Title: Explorations in Numerical Relativity (PHYS 642) - Lecture 2

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Abstract:

1-D Wave Equation: Crank-Nicholson Scheme

- Written out in full, this is

$$\frac{\Phi_j^{n+1} - \Phi_j^n}{\triangle t} = \frac{1}{2}\left[\frac{\Pi_{j+1}^{n+1} - \Pi_{j-1}^{n+1}}{2\,\triangle x} + \frac{\Pi_{j+1}^{n} - \Pi_{j-1}^{n}}{2\,\triangle x}\right] \tag{41}$$

- Note that the Crank-Nicholson scheme immediately generalizes to any equation that can be written in the form

$$u_t = L[u] \tag{42}$$

where is L is some spatial operator. A Crank-Nicholson FDA of (42) is

$$\frac{u_j^{n+1} - u_j^n}{\triangle t} = \frac{1}{2}\left(L^h\left[u^{n+1}\right] + L^h\left[u^n\right]\right) \tag{43}$$

where L^h is some discretization of L, not necessarily second order

- Also observe that Crank-Nicholson scheme is a two-level method (couples

FDAs: Back to the Basics—Concepts & Definitions

- Will be considering the finite-difference approximation (FDA) of PDEs-0—will generally be interested in the continuum limit, where the *mesh spacing*, or *grid spacing*, usually denoted h, tends to 0.
- Because any specific calculation must necessarily be performed at some specific, *finite* value of h, we will also be (extremely!) interested in the way that our discrete solution varies as a function of h.
- Will *always* view h as the basic "control" parameter of a typical FDA.
- Fundamentally, for sensibly constructed FDAs, we expect the error in the approximation to go to 0, as h goes to 0.

Some Basic Concepts, Definitions and Techniques

- Let
$$Lu = f \tag{54}$$
denote a general *differential* system.

- For simplicity, concreteness, can think of $u = u(x, t)$ as a single function of one space variable and time,

- Discussion applies to cases in more independent variables ($u(x, y, t)$, $u(x, y, z, t)$ $\cdots$ etc.), as well as multiple *dependent* variables ($u = \mathbf{u} = [u_1, u_2, \cdots, u_n]$).

- In (54), L is some differential operator (such as $\partial_{tt} - \partial_{xx}$) in our wave equation example), u is the unknown, and f is some specified function (frequently called a *source* function) of the independent variables.

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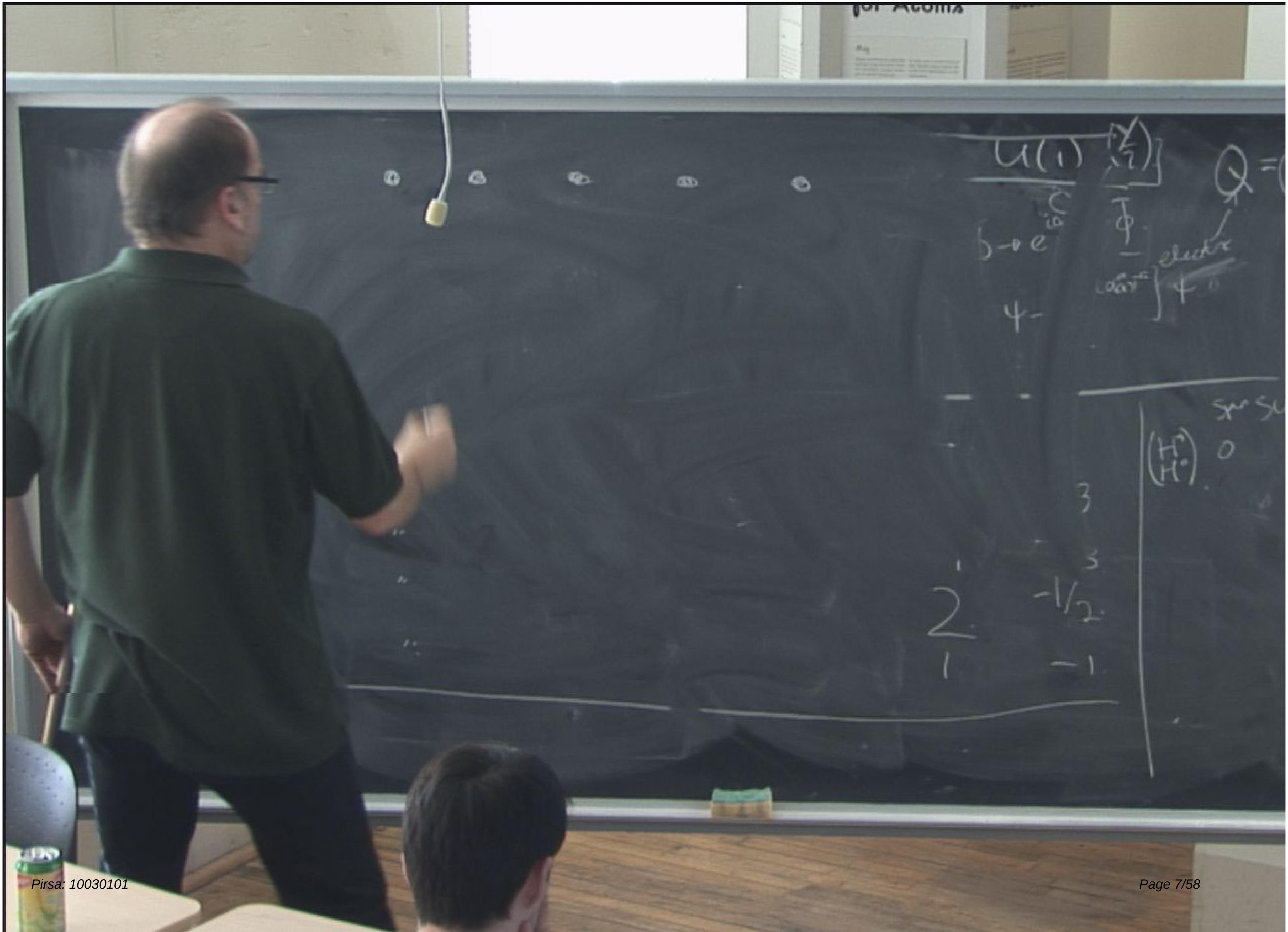
Some Basic Concepts, Definitions and Techniques

- Here and in the following, will *sometimes* be convenient use notation where a superscript h on a symbol indicates that it is discrete, or associated with the FDA, rather than the continuum.

