Numerical Solutions to PDEs

Lecture Notes #18 — Well-Posed and Stable Initial-Boundary Value Problems, Part 1

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Outline

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A Quick Look in the Rear-View Mirror

In the last two lectures we covered [1] **Analysis of Well-Posed and Stable Problems** and [2] **Convergence Estimates for Initial Value Problems**.

Topic [1] is **model-related** and gave us a firmer theoretical foundation in regards to what the potential usefulness of various PDE models in relation to *"well-behaved" physical phenomena.* The key considerations were continuous dependence on initial data, and robustness in terms of perturbations in (or introduction of) lower order terms.

Topic [2] is **numerics-related** and gave us guidelines for how lack of smoothness in the initial data may degrade the convergence rate of our finite difference schemes. We have very clear results (theorems), for both hyperbolic and parabolic problems, describing how much smoothness is required to achieve the full convergence rate of the scheme, and exactly to what degree non-smoothness degrades convergence.

Looking Forward: Well-Posed and Stable IBVP

We now look at two topics which relate directly to the previous two lectures, and provide the final piece to the puzzle describing hyperbolic and parabolic problems in **finite domains:**

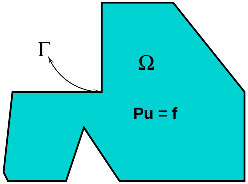
- the **well-posedness of boundary conditions for PDEs** (**model-centric**), and
- the **analysis of boundary conditions for finite difference schemes** (**numerics-centric**).

Our main theoretical tool/toy is the **Laplace transform** (which can be viewed as a special case of the Fourier transform.)

This two-part lecture concludes our quick theoretical "detour," which is meant to serve two purposes: [A] to high-light the main theoretical results pertaining to our computational goals; and [B] to give some indication of the areas of (more) theoretical mathematics which are directly useful for computational sciences.

Introduction: The IBVP

PDE / Finite Difference Scheme



We consider an initial-boundary value problem

$$Pu = f, \quad \text{or} \quad P_{h,k}v = R_{h,k}f,$$

on some domain $\Omega \subseteq \mathbb{R}^n$ with given initial conditions

$$u(0,x) = u_0(x), \quad \text{or} \quad v_m^0 = u_0(x_m),$$

and boundary ($\Gamma = \partial\Omega$) conditions

$$Bu(t,x) = \beta(t,x),\ x \in \Gamma, \quad \text{or} \quad Bv_m^n = \beta(t_n, x_m),\ x_m \in \Gamma.$$

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"Massaging" the Problem...

Simplification #1:

We assume that there is an extension of the model equation $Pu = f$ and the associated initial data $u_0(x)$ to all of $\mathbb{R}^n$, so that the resulting initial value problem is $[1]$ Well-posed for the PDE; $[2]$ Stable for the FDS.

We let w denote the solution to the extended problem. By expressing the solution to the original problem as $u = w + u'$, we realize that the "missing part" u' is given by the IBVP where $f \equiv 0$, and $u_0(x) \equiv 0$, *i.e.* the only non-zero data determining u' is the boundary conditions $Bu'(t,x) = \beta(t,x)$

Simplification #2:

We extend the time-interval from $(0,\infty)$ to $(-\infty,\infty)$, which will simplify the analysis...

"Massaging" the Problem...

Simplification #3:

Well-posedness of boundary conditions of PDEs is essentially a **local property** — we need only consider the PDE and BC at each boundary point (separately), and if the problem is well-posed at each point, the global problem is well-posed.

This allows us to only consider the **frozen coefficient problems** — when Γ is smooth enough the analysis of the IBVP at the boundary point x_0 at time t_0 is reduced to considering the PDE with coefficients fixed at (t_0, x_0), and Ω replaced by half-space (illustrated on slide 8). We end up with a constant-coefficient problem on a half-space, which may be a tremendous simplification over a variable coefficient problem on a complicated domain.

This simplification extends to some degree to finite difference schemes; however, the theory is not as complete as it is for PDEs.

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"Massaging" the Problem...

