Explorations in Gravitational Physics–Numerical Relativity

Matt Choptuik, UBC
Luis Lehner, Perimeter/Guelph
Frans Pretorius, Princeton

Perimeter Institute
Waterloo, ON
March 15–April 2, 2010

`http://bh0.phas.ubc.ca/pi-nr/www/`

Course Outline

- Solution of Classical Field Equations Using Finite Difference Techniques (Matt)

  1. Solving the wave equation using finite difference techniques
  2. $3 + 1$ approach to the Einstein equations
  3. Dynamical spherically symmetric spacetimes
  4. Spherically symmetric Einstein-Klein-Gordon Evolution
  5. Introduction to Black Hole Critical Phenomena

- General Relativistic Hydrodynamics Using Gudonov/HRSC Schemes (Luis)

  1. Mathematical structure; Linearly degenerate vs truly nonlinear eqns
  2. Burgers eqn; Godunov Methods & the Riemann problem
  3. $3 + 1$ Approach to GRHydrodynamics
  4. Stationary solutions, TOV stars & perturbations
  5. Magnetohydrodynamics & miscellaneous topics

- Topics in Numerical Relativity (Frans)

  1. Gravitational waves overview (nature in GR & sources)
  2. Newman Penrose formalism, Teukolsky equation
  3. BSSN/generalized harmonic evolution
  4. Adaptive mesh refinement (AMR)/parallel computation
  5. Miscellaneous topics: excision, apparent horizon finders, GW extraction

Week 1

Solution of Classical Field Equations Using Finite Difference Techniques

Week 1: References

- Mitchell, A. R., and D. F. Griffiths, **The Finite Difference Method in Partial Differential Equations**, New York: Wiley (1980)
- Richtmeyer, R. D., and Morton, K. W., **Difference Methods for Initial-Value Problems**, New York: Interscience (1967)
- H.-O. Kreiss and J. Oliger, **Methods for the Approximate Solution of Time Dependent Problems**, GARP Publications Series No. 10, (1973)
- Gustatsson, B., H. Kreiss and J. Oliger, **Time-Dependent Problems and Difference Methods**, New York: Wiley (1995)

Solution of Classical Field Equations Using Finite Difference Techniques

1. Solving the wave equation using finite difference techniques

Preliminaries

- Classical field equations $\equiv$ time dependent partial differential equations (PDEs)

- Can divide time-dependent PDEs into two broad classes:

  1. **Initial-value Problems (Cauchy Problems)**, spatial domain has no boundaries (either infinite or "closed"—e.g. "periodic boundary conditions")
  2. **Initial-Boundary-Value Problems**, spatial domain *finite*, need to specify boundary conditions

- **Note:** Even if *physical* problem is really of type 1, finite computational resources $\longrightarrow$ finite spatial domain $\longrightarrow$ approximate as type 2; will hereafter loosely refer to either type as an IVP.

- *Working Definition:* **Initial Value Problem**

  - State of physical system arbitrarily (usually) specified at some initial time $t = t_0$.
  - Solution exists for $t \geq t_0$; uniquely determined by equations of motion (EOM) and boundary conditions (BCs).

Preliminaries

- Approximate solution of initial value problems using *any* numerical method, including finite differencing, will always involve three key steps

  1. Complete mathematical specification of system of PDEs, including boundary conditions and initial conditions
  2. Discretization of the system: replacement of continuous domain by discrete domain, and approximation of differential equations by algebraic equations for discrete unknowns
  3. Solution of discrete algebraic equations

- Will assume that the set of PDEs has a unique solution for given initial conditions and boundary conditions, and that the solution does not "blow up" in time, unless such blow up is expected from the physics

- Whenever this last condition holds for an initial value problem, we say that the problem is well posed

- Note that this is a non-trivial issue in general relativity, since there are in practice *many* distinct forms the PDEs can take for a given physical scenario (in principle infinitely many), and not all will be well-posed in general

Why Finite Differencing?

- There are several general approaches to the numerical solution of time dependent PDEs, including

  1. Finite differences
  2. Finite volume
  3. Finite elements
  4. Spectral

- Finite difference (FD) methods are particularly appropriate when the solution is expected to be smooth (infinitely differentiable) given that the initial data is smooth

- This is the case for many classical field theories including those for a scalar (linear/nonlinear Klein Gordon), vector (electromagnetism [Maxwell]), rank-2 symmetric tensor (general relativity [Einstein])

- In cases where solutions do *not* remain smooth, even if the initial data is—as happens in compressible hydrodynamics, for example, where shocks can form—the finite volume approach is the method of choice (next week)

Why Finite Differencing?

- Accessibility: Requires a minimum of mathematical background: if you're mathematically mature enough to understand the nature of the PDEs you need to solve, you're mathematically mature enough to understand finite differencing

- Flexibility: Technique can be used for essentially any system of PDEs that has smooth solutions, irrespective of

  - Number of dependent variables (unknown functions)
  - Number of independent variables (a.k.a. "dimensionality" of the system: nomenclature "1-D" means dependence on one spatial dimension plus time, "2-D", "3-D" similarly mean dependence on two/three dimensions, plus time, respectively)
  - Nonlinearity
  - Form of equations: technique does not require that the system of equations has any particular/special form (contrast with finite volume methods where one generally wants to cast the equations in so-called conservation-law form)

Why Finite Differencing?

- Error analysis:
  - Mathematically rigorous: Quite difficult
  - Practical/empirical: Extremely straightforward—basic principle is to compute multiple solutions using same initial data and problem parameters, but differing fundamental discretization scales. Comparison of solutions provides direct estimate of error in solutions

- Adaptivity: Can combine basic method with changes in
  - Local scale of discretization
  - Order of approximation

  in order to maximize increase in solution accuracy as a function of computational work invested (e.g. adaptive mesh refinement, week 3)

- Parallelization: Due to “locality of influence” in finite difference schemes, it is relatively easy to write FD codes than run efficiently on large distributed memory computer clusters having 1000s or cores (these days 10,000s or even 100,000s!)

