Numerical Solutions to PDEs

Lecture Notes #17

Convergence Estimates for Initial Value Problems

Peter Blomgren,
⟨blomgren.peter@gmail.com⟩

Department of Mathematics and Statistics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720

http://terminus.sdsu.edu/

Spring 2018

Outline

Convergence Estimates for Initial Value Problems

We show some estimates for the convergence of solutions of finite difference schemes.

We are interested in the **rate**, $\mathcal{O}(h^r)$, of convergence of the scheme to the solution of the PDE.

Breaking News!!!

The regularity (smoothness) of the initial condition(s) impacts the convergence rate.

The discussion is restricted to one-step schemes for first-order (time) scalar equations with constant coefficients. Most of the results can (with "some work") be extended to multi-step schemes, systems, higher-order equations, and variable coefficient problems.

Truncation: From Continuous Functions to the Grid

Definition (Truncation Operator, $\mathcal{T} : L^2(\mathbb{R}) \to L^2(h\mathbb{Z})$)

The truncation operator $\mathcal{T}$ maps functions in $L^2(\mathbb{R})$ to functions on $L^2(h\mathbb{Z})$. Given $u \in L^2(\mathbb{R})$, we have

$$u(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ix\xi}\, \widehat{u}(\xi)\, d\xi,$$

and $\mathcal{T}u$ is defined as

$$\mathcal{T}u_m = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} e^{imh\xi}\, \widehat{u}(\xi)\, d\xi,$$

for each grid point $mh \in h\mathbb{Z}$. Alternatively, the Fourier transform of $\mathcal{T}u$ is given by

$$\widehat{\mathcal{T}u}(\xi) = \widehat{u}(\xi), \text{ for } |\xi| \leq \frac{\pi}{h}. \quad [\text{Lowpass Filter}]$$

Illustration: The Truncation Operator

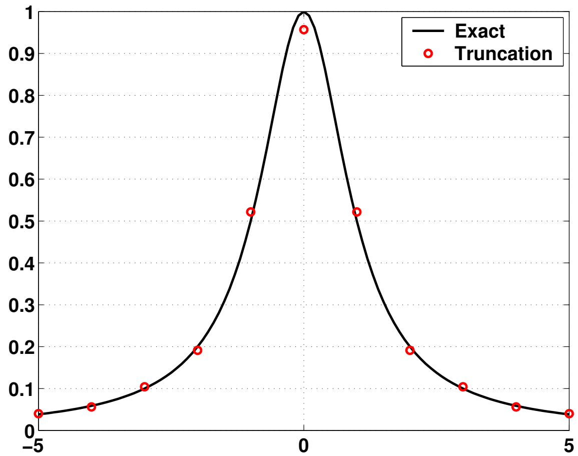


Figure: A scaled version of Runge's function: $u(x) = \frac{1}{1+x^2}$ truncated to the grid $h\mathbb{Z}$, where $h = 1.0$. The largest mismatch between $u(x_m)$ and $\mathcal{T}u_m$ is at $x_m = 0$. **Notice** that truncation is not the same thing as point-wise evaluation!

Interpolation: From the Grid to Continuous Functions

Definition (Interpolation Operator, $\mathcal{S} : L^2(h\mathbb{Z}) \to L^2(\mathbb{R})$)

The interpolation operator $\mathcal{S}$ maps functions in $L^2(h\mathbb{Z})$ to functions on $L^2(\mathbb{R})$. Given $v \in L^2(h\mathbb{Z})$, we have

$$v_m = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} e^{imh\xi}\, \widehat{v}(\xi)\, d\xi,$$

and $\mathcal{S}v(x)$ is defined as

$$\mathcal{S}v(x) = \frac{1}{\sqrt{2\pi}} \int_{-\pi/h}^{\pi/h} e^{ix\xi}\, \widehat{v}(\xi)\, d\xi,$$

for each $x \in \mathbb{R}$. Alternatively, the Fourier transform of $\mathcal{S}v(x)$ is given by

$$\widehat{\mathcal{S}v}(\xi) = \begin{cases} \widehat{v}(\xi) & \text{if } |\xi| \leq \pi/h \\ 0 & \text{if } |\xi| > \pi/h. \end{cases}$$

