
Introduction to Numerical Field Theory II
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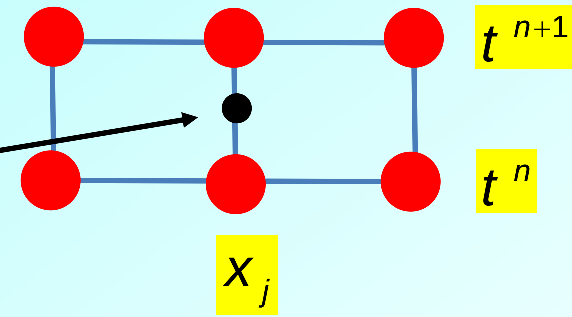
Overview / Summary

- Today
  - Review of CN differencing
  - CN FDA for nonlinear Klein-Gordon eqn (NKG)
  - Sample evolution (numerical solution) of NKG
  - **Convergence testing & validation of implementation / results**
    - Basic concepts, definitions & techniques for convergence testing FDAs

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



- 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

- Adopting the standard finite difference notation introduced previously

$$f_j^n \equiv f\left(n\Delta t,\ \left(j-1\right)\Delta r\right)$$

we now define various finite difference operators as follows

$$D_t\ f_j^n \equiv \frac{f_j^{n+1} - f_j^n}{\Delta t} = \left(\partial_t f\right)_j^{n+1/2} + O(h^2)$$

$$\mu_t\ f_j^n \equiv \frac{f_j^{n+1} + f_j^n}{2} = \left(f\right)_j^{n+1/2} + O(h^2)$$

$$D_{r^3}^0\ f_j^n \equiv \frac{r_{j+1/2}^2\left(f_{j+1}^n - f_j^n\right) - r_{j-1/2}^2\left(f_j^n - f_{j-1}^n\right)}{r_{j+1/2}^3 - r_{j-1/2}^3} = \frac{\partial}{\partial(r^3)}\left(r^2 f\right)_j^n + O(h^2)$$

$$D_r^F\ f_j^n \equiv \frac{-f_{j+2}^n + 4f_{j+1}^n - 3f_j^n}{2\Delta r} = \left(\partial_r f\right)_j^n + O(h^2)$$

$$D_r^B\ f_j^n \equiv \frac{f_{j-2}^n - 4f_{j-1}^n + 3f_j^n}{2\Delta r} = \left(\partial_r f\right)_j^n + O(h^2)$$

- In terms of these difference operators, our (Crank-Nicholson) discretizations of the four PDEs comprising the NKG equation are then

$$D_t\, \phi_1 = \mu_t\, \Pi_1$$
$$D_t\, \Pi_1 = 3\, \mu_t \left[D^0_{r^3}\, (r^2 \phi_1) \right] - \mu_t \left[\left(c_1 + (c_2 + c_3\, |\, \phi\, |)\, |\, \phi\, | \right) \phi_1 \right]$$
$$D_t\, \phi_2 = \mu_t\, \Pi_2$$
$$D_t\, \Pi_2 = 3\, \mu_t \left[D^0_{r^3}\, (r^2 \phi_2) \right] - \mu_t \left[\left(c_1 + (c_2 + c_3\, |\, \phi\, |)\, |\, \phi\, | \right) \phi_2 \right]$$

- The boundary conditions are

$$\left[D^F_r\, \phi_1 \right]^{n+1}_1 = \left[D^F_r\, \phi_2 \right]^{n+1}_1 = \left[D^F_r\, \Pi_1 \right]^{n+1}_1 = \left[D^F_r\, \Pi_2 \right]^{n+1}_1 = 0$$
$$\left[D_t\, \phi_1 \right]^n_J = -\mu_t \left[D^B_r\, \phi_1 \right]^n_J$$
$$\left[D_t\, \phi_2 \right]^n_J = -\mu_t \left[D^B_r\, \phi_2 \right]^n_J$$
$$\left[D_t\, \Pi_1 \right]^n_J = -\mu_t \left[D^B_r\, \phi_1 \right]^n_J$$
$$\left[D_t\, \Pi_2 \right]^n_J = -\mu_t \left[D^B_r\, \phi_2 \right]^n_J$$

