Introduction to Numerical Field Theory I

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Overview / Summary

- Today
  - Discretization
  - Brief overview of finite difference approximation, including rationale for its adoption, given other available discretization techniques
  - Brief discussion of derivation of FDAs
  - Prototype classical nonlinear field theory
    - Nonlinear Klein Gordon equation
      - Spherical symmetriy
      - Solution using FDA

Discretization

- In numerical analysis one can often approximately solve continuum systems—typically differential equations—through a process known as discretization

- In the continuum case, the unknown function(s), for example, will typically be defined on some interval $0 \le t \le t_{\max}$ of the real number line and will thus constitute an infinite number of values (the same infinity as that associated with the entire real number line, or any interval thereof)

- In the discrete case, the unknown function will typically be defined only at a finite (or at most countable, i.e. having the infinity of the integers) number of values $t_n,\ n = 1, 2, \ldots, n_t$

Discretization (continued)

- 1st FUNDAMENTAL PURPOSE OF DISCRETIZATION
  - Reduce infinite number of “degrees of freedom” to finite number
- WHY?
  - Computational resources are finite
- 2nd FUNDAMENTAL PURPOSE OF DISCRETIZATION
  - Replace differential equations with algebraic equations
- WHY?
  - Can solve algebraic equations (linear or non-linear) computationally

Finite Difference Approximation

- Finite difference approximation (FDA) is one specific approach to the discretization of continuum systems such as differential equations
- We choose to focus on it here for several reasons
  - Accessibility (requires a minimum of mathematical background)
  - Generality (can be applied to virtually any system of differential equations)
  - Simplicity (relatively easy to apply in many cases)
  - Sufficiency (for many problems, produces results of acceptable accuracy with reasonable computational cost)
- Other important approaches that we will not discuss
  - Finite element approximation
  - Spectral approximation

Finite Difference Approximation (continued)

- BASIC IDEA
  - Derivatives are replaced with algebraic “difference quotients”, very similar in spirit to algebraic expressions that are encountered in the standard definition of a derivative in calculus

$$\frac{df(x)}{dx} \equiv f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

  - In the above

$$\frac{f(x+h) - f(x)}{h}$$

    is a finite difference approximation of $f'(x)$

Key Steps in Solution of Differential Systems Using FDA

1. Formulate precise and complete mathematical description of the problem to solve, including
   - Specification of independent variables (coordinates)

     $t,\ x,\ (t,x),\ (t,x,y),\ \ldots$

   - Specification of solution domain in terms of ind. Vars.

     $0 \le t \le t_{max},\ [0 \le t \le t_{max},\ 0 \le x \le 1],\ \ldots$

   - Specification of dependent variables and their type (e.g. scalar or vector, real or complex ...)

     $u(t),\ f(x),\ \psi(t,x),\ u(x,y),\ \vec{r}_i(t),\ \ldots$

   - Specification of differential equations governing dependent variables

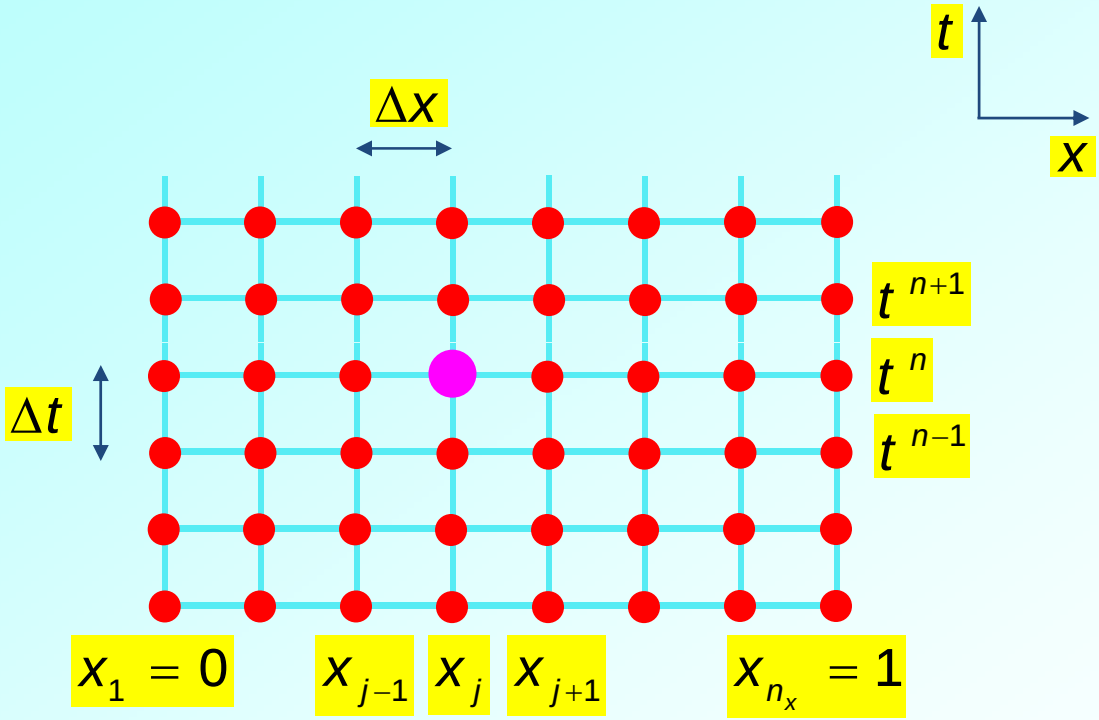
   - Specification of sufficient initial and/or boundary conditions to ensure that the problem has a unique solution.