Interpolation Operator — Implementation

Note that in order to implement the Interpolation Operator, we either need

- The analytic expression for $\widehat{v}(\xi)$ (which is probably cheating?), or
- The expression from [LECTURE #4]: — For a grid function v_m defined for all integers coordinates m, the Fourier transform is given by

$$\widehat{v}(\xi) = \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-im\xi}\, v_m.$$

Illustration: The Interpolation Operator

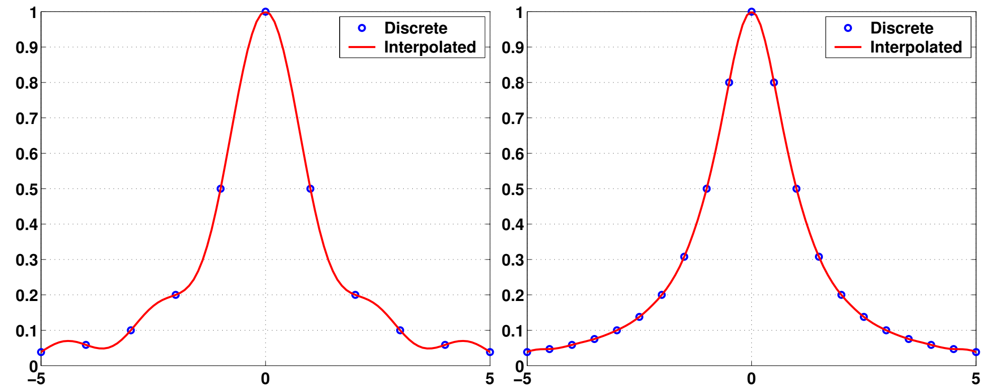


Figure: The interpolation operator applied to two grid functions, on the left $h = 1.0$, and on the right $h = 0.5$.

Evaluation: From Continuous Functions to the Grid

For completeness, we also include the Evaluation operator in our discussion

Definition (Evaluation Operator, $\mathcal{E} : F(\mathbb{R}) \to F(h\mathbb{Z})$)

The evaluation operator $\mathcal{E}$ maps functions on $\mathbb{R}$ to functions on the grid $h\mathbb{Z}$. Given $u(x)$, the evaluation operator is defined by

$$\mathcal{E}u = u(mh), \quad m \in \mathbb{Z}.$$

Usually, we use $v_m^0 = \mathcal{E}u_0 = u_0(mh)$ as the initial conditions for our numerical schemes.

Numerical Schemes for PDEs

We now consider finite difference schemes for PDEs in the form

$$\widehat{u}_t = q(\omega)\widehat{u}.$$

As initial data we take the values given by the **truncation operator**, *i.e.*

$$v_m^0 = [\mathcal{T}u_0]_m.$$

Usually, this in not what we do in practice. However, this initial data gives the "cleanest" results.

Next, we redefine the order of accuracy in such a way that we can quantify how much smoothness we must require of the initial data in order for the **order of accuracy of the solutions** (global result) of the scheme to equal the **order of accuracy of the scheme** (local result, Taylor expansion).

Order of Accuracy — Old and New

Old Defintion: Order of Accuracy

A scheme $P_{k,h}v = R_{k,h}f$ with $k = \Lambda(h)$ that is consistent with the differential equation $Pu = f$ is accurate of order r if for any smooth function $\Phi(t,x)$,

$$P_{k,h}\Phi - R_{k,h}P\Phi = \mathcal{O}(h^r).$$

Definition: Order of Accuracy

A one-step scheme for a first-order system in the form $\widehat{u}_t = q(\omega)\widehat{u}$ with $k = \Lambda(h)$ is accurate of order $[\mathbf{r}, \rho]$ if there is a constant C such that for $|h\xi| \le \pi$

$$\left| \frac{e^{kq(\xi)} - g(h\xi, k, h)}{k} \right| \le Ch^{\mathbf{r}}(1 + |\xi|)^{\rho}.$$

Old Accuracy to New Accuracy...

Theorem

If a one-step finite difference scheme for a well-posed IVP is accurate of order r according to the "old definition" then there is a non-negative integer ρ such that the scheme is accurate of order $[r, \rho]$ according to the "new definition."