- With this notation, we will generically denote an FDA of (54) by

$$L^h u^h = f^h \tag{55}$$

where u^h is the discrete solution, f^h is the specified function evaluated on the finite-difference mesh, and L^h is the finite-difference approximation of L.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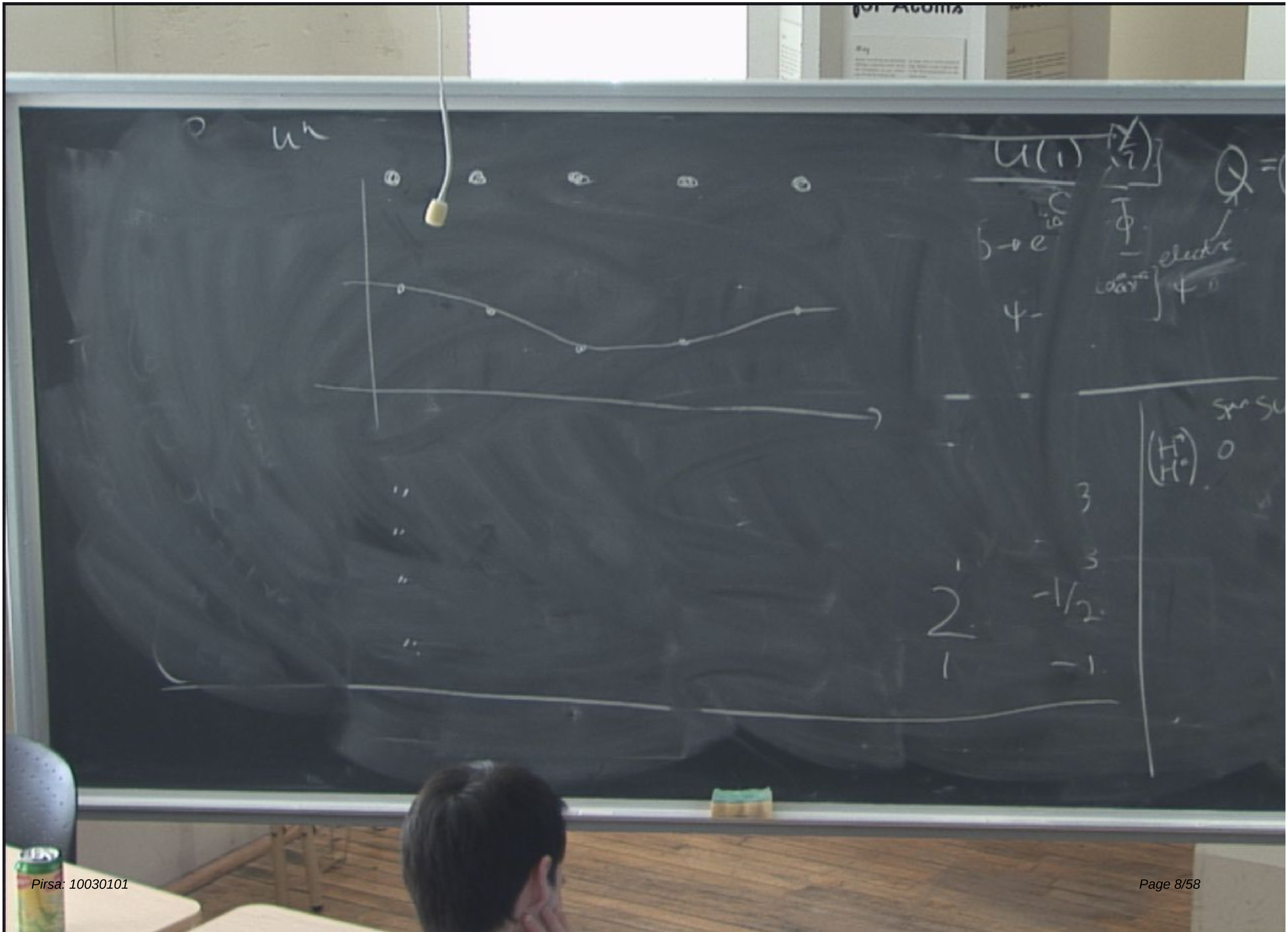

Residual

- Note that another way of writing our FDA is

$$L^h u^h - f^h = 0 \tag{56}$$

- Often useful to view FDAs in this form for following reasons
  - Have a canonical view of what it means to solve the FDA—"drive the left-hand side to 0".
  - For iterative approaches to the solution of the FDA (which are common, since it may be too expensive to solve the algebraic equations directly), are naturally lead to the concept of a *residual*.
  - Residual is simply the level of "non-satisfaction" of our FDA (and, indeed, of any algebraic expression).
  - Specifically, if $\tilde{u}^h$ is some approximation to the true solution of the FDA, u^h, then the residual, r^h, associated with $\tilde{u}^h$ is just

$$r^h \equiv L^h \tilde{u}^h - f^h \tag{57}$$

- Leads to the view of a convergent, iterative process as being one which "drives

Truncation Error

- *Truncation error*, τ^h, of an FDA is defined by

$$\tau^h \equiv L^h u - f^h \tag{58}$$

where u satisfies the continuum PDE (54).