- The specific initial conditions we will consider for testing (development purposes) are as follows. First, we define an auxiliary function

$$\phi_0(r) \equiv \phi_0(r;\ A, r_0, \delta) = A \exp\left[-\left(\left(r - r_0\right) / \delta\right)^2\right]$$

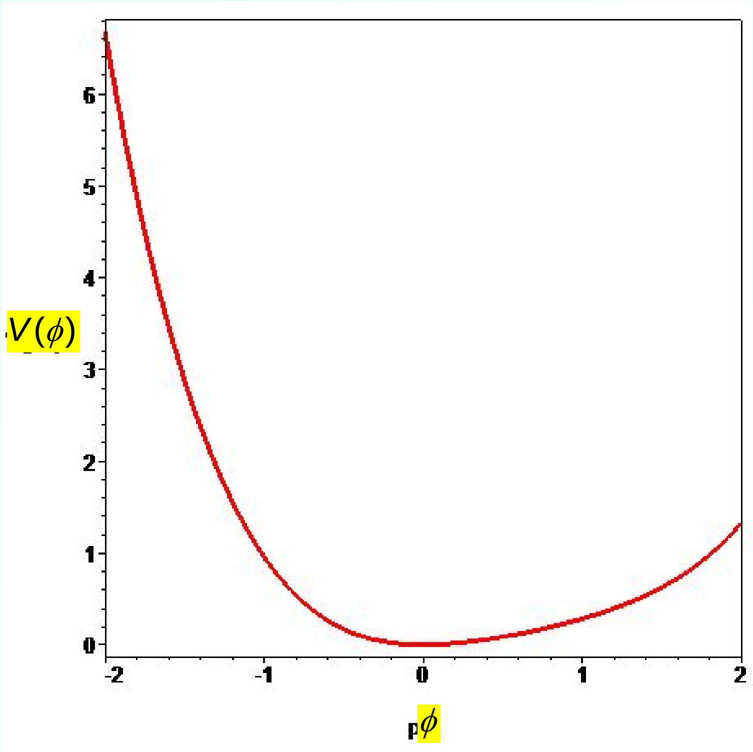
- We then set

$$\begin{aligned}
\phi_1(0,r) &\equiv \phi_0(r) \\
\phi_2(0,r) &= 0 \\
\Pi_1(0,r) &\equiv 0 \\
\Pi_2(0,r) &\equiv \phi_o(r)
\end{aligned}$$

and we now have completely specified the discrete equations of motion for the discrete unknowns

$$\left\{\phi_1(t,r),\ \phi_2(t,r),\ \Pi_1(t,r),\ \Pi_2(t,r)\right\}$$

- Typical results from implementation of the difference equations as detailed above