Key Steps in Solution of Differential System Using FDA

2. Discretization: Step 1

- Define finite difference grid (mesh, lattice) that replaces continuum solution domain with finite set of grid points at which discrete solution is to be computed
- Mesh will be characterized be a set of spacings between adjacent points in each of the coordinate directions; in this course will typically assume that these are constants (so meshes will be called uniform)
- Mesh spacings constitute fundamental parameters that control accuracy of particular FDA
- Working assumption is that in the limit that the spacings tend to 0, the finite difference solution will converge to the continuum solution

Schematic of Typical Uniform Finite Difference Mesh



Notation : $f_j^n \equiv f(n\Delta t,\ j\Delta x)$

Terminology : $f_j^n \equiv$ grid function

Key Steps in Solution of Differential System Using FDA

3. Discretization: Step 2

   - Replace all derivatives—including any involved in the initial or boundary conditions—with finite difference approximations
   - This process yields a set of algebraic equations (linear or non-linear) for the discrete unknowns

4. Solution of algebraic equations

   - The solution of the algebraic equations is then accomplished computationally
   - Depending on the nature of the differential equations as well as the FDA used the sophistication/complexity of the algorithms required to do this efficiently can vary widely

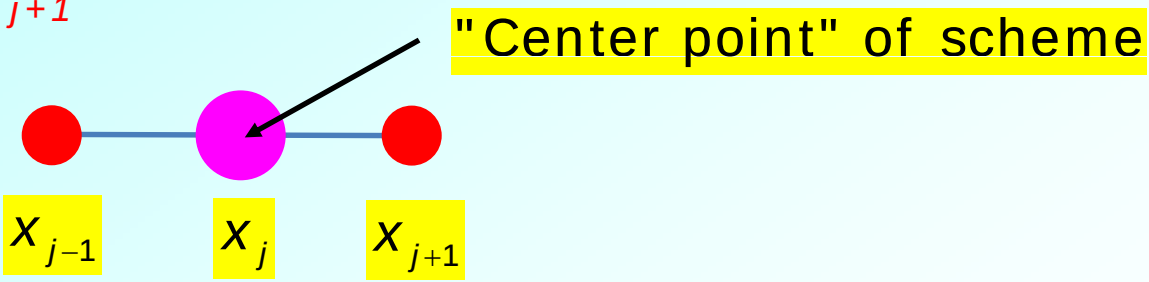
Key Steps in Solution of Differential System Using FDA

5. Convergence testing / error analysis

   - Extremely important part of solution process (difficult to overemphasize importance)
   - Basic idea is to repeat calculations using same basic problem parameters, initial data, boundary conditions etc., but with varying mesh sizes (grid spacings)
   - Investigation of behaviour of finite difference solution as a function of mesh size allows us to estimate (and ultimately control) the accuracy of the solution, and to establish that the solution is converging to the desired continuum limit

Derivation of FDAs

- Straightforward (“brute-force”) approach: Taylor series
- Example: Consider derivation of FDA for second derivative of a function, given grid function value, f_j , and nearest neighbors , f_{j-1} and f_{j+1}



- Taylor expand about $x = x_j$ with $x_{j+1} - x_j = h$

$$f_{j-1} = f(x_j - h) = f_j - h\left[f'\right]_j + \frac{1}{2}h^2[f'']_j - \frac{1}{6}h^3[f''']_j + \frac{1}{24}h^4[f'''']_j + O(h^5)$$

$$f_j = f_j$$

$$f_{j+1} = f(x_j + h) = f_j + h\left[f'\right]_j + \frac{1}{2}h^2[f'']_j + \frac{1}{6}h^3[f''']_j + \frac{1}{24}h^4[f'''']_j + O(h^5)$$

