)^{n-1}, \qquad (4)$$

where $A(\xi)$, and $B(\xi)$ are related to $\hat{v}^0(\xi)$, and $\hat{v}^1(\xi)$ by

$$\begin{aligned}
A(\xi) &= \hat{v}^0(\xi) \\
B(\xi) &= \hat{v}^1(\xi) - \hat{v}^0(\xi)g(h\xi). \qquad (5)
\end{aligned}$$

We will refer back to these expressions when we analyze the stability of the scheme.

Stability for the Leapfrog Scheme

We discuss the stability in terms of

Definition (Stable Scheme)

A finite difference scheme $P_{k,h}v_m^n = 0$ for a first-order equation is **stable** in a stability region Λ if there is an integer J such that for any positive time T, there is a constant C_T such that

$$h \sum_{m=-\infty}^{\infty} |v_m^n|^2 \leq C_T h \sum_{j=0}^{J} \sum_{m=-\infty}^{\infty} \left|v_m^j\right|^2,$$

for $0 \leq nk \leq T$, with $(k,h) \in \Lambda$.

with the integer $\mathbf{J} = \mathbf{1}$.

First, we consider the case where $g_+ \neq g_-$, and **choose** the initial conditions so that $B(\xi) \equiv 0$.

Stability for the Leapfrog Scheme

Now, with this setup and using (3) we have

$$|\widehat{v}^n(\xi)| = |A(\xi)| \cdot |g_+(h\xi)|^n,$$

and it follows that we must require

$$|g_+(h\xi)| \leq 1 + Kk,$$

for stability. Application with different initial conditions (such that $A(\xi) \equiv 0$) gives the same restriction on $g_-(h\xi)$.

When λ is constant, the restricted conditions

$$|g_\pm(h\xi)| \leq 1,$$

apply.

Stability for the Leapfrog Scheme

From (1), with $|\mathbf{a}\lambda| \leq \mathbf{1}$ we have that

$$|g_\pm|^2 = 1 - (a\lambda)^2 \sin^2(\theta) + (a\lambda)^2 \sin^2(\theta) = 1,$$

and when $|\mathbf{a}\lambda| > \mathbf{1}$, we get

$$|g_-(\pi/2)| = |a\lambda| + \sqrt{(a\lambda)^2 - 1} \geq |a\lambda| > 1.$$

Hence, $|\mathbf{a}\lambda| \leq \mathbf{1}$ **is a necessary condition for stability.**

But... We're not done. — We must also look at the case $g_+ = g_-$. This equality holds only when $|a\lambda| = 1$, and $\theta = \pm\pi/2$. For these two values we get $g = \pm i$, and the solutions

$$\widehat{v}^n\left(\pm\pi/2h\right) = A\left(\pm\pi/2h\right)(\mp i)^n + \mathbf{n} \cdot B\left(\pm\pi/2h\right)(\mp i)^{n-1}.$$

Since this term grows linearly in n, the leapfrog scheme is unstable for $|a\lambda| = 1$. **Hence, the leapfrog scheme is stable** $\Leftrightarrow$ $|\mathbf{a}\lambda| < \mathbf{1}$.

Initializing the Leapfrog Scheme

The Leapfrog scheme (and other two-step schemes) require that in addition to the initial values v_m^0, the first time level v_m^1 must also be initialized.

Any consistent one-step scheme, **even an unstable one**, can be used to initialize v_m^1. Since the unstable scheme is applied only once, the error growth is minimal.

Further, if the grid parameter λ is constant, then the initialization scheme can be **accurate of one order less** than that of the two-step scheme, without degrading the overall accuracy of the scheme.

Thus, we have found a potential use for the unstable forward-time central-space scheme; — as an initializer for the leap-frog scheme.

Parasitic Modes of the Leapfrog Scheme

From the expressions

$$\begin{aligned} \widehat{v}^n(\xi) &= A_+(\xi) g_+(h\xi)^n + A_-(\xi) g_-(h\xi)^n, \\ g_\pm(\theta) &= -ia\lambda \sin(\theta) \pm \sqrt{1-(a\lambda)^2 \sin^2(\theta)}, \end{aligned}$$

we see that the solution of the leapfrog scheme consists of two parts, associated with $g_+(\theta)$, and $g_-(\theta)$. We note that $g_+(0) = 1$, and $g_-(0) = -1$.