Why Finite Differencing?

- Sufficiency: FD techniques are often sufficient to generate solutions of acceptable accuracy, again assuming that solutions are smooth
  - Will usually not be the most efficient and/or accurate among possible approaches, but when one is looking for a solution for the first time (science vs engineering/technology), such considerations are often not very important
- Now proceed to illustration of finite difference technique through the solution of the simple and familiar 1-D wave equation

1. Mathematical Formulation

The 1-D Wave Equation

- Consider the following initial value (Cauchy) problem for the scalar function $\phi(t,x)$

$$\phi_{tt} = c^2 \phi_{xx}\,, \quad -\infty \le x \le \infty\,, \quad t \ge 0 \tag{1}$$

$$\phi(0,x) = \phi_0(x) \tag{2}$$

$$\phi_t(0,x) = \Pi_0(x) \tag{3}$$

  where c is a positive constant, we have adopted the subscript notation for partial differentiation, e.g. $\phi_{tt} \equiv \partial^2 \phi / \partial t^2$, and we wish to determine $\phi(t,x)$ in the solution domain from the initial conditions (2–3) and the governing equation (1)

- Note the following:
  - Since the spatial domain is unbounded, there are *no* boundary conditions
  - Since the equation is second order in time, two functions-worth of initial data must be specified: the initial scalar field profile, $\phi_0(x)$, and the initial time derivative, $\Pi_0(x)$
  - This system is well posed, and if the initial conditions $\phi_0(x)$ and $\Pi_0(x)$ are smooth—which we will hereafter assume—so is the complete solution $\phi(t,x)$

The 1-D Wave Equation

- Eqn. (1) is a *hyperbolic* PDE, and as such, its solutions generically describe the propagation of disturbances at some finite speed(s), which in this case is c

- Without loss of generality, we can assume that we have adopted units in which this speed satisfies $c = 1$. Our problem then becomes

$$\phi_{tt} = \phi_{xx}\,, \quad -\infty \le x \le \infty\,, \quad t \ge 0 \tag{4}$$

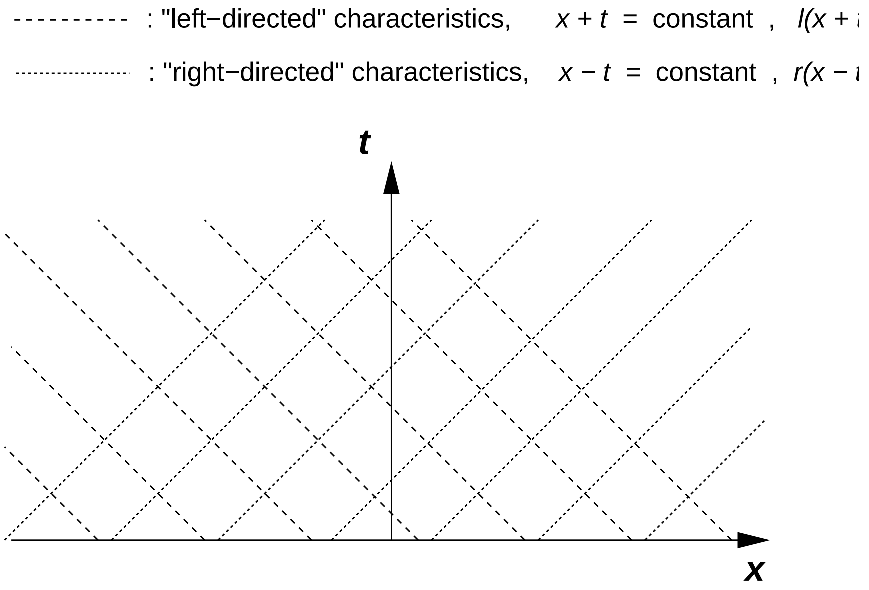
$$\phi(0,x) = \phi_0(x) \tag{5}$$

$$\phi_t(0,x) = \Pi_0(x) \tag{6}$$

- In the study of the solutions of hyperbolic PDEs, using either closed form (preferred to "analytic") or numerical approaches, the concept of characteristic is crucial

- Loosely, in a spacetime diagram, characteristics are the lines/surfaces along which information/signals propagate(s).

The 1-D Wave Equation


- - - - - : "left−directed" characteristics, x + t = constant , l(x +
········ : "right−directed" characteristics, x − t = constant , r(x −
t
x

- General solution of (4) is a superposition of an arbitrary *left-moving* profile ($v = -c = -1$), and an arbitrary *right-moving* profile ($v = +c = +1$); i.e.

$$\phi(t, x) = \ell(x + t) + r(x - t) \tag{7}$$

where

$$\begin{aligned} \ell &: \quad \text{constant along “left-directed” characteristics} \\ r &: \quad \text{constant along “right-directed” characteristics} \end{aligned}$$

The 1-D Wave Equation

- Observation provides alternative way of specifying initial values—often convenient in practice

- Rather than specifying $u(x, 0)$ and $u_t(x, 0)$ directly, specify *initial* left-moving and right-moving parts of the solution, $\ell(x)$ and $r(x)$

- Specifically, set

$$
\begin{aligned}
\phi(x,0) &= \ell(x) + r(x) && (8) \\
\phi_t(x,0) &= \ell'(x) - r'(x) \equiv \frac{d\ell}{dx}(x) - \frac{dr}{dx}(x) && (9)
\end{aligned}
$$

- For illustrative purposes will frequently take profile functions $\phi_0(x)$, $\ell(x)$, $r(x)$ to be "gaussians", e.g.

$$
\phi_0(x) = A \exp\left[- \left(\left(x - x_0 \right) / \delta \right)^2 \right] \qquad (10)
$$

where A, x_0 and δ are viewed as adjustable parameters that control the overall size/height of the profile (A), its centre point (x_0) and its effective width (δ)