- Now look for linear combination

$$c_- f_{j-1} + c_0 f_j + c_+ f_{j+1}$$

of the three grid function values that provides approximation of $[f\,'']_j = f\,''(x_j)$

- Get one linear equation at each order in $h \equiv \Delta x$

$$\begin{aligned} O(1): &\quad c_- + c_0 + c_+ = 0 \\ O(h): &\quad -c_- + c_+ = 0 \\ O(h^2): &\quad \frac{1}{2}h^2 c_- + \frac{1}{2}h^2 c_+ = 1 \end{aligned}$$

- Solving this system we find

$$c_- = c_+ = h^{-2}$$
$$c_0 = -2h^{-2}$$

so our desired finite difference approximation is

$$[f\,'']_j \approx \frac{f_{j-1} - 2f_j + f_{j+1}}{h^2}$$

- **Exercise:** Show that

$$\frac{f_{j-1} - 2f_j + f_{j+1}}{h^2} = [f\,'']_j + \frac{1}{12}h^2[f\,'''']_j + O(h^4)$$

- Terminology: Since the leading order error term is quadratic in the mesh spacing, the approximation is said to be "second order accurate", or simply "second order"

Prototype Classical Field Theory
Nonlinear Klein Gordon Equation

- Motivation
  - Relatively simple time dependent PDE that is straightforward to solve using FDA (good model problem)
  - Nonlinearity appears in the form of self interaction potential
  - With suitable choice of potential, get surprisingly rich phenomenology

Prototype Classical Field Theory
Nonlinear Klein Gordon Equation

- Approach
  - Will consider following cases
    1. Spherical symmetry (PDEs in 1 space + 1 time dimension)
       1. Time dependent [today]
       2. Time independent (static) — “q-balls” [tomorrow]
    2. No symmetry (PDEs in 3 space + 1 time dimension [tomorrow or Wed.])

Nonlinear Klein Gordon Equation in Spherical Symmetry

- Nonlinear Klein Gordon (NKG) equation

$$\nabla^{\mu}\nabla_{\mu}\phi = \frac{dV}{d\phi}$$

where $\phi \equiv \phi_1 + i\phi_2$ is *complex* and ϕ_1 and ϕ_2 are real

- For concreteness, will take

$$V(\phi) \equiv V(|\phi|) = \frac{c_1}{2}|\phi|^2 + \frac{c_2}{3}|\phi|^3 + \frac{c_3}{4}|\phi|^4$$

$$\frac{dV}{d\phi} = c_1\phi + c_2|\phi|\phi + c_3|\phi|^2\phi$$

c_1, c_2 and c_3 : adjustable parameters (constants)

(will discuss motivation in subsequent lecture)

- Specialize to spherical symmetry
  - Coordinates

$$x^{\mu} \equiv (t, r, \theta, \varphi)$$

  - Klein Gordon field

$$\phi \equiv \phi(t, r) \equiv \phi_1(t, r) + i\phi_2(t, r)$$

  - Metric (flat)

$$g_{\mu\nu} = f_{\mu\nu} = \text{diag}(-1,\ 1,\ r^2,\ r^2 \sin^2\theta)$$

$$g \equiv \det(g_{\mu\nu}) = -r^4 \sin^2\theta$$

- Wave operator in spherical symmetry

$$\nabla^\mu \nabla_\mu \phi = \frac{1}{\sqrt{-g}} \partial_\mu \left(\sqrt{-g} g^{\mu\nu} \partial_\nu \phi \right) = \frac{1}{r^2 \sin\theta} \partial_\mu \left(r^2 \sin\theta \, g^{\mu\nu} \partial_\nu \phi \right)$$

$$= \frac{1}{r^2} \partial_t \left(r^2 (-1) \partial_t \phi \right) + \frac{1}{r^2} \partial_r \left(r^2 (1) \partial_r \phi \right)$$

$$= -\partial_{tt} \phi + \frac{1}{r^2} \left(r^2 \phi_r \right)_r$$

- Easy to show the following (**exercise**)

$$r \, \nabla^\mu \nabla_\mu \phi = -\left(r\phi \right)_{tt} + \left(r\phi \right)_{rr}$$

which we will use in our testing of the numerical implementation

- We thus have

$$\nabla^{\mu}\nabla_{\mu}\phi = \frac{dV}{d\phi} \quad \rightarrow \quad -\phi_{tt} + \frac{1}{r^2}\left(r^2\phi_r\right)_r = \frac{dV}{d\phi}$$