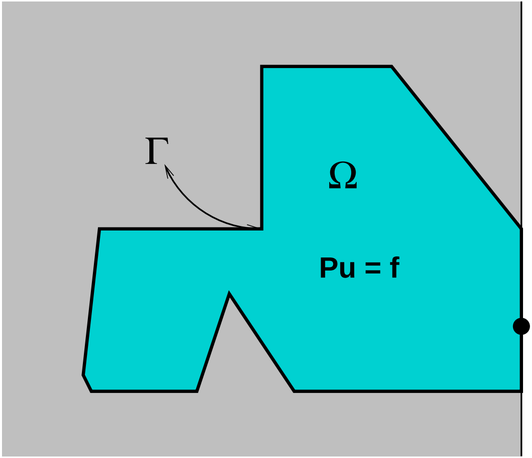


Figure: Illustration of the extension of Ω to the appropriate half-space, formed by the tangent-plane at $x_0 \in \Gamma$, and the interior normal $\bar{\mathbf{n}}$ at x_0.

The Laplace Transform

Strikwerda's Version

There are several ways to define the Laplace transform. Here, we use Strikwerda's choice:

Definition (The Laplace Transform)

The Laplace transform $\tilde{u}(s)$ is equal to the Fourier transform of $e^{-\eta t}u(t)$ with the dual variable τ, *i.e.*

$$\tilde{u}(s) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-(\eta+i\tau)t}\, u(t)\, dt$$

where $s = \eta + i\tau$.

Most definitions of the Laplace transform do not include $\frac{1}{\sqrt{2\pi}}$ (we include it for symmetry with the Fourier transform); and often you see it expressed only at $\tau \equiv 0$, and for functions $u(t)$ for which $u(t) \equiv 0$ for $t < 0$.

The Laplace Inversion Formula

Based on what we know about the Fourier inversion formula, and variable substitution we get

$$u(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{(\eta + i\tau)t}\, \tilde{u}(n + i\tau)\, d\tau = \frac{1}{i\sqrt{2\pi}} \int_{\eta - i\infty}^{\eta + i\infty} e^{st}\, \tilde{u}(s)\, ds$$

This latter integral is known as the **Bromwich integral** or the **Fourier-Mellin integral**. The path of integration is a vertical contour in the complex plane chosen so that all singularities of $u(s)$ are to the left of it.

Since we are interested in positive time, we are always going to have $\eta > 0$.

The Discrete Laplace Transform

See also "Z-transform"

Definition (The Discrete Laplace Transform)

The Laplace transform of a discrete function v_m^n on a grid with time-spacing k is defined by

$$\tilde{v}(s) = \frac{k}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} e^{-(\eta+i\tau)nk}\, v^n,$$

With $z = e^{(\eta+i\tau)k}$ and a slight abuse of notation [n both a power and time-superscript], we have

$$\tilde{v}(z) = \frac{k}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} z^{-n} v^n,$$

with the inversion formula

$$v^n = \frac{1}{2\pi} \int_{-\pi/k}^{\pi/k} e^{snk}\, \tilde{v}(s)\, d\tau = \frac{1}{ik\sqrt{2\pi}} \oint_{|z|=e^{\eta k}} z^{(n-1)}\, \tilde{v}(z)\, dz.$$

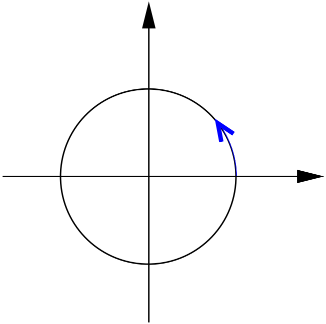
The Discrete Laplace Transform: Notes

The condition $\mathrm{Re}(\eta) \geq 0$ is equivalent to $|z| \geq 1$.

The contour/circle integral

$$\oint_{|z|=e^{\eta k}} z^{(n-1)}\, \tilde{v}(z)\, dz$$

is the integral in the complex plan over the circle with radius $e^{\eta k}$.



Energy Estimates — Parseval — Fourier — Laplace

From Parseval's relation for the Fourier transform, we have

$$\|u\|_\eta^2 = \int_{-\infty}^{\infty} e^{-2\eta t}\,|u(t)|^2\,dt = \int_{-\infty}^{\infty} |\tilde{u}(\eta+i\tau)|^2\,d\tau.$$

$$\|v\|_{\eta,k}^2 = k\sum_{n=-\infty}^{\infty} e^{-2\eta k n}\,|v^n|^2 = \int_{-\pi/k}^{\pi/k} |\tilde{v}(\eta+i\tau)|^2\,d\tau$$

$$\equiv k\sum_{n=-\infty}^{\infty} z^{-2n}\,|v^n|^2 = \frac{1}{k}\oint_{|z|=e^{\eta k}} |\tilde{v}(z)|^2\,d\theta.$$

where $z = e^{\eta k}e^{i\theta}$, *i.e.* $\theta = \tau k$.

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Boundary "Energy" and Well-Posedness

For both time and space dimensions we can define

$$\begin{aligned} |||u|||_\eta^2 &= \int_{-\infty}^{\infty}\int_0^{\infty}\int_{-\infty}^{\infty} e^{-2\eta t}\,|u(t,x,y)|^2\,dt\,dx\,dy \\ &= \int_{-\infty}^{\infty}\int_0^{\infty}\int_{-\infty}^{\infty} |\widehat{u}(\eta+i\tau,x,\omega_y)|^2\,d\tau\,dx\,d\omega_y, \end{aligned}$$

and for norms over the boundary we use

$$\begin{aligned} |\beta|_\eta^2 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-2\eta t}\,|\beta(t,y)|^2\,dt\,dy \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\widehat{\beta}(\eta+i\tau,\omega)|^2\,d\tau\,d\omega. \end{aligned}$$

We express **well-posedness** for IBVPs

$$|||u|||_\eta^2 + |u|_\eta^2 \le C(\eta)\left(|\beta|_\eta^2 + |||f|||_\eta^2 + \|u_0\|^2\right).$$

Boundary Conditions for the Leapfrog Scheme

With the theoretical machinery in place, we now analyze boundary conditions for the leapfrog scheme for $u_t - au_x = 0$, $a > 0$, *i.e.*

$$v_m^{n+1} = v_m^{n-1} + a\lambda(v_{m+1}^n - v_{m-1}^n),$$

we consider the spatial region $\mathbb{R}^+ = [0, \infty)$, for $t \in (-\infty, \infty)$, we consider the following numerical boundary conditions at x_0:

$$v_0^{n+1} = v_1^{n+1} + \beta^{n+1} \tag{11.2.2a}$$

$$v_0^{n+1} = v_1^n + \beta^{n+1} \tag{11.2.2b}$$

$$v_0^{n+1} = v_0^{n-1} + 2a\lambda(v_1^n - v_0^n) + \beta^{n+1} \tag{11.2.2c}$$

$$v_0^{n+1} = v_0^n + a\lambda(v_1^n - v_0^n) + \beta^{n+1} \tag{11.2.2d}$$

Boundary Conditions for the Leapfrog Scheme

Replacing $v_m^n \rightsquigarrow z^n \kappa^m$ in the scheme, gives us (after division by $z^n \kappa^m$)

$$z - \frac{1}{z} = a\lambda \left(\kappa - \frac{1}{\kappa} \right),$$

this equation has two roots $\kappa_\pm(z)$ which are continuous functions of z; when $\kappa_+ \neq \kappa_-$ the general solution is in the form

$$\tilde{v}_m = A\kappa_-(z)^m + B\kappa_+(z)^m.$$

Result #1: When $|z| > 1$, we have $|\kappa_-(z)| < 1$ and $|\kappa_+(z)| > 1$. Since we are only interested in the finite-energy solutions in $L^2(h\mathbb{Z}^+)$, the general form of $\tilde{v}_m$ for $|z| > 1$ is

$$\tilde{v}_m = A(z)\kappa_-(z)^m;$$

$A(z)$ is determined by the transform of the boundary function, $\tilde{\beta}(z)$.

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Boundary Conditions for the Leapfrog Scheme

Using this representation in the boundary expressions (11.2.2a–11.2.2d), we get

$$A(z)\,[1-\kappa_-(z)] = \tilde{\beta}(z) \tag{11.2.6a}$$

$$A(z)\,[z-\kappa_-(z)] = z\tilde{\beta}(z) \tag{11.2.6b}$$

$$A(z)\,\left[z - z^{-1} - 2a\lambda\,[\kappa_-(z)-1]\right] = z\tilde{\beta}(z) \tag{11.2.6c}$$

$$A(z)\,[z - 1 - a\lambda\,[\kappa_-(z)-1]] = z\tilde{\beta}(z) \tag{11.2.6d}$$

The norm of $\tilde{v}_m$ in $L^2(h\mathbb{Z}^+)$ is given by

$$\|\tilde{v}(z)\|^2 = h\sum_{m=0}^{\infty}|\tilde{v}_m|^2 = h|A(z)|^2\sum_{m=0}^{\infty}|\kappa_-(z)|^{2m} = \frac{h\,|A(z)|^2}{1-|\kappa_-(z)|^2},$$

and, with $s=\eta+i\tau$, in terms of the function v_m^n

$$\|v\|_{\eta,h}^2 = \int_{-\pi/k}^{\pi/k} \frac{h\,|A(e^{sk})|^2}{1-|\kappa_-(e^{sk})|^2}\,d\tau.$$

Boundary Conditions for the Leapfrog Scheme

In order to get an estimate of the form $\|v\|^2_{\eta,h} \leq C|\beta|^2_{\eta,h}$, we substitute the expressions for $A(z)$. *E.g.* for boundary conditions (11.2.2a) and (11.2.2b), we have from (11.2.6a) and (11.2.6b)

$$\|v\|^2_{\eta,h} = \int_{-\pi/k}^{\pi/k} \frac{|\tilde{\beta}(e^{sk})|^2}{|1-\kappa_-(e^{sk})|^2} \, \frac{h}{1-|\kappa_-(e^{sk})|^2} d\tau \qquad (11.2.8a)$$

$$\|v\|^2_{\eta,h} = \int_{-\pi/k}^{\pi/k} \frac{|z|^2\,|\tilde{\beta}(e^{sk})|^2}{|e^{sk}-\kappa_-(e^{sk})|^2} \, \frac{h}{1-|\kappa_-(e^{sk})|^2} d\tau \qquad (11.2.8b)$$

For (11.2.8a) we must find a lower bound on $|1-\kappa_-|$, and for (11.2.8b) we must find a lower bound on $|e^{sk}-\kappa_-(e^{sk})|$.

Since we choose $\eta > 0$, we have $|z| > 1$, and $|\kappa_-| < 1$, therefore neither $|1-\kappa_-|$ nor $|z-\kappa_-|$ is zero, but, as $k \to 0$ ($|z| \to 1$). Hence we analyze the behavior of $\kappa_-(z)$ for $|z| = 1$, the behavior for $|z| > 1$ can then be determined by, *e.g.* Taylor series.

Boundary Conditions for the Leapfrog Scheme

The analysis reduces to checking for **non-trivial solutions** of the form $\tilde{v}_m = A(z)\kappa_-(z)^m$, which solve the homogeneous boundary conditions; we must check if there is a $\kappa_-(z)$ such that

$$A(z)[1-\kappa_z] = 0 \qquad (11.2.9a)$$

$$A(z)[z-\kappa_z] = 0 \qquad (11.2.9b)$$

for the boundary conditions (11.2.2a) and (11.2.2b) respectively.

To analyze boundary conditions (11.2.2a)–(11.2.2d), we first set $\kappa = 1$ in $z - \frac{1}{z} = a\lambda\left(\kappa - \frac{1}{\kappa}\right)$, and notice that $z = \pm 1$ are roots, and conversely if $z = \pm 1$, then $\kappa = \pm 1$ are roots. By expansion $z = \pm(1+\epsilon)$, and $\kappa = (1+\delta)$ it is quite straight forward to identify which root (κ_- or κ_+) approaches ± 1 in each case. See figure on slide 20.

Boundary Conditions for the Leapfrog Scheme

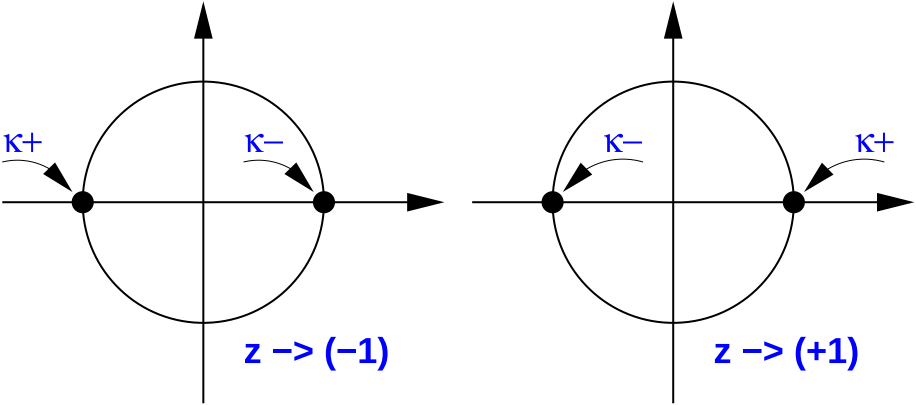

Figure: The behavior of the roots $\kappa_-(z)$ and $\kappa_+(z)$ as [LEFT PANEL] $z \to -1$, and [RIGHT PANEL] $z \to +1$.

We show the analysis for $z \to -1$ ($\kappa_- \to 1$), which ties in directly to an expression for the lower bound of $1 - \kappa_-$...

Boundary Conditions for the Leapfrog Scheme

We set $z = -(1+\epsilon)$, and $\kappa = 1+\delta$, and get

$$\begin{aligned} z - z^{-1} &= -2\epsilon + \mathcal{O}\left(\epsilon^2\right) \\ a\lambda(\kappa - \kappa^{-1}) &= 2a\lambda\delta + \mathcal{O}\left(\delta^2\right) \end{aligned}$$

Since $a\lambda > 0$, $\epsilon > 0 \Rightarrow \delta < 0$, thus $\kappa_-(-1) = 1$.

For $z \approx -1$, $(1-\kappa_-) \sim -\delta = \mathcal{O}(\epsilon) = \mathcal{O}(|z|-1) = \mathcal{O}(k\eta)$, hence*

$$|\mathbf{1} - \kappa_-(\mathbf{z})| \geq \mathbf{c}\eta\mathbf{k}.$$

Unfortunately, this is a **best possible estimate** for the denominator, only achieved on the real line (at $\tau = \pm\pi/k$). We will **not** be able to use this to get a stability bound for boundary condition (11.2.2a).

Boundary Conditions for the Leapfrog Scheme

For boundary condition (11.2.2b) we need a lower bound for $|z - \kappa_-(z)|$: to see if this quantity can be small, we set $\kappa = z$ and get

$$z - \frac{1}{z} = a\lambda \left(z - \frac{1}{z} \right);$$

since $a\lambda < 1$ (stability of the scheme), this is only satisfied when $z = \pm 1$, but from the previous analysis $\kappa_-(\pm 1) = \mp 1$, so independent of k

$$|\mathbf{z} - \kappa_-(\mathbf{z})| \geq \mathbf{c},$$

for $|z| \geq 1$.

Boundary Conditions for the Leapfrog Scheme

We are now well on our way of getting estimates for the boundary conditions (11.2.2a)/(11.2.8a) and (11.2.2b)/(11.2.8b)

$$\|v\|_{\eta,h}^2 \leq \frac{1}{c^2 k^2} \int_{-\pi/k}^{\pi/k} \frac{|\beta|^2 h}{1-|\kappa_-|^2} d\tau \qquad (11.2.11a)$$

$$\|v\|_{\eta,h}^2 \leq \frac{1}{c^2} \int_{-\pi/k}^{\pi/k} \frac{|\beta|^2 h}{1-|\kappa_-|^2} d\tau \qquad (11.2.11b)$$

with the caveat that (11.2.11a) is a best-case estimate.

It now remains to estimate the term

$$\frac{h}{1-|\kappa_-(z)|^2}.$$

Boundary Conditions for the Leapfrog Scheme

We set $z = e^{sk} = e^{i\tau}(1 + \eta k + \mathcal{O}\left(\eta^2 k^2\right))$, and consider two cases: Either $|\kappa_-(z)| = 1$ for $k\eta = 0$, or $|\kappa_-(z)| < 1$ for $k\eta = 0$. In the first case $\kappa_-(z) = e^{i\varphi}(1-\delta)$, and from

$$z - \frac{1}{z} = a\lambda\left(\kappa - \frac{1}{\kappa}\right),$$

we get

$$2i\sin\tau + 2k\eta\cos\tau + \mathcal{O}\left(k^2\eta^2\right) = a\lambda\left(2i\sin\varphi + 2\delta\cos\varphi + \mathcal{O}\left(\delta^2\right)\right),$$

so that $\sin\tau = a\lambda\sin\varphi$, and $|\sin\tau| \leq |a\lambda|$, and $|\cos\tau| \geq \sqrt{1-(a\lambda)^2}$. Thus,

$$\delta = \frac{\cos\tau}{\cos\varphi}\,k\eta + \mathcal{O}\left(k^2\eta^2\right) \geq \sqrt{1-(a\lambda)^2}\,k\eta + \mathcal{O}\left(k^2\eta^2\right).$$

Boundary Conditions for the Leapfrog Scheme

For $|\sin\tau| > a\lambda$, $|\kappa_-(z)| < 1$. Therefore, for $\eta > 0$ and $k \in (0, k_0(\eta)]$, we have $1 - |k_-(z)| \geq c_0 k\eta$, and

$$\frac{h}{1 - |\kappa_-(z)|^2} \leq \frac{h}{1 - |\kappa_-(z)|} \leq \frac{c}{\eta},$$

and now we have,

$$\|v\|^2_{\eta,h} \leq \frac{c_1^*}{k^2\eta} |\beta|^2_{\eta,h} \tag{11.2.14a}$$

$$\|v\|^2_{\eta,h} \leq \frac{c_2^*}{\eta} |\beta|^2_{\eta,h} \tag{11.2.14b}$$

where, again (11.2.14a) is a best-case estimate, so boundary condition (11.2.2a) $v_0^{n+1} = v_1^{n+1} + \beta^{n+1}$ is unstable.

(11.2.14b) shows that boundary condition (11.2.2b) $v_0^{n+1} = v_1^n + \beta^{n+1}$ is stable.

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Boundary Conditions for the Leapfrog Scheme

We have 2 more boundary conditions to analyze

$$\begin{aligned} &(11.2.2c) \qquad v_0^{n+1} = v_0^{n-1} + 2a\lambda(v_1^n - v_0^n) + \beta^{n+1} \\ &(11.2.2d) \qquad v_0^{n+1} = v_0^{n} + a\lambda(v_1^n - v_0^n) + \beta^{n+1} \end{aligned}$$

(11.2.2c) gives the equation

$$z - z^{-1} = 2a\lambda(\kappa_- - 1), \qquad (11.2.9c)$$

as the equation to be solved if there is to be a non-trivial solution to the homogeneous BVP; and (11.2.2d) gives the equation

$$z - 1 = 2a\lambda(\kappa_- - 1). \qquad (11.2.9d)$$

Boundary Conditions for the Leapfrog Scheme

Using the relation $z - z^{-1} = a\lambda\left(\kappa - \kappa^{-1}\right)$ and (11.2.9c) gives us

$$2a\lambda(\kappa_- - 1) = a\lambda\left(\kappa - \kappa^{-1}\right)$$

which has $\kappa_- = 1$ as the only solution (corresponding to $z = -1$); since there is a solution, boundary condition (11.2.2c) $v_0^{n+1} = v_0^{n-1} + 2a\lambda(v_1^n - v_0^n) + \beta^{n+1}$ is unstable.

Similarly dividing the relation (top of slide) by (11.2.9d) gives us

$$\frac{z - z^{-1}}{z - 1} = \frac{\mathbf{z+1}}{\mathbf{z}} = \frac{a\lambda(\kappa_- - \kappa_-^{-1})}{a\lambda(\kappa_- - 1)} = \frac{\kappa_- + \mathbf{1}}{\kappa_-}$$

implying that $z = \kappa_-$, however the previous analysis showed that this is not true; thus there is no solution to (11.2.9d), and therefore boundary condition (11.2.2d) $v_0^{n+1} = v_0^n + a\lambda(v_1^n - v_0^n) + \beta^{n+1}$ is stable.

Boundary Conditions for the Leapfrog Scheme

$$
\begin{aligned}
v_0^{n+1} &= v_1^{n+1} + \beta^{n+1} && \text{unstable} \\
v_0^{n+1} &= v_1^{n} + \beta^{n+1} && \text{stable} \\
v_0^{n+1} &= v_0^{n-1} + 2a\lambda(v_1^n - v_0^n) + \beta^{n+1} && \text{unstable} \\
v_0^{n+1} &= v_0^{n} + a\lambda(v_1^n - v_0^n) + \beta^{n+1} && \text{stable}
\end{aligned}
$$

Movies:

leapfrog_bc_1122a.mpg, **leapfrog_bc_1122b.mpg**,
leapfrog_bc_1122c.mpg, **leapfrog_bc_1122d.mpg**

Next time, we state some general results for the stability of boundary conditions...