- Note that the *form* of the truncation error can always be computed (typically using Taylor series) from the finite difference approximation and the differential equations.

Convergence

- Assume FDA is characterized by a *single* discretization scale, h,
- we say that the approximation *converges* if and only if

$$u^h \to u \quad \text{as} \quad h \to 0. \tag{59}$$

- In practice, convergence is clearly our chief concern as numerical analysts, particularly if there is reason to suspect that the solutions of our PDEs are good models for real phenomena.
- Note that this is believed to be the case for many interesting problems in general relativistic astrophysics—the two black hole problem being an excellent example.

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Consistency

- Assume FDA with truncation error τ^h is characterized by a single discretization scale, h,
- Say that the FDA is *consistent* if

$$\tau^h \to 0 \quad \text{as} \quad h \to 0. \tag{60}$$

- Consistency is obviously a necessary condition for convergence.

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Order of an FDA

- Assume FDA is characterized by a single discretization scale, h
- Say that the FDA is p-*th order accurate* or simply p-*th order* if

$$\lim_{h \to 0} \tau^h = O(h^p) \qquad \text{for some integer } p \tag{61}$$

Solution Error

- Solution error, e^h, associated with an FDA is defined by

$$e^h \equiv u - u^h \tag{62}$$

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Relation Between Truncation Error and Solution Error

- Common to tacitly assume that

$$\tau^h = O(h^p) \qquad \longrightarrow \qquad e^h = O(h^p)$$

- Assumption is often warranted, but is extremely instructive to consider *why* it is warranted and to investigate (following Richardson 1910 (!)) in some detail the *nature* of the solution error.

- Will return to this issue in more detail later.

Error Analysis and Convergence Tests

- Discussion here applies to essentially *any* continuum problem which is solved using FDAs on a *uniform* mesh structure.
- In particular, applies to the treatment of ODEs and elliptic problems
- For such problems convergence is often easier to achieve due to fact that the FDAs are typically intrinsically stable
- Also note that departures from non-uniformity in the mesh do not, in general, complete destroy the picture: however, do tend to distort it in ways that are beyond the scope of these notes.
- Difficult to overstate importance of convergence studies

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Sample Analysis: The Advection Equation

- Consider solution of *advection equation*,

$$
\begin{aligned}
u_t &= a\,u_x \quad (a > 0) \qquad 0 \le x \le 1, \quad t \ge 0 \\
u(x,0) &= u_0(x)
\end{aligned}
\tag{63}
$$

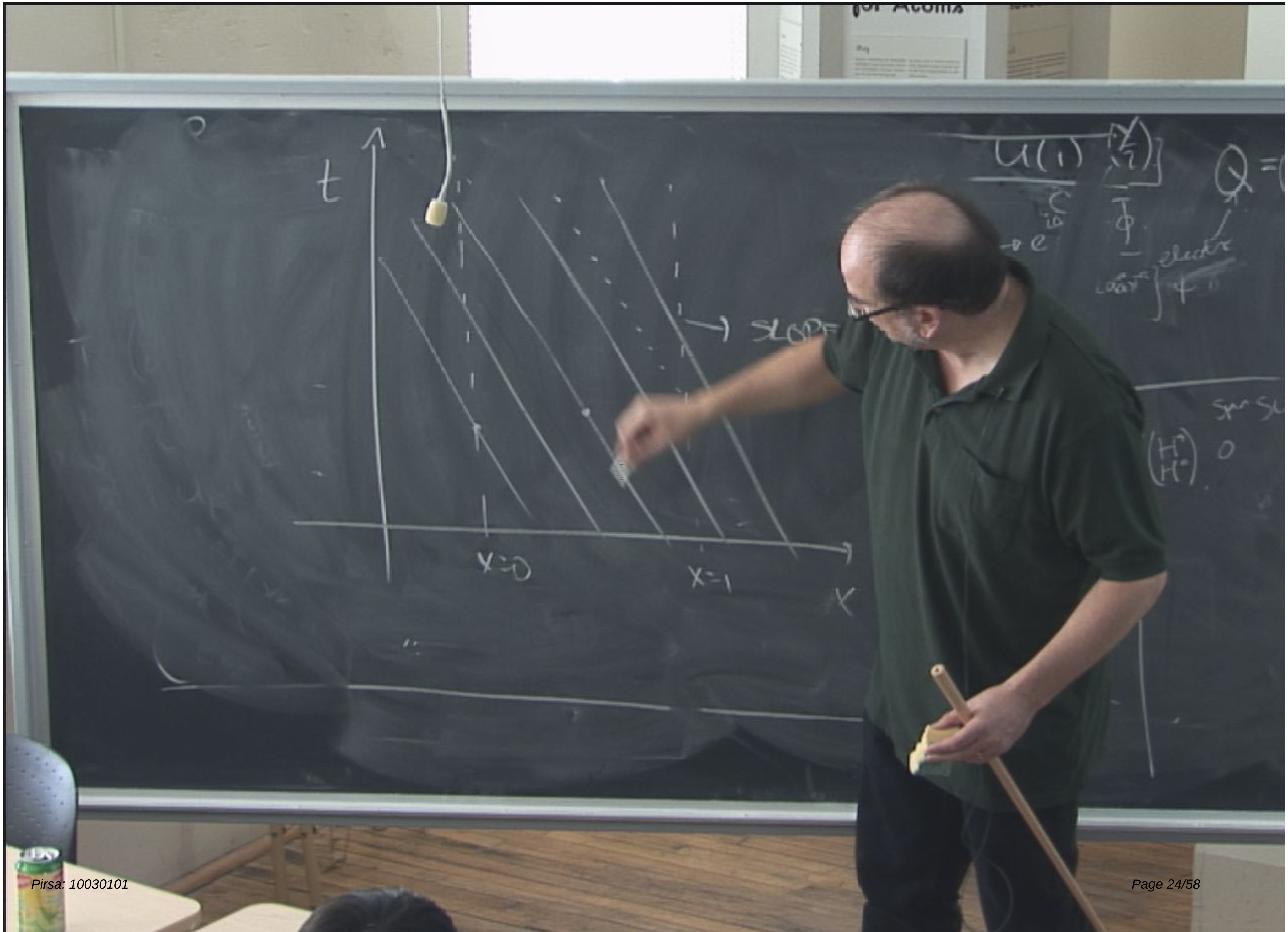
with periodic boundary conditions; i.e. $x = 0$ and $x = 1$ identified

- Note that initial conditions $u_0(x)$ must be compatible with periodicity, i.e must specify *periodic* initial data.