2. Discretization

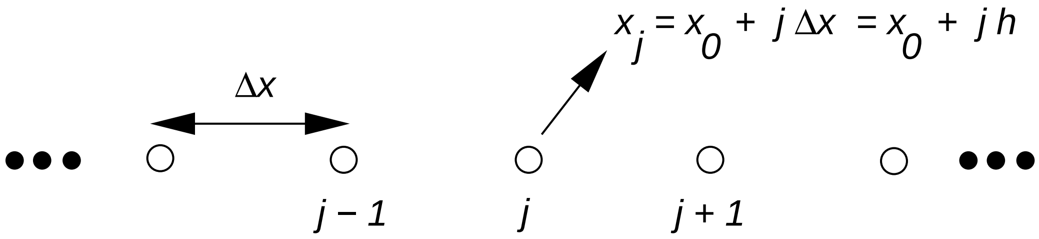
Deriving Finite Difference Formulae

- Essence of finite-difference approximation of a PDE:
  - Replacement of the continuum by a discrete lattice of grid points
  - Replacement of derivatives/differential operators by finite-difference expressions

- Finite-difference expressions (finite-difference quotients) approximate the derivatives of functions at grid points, using the grid values themselves. All operators and expressions needed here can easily be worked out using Taylor series techniques.

- Example: Consider task of approximating the first derivative $u_x(x)$ of a function $u(x)$, given a discrete set of values $u_j \equiv u(jh)$

Deriving Finite Difference Formulae



- One-dimensional, uniform finite difference mesh.

- Note that the spacing, $\Delta x = h$, between adjacent mesh points is *constant*.

- Will tacitly assume that the origin, x_0, of coordinate system is $x_0 = 0$.

Deriving Finite Difference Formulae

- Given the three values $u(x_j - h), u(x_j)$ and $u(x_j + h)$, denoted u_{j-1}, u_j, and u_{j+1} respectively, can compute an $O(h^2)$ approximation to $u_x(x_j) \equiv (u_x)_j$ as follows

- Taylor expanding, have

$$\begin{aligned}
u_{j-1} &= u_j - h(u_x)_j + \frac{1}{2}h^2(u_{xx})_j - \frac{1}{6}h^3(u_{xxx})_j + \frac{1}{24}h^4(u_{xxxx})_j + O(h^5) \\
u_j &= u_j \\
u_{j+1} &= u_j + h(u_x)_j + \frac{1}{2}h^2(u_{xx})_j + \frac{1}{6}h^3(u_{xxx})_j + \frac{1}{24}h^4(u_{xxxx})_j + O(h^5)
\end{aligned}$$

- Now seek a linear combination of u_{j-1}, u_j, and u_{j+1} which yields $(u_x)_j$ to $O(h^2)$ accuracy, i.e. we seek c_-, c_0 and c_+ such that

$$c_- \, u_{j-1} + c_0 \, u_j + c_+ \, u_{j+1} = (u_x)_j + O(h^2)$$

Deriving Finite Difference Formulae

- Results in a system of three linear equations for u_{j-1}, u_j, and u_{j+1}:

$$\begin{aligned} c_- + c_0 + c_+ &= 0 \\ -hc_- + hc_+ &= 1 \\ \frac{1}{2}h^2 c_- + \frac{1}{2}h^2 c_+ &= 0 \end{aligned}$$

which has the solution

$$\begin{aligned} c_- &= -\frac{1}{2h} \\ c_0 &= 0 \\ c_+ &= +\frac{1}{2h} \end{aligned}$$

- Thus, $O(h^2)$ FDA (finite difference approximation) for the first derivative is

$$\frac{u(x+h) - u(x-h)}{2h} = u_x(x) + O(h^2) \tag{11}$$

Deriving Finite Difference Formulae

- May not be obvious *a priori*, that the truncation error of approximation *is* $O(h^2)$
- Naive consideration of the number of terms in the Taylor series expansion which can be eliminated using 2 values (namely $u(x+h)$ and $u(x-h)$) suggests that the error might be $O(h)$.
- Fact that the $O(h)$ term "drops out" a consequence of the *symmetry*, or *centering* of the stencil: common theme in such FDA, called *centred* difference approximations
- Using same technique, can easily generate $O(h^2)$ expression for the *second* derivative, which uses the same difference stencil as the above approximation for the first derivative.

$$\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} = u_{xx}(x) + O(h^2) \qquad (12)$$

- *Exercise:* Compute the precise form of the $O(h^2)$ terms in expressions (11) and (12).

Sample FDA for the 1-D Wave Equation

- Let us consider the 1-D wave equation again, but this time on the finite spatial domain, $0 \le x \le 1$, where we will prescribe fixed (Dirichlet) boundary conditions

- Then we wish to solve

$$\begin{aligned}
\phi_{tt} &= \phi_{xx} \qquad (c = 1) \qquad 0 \le x \le 1, \quad t \ge 0 && (13) \\
\phi(0, x) &= \phi_0(x) \\
\phi_t(0, x) &= \Pi_0(x) \\
\phi(t, 0) &= \phi(t, 1) = 0 && (14)
\end{aligned}$$

- We will again require that the initial data functions, $\phi_0(x)$ and $\Pi_0(x)$ be smooth

- Moreover, in order to ensure a smooth solution everywhere, the initial values must be compatible with the boundary conditions, i.e.