Examples: Applied to the one-way wave-equation —

Scheme	Old Accuracy	New Accuracy
Lax-Friedrichs	1	$[1, 2]$
Lax-Wendroff	2	$[2, 3]$

Key Result: Numerical Solution ↔ Solution of PDE

Theorem

If the IVP for a PDE of the form $\widehat{u}_t = q(\omega)\widehat{u}$, for which the IVP is well-posed, is approximated by a stable one-step finite difference scheme that is accurate of order $[r, \rho]$ with $r \le \rho$, and the initial function is $\mathcal{T}u_0$, where u_0 is the initial function for the differential equation, then for each time T there exists a constant C_T such that

$$\|u(t_n, \circ) - \mathcal{S}v^n\| \le C_T h^r \|u_0\|_{H^\rho}$$

holds for all initial data u_0 and for each $t_n = nk$ with $0 \le t_n \le T$, and $(h, k) \in \Lambda$.

Comments

- The initial function must be in H^ρ, *i.e.* it must be smooth enough that
$$\int_{-\infty}^{\infty} \left| \frac{\partial^j}{\partial x^j} u_0(x) \right|^2 dx < \infty, \quad j = 0, 1, \dots, \rho$$
- If $u_0 \notin H^\rho$, but $u_0 \in H^p$ for some $p < \rho$ the convergence rate will be **less than** r.
- The initial condition $\mathcal{T}u_0$ is not "natural," in that we prefer to use $\mathcal{E}u_0$.
- The comparison of u with $\mathcal{S}v$ is also somewhat artificial.

We need to consider the effects of using the $\mathcal{E}u_0$ initial condition and the comparison of $u(t_n, x_m)$ with v_m^n...

Truncation ICs ⇝ Evaluation ICs

If a function just has "a little" more smoothness than being in $L^2(\mathbb{R})$, then it can be shown that the difference between the evaluation operator and the truncation operator applied to that function is bounded by the level of smoothness... Formally:

Theorem

If $\|D^\sigma u\| < \infty$ for $\sigma > 1/2$, then

$$\|\mathcal{E}u - \mathcal{T}u\|_h \le C(\sigma) h^\sigma \|D^\sigma u\|.$$

I.e. if the function has **more than half a derivative in** L_2, then the evaluation operator is well-defined, and the estimate in the theorem holds.

"Half a derivative" may seem strange in physical space, but it makes sense in the Fourier domain, where the existence of any fractional derivative can be guaranteed by

$$u \in H^\sigma(\mathbb{R}) \;\Leftrightarrow\; \int_{-\infty}^{\infty} |\xi|^{2\sigma}\, |\widehat{u}(\xi)|^2\, d\xi < \infty.$$

The Theorem, Now with Standard Initial Conditions

Theorem

*If the IVP for a PDE of the form $\widehat{u}_t = q(\omega)\widehat{u}$, for which the IVP is well-posed, is approximated by a stable one-step finite difference scheme that is accurate of order $[r, \rho]$ with $\rho > \mathbf{1/2}$, **and** $r \le \rho$, and the initial function $\mathbf{v_m^0 = u_0(mh)}$, where u_0 is **in** $\mathbf{H}^\rho$, then for each time $T > 0$ there exists a constant C_T such that*

$$\|\mathcal{E}u(t_n, \circ) - v^n\|_h \le C_T h^r \|u_0\|_{H^\rho}$$

for each $t_n = nk$ with $0 \le t_n \le T$, and $(h, k) \in \Lambda$.

$\rho > 1/2$ in the order of accuracy is not really a restriction (since we usually want $r \ge 2$, and we must have $\rho \ge r$...

However, requiring $u_0 \in H^\rho(\mathbb{R})$ with $\rho \ge 2$, can be quite restrictive.

Non-Smooth Initial Data

Clearly, **"what happens when the initial data is not smooth enough?"** is the next question to ask...

We address this question for one-step schemes for first-order equations satisfying $|e^{tq(\xi)}| \leq 1$ and $|g(h\xi)| \leq 1$.

Now, we have $\|u_0\|_{H^\rho} = \infty$ (not enough smoothness), but for some $\sigma < \rho$, $\|u_0\|_{H^\sigma} < \infty$.

The answer is...