- Given initial data, $u_0(x)$, can immediately write down the full solution

$$
u(x,t) = u_0(x + a\,t \bmod 1) \tag{64}
$$

where mod is the modulus function which "wraps" $x + a\,t$, $t > 0$ onto the unit interval.



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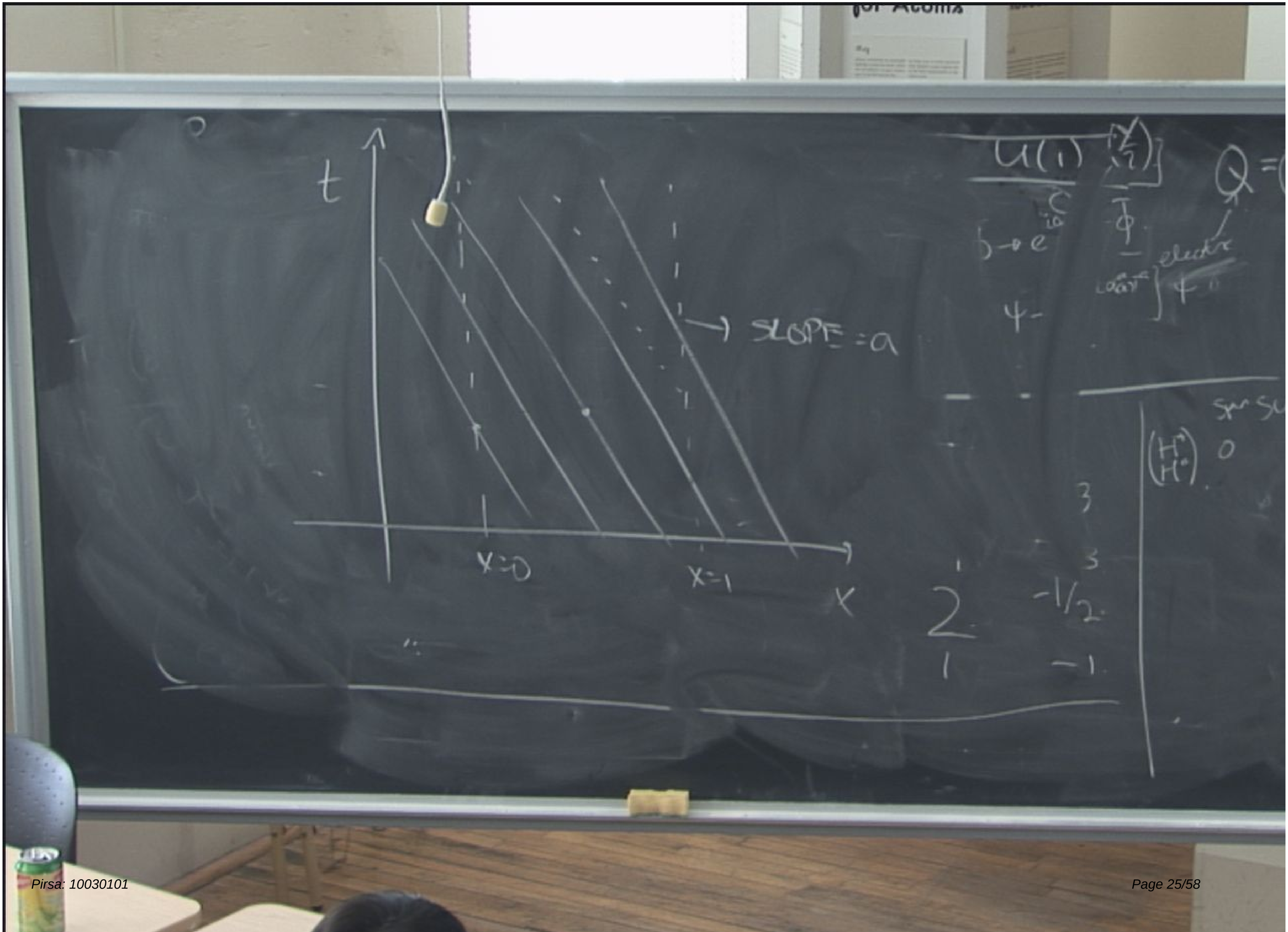
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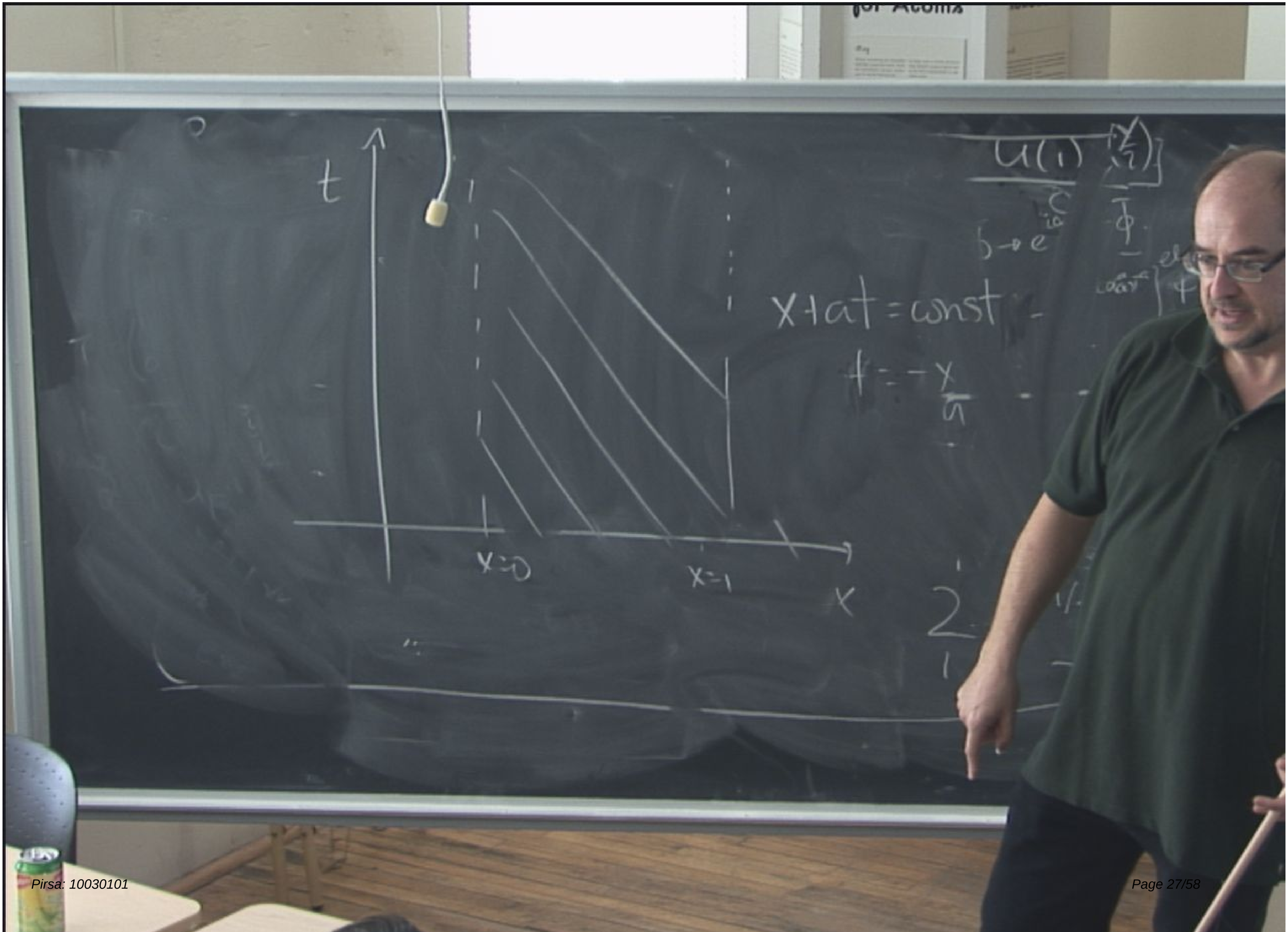
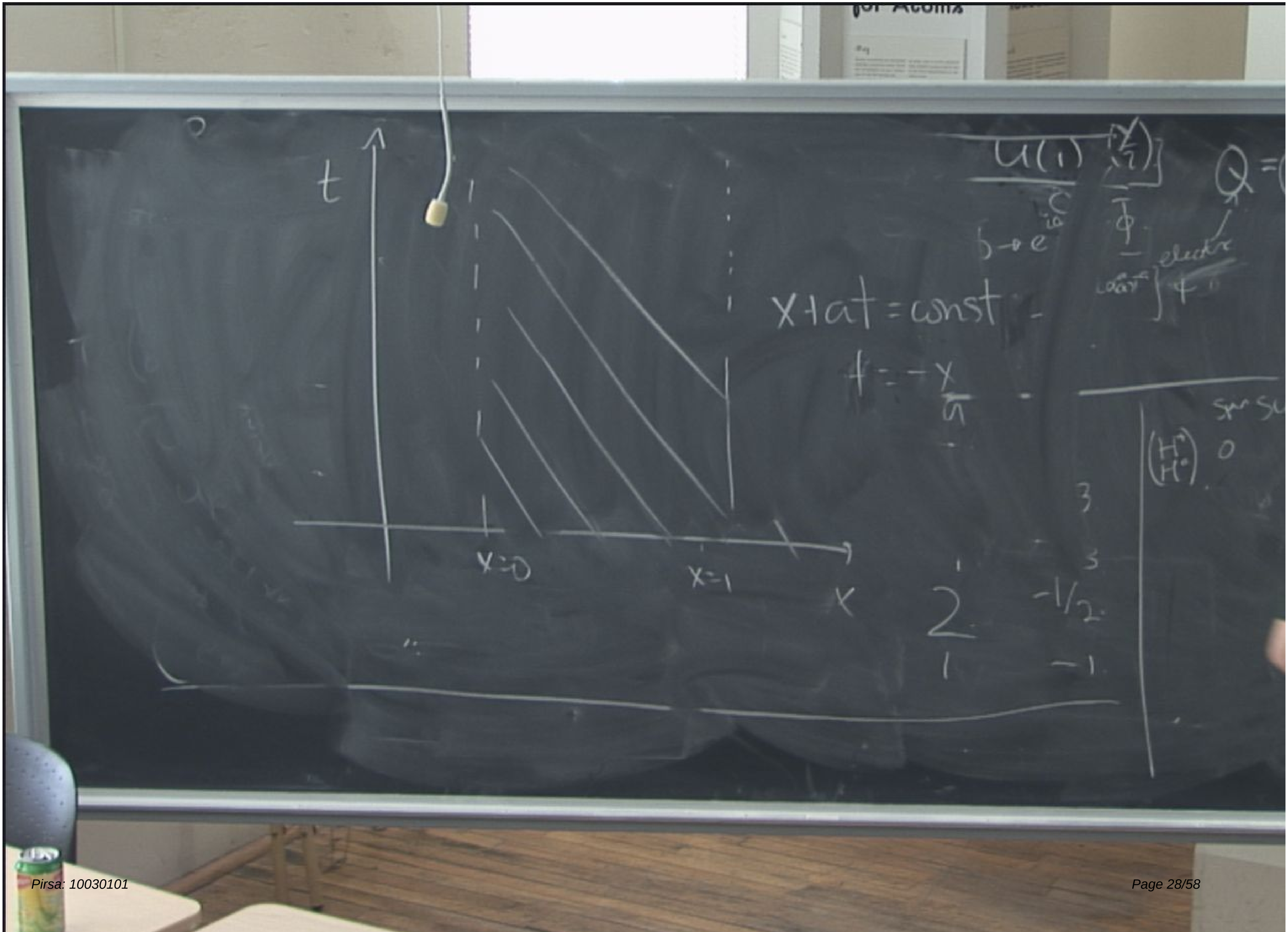