$$\phi_0(0) = \phi_0(1) = \Pi_0(0) = \Pi_0(1) = 0 \qquad (15)$$

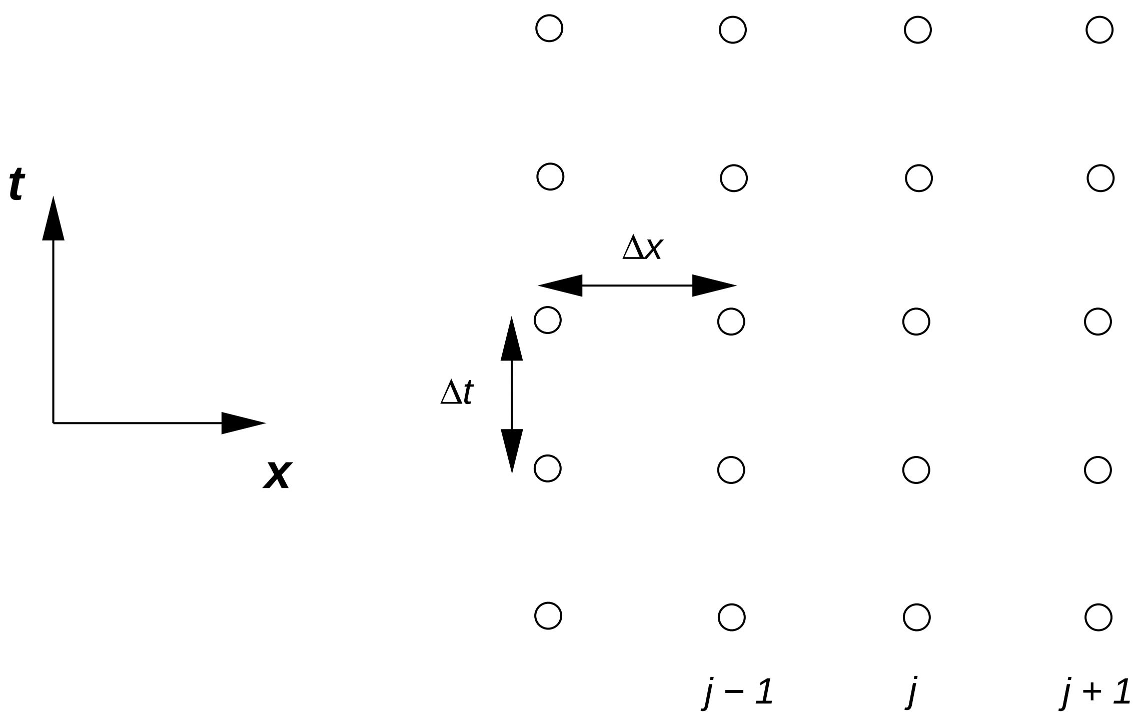
Sample FDA for the 1-D Wave Equation

- As always, we begin the discretization process by replacing the continuum solution domain with a finite difference mesh, whose typical element (point/event) we will denote by (x_j, t^n):

$$\begin{aligned} t^n &\equiv n\,\triangle t\,, \qquad n = 0, 1, 2, \cdots \\ x_j &\equiv (j-1)\,\triangle x\,, \qquad j = 1, 2, \cdots J \\ \phi^n_j &\equiv \phi(n\,\triangle t\,, (j-1)\,\triangle x\,) \\ \triangle x &= (J-1)^{-1} \\ \triangle t &= \lambda\,\triangle x \qquad \lambda \equiv \text{“Courant number”} \end{aligned}$$

- We note in passing that the quantity λ defined above is often called the Courant number or Courant factor, after the great 20th century mathematician Richard Courant who was a pioneer in the study of finite difference solutions of time dependent PDEs (in particular, in the use of FD techniques to establish existence and uniqueness of such PDEs))

Uniform Grid for 1-D Wave Equation

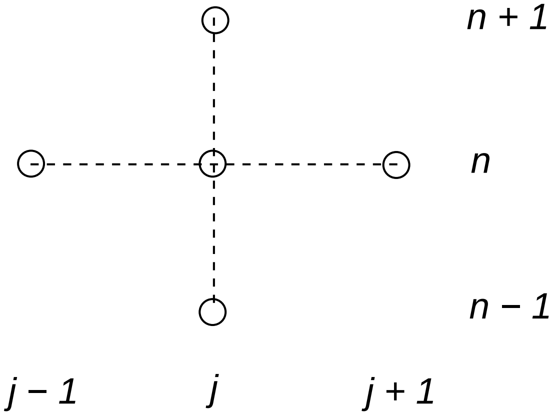


- When solving wave equations using FDAs, typically keep λ constant when $\triangle x$ varied.

- FDA will always be characterized by the *single* discretization scale, h.

$$\begin{aligned} \triangle x &\equiv h \\ \triangle t &\equiv \lambda h \end{aligned}$$

Stencil for "Standard" $O(h^2)$ Approximation of 1-D Wave Equation



FDA for 1-D Wave Equation

- Discretized Interior equation

$$
\begin{aligned}
(\triangle t)^{-2}\left(\phi_j^{n+1} - 2\phi_j^n + \phi_j^{n-1}\right) &= (\phi_{tt})_j^n + \frac{1}{12}\triangle t^{\,2}(\phi_{tttt})_j^n + O(\triangle t^{\,4}) \\
&= (\phi_{tt})_j^n + O(h^2) \\
(\triangle x)^{-2}\left(\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n\right) &= (\phi_{xx})_j^n + \frac{1}{12}\triangle x^{\,2}(\phi_{xxxx})_j^n + O(\triangle x^{\,4}) \\
&= (\phi_{xx})_j^n + O(h^2)
\end{aligned}
$$

Putting these two together, get $O(h^2)$ approximation

$$
\frac{\phi_j^{n+1} - 2\phi_j^n + \phi_j^{n-1}}{\triangle t^{\,2}} = \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\triangle x^{\,2}} \qquad j = 2, 3, \cdots, J-1 \qquad (16)
$$

- Scheme such as (16) often called a *three level scheme* since couples *three "time levels"* of data (i.e. unknowns at three distinct, discrete times t^{n-1}, t^n, t^{n+1}.