San Diego State University

Accuracy for Non-Smooth Initial Data

Theorem

If a stable one-step finite difference scheme is accurate of order $[r, \rho]$, with $r \leq \rho$, the initial condition to the PDE is u_0 with $\|D^\sigma u_0\| < \infty$ and $\sigma < \rho$, and the initial condition for the scheme v_m^0 is $\mathcal{T} u_0$, then the solution v^n to the finite difference scheme satisfies

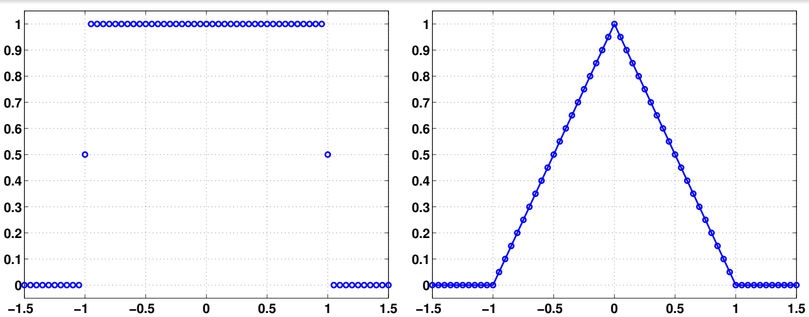
$$\|u(t_n, \circ) - \mathcal{S} v^n\| \leq C_2 h^\beta \|u_0\|_{H^\sigma},$$

where $\beta = r\sigma/\rho$. If $\sigma > 1/2$ and the initial function is either $\mathcal{E} u_0$ or $\mathcal{T} u_0$, then in addition

$$\|\mathcal{E} u^n - v^n\|_h \leq C_1 h^\beta \|u_0\|_{H^\sigma}.$$

San Diego State University

Examples: Non-Smooth Functions



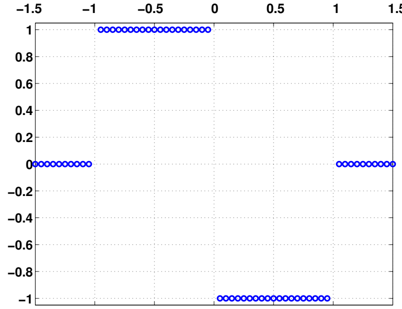
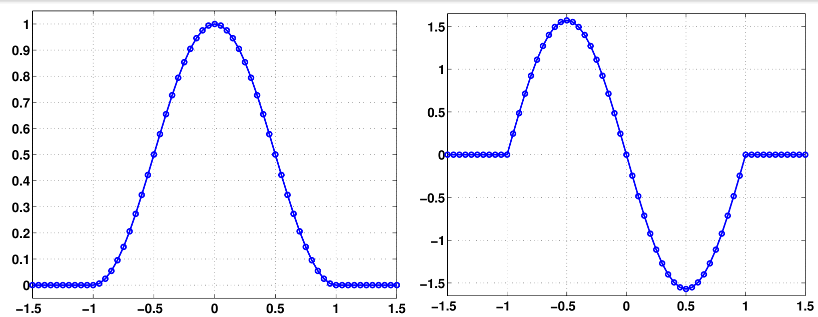


Figure: In the top-left panel we have $u_1(x) = \{1 \text{ if } |x| < 1,\ \frac{1}{2} \text{ if } |x| = 1,\ 0 \text{ otherwise}\}$; in the top-right panel we have $u_2(x) = \{1 - |x| \text{ if } |x| \leq 1,\ 0 \text{ otherwise}\}$; and in the right panel we have $\partial_x u_2(x)$. The piecewise constant function $u_1(x) \in H^{\sigma_1}$ for $\sigma_1 < 1/2$; the piecewise linear $u_2(x) \in H^{\sigma_2}$ for $\sigma_2 < 3/2$.

San Diego State University

Examples: Non-Smooth Functions



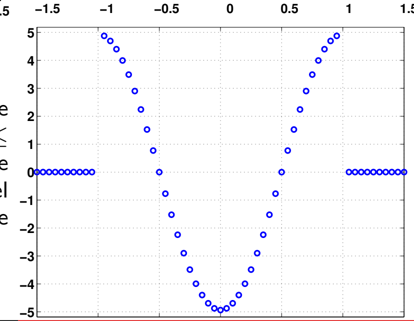
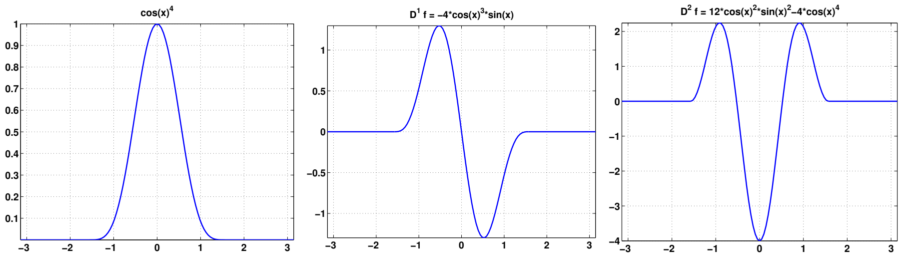