t
x
x=0
x=1
x+at=const
t = −x/a


t
x+at = const
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x=1
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U(1)
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-1/2
-1

Sample Analysis: The Advection Equation

- Due to the simplicity and solubility of this problem, will see that can perform a rather complete closed-form ("analytic") treatment of the convergence of simple FDAs of (63).

- Point of the exercise, however, is *not* to advocate parallel closed-form treatments for more complicated problems.

- Rather, key idea to be extracted that, in principle (always), and in practice (almost always, i.e. I've never seen a case where it *didn't* work, but then there's a lot of computations I haven't seen):

  The error, e^h, of an FDA is no less computable than the solution, u^h itself.

- Has widespread ramifications, one of which is that there is no excuse for publishing solutions of FDAs without error bars, or their equivalents!

Sample Analysis: The Advection Equation

- First introduce some difference operators for the usual $O(h^2)$ centred approximations of ∂_x and ∂_t:

$$D_x\, u_j^n \equiv \frac{u_{j+1}^n - u_{j-1}^n}{2\,\triangle x} \quad (65)$$

$$D_t\, u_j^n \equiv \frac{u_j^{n+1} - u_j^{n-1}}{2\,\triangle t} \quad (66)$$

- Again take

$$\triangle x \equiv h \qquad \triangle t \equiv \lambda\, \triangle x = \lambda\, h$$

and hold λ fixed as h varies, so that, as usual, FDA is characterized by the single scale parameter, h.

- First key idea behind error analysis: want to view the solution of the FDA as a *continuum* problem,

- Hence express both the difference operators and the FDA solution as asymptotic series (in h) of differential operators, and continuum functions, respectively.

Sample Analysis: The Advection Equation

- Have the following expansions for D_x and D_t:

$$D_x = \partial_x + \frac{1}{6}h^2\,\partial_{xxx} + O(h^4) \tag{67}$$

$$D_t = \partial_t + \frac{1}{6}\lambda^2 h^2\,\partial_{ttt} + O(h^4) \tag{68}$$

- In terms of the general, abstract formulation discussed earlier, have

$$L\,u - f = 0 \quad \Longleftrightarrow \quad (\partial_t - a\,\partial_x)\,u = 0$$

$$L^h u^h - f^h = 0 \quad \Longleftrightarrow \quad (D_t - a\,D_x)\,u^h = 0$$

$$L^h u - f^h \equiv \tau^h \quad \Longleftrightarrow \quad (D_t - a\,D_x)\,u \equiv \tau^h = \frac{1}{6}h^2\left(\lambda^2\partial_{ttt} - a\,\partial_{xxx}\right)u + O(h^4$$

Sample Analysis: The Advection Equation

- Second key idea behind error analysis: *The Richardson ansatz:* Appeal to L.F. Richardson's old observation (*ansatz*), that the solution, u^h, of *any* FDA which

  1. Uses a uniform mesh structure with scale parameter h,
  2. Is completely centred

  should have the following expansion in the limit $h \to 0$:

$$u^h(x,t) = u(x,t) + h^2 e_2(x,t) + h^4 e_4(x,t) + \cdots \qquad (72)$$

- Here u is the continuum solution, while e_2, e_4, $\cdots$ are (continuum) *error functions* which *do not depend on* h.

- The Richardson expansion (72), is *the* key expression from which almost all error analysis of FDAs derives.

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Sample Analysis: The Advection Equation

- In the case that the FDA is *not* completely centred, we will have to modify the *ansatz*.

- In particular, for first order schemes, will have

$$u^h(x,t) = u(x,t) + he_1(x,t) + h^2 e_x(x,t) + h^3 e_3(x,t) + \cdots \tag{73}$$

- Also note that Richardson expansion is completely compatible with the assertion discussed previously namely that

$$\tau^h = O(h^2) \quad \longrightarrow \quad e^h \equiv u - u^h = O(h^2) \tag{74}$$

- However, Richardson form contains much more information than "second-order truncation error should imply second-order solution error"

- Dictates the precise form of the h dependence of u^h.

Sample Analysis: The Advection Equation

- Given the Richardson expansion, can proceed with error analysis.
- Start from the FDA, $L^h u^h - f^h = 0$, and replace both L^h and u^h with continuum expansions:

$$
\begin{aligned}
L^h u^h = 0 \quad & \longrightarrow \quad (D_t - a\,D_x)\left(u + h^2 e_2 + \cdots\right) = 0 \\
& \longrightarrow \quad \left(\partial_t + \frac{1}{6}\lambda^2 h^2 \partial_{ttt} - a\,\partial_x - \frac{1}{6} a h^2\,\partial_{xxx} + \cdots\right) \\
& \qquad \times \left(u + h^2 e_2 + \cdots\right) = 0
\end{aligned}
$$

- Now demand that terms in above vanish order-by-order in h
- At $O(1)$ (zeroth-order), have

$$
(\partial_t - a\,\partial_x)\,u = 0 \tag{75}
$$

which is simply a statement of the *consistency* of the difference approximation.