  - Spatial domain

    $$0 \le r \le 5$$

  - Potential parameters

    $$c_1 = 1 \quad c_2 = -1 \quad c_3 = 1/2$$

  - Initial pulse profile

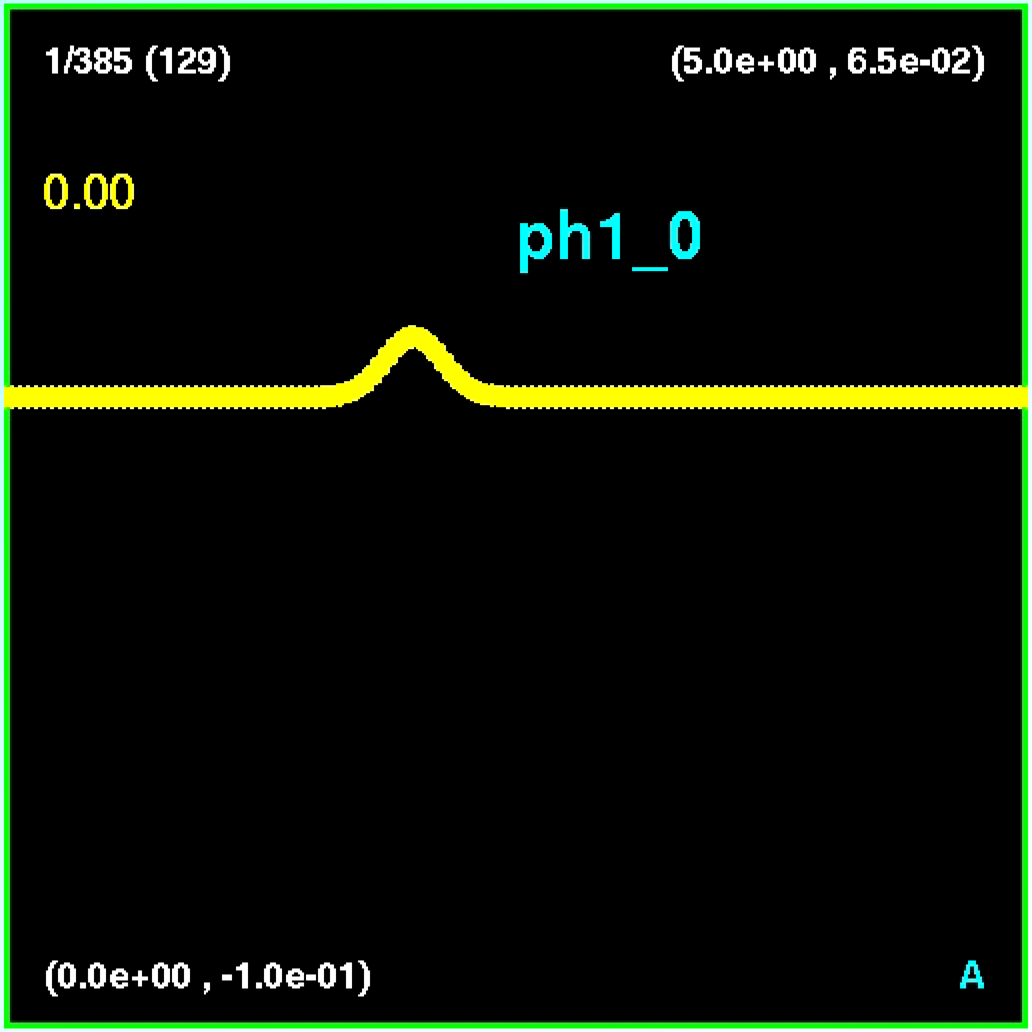
    $$\phi_0(r) \equiv \phi_0(r;\ A, r_0, \delta) = 0.01 \exp\left[-\left(\left(r-2\right)/0.2\right)^2\right]$$