Figure: In the top-left panel we have $u_3(x) = \{\cos^2(\frac{\pi x}{2}) \text{ if } |x| \leq 1,\ 0 \text{ otherwise}\}$; in the top-right we have $\partial_x u_3(x)$, and in the right panel we have $\partial_{xx} u_3(x)$. The piecewise quadratic $u_3(x) \in H^{\sigma_3}$ for $\sigma_3 < 5/2$.

San Diego State University

Examples: Non-Smooth Functions 3 of 3



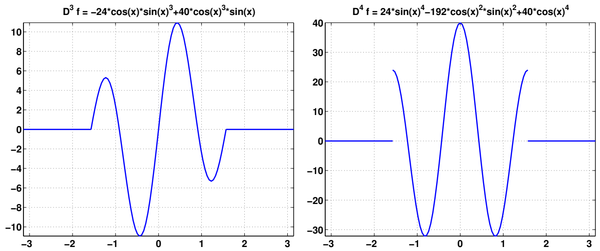


Figure: $\cos^4(x) \in H^{\sigma_4}$ for $\sigma_4 < 9/2$.

SAN DIEGO STATE UNIVERSITY

Forward-Time-Backward-Space

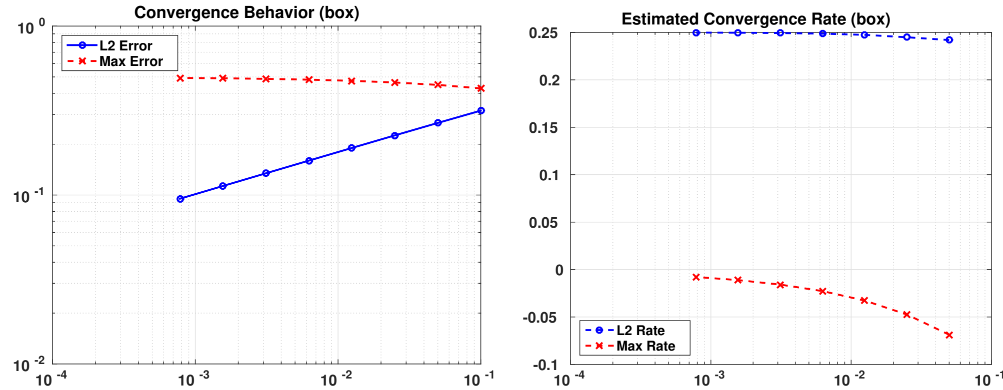


Figure: "Box" Initial condition, $\sigma < 1/2$. Observed convergence rate $\mathcal{O}\left(h^{1/4}\right)$...
$\Rightarrow$ FTBS is $\mathcal{O}\left(h^1(1+|\xi|)^2\right)$, since $(r,\sigma,\rho) = (1, 1/2, 2)$ gives $\beta = r\sigma/\rho = 1/4$.

SAN DIEGO STATE UNIVERSITY

Forward-Time-Backward-Space

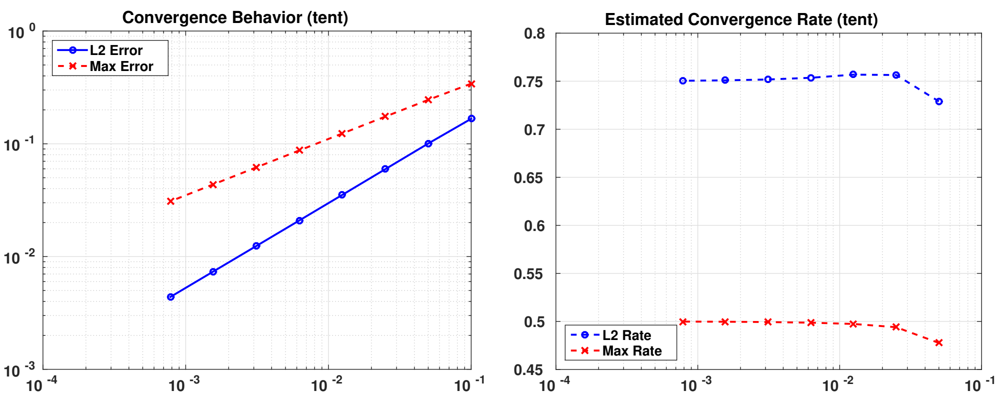


Figure: "Tent" Initial condition, $\sigma < 3/2$. Observed convergence rate $\mathcal{O}\left(h^{3/4}\right)$...
$\Rightarrow$ FTBS is $\mathcal{O}\left(h^1(1+|\xi|)^2\right)$, since $(r,\sigma,\rho) = (1, 3/2, 2)$ gives $\beta = r\sigma/\rho = 3/4$.

SAN DIEGO STATE UNIVERSITY

Forward-Time-Backward-Space

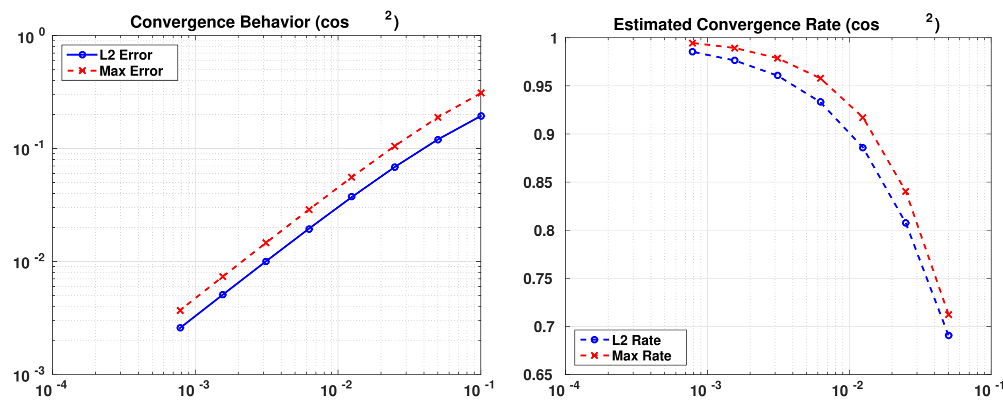


Figure: "$\cos^2(\cdot)$" Initial condition, $\sigma < 5/2$. Observed convergence rate $\mathcal{O}\left(h^1\right)$...
$(r,\sigma,\rho) = (1, 5/2, 2)$.

SAN DIEGO STATE UNIVERSITY

Parabolic Equations

The main "feature" of parabolic equations is that the initial data gets smoothed very quickly as time increases. In this scenario it seems unlikely that non-smooth initial conditions would seriously degrade the rate of convergence of finite difference solutions to solutions of the PDE.

The previous theorems are indeed much too pessimistic for parabolic problems, as long as we use dissipative schemes.

SAN DIEGO STATE UNIVERSITY

Convergence for Parabolic Equations

Theorem

If a one-step scheme that approximates an IVP for a parabolic equation is accurate of order $[r, \rho]$, for $\rho \geq r+2$, and dissipative of order 2, with $\mu = kh^{-2}$ constant, then for each time T, there is a constant C_T such that for any t with $nk = t \leq T$ and $(h,k) \in \Lambda$,

$$\|u(t,\circ) - \mathcal{S}v^n\| \leq C_T\left(1 + t^{-(\rho-1)/2}\right) h^r \, \|u_0\|,$$

and

$$\|\mathcal{E}u^n - v^n\|_h \leq C_T\left(1 + t^{-(\rho-1)/2}\right) h^r \, \|u_0\|.$$

Notice that the only requirement on u_0 is that $u_0 \in L^2(\mathbb{R})$, which does not impose any "extra" smoothness on u_0.

SAN DIEGO STATE UNIVERSITY

Recommended Reading...

10.5: The Lax-Richtmyer Equivalence Theorem

"A consistent one-step scheme for a well-posed IVP for a PDE is convergent if and only if it is stable."

10.6: Analysis of Multistep Schemes

Extension of the ideas and results in this lecture to multistep schemes. Initialization issues.

10.7: Convergence Estimates for Second Order Equations

Extension of the ideas and results in this lecture (and the multistep results) to second-order equations.

SAN DIEGO STATE UNIVERSITY