Sample Analysis: The Advection Equation

- More interestingly, at $O(h^2)$ (second-order), find

$$(\partial_t - a\,\partial_x)\,e_2 = \frac{1}{6}\left(a\partial_{xxx} - \lambda^2\partial_{ttt}\right)u \tag{76}$$

- View u as a "known" function, then this is simply a PDE for the leading order error function, e_2.
- Moreover, the PDE governing e_2 is of *precisely* the same nature as the original PDE, $(\partial_t - a\partial_x)u = 0$

Sample Analysis: The Advection Equation

- In fact, can *solve* (76) for e_2.
- Given the "natural" initial conditions

$$e_2(x,0) = 0$$

(i.e. we initialize the FDA with the exact solution so that $u^h = u$ at $t = 0$), and defining $q(x+at)$:

$$q(x+at) \equiv \frac{1}{6} a \left(1 - \lambda^2 a^2\right) \partial_{xxx} u(x,t)$$

have

$$e_2(x,t) = t\, q(x + at \bmod 1) \tag{77}$$

- Note that, as is typical for leap-frog, we have *linear* growth of the finite difference error with time (to leading order in h).

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Sample Analysis: The Advection Equation

- Also note that analysis can be extended to higher order in h—what results, then, is an entire *hierarchy* of differential equations for u and the error functions $e_2, e_4, e_6, \cdots$.

- Indeed, useful to keep following view in mind:

  When one solves an FDA of a PDE, one is *not* solving some system which is "simplified" relative to the PDE, rather, one is solving a much *richer* system consisting of an (infinite) hierarchy of PDEs, one for each function appearing in the Richardson expansion (72).

Convergence Tests

- In general case we will not be able to solve the PDE governing u, let alone that governing e_2—otherwise we wouldn't be considering the FDA in the first place!
- Is precisely in this instance where the true power of Richardson's observation is evident!
- The key observation is that starting from (72), and computing FD solutions using the same initial data, but with differing values of h, can learn a great deal about the error in FD approximations.
- The whole game of investigating the manner in which a particular FDA converges or doesn't (i.e. looking at what happens as one varies h) is known as *convergence testing*.
- Important to realize that there are no hard and fast rules for convergence testing; rather, one tends to tailor the tests to the specifics of the problem at hand, and, being largely an empirical approach, one gains experience and intuition as one works through more and more problems.
- However, the Richardson expansion, in some form or other, *always* underlies convergence analysis of FDAs.

Convergence Tests

- A simple example of a convergence test, and one commonly used in practice is as follows.
- Compute three distinct FD solutions u^h, u^{2h}, u^{4h} at resolutions h, $2h$ and $4h$ respectively, but using the same initial data (as naturally expressed on the 3 distinct FD meshes).
- Also assume that the finite difference meshes "line up", i.e. that the $4h$ grid points are a subset of the $2h$ points which are a subset of the h points
- Thus, the $4h$ points constitute a common set of events (x_j, t^n) at which specific grid function values can be directly (i.e. no interpolation required) and meaningfully compared to one another.

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Convergence Tests

- From the Richardson *ansatz* (72), expect:

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\begin{aligned}
u^h &= u + h^2 e_2 + h^4 e_4 + \cdots \\
u^{2h} &= u + (2h)^2 e_2 + (2h)^4 e_4 + \cdots \\
u^{4h} &= u + (4h)^2 e_2 + (4h)^4 e_4 + \cdots
\end{aligned}
$$

- Then compute a quantity $Q(t)$, which will call a *convergence factor*, as follows:

$$Q(t) \equiv \frac{\|u^{4h} - u^{2h}\|_x}{\|u^{2h} - u^h\|_x} \tag{78}$$

where $\|\cdot\|_x$ is any suitable discrete spatial norm, such as the ℓ_2 norm, $\|\cdot\|_2$:

$$\|u^h\|_2 = \left(J^{-1} \sum_{j=1}^{J} \left(u_j^h\right)^2 \right)^{1/2} \tag{79}$$

- Subtractions in (78) can be taken to involve the sets of mesh points which are

Convergence Tests

- Is simple to show that, if the FD scheme is converging, then should find:

$$\lim_{h \to 0} Q(t) = 4. \tag{80}$$

- In practice, can use additional levels of discretization, $8h$, $16h$, etc. to extend this test to look for "trends" in $Q(t)$ and, in short, to convince oneself (and, with luck, others), that the FDA really *is* converging.

- Additionally, once convergence of an FDA has been established, then point-wise subtraction of any two solutions computed at different resolutions, immediately provides an estimate of the level of error in both.

- For example, if one has u^h and u^{2h}, then, again by the Richardson *ansatz* have

$$u^{2h} - u^h = \left(\left(u + (2h)^2 e_2 + \cdots\right) - \left(u + h^2 e_2 + \cdots\right)\right) \tag{81}$$

$$= 3h^2 e_2 + O(h^4) \sim 3e^h \sim \frac{3}{4} e^{2h} \tag{82}$$

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- Additionally, once convergence of an FDA has been established, then point-wise subtraction of any two solutions computed at different resolutions, immediately provides an estimate of the level of error in both.

- For example, if one has u^h and u^{2h}, then, again by the Richardson *ansatz* have

$$u^{2h} - u^h = \left(\left(u + (2h)^2 e_2 + \cdots\right) - \left(u + h^2 e_2 + \cdots\right)\right) \tag{81}$$

$$= 3h^2 e_2 + O(h^4) \sim 3e^h \sim \frac{3}{4} e^{2h} \tag{82}$$

Convergence Tests

- Is simple to show that, if the FD scheme is converging, then should find:

$$\lim_{h \to 0} Q(t) = 4. \qquad (80)$$

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Richardson Extrapolation

- *Richardson extrapolation:* Richardson's observation (72) also provides the basis for all the techniques of *Richardson extrapolation*

- Solutions computed at different resolutions are linearly combined so as to *eliminate* leading order error terms, providing more accurate solutions.