We examine how the two parts contribute to the solution.

If we use the forward-time central-space scheme for initialization, then we have

$$\widehat{v}^1(\xi) = (1 - ia\lambda \sin(\theta))\widehat{v}^0(\xi).$$

Parasitic Modes of the Leapfrog Scheme

Based on taking the first step using the forward-time central-space scheme, and Taylor expanding the square roots in the expressions for $g_\pm(\theta)$:

$$\begin{aligned} g_+(\theta) &= 1 - ia\lambda \sin(\theta) - \frac{1}{2} a^2 \lambda^2 \sin^2(\theta) + \mathcal{O}\left(h^4\right), \\ g_-(\theta) &= -1 - ia\lambda \sin(\theta) + \frac{1}{2} a^2 \lambda^2 \sin^2(\theta) + \mathcal{O}\left(h^4\right), \end{aligned}$$

now, using (5), we get

$$B(\xi) = \left[\frac{1}{2} a^2 \lambda^2 \sin^2(\theta) + \mathcal{O}\left(\theta^4\right) \right] \widehat{v}^0(\xi).$$

For $|\theta|$ small, $|B(\xi)| = \mathcal{O}\left(\theta^2\right)$, *i.e.* small, the scheme behaves like a one-step scheme with amplification factor $g_+(\theta)$.

Parasitic Modes of the Leapfrog Scheme

When $|\theta|$ is not small, $B(\xi)$ is not necessarily small, and the effect of the second amplification factor $g_-(\theta)$ is felt.

The portion of the solution associated with $g_-(\theta)$ is called the **parasitic mode**. Since $g_-(0) = -1$, the parasitic mode induces rapid **oscillations** in time.

The parasitic mode **travels in the wrong direction**. When a is positive, the parasitic mode travels to the left, and when a is negative it travels to the right.

Example: Parasitic Modes

We consider the one-way wave-equation, with constant speed $a = 1$, in the interval $[-1, 1]$, with initial conditions

$$v_m^0 = \begin{cases} \cos^2(\pi x_m) & \text{if } |x_m| \le \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

At the left boundary ($x = -1$) we set $v_0^n = 0$ (which is consistent with the equation), and at the right boundary ($x = 1$) we also set $v_M^0 = 0$ (which is inconsistent with the equation).

The inconsistent boundary condition will transfer energy into the parasitic mode.

We set the grid parameter $\lambda = 0.9$, and $h = 1/20$.

Example: Parasitic Modes

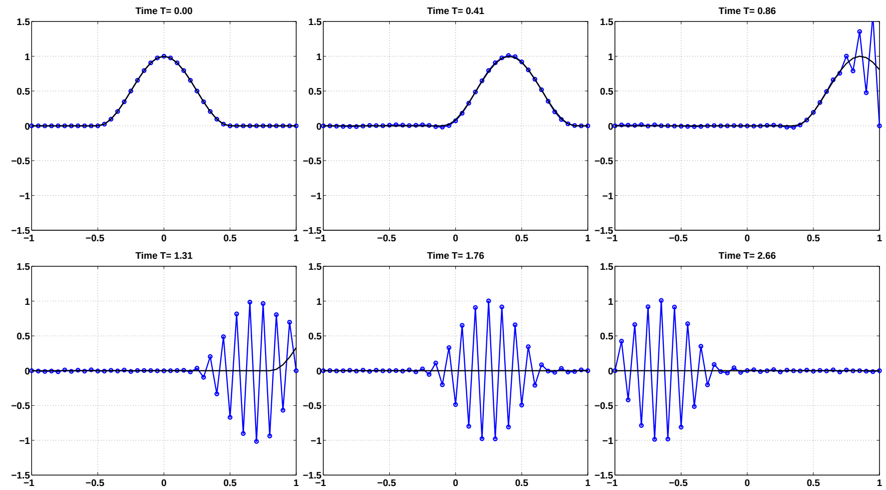


Figure: The exact (black solid), and the numerical (**blue**, with ○-markers) solutions. At time T=0.86 (3rd panel), the exact solution is leaving the domain, but the inconsistent boundary condition is starting to pump energy into the parasitic mode, which propagates to the left (panels 4–6).

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Example: Parasitic Modes

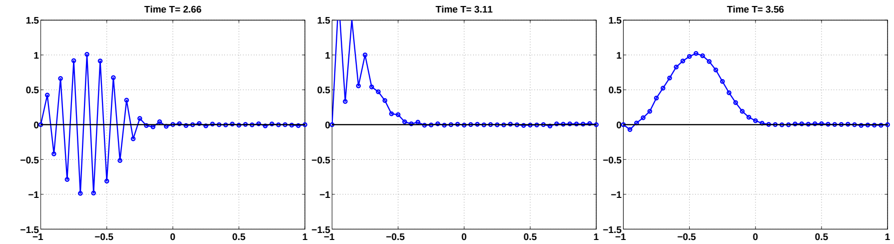

Figure: The exact (black solid), and the numerical (**blue**, with ○-markers) solutions. At time T=2.66 (1st panel), the parasitic mode hits the right boundary and bounces back (T=3.11, 2nd panel), and the reflected energy almost perfectly restores the initial shape of the pulse (T=3.56, 3rd panel). We note that Dirichlet-type (fixed) boundary conditions are **reflecting** for the wave-equation.

The effects of parasitic modes can be reduced by the use of (numerical) dissipation, which we will discuss next week.

See also **Movie: leapfrog_ftcs.mpg**.

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Example: Other Boundary Conditions

We re-run the same problem with different boundary conditions:

Eqn	Boundary Condition	Movie
3.4.1a	$v_M^{n+1} = v_{M-1}^{n+1}$	**leapfrog_ftcs_341a.mpg**
3.4.1b	$v_M^{n+1} = 2v_{M-1}^{n+1} - v_{M-2}^{n+1}$	**leapfrog_ftcs_341b.mpg**
3.4.1c	$v_M^{n+1} = v_{M-1}^{n}$	**leapfrog_ftcs_341c.mpg**
3.4.1d	$v_M^{n+1} = 2v_{M-1}^{n} - v_{M-2}^{n-1}$	**leapfrog_ftcs_341d.mpg**

At first glance (wave leaving the domain) **3.4.1a** and **3.4.1b** seem to perform OK; however, the instability causes the numerical solution to blow up rapidly.

Boundary conditions **3.4.1c 3.4.1d** are stable, and after the solution leaves the domain only some very minor oscillations remain.

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Stability for General Multistep Schemes

"The Return of the Symbol"

We can express the stability of a multistep scheme in several ways, including using the symbol of the scheme:

The stability of a multistep scheme $P_{k,h}v = R_{k,h}f$ is determined by the roots of the amplification polynomial

$$\Phi(g,\theta) = k\, p_{k,h}\left(\frac{\ln(g)}{k}, \frac{\theta}{h}\right),$$

or, equivalently

$$\Phi\left(e^{sk}, h\xi\right) = k\, p_{k,h}(s,\xi).$$

Alternatively, and more familiarly, Φ can be obtained by requiring that $v_m^n = g^n e^{im\theta}$ is a solution to $P_{k,h}v = 0$, and $\Phi(g,\theta)$ is the polynomial of which g must be a root so that $v_m^n = g^n e^{im\theta}$ is a solution of $P_{k,h}v = R_{k,h}f$.

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Stability for General Multistep Schemes

We assume that the scheme involves $\sigma + 1$ time-levels, and therefore Φ is a polynomial of degree σ. The integer J in the stability definition is taken to be σ.

For now, we will largely ignore the relation between Φ and the symbol $p(s, \xi)$. This relation will, however, be important when we later discuss convergence of multi-step schemes.

OK, our old trick $v_m^n \rightsquigarrow g^n e^{im\theta}$, and eliminating common factors will work (phew!).

Still we will run into some trouble.

A Simple? Example

Consider the multistep scheme for the one-way wave equation

$$\frac{3v_m^{n+1} - 4v_m^n + v_m^{n-1}}{2k} + a\frac{v_{m+1}^{n+1} - v_{m-1}^{n+1}}{2h} = f_m^{n+1}$$

— this scheme is order-(2,2) and unconditionally stable.

The amplification polynomial is

$$\Phi(g, \theta) = \left[\frac{3 + 2ia\lambda\sin(\theta)}{2}\right] g^2 - 2g + \frac{1}{2}.$$

Fantastic! — A second order polynomial with a complex coefficient on the quadratic term; which should be investigated $\forall\theta$.