FDA for 1-D Wave Equation

- Discretized Boundary conditions

$$\phi_1^{n+1} = \phi_J^{n+1} = 0$$

- Discretized Initial conditions

  - Need to specify *two* “time levels” of data (effectively $\phi(x,0)$ and $\phi_t(x,0)$), i.e. we must specify

$$\begin{array}{lcl} \phi_j^0 & , & j = 1, 2, \cdots, J \\ \phi_j^1 & , & j = 1, 2, \cdots, J \end{array}$$

  ensuring that the initial values are compatible with the boundary conditions.

- Can solve (16) *explicitly* for ϕ_j^{n+1}:

$$\phi_j^{n+1} = 2\phi_j^n - \phi_j^{n-1} + \lambda^2 \left(\phi_{j+1}^n - 2\phi_j^n + \phi_j^{n-1}\right) \qquad (17)$$

FDA for 1-D Wave Equation

- Also note that (17) is actually a *linear system* for the unknowns $\phi_j^{n+1},\ j = 1, 2, \cdots, J$; in combination with the discrete boundary conditions can write
$$\mathbf{A}\ \phi^{n+1} = \mathbf{b} \tag{18}$$
where $\mathbf{A}$ is a *diagonal* $J \times J$ matrix and ϕ^{n+1} and $\mathbf{b}$ are vectors of length J.

- Such a difference scheme for an IVP is called an *explicit* scheme.

3. Solution of Discrete Equations

Will not discuss in any detail until later this week

1-D Wave Equation: 1st Order Form

- Let us again consider the 1-D wave equation, solved on the spatial domain $0 \le x \le 1$, and where we will delay the specification of the boundary conditions for the time being

- We have

$$\begin{aligned} \phi_{tt} &= \phi_{xx}\,, \quad 0 \le x \le 1\,, \quad t \ge 0 && (19) \\ \phi(0,x) &= \phi_0(x) && (20) \\ \phi_t(0,x) &= \Pi_0(x) && (21) \end{aligned}$$

- We rewrite (19) in a form that involves only first time derivatives by defining the following auxiliary variables

$$\begin{aligned} \Phi(t,x) &\equiv \phi_x && (22) \\ \Pi(t,x) &\equiv \phi_t && (23) \end{aligned}$$

1-D Wave Equation: 1st Order Form

- Using the commutativity of (mixed) partial derivatives, it is easy to show that (19) is equivalent to the following system

$$\begin{aligned} \Phi_t &= \Pi_x && (24) \\ \Pi_t &= \Phi_x && (25) \end{aligned}$$

- The initial conditions are then given by

$$\begin{aligned} \Phi(0,x) &= \frac{d}{dx}\phi_0(x) && (26) \\ \Pi(0,x) &= \Pi_0(x) && (27) \end{aligned}$$

- We also note that if we are not concerned with actually computing values of the scalar field, $\phi(t,x)$ itself (and in this treatment we will *not* be), then we can equally well replace (26) with

$$\Phi(0,x) = \Phi_0(x) \qquad (28)$$

i.e. we can specify the initial values of $\Phi \equiv \phi_x$ *directly*

1-D Wave Equation: 1st Order Form

- We now return to the issue of boundary conditions: we wish to illustrate a type of boundary condition which is often imposed when a (pure) initial-value problem for a hyperbolic system has been converted into an initial-boundary-value problem by truncation of the solution domain to some finite extent

- Thus, although we will solve the wave equation on the spatial domain $0 \le x \le 1$, we want the solution to approximate the one that we would get if we were able to solve on the unbounded domain $-\infty < x < \infty$

- We assume that the initial conditions represent some set of disturbances which are localized in space, well away from the boundaries $x = 0$ and $x = 1$, and that the subsequent dynamics describes the propagation of these disturbances in and away from the interval in which they are initially localized

- We recall that the general solution of the wave equation can be written in the form

$$\phi(t, x) \sim \ell(x + t) + r(x - t) \tag{29}$$

where ℓ and r are the left- and right-moving parts of the solution, respectively

1-D Wave Equation: 1st Order Form

- We further observe that it follows from (29) and the definitions of Φ and Π that $\Phi \equiv \phi_x$ and $\Pi \equiv \phi_t$ can also be written as a linear combination of right- and left-moving pieces

- The boundary condition we now wish to employ is often called a radiation condition, or Sommerfeld condition, and is equivalent to the demand that there be no incoming radiation (disturbances) at the boundaries of the solution domain

- This means that at $x = 0$ we must have only left-moving signals, so that $\Phi(t,x) \sim \Phi(x+t)$ and $\Pi(t,x) \sim \Pi(x+t)$, or

$$\begin{aligned} \Phi_t(t,0) &= \Phi_x(t,0) \qquad (30) \\ \Pi_t(t,0) &= \Pi_x(t,0) \qquad (31) \end{aligned}$$

- Similarly, at $x = 1$ we require only left-moving waves, so that $\Phi(t,x) \sim \Phi(x-t)$ and $\Pi(t,x) \sim \Pi(x-t)$, or

$$\begin{aligned} \Phi_t(t,1) &= -\Phi_x(t,1) \qquad (32) \\ \Pi_t(t,1) &= -\Pi_x(t,1) \qquad (33) \end{aligned}$$

1-D Wave Equation: Crank-Nicholson Scheme

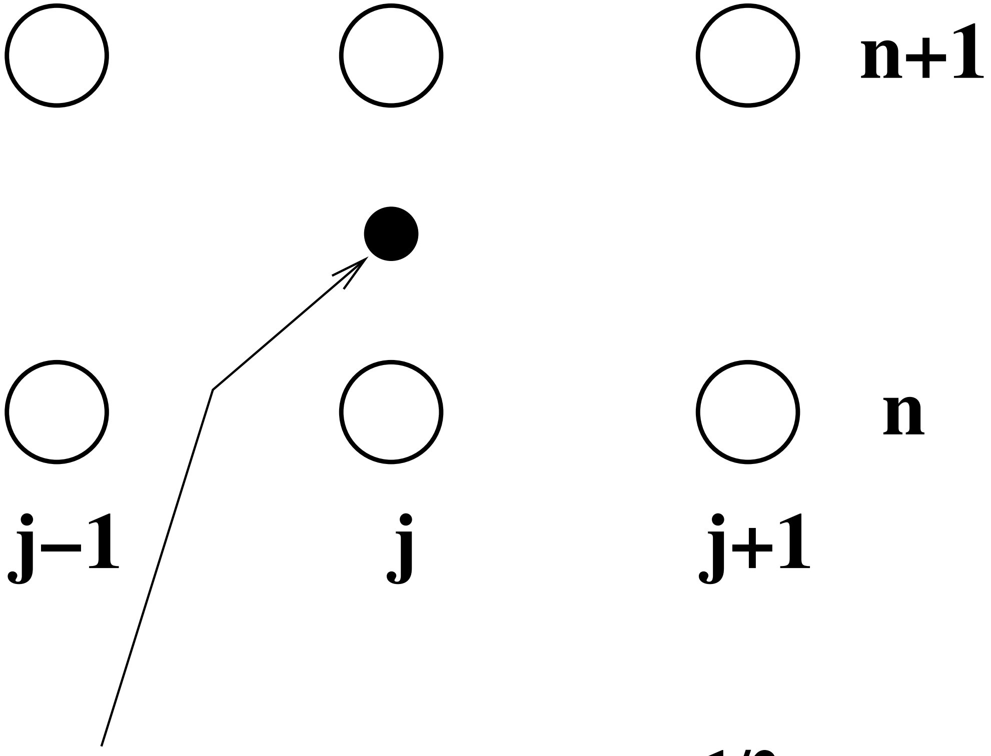
- We now discuss the Crank-Nicholson discretization scheme for the 1-D wave equation as written in the first order form defined above: variations on this theme will be used extensively in this week's lectures and tutorial sessions

- We adopt the same uniform grid structure (in space and time) as previously, but now use the stencil illustrated on the next page for our PDEs

$$\begin{aligned} \Phi_t &= \Pi_x \\ \Pi_t &= \Phi_x \end{aligned}$$

- In our description of the Crank Nicholson FDA we will also introduce the notion of finite difference operators, which provide a compact way of denoting many FDAs, and which play a central role in the special purpose programming language, RNPL, that we will use in the tutorial sessions

Stencil for $O(h^2)$ Crank-Nicholson Approximation of 1-D Wave Equation



Scheme is centred at $t^{n+1/2}$, x_j

1-D Wave Equation: Crank-Nicholson Scheme

- To illustrate the scheme, it will suffice to consider one of the two first-order PDEs that together constitute the wave equation: for specificity we focus on

$$\Phi_t = \Pi_x \tag{34}$$

- The time derivative of Φ is approximated using

$$\begin{aligned} \triangle t^{-1} \left(\Phi_j^{n+1} - \Phi_j^n \right) &= \left(\Phi_t \right)_j^{n+\frac{1}{2}} + \frac{1}{24} \triangle t^2 \left(\Phi_{ttt} \right)_j^{n+\frac{1}{2}} + O(\triangle t^4) \\ &= \left(\Phi_t \right)_j^{n+\frac{1}{2}} + O(\triangle t^2) \end{aligned} \tag{35}$$

- To approximate Π_x, we write the usual $O(h^2)$ centred approximation for the first derivative in operator form as

$$D_x \Pi_j^n \equiv (2 \triangle x)^{-1} \left(\Pi_{j+1}^n - \Pi_{j-1}^n \right) \tag{36}$$

$$D_x = \partial_x + \frac{1}{6} \triangle x^2 \partial_{xxx} + O(\triangle x^4) \tag{37}$$

1-D Wave Equation: Crank-Nicholson Scheme

- We further introduce the (forward) time-averaging operator, μ_t:

$$\begin{aligned} \mu_t \, u_j^n &\equiv \frac{1}{2}\left(u_j^{n+1} + u_j^n\right) = u_j^{n+\frac{1}{2}} + \frac{1}{8}\triangle t^{\,2}\,(u_{tt})_j^{\,n+\frac{1}{2}} + O(\,\triangle t^{\,4}) & (38) \\ \mu_t &= \left[I + \frac{1}{8}\triangle t^{\,2}\,\partial_{tt} + O(\,\triangle t^{\,4}) \right]_{t=t^{n+1/2}} & (39) \end{aligned}$$

  where I is the identity operator.

- Assuming that $\triangle t = O(\,\triangle x\,) = O(h)$, it is easy to show (exercise) that

$$\mu_t\left[D_x\,\Pi_j^n\right] = (\Pi_x)_j^{\,n+\frac{1}{2}} + O(h^2)$$

- Putting above results together, we get the $(O(h^2))$ Crank-Nicholson approximation of $\Phi_t = \Pi_x$

$$\frac{\Phi_j^{n+1} - \Phi_j^n}{\triangle t} = \mu_t\left[D_x\,\Pi_j^n\right] \qquad (40)$$

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 unknowns at two discrete time steps)

1-D Wave Equation: Crank-Nicholson Scheme

- The difference equations (40) can be applied at grid points labelled by $j = 2, 3, \ldots, J-1$ (the interior points)

- For $j = 1$ and $j = J$ we use discretized versions of the radiation (Sommerfeld) boundary conditions

$$\begin{aligned} \Phi_t(t,0) &= \Phi_x(t,0) && (44) \\ \Phi_t(t,1) &= -\Phi_x(t,1) && (45) \end{aligned}$$