  - Base (coarsest) resolution

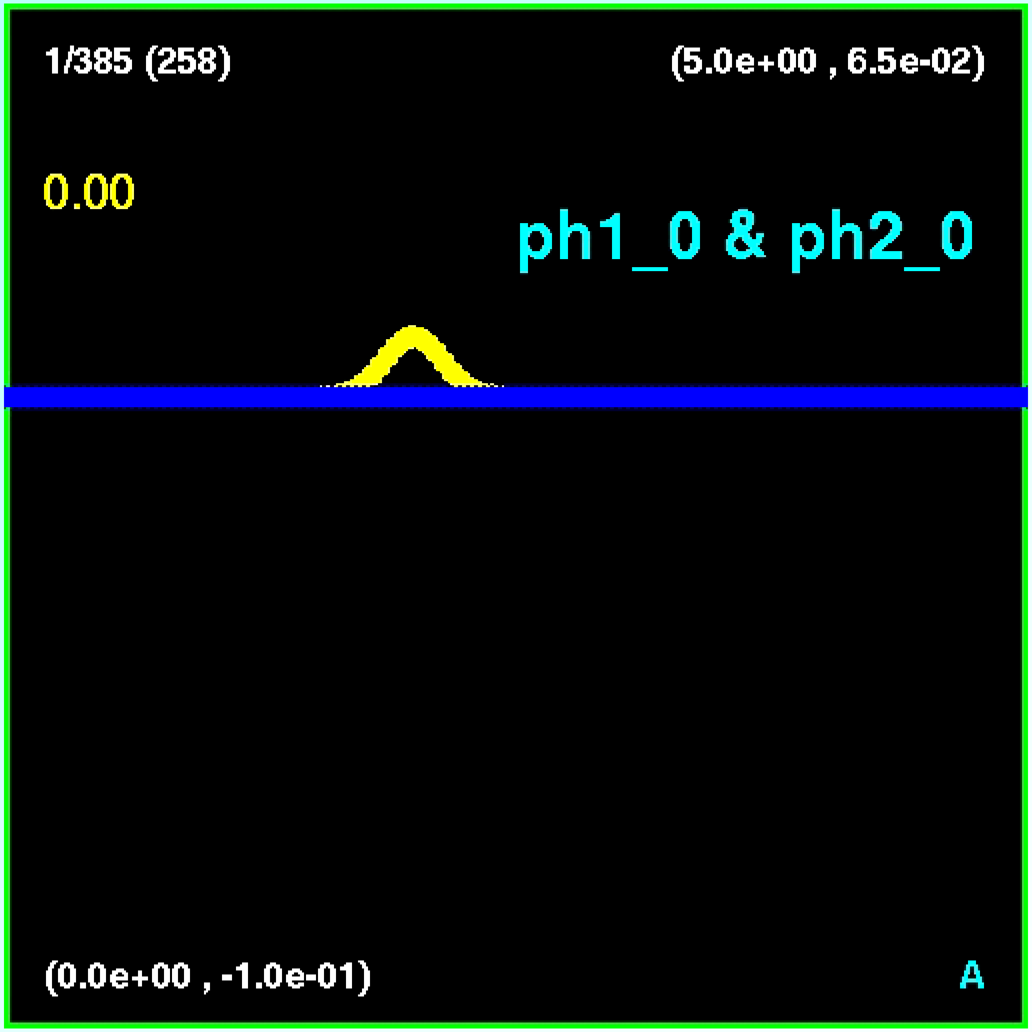
    $$J = N_r = 129$$

    $$N = N_t = 384 \;\rightarrow\; t_{\max} \approx 7.5$$

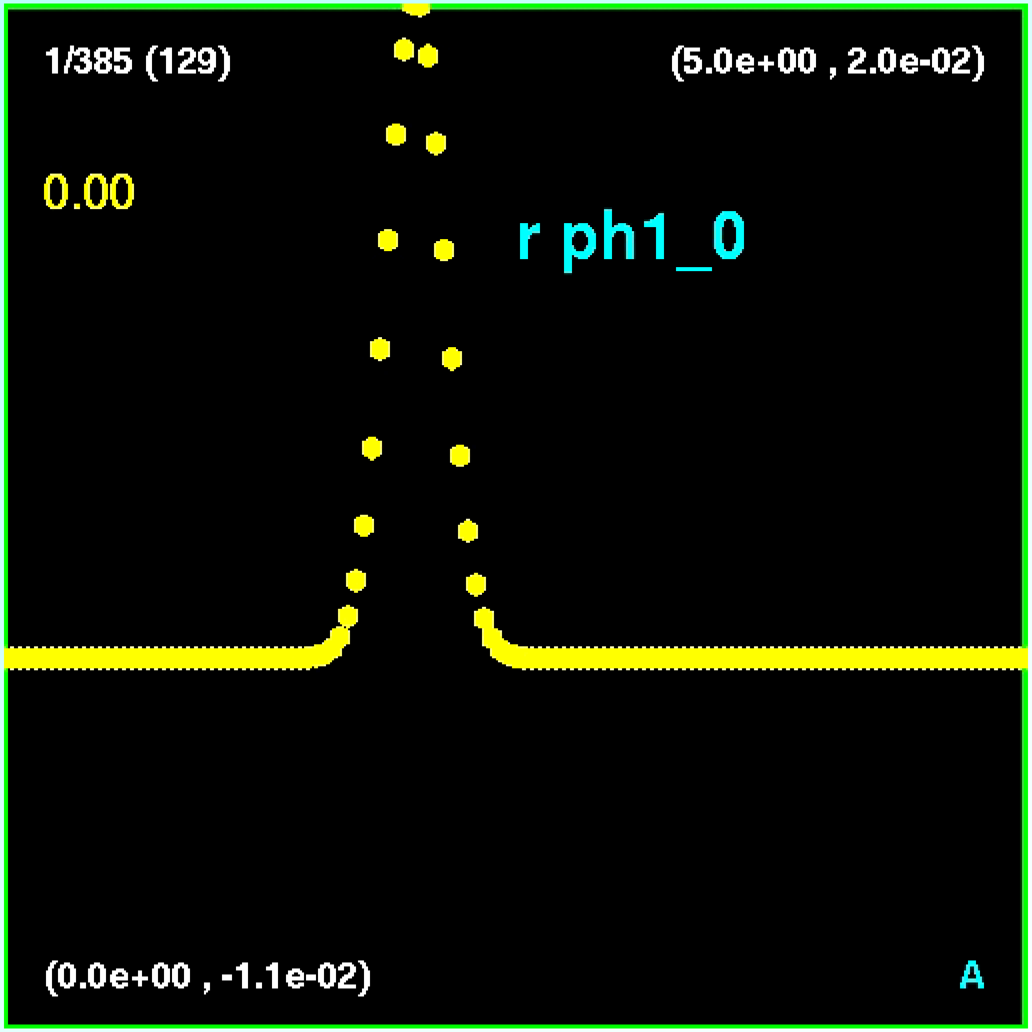
$\phi_1(t, r)$



$\phi_1(t,r)$ and $\phi_2(t,r)$



$r\phi_1(t,r)$



Convergence Testing & Validation of Results

Some Basic Concepts & Definitions

- Let

$$L\,u = f$$

denote a general *differential* system

- For simplicity, concretness, can think of $u \equiv u(t, r)$ as a single function of time and one space vbl
- However, discussion applies to cases in more independent vbls as well as multiple *dependent* vbls
- In the above, L is some differential operator, u is the unknown solution of the PDE, and f is some specified fcn (frequently called a *source* fcn) of the independent vars

- Here, and in the following, will often be convenient to use a notation where a subscript *h* on a quantity indicates that it is *discrete*, or associated with the FDA, rather than the continuum

- With this notation, we will generically denote an FDA of our PDE by

$$L^h u^h = f^h$$

where u^h is the discrete soln, f^h is the source fcn evaluated on the FD mesh, and L^h is the FD approximation of L

Residual

- Note that another way of writing our FDA is

$$L^h u^h - f^h = 0$$

- Often useful to view FDAs in this form for following reasons:

1. Yields a canonical view of what it means to solve the FDA: "drive the residual to 0"
2. For iterative approaches to the soln of the FDA (which are common, since it may be too expensive to solve the algebraic equations directly), we are naturally lead to the concept of a residual
3. Residual is simple the level of "non-satisfaction" of our FDA (and, in fact, of *any* algebraic expression)

4. Specifically, if $\tilde{u}^h$ is some approximation to the true solution of the FDA, u^h , then the residual, , associated with $\tilde{u}^h$ is just

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

- Leads to the view of a convergent iterative procedure as being one which "drives the residual to 0"

Truncation Error

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

$$\tau^h \equiv L^h u - f^h$$

  where u satisfies the *continuum PDE.*