The analysis of this scheme is much harder than that of the leapfrog scheme; we need additional tools from complex analysis and the concepts of Schur, and von Neumann polynomials. This will all be developed in next lecture.

Moving Along...

Still, we can talk about the stability in general terms: —

If the roots, g_ν of $\Phi(g, \theta)$ are **distinct**, then the solution to the homogeneous difference scheme is given by

$$\widehat{v}^n = \sum_{\nu=1}^{\sigma} g_\nu(h\xi)^n A_\nu(\xi), \quad A_\nu(\xi) \text{ determined by initial conditions.}$$

The stability condition is

$$|g_\nu(h\xi)| \leq 1 + Kk, \quad \nu = 1, \ldots, \sigma.$$

When $\Phi(g, \theta)$ is independent of k and h, we can set $K = 0$.

Roots of Multiplicity > 1

We now look at the case when $\Phi(g, \theta)$ has **roots of higher multiplicity**. For simplicity, lets assume that $\Phi(g, \theta)$ is independent of k and h so that the restricted stability criterion can be used.

Suppose $g_1(\theta_0)$ is a multiple root of $\Phi(g, \theta)$ at θ_0; then

$$\widehat{v}_m^n = \left[g_1(\theta_0)^n B_0 + n g_1(\theta_0)^{n-1} B_1\right] e^{im\theta_0},$$

is a solution of the difference equation.

If $B_0 = 0$ (carefully selected initial conditions), then

$$|\widehat{v}_m^n| = n|g_1(\theta_0)|^{n-1}|B_1|.$$

When $|\mathbf{g_1}(\boldsymbol{\theta_0})| < \mathbf{1}$, we have

$$|\widehat{v}_m^n| \leq C\left[|g_1(\theta_0)| \log\left(\frac{1}{|g_1(\theta_0)|}\right)\right]^{-1} |B_1|.$$

Roots of Multiplicity > 1

When $|\mathbf{g_1}(\theta_0)| = \mathbf{1}$, we cannot find a bound on $|\widehat{v}_m^n|$, and there exists a solution which is linearly unbounded; hence the scheme is unstable in this case.

We have the following

Theorem (Stability of Multistep Schemes)

If the amplification polynomial $\Phi(g,\theta)$ is explicitly independent of h and k, then the necessary and sufficient condition for the finite difference scheme to be stable is that all roots, $g_\nu(\theta)$, satisfy the following conditions:

(a) $|g_\nu(\theta)| \le 1$, *and*

(b) *if* $|g_\nu(\theta)| = 1$, *then* $g_\nu(\theta)$ *must be a simple root.*

A More General Stability Theorem

Theorem (Stability of Multistep Schemes)

A finite difference scheme for a scalar equation is stable if and only if all the roots, $g_\nu(\theta)$, of the amplification polynomial $\Phi(g,\theta,k,h)$ satisfy the following conditions:

(a) *There is a constant K such that $|g_\nu| \le 1 + Kk$.*

(b) *There are positive constants c_0 and c_1 such that if $c_0 \le |g_\nu| \le 1 + Kk$, then g_ν is a simple root, and for any other root g_μ, the relation*

$$|g_\nu - g_\mu| \ge c_1$$

holds for h and k sufficiently small.

Illustration of the Theorem

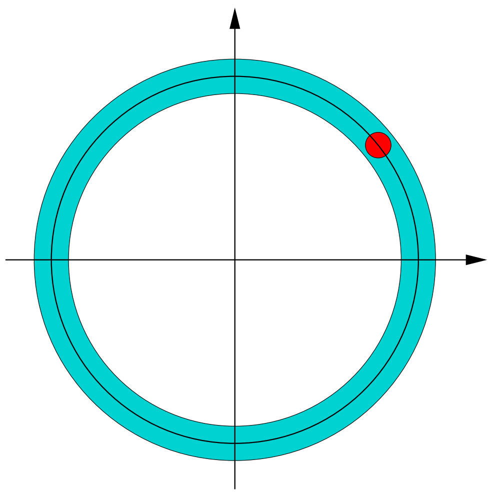

Figure: In the band $c_0 \le r \le 1 + Kk$, we can only have simple roots; and the minimal distance between a root in this band and another root is c_1.

Example: The Leapfrog Scheme

$a\lambda \in \{0.9, 0.99, 1.0, 1.05\}$