- The time derivatives are approximated as previously, and for the space derivatives we use second order, forward and backward (“off-centred”) difference approximations defined by

$$\begin{aligned} D_x^F \, \Phi_j^n &\equiv (2\,\triangle x\,)^{-1} \left(-3\Phi_j^n + 4\Phi_{j+1}^n - \Phi_{j+2}^n \right) && (46) \\ D_x^F &= \partial_x + O(\,\triangle x\,^2) \quad \text{exercise} && (47) \\ D_x^B \, \Phi_j^n &\equiv (2\,\triangle x\,)^{-1} \left(3\Phi_j^n - 4\Phi_{j-1}^n + \Phi_{j-2}^n \right) && (48) \\ D_x^B &= \partial_x + O(\,\triangle x\,^2) \quad \text{exercise} && (49) \end{aligned}$$

1-D Wave Equation: Crank-Nicholson Scheme

- Employing the time-averaging operator, μ_t, defined previously, the FDAs for the outgoing-radiation boundary conditions are

$$
\begin{aligned}
\frac{\Phi_j^{n+1} - \Phi_j^n}{\triangle t} &= \mu_t \left[D_x^F \, \Phi_j^n \right] \quad j = 1 && (50) \\
\frac{\Phi_j^{n+1} - \Phi_j^n}{\triangle t} &= -\mu_t \left[D_x^B \, \Phi_j^n \right] \quad j = J && (51)
\end{aligned}
$$

- Finally, in our `RNPL` implementation of this scheme, we will set initial data of the form

$$
\begin{aligned}
\Phi_j^0 &= A \exp \left[- \left((x - x_0) / \delta \right)^2 \right] && (52) \\
\Pi_j^0 &= \sigma \Phi_j^0 && (53)
\end{aligned}
$$

where $\sigma = -1, 0, 1$ will generate purely left-moving, left-moving/right-moving (time symmetric) or purely right-moving data, respectively, and where A, x_0 and δ are adjustable parameters of the gaussian pulse shape

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.

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.

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 the residual to 0".

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.

Consistency

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

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

- Consistency is obviously a necessary condition for convergence.

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

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

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

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.

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:

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

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

- Again take

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

  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

$$\begin{aligned}
L\,u - f = 0 \quad &\Longleftrightarrow \quad (\partial_t - a\,\partial_x)\,u = 0 \\
L^h u^h - f^h = 0 \quad &\Longleftrightarrow \quad (D_t - a\,D_x)\,u^h = 0 \\
L^h u - f^h \equiv \tau^h \quad &\Longleftrightarrow \quad (D_t - a\,D_x)\,u \equiv \tau^h = \frac{1}{6} h^2 \left(\lambda^2 \partial_{ttt} - a\,\partial_{xxx}\right) u + O(h^4)
\end{aligned}$$

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 $h \to 0$:

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

- 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.

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:

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

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

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

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).

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.

Convergence Tests

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

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

- 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 common between u^{4h} and u^{2h}, and between u^{2h} and u^h.

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

$$\begin{aligned} u^{2h} - u^h &= \left(\left(u + (2h)^2 e_2 + \cdots\right) - \left(u + h^2 e_2 + \cdots\right)\right) \qquad (81) \\ &= 3h^2 e_2 + O(h^4) \;\sim\; 3e^h \;\sim\; \frac{3}{4} e^{2h} \qquad (82) \end{aligned}$$

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!

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

Richardson Extrapolation

- When it works, Richardson extrapolation has an almost magical quality about it
- However, generally have to start with fairly accurate (on the order of a few %) solutions in order to see the dramatic improvement in accuracy suggested by (84).
- Still a struggle to achieve that sort of accuracy (i.e. a few %) for *any* computation in many areas of numerical relativity/astrophysics *and* keep the error smooth (which is necessary for Richardson extrapolation to be effective)
- Thus, techniques based on Richardson extrapolation have not had a major impact in this context, although higher-order $O(h^4)$, $O(h^6)$ etc. finite difference methods *are* increasingly common for the vacuum Einstein equations

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 $h \to 0$.

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

$$u^h = u + e_0 + he_1 + h^2 e_2 + \cdots \tag{94}$$

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

- In this case, will compute

$$\begin{aligned}
\tilde{L}^h u^h &= \left(L + h^2 E_2 + O(h^4)\right)\left(u + e_0 + he_1 + h^2 e_2 + O(h^4)\right) \\
&= Lu + Le_0 + hLe_1 + O(h^2) \\
&= Le_0 + O(h)
\end{aligned}$$

- Unless one is *extraordinarily* (un) lucky, and $L\, e_0$ vanishes, will *not* observe the expected convergence

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:

$$\|u(x,t)\| \equiv \left(\int_0^1 u(x,t)^2\,dx\right)^{1/2} . \tag{96}$$

Stability Analysis

- Will use the property captured by (95) as working definition of stability.

- In particular, if you believe (95) is true for the wave equation, then you believe the wave equation is stable.

- Fundamentally, if FDA approximation *converges*, then expect the same behaviour for the difference solution:

$$\|u_j^n\| \sim \|u_j^0\| \,. \tag{97}$$

- FD solution constructed by *iterating in time*, generating

$$u_j^0,\ u_j^1,\ u_j^2,\ u_j^3,\ u_j^4,\ \cdots$$

in succession, using the FD equation

$$u_j^{n+1} = 2u_j^n - u_j^{n-1} + \lambda^2 \left(u_{j+1}^n - 2u_j^n + u_{j-1}^n \right) \,.$$

Stability Analysis

- *Not* guaranteed that (97) holds for all values of $\lambda \equiv \triangle t \,/\, \triangle x$.

- For certain λ, have
$$\|u_j^n\| \gg \|u_j^0\| \,,$$
and for those λ, $\|u^n\|$ *diverges* from u, even (especially!) as $h \to 0$—that is, the difference scheme is *unstable*.

- For many wave problems (including all linear problems), given that a FD scheme is *consistent* (i.e. so that $\hat{\tau} \to 0$ as $h \to 0$), *stability is the necessary and sufficient condition for convergence* (Lax's theorem).

Heuristic Stability Analysis

- Write general time-dependent FDA in the form

$$\mathbf{u}^{n+1} = \mathbf{G}[\mathbf{u}^n] \, , \tag{98}$$

- $\mathbf{G}$ is some *update operator* (linear in our example problem)
- $\mathbf{u}$ is a column vector containing sufficient unknowns to write the problem in first-order-in-time form.
- Example: introduce new, auxiliary set of unknowns, v^n_j, defined by

$$v^n_j = u^{n-1}_j \, ,$$

then can rewrite differenced-wave-equation (16) as

$$\begin{aligned} u^{n+1}_j &= 2u^n_j - v^n_j + \lambda^2 \left(u^n_{j+1} - 2u^n_j + u^n_{j-1} \right) \, , && (99) \\ v^{n+1}_j &= u^n_j \, , && (100) \end{aligned}$$

Heuristic Stability Analysis

- Thus with

  $$\mathbf{u}^n = [u_1^n, v_1^n,\ u_2^n, v_2^n,\ \cdots\ u_J^n, v_J^n]\,,$$

  (for example), (99-100) is of the form (98).

- Equation (98) provides compact way of describing the FDA solution.

- Given initial data, $\mathbf{u}^0$, solution after n time-steps is

  $$\mathbf{u}^n = \mathbf{G}^n \mathbf{u}^0\,, \qquad (101)$$

  where $\mathbf{G}^n$ is the n-th power of the matrix $\mathbf{G}$.

- Assume that $\mathbf{G}$ has a complete set of orthonormal eigenvectors

  $$\mathbf{e}_k, \quad k = 1, 2, \cdots J\,,$$

  and corresponding eigenvalues

  $$\mu_k, \quad k = 1, 2, \cdots J\,,$$

Heuristic Stability Analysis

- Thus have

$$\mathbf{G}\,\mathbf{e}_k = \mu_k\,\mathbf{e}_k, \quad k = 1, 2, \cdots J\,.$$

- Can then write initial data as (spectral decomposition):

$$\mathbf{u}^0 = \sum_{k=1}^{J} c_k^0\,\mathbf{e}_k\,,$$

where the c_k^0 are coefficients.

- Using (101), solution at time-step n is

$$\begin{aligned} \mathbf{u}^n &= \mathbf{G}^n \left(\sum_{k=1}^{J} c_k^0\,\mathbf{e}_k \right) && (102) \\ &= \sum_{k=1}^{J} c_k^0\,(\mu_k)^n\,\mathbf{e}_k\,. && (103) \end{aligned}$$

Heuristic Stability Analysis

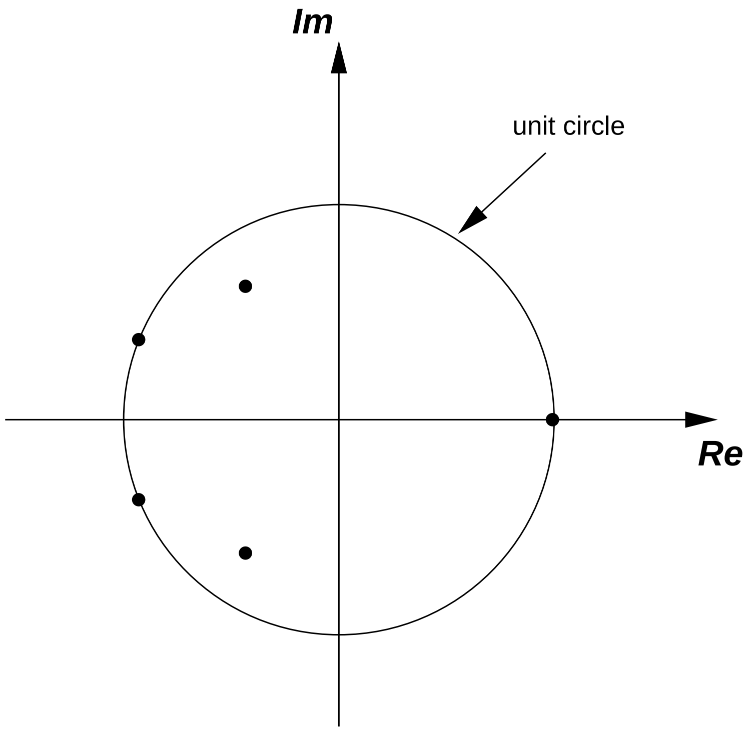
- If difference scheme is to be stable, must have

$$|\mu_k| \leq 1 \qquad k = 1, 2, \cdots J \tag{104}$$

(Note: μ_k will be complex in general, so $|\mu|$ denotes the complex modulus, $|\mu| \equiv \sqrt{\mu\mu^\star}$).

- Geometric interpretation: eigenvalues of the update matrix must lie on or within the unit circle

Heuristic Stability Analysis



- Schematic illustration of location in complex plane of eigenvalues of update matrix **G**.

- In this case, all eigenvalues (dots) lie on or within the unit circle, indicating that the corresponding finite difference scheme is stable.

Von-Neumann (Fourier) Stability Analysis (Summary)

- Von-Neumann (VN) stability analysis based on the ideas sketched above
- Assumes that difference equation is linear with constant coefficients, periodic boundary conditions boundary conditions are periodic
- Can then use Fourier analysis: difference operators in real-space variable $x \longrightarrow$ algebraic operations in Fourier-space variable k
- VN applied to wave-equation example shows that must have

  $$\lambda \equiv \frac{\triangle t}{\triangle x} \le 1\,,$$

  for stability of scheme (16).
- Condition is often called the CFL condition—after Courant, Friedrichs and Lewy who derived it in 1928
- This type of instability has "physical" interpretation, often summarized by the statement *the numerical domain of dependence of an explicit difference scheme must contain the physical domain of dependence.*