- Note that the *form* of the truncation error can always be computed (typically using Taylor series) from the FDA and the PDE

Convergence

- Assume FDA is characterized by a *single* discretization scale, h

- We say that the FDA *converges* if and only if

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

- In practice, convergence is our primary concern as numerical analysts, particularly if there is reason to suspect that the solutions of our PDEs are good models for real phenomena:

  i.e. that we are *not* "simulating" physics, but are solving PDEs whose solutions are expected to accurately reflect the real world

- For example, modulo general relativity *not* being an accurate theory in the strong, dynamical limit, expect solutions of Einstein's equations for colliding black holes to model the astrophysics to very high precision

Consistency

- Assume FDA with truncation error τ^h is characterized by a single discretization scale, *h*

- We say that the FDA is *consistent* if

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

- Consistency is obviously a *necessary* condition for convergence

Solution Error

- The *solution error,* e^h , associated with an FDA is defined by

$$e^h \equiv u - u^h$$

Relation Between Truncation & Solution Errors

- Standard (naïve) approach—*assume* that

$$e^h \equiv u - u^h$$

  is of the same order in the mesh spacing, *h*, as the truncation error, τ^h

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

- Will return to this issue in the last lecture

Error Analysis & Convergence Tests

- Discussion here applies to essentially *any* continuum problem that is solved with using FDAs on a *uniform* mesh structure

- In particular, also applies to the treatment of ODEs and elliptic PDEs as well as PDEs of evolution type (hyperbolic/wave, diffusion, Schrodinger ...)

  - For ODEs and elliptic PDEs convergence is often easier to achieve due to the fact that the FDAs are typically intrinsically stable

- We also note that departures from non-uniformity in the FD mesh do not, in general, completely destroy the picture—however do tend to distort it in ways that are beyond the scope of these lectures

- **IMPOSSIBLE TO OVERSTATE IMPORTANCE OF CONVERGENCE STUDIES!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!**