- Solution domain

$$[0 \le t \le t_{\max},\ 0 \le r \le r_{\max}]$$

- Will need initial conditions …

$$\phi_1(0,r),\ \ \phi_2(0,r),\ \ \frac{\partial\phi_1}{\partial t}(0,r) \text{ and } \frac{\partial\phi_2}{\partial t}(0,r)$$

- … and boundary conditions …
  - Inner: regularity conditions—*r=0* is *not* a true boundary
    - Smoothness (regularity) at the origin dictates that

$$\lim_{r\to 0}\phi_1(t,r)=\phi_{10}(t)+r^2\phi_{12}(t)+O(r^4)$$
$$\lim_{r\to 0}\phi_2(t,r)=\phi_{20}(t)+r^2\phi_{22}(t)+O(r^4)$$

from which it follows that

$$\frac{\partial\phi_1}{\partial r}(t,0)=0$$
$$\frac{\partial\phi_2}{\partial r}(t,0)=0$$

- ... boundary conditions continued ...

  - Outer: will impose (approximate) outgoing radiation conditions (Sommerfeld conditions) based on the observation that at large distances, disturbances in a scalar field *with no potential* propagate as outgoing waves with amplitudes that fall off like 1/*r*

$$\lim_{r\to\infty}\left(r\phi_1(t,r)\right) \sim f_1(t-r)$$
$$\lim_{r\to\infty}\left(r\phi_2(t,r)\right) \sim f_2(t-r)$$

from which we readily derive

$$\left[\left(r\phi_1\right)_t + \left(r\phi_1\right)_r\right](t, r_{\max}) \sim 0$$
$$\left[\left(r\phi_2\right)_t + \left(r\phi_2\right)_r\right](t, r_{\max}) \sim 0$$

- For the numerical analysis, it will prove convenient to rewrite the NKG equation in first-order-in-time form by introducing the following auxiliary variables

$$\Pi_1(t,r) \equiv \frac{\partial \phi_1}{\partial t}$$

$$\Pi_2(t,r) \equiv \frac{\partial \phi_2}{\partial t}$$

- In addition, for the purposes of maintaining regularity at the origin in the numerical solution, it is advantageous to use the following identity that follows immediately from the chain rule

$$\frac{1}{r^2}\left(r^2 f_r\right)_r = 3\left(r^2 f_r\right)_{r^3} \equiv 3\frac{\partial}{\partial r^3}\left(r^2 f_r\right)$$

- We can then rewrite the NKG equation as the following system of 4 first-order-in-time PDEs

$$\frac{\partial \phi_1}{\partial t} = \Pi_1$$

$$\frac{\partial \Pi_1}{\partial t} = 3\frac{\partial}{\partial (r^3)}\left(r^2 \frac{\partial \phi_1}{\partial r}\right) - \frac{\partial V}{\partial \phi_1} = 3\frac{\partial}{\partial (r^3)}\left(r^2 \frac{\partial \phi_1}{\partial r}\right) - \left(c_1 + (c_2 + c_3 \mid \phi \mid) \mid \phi \mid\right)\phi_1$$

$$\frac{\partial \phi_2}{\partial t} = \Pi_2$$

$$\frac{\partial \Pi_2}{\partial t} = 3\frac{\partial}{\partial (r^3)}\left(r^2 \frac{\partial \phi_2}{\partial r}\right) - \frac{\partial V}{\partial \phi_2} = 3\frac{\partial}{\partial (r^3)}\left(r^2 \frac{\partial \phi_2}{\partial r}\right) - \left(c_1 + (c_2 + c_3 \mid \phi \mid) \mid \phi \mid\right)\phi_2$$

- Initial conditions (4 freely specifiable functions – will typically demand that initial data be *smooth* – i.e. ifinitely differentiable):

$$\phi_1(0, r) = \phi_1^0(r)$$

$$\Pi_1(0, r) = \Pi_1^0(r)$$

$$\phi_2(0, r) = \phi_2^0(r)$$

$$\Pi_2(0, r) = \Pi_2^0(r)$$

- Boundary conditions
  - Inner (regularity)

$$\frac{\partial \phi_1}{\partial r}(t,0) = \frac{\partial \phi_2}{\partial r}(t,0) = \frac{\partial \Pi_1}{\partial r}(t,0) = \frac{\partial \Pi_2}{\partial r}(t,0) = 0$$

  - Outer (outgoing radiation / Sommerfeld condition: note that these conditions are exact *only* for the case of no potential)

$$\left[\frac{\partial}{\partial t}(r\phi_1) + \frac{\partial}{\partial r}(r\phi_1)\right](t, r_{\max}) = 0$$

$$\left[\frac{\partial}{\partial t}(r\Pi_1) + \frac{\partial}{\partial r}(r\Pi_1)\right](t, r_{\max}) = 0$$

$$\left[\frac{\partial}{\partial t}(r\phi_2) + \frac{\partial}{\partial r}(r\phi_2)\right](t, r_{\max}) = 0$$

$$\left[\frac{\partial}{\partial t}(r\Pi_1) + \frac{\partial}{\partial r}(r\Pi_2)\right](t, r_{\max}) = 0$$

- This finishes the complete mathematical specification of the system of PDEs that we must solve (including initial and boundary conditions)

- We can now proceed with the discretization of the problem using finite difference techniques

- We replace the continuum domain with a finite difference mesh having constant spacing in each of the two coordinate directions

$$0 \le r \le r_{\max} \times \; 0 \le t \le t_{\max} \;\rightarrow \left(t^n, r_j\right),\; n = 0,1,\ldots N,\;\; j = 1,2,\ldots,J$$

where J and $N+1$ are the numbers of mesh points in the space (r) and time (t) directions, respectively, and

$$r_{j+1} - r_j = \text{const.} \equiv \Delta r \equiv h$$

$$t^{n+1} - t^n = \text{const.} \equiv \Delta t \equiv \lambda h$$

- In the above, λ is the so-called Courant number defined by

$$\lambda \equiv \frac{\Delta t}{\Delta r}$$

- For the type of finite difference scheme that we will be adopting, the condition

$$\lambda \leq 1$$

is often required for *stability* (equivalently *convergence*), while the condition

$$\lambda = O(1)$$

is generally dictated by accuracy (assuming that the truncation error orders of the temporal and spatial derivatives are the same)

- In practice, we will typically choose $\lambda = 1 / 2$

Crank-Nicholson Differencing

- Finite difference scheme applicable to any first-order-in-time PDE: originally developed for diffusion equation, but has proven useful for hyperbolic / wave equations, due to its good stability properties (numerical instability of FDAs of time dependent PDEs is a chronic problem), and the fact that the systems of equations that result can frequently be efficiently solved using a simple iterative technique

- Consider general first-order-in-time PDE

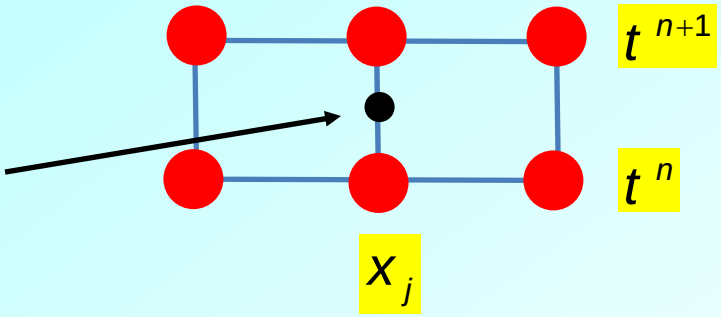
$$\frac{\partial u}{\partial t} = L[u]$$

  where $L[\cdot]$ is some spatial differential operator

- BASIC IDEA: "Centre" FDA at fictitious grid point

$$\left(t^{n+1/2}, x_j\right) = \left(t^n + \frac{\Delta t}{2}, x_j\right)$$

$$\left(t^{n+1/2}, x_j\right) = \left(t^n + \frac{\Delta t}{2}, x_j\right)$$



- Approximate time derivative using

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \left(\frac{\partial u}{\partial t}\right)_j^{n+1/2} + O(\Delta t^2)$$

and "average" action of $L[\cdot]$ on u_j^n and u_j^{n+1}

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

where L^h is the FDA of the spatial operator L

- If L^h is a second order approximation, so that

$$L^h = L + O(h^2)$$

  then the overall scheme will be second order in both space and time.

- Note that Crank-Nicholson finite-differencing generically leads to a *coupled system* for the advanced time unknowns u_j^{n+1}

- For many hyperbolic/wave-like equations, such as the nonlinear Klein Gordon equation, a simple relaxation technique provides a robust and efficient method of solving the system of equations