- As an example, given u^h and u^{2h} which satisfy (72), can take the linear combination

$$\bar{u}^h \equiv \frac{4u^h - u^{2h}}{3} \tag{83}$$

which, by (72), is easily seen to be $O(h^4)$, i.e. *fourth*-order accurate!

$$\begin{aligned} \bar{u}^h &\equiv \frac{4u^h - u^{2h}}{3} = \frac{4\left(u + h^2 e_2 + h^4 e_4 + \cdots\right) - \left(u + 4h^2 e_2 + 16h^4 e_4 + \cdots\right)}{3} \\ &= -4h^4 e_4 + O(h^6) = O(h^4) \end{aligned} \tag{84}$$

Independent Residual Evaluation

- Question that often arises in convergence testing: is the following:

  "OK, you've established that u^h is converging as $h \to 0$, but how do you know you're converging to u, the solution of the continuum problem?"

- Here, notion of an independent residual evaluation is very useful.

- Idea is as follows: have continuum PDE

$$Lu - f = 0 \tag{85}$$

  and FDA

$$L^h u^h - f^h = 0 \tag{86}$$

- Assume that u^h is apparently converging from, for example, computation of convergence factor (78) that looks like it tends to 4 as h tends to 0.

- However, do not know if we have derived and/or implemented our discrete operator L^h correctly.

Independent Residual Evaluation

- Note that implicit in the "implementation" is the fact that, particularly for multi-dimensional and/or implicit and/or multi-component FDAs, considerable "work" (i.e. analysis and coding) may be involved in setting up and solving the algebraic equations for u^h.

- As a check that solution *is* converging to u, consider a *distinct* (i.e. independent) discretization of the PDE:

$$\tilde{L}^h \tilde{u}^h - f^h = 0 \tag{87}$$

- Only thing needed from this FDA for the purposes of the independent residual test is the new FD operator $\tilde{L}^h$.

- As with L^h, can expand $\tilde{L}^h$ in powers of the mesh spacing:

$$\tilde{L}^h = L + h^2 E_2 + h^4 E_4 + \cdots \tag{88}$$

where E_2, E_4, $\cdots$ are higher order (involve higher order derivatives than L) differential operators.

Independent Residual Evaluation

- Now simply apply the new operator $\tilde{L}^h$ to our FDA u^h and investigate what happens as $h \to 0$.
- If u^h *is* converging to the continuum solution, u, will have

$$u^h = u + h^2 e_2 + O(h^4) \tag{89}$$

and will compute

$$\begin{aligned} \tilde{L}^h u^h &= \left(L + h^2 E_2 + O(h^4)\right)\left(u + h^2 e_2 + O(h^4)\right) && (90) \\ &= Lu + h^2(E_2 u + L e_2) && (91) \\ &= O(h^2) && (92) \end{aligned}$$

- That is $\tilde{L}^h u^h$ will be a residual-like quantity that converges quadratically as $h \to 0$.

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Independent Residual Evaluation

- Conversely, assume there is a problem in the derivation and/or implementation of $L^h u^h = f^h = 0$, but there is still convergence; i.e. for example,

$$u^{2h} - u^h \to 0 \quad \text{as} \quad h \to 0 \tag{93}$$

- Then must have something like

$$u^h = u + e_0 + h e_1 + h^2 e_2 + \cdots \tag{94}$$

where crucial fact is that the error must have an $O(1)$ component, e_0.

- In this case, will compute

$$\begin{aligned} \tilde{L}^h u^h &= \left(L + h^2 E_2 + O(h^4)\right)\left(u + e_0 + h e_1 + h^2 e_2 + O(h^4)\right) \\ &= Lu + Le_0 + hLe_1 + O(h^2) \\ &= Le_0 + O(h) \end{aligned}$$

- Unless one is *extraordinarily* (un) lucky, and Le_0 vanishes, will *not* observe the

Independent Residual Evaluation

- Instead, will see $\tilde{L}^h u^h - f^h$ tending to a *finite* ($O(1)$) value—a sure sign that something is wrong.

- Possible problem: might have slipped up in our implementation of the "independent residual evaluator", $\tilde{L}^h$

- In this case, results from test will be ambiguous at best!

- However, a key point here is that because $\tilde{L}^h$ is only used *a posterior* on a computed solution (never used to compute $\tilde{u}^h$, for example) it is a relatively easy matter to ensure that $\tilde{L}^h$ has been implemented in an error-free fashion (perhaps using symbolic manipulation facilities).

- Also, many of the restrictions commonly placed on the "real" discretization (such as stability and the ease of solution of the resulting algebraic equations) do not apply to $\tilde{L}^h$.

- Finally, note that although have assumed in the above that L, L^h and $\tilde{L}^h$ are *linear*, the technique of independent residual evaluation works equally well for non-linear problems.

Stability Analysis

- One of the most frustrating/fascinating features of FD solutions of time dependent problems: discrete solutions often "blow up"—e.g. floating-point overflows are generated at some point in the evolution

- 'Blow-ups" can sometimes be caused by legitimate (!) "bugs"—i.e. an incorrect implementation—at other times it is simply the *nature of the FD scheme* which causes problems.

- Are thus lead to consider the *stability* of solutions of difference equations

- Again consider the 1-d wave equation, $u_{tt} = u_{xx}$

- Note that it is a *linear, non-dispersive* wave equation

- Thus the "size" of the solution does *not* change with time:

$$\|u(x,t)\| \sim \|u(x,0)\|, \tag{95}$$

where $\|\cdot\|$ is an suitable norm, such as the L_2 norm: