Lecture No. 10

References: Celia and Gray, 214-253; Roache, 33-91; Pinder and Gray, 150-157.

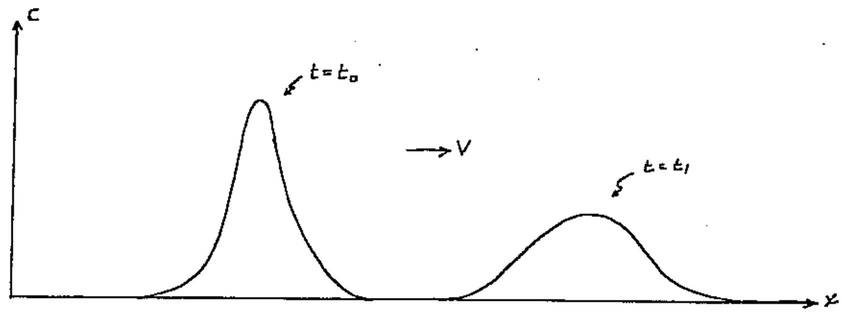
Convection-Diffusion Equation

$$\frac{\partial u}{\partial t}+V\frac{\partial u}{\partial x} = D\frac{\partial^2 u}{\partial x^2}$$

V = velocity (convection or advection)

D = diffusion

- Model equation for computational fluid mechanics
- Represents convective and diffusive transport



The convection-diffusion equations represents:

- Transport of pollutants
- Transport of momentum (Burgers and Navier-Stokes equations)
- Transport of turbulence

Numerical Solution to this equation is plagued by various numerical accuracy and/ or stability problems. Typically these problems arise when convection dominates diffusion in which case wiggles or node to node type oscillations appear in the solution.

Oscillations appear when

$$\mathbf{P_e} = \frac{V\Delta x}{D} > 2$$

where $\mathbf{P_e}$ = Peclet number (equals cell Reynolds number in the case of the Navier-Stokes equations).

In addition the peak is damped and phase lag of the distribution may be seen.

<u>Explicit Solution to the Convection-Diffusion Equation</u>

Let us examine the use of the <u>forward in time central in space (FTCS)</u> FD solution to the convection-diffusion (C-D) equation (i.e. the explicit solution):

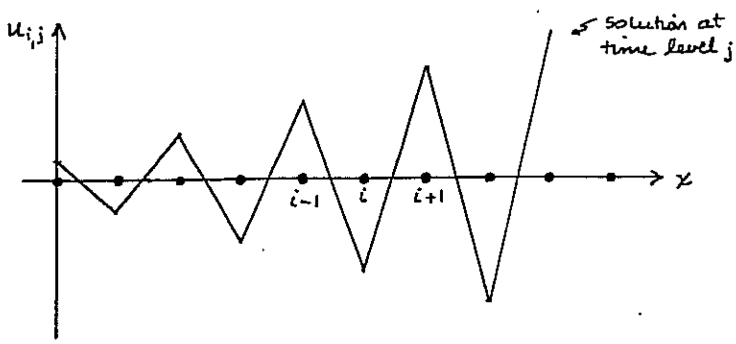
$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = -V\frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + D\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2}$$

<u>Heuristic Approach to Stability of the Explicitly Discretized C-D Equation</u>

The explicit solution to the C-D equation can be re-written as:

$$u_{i,j+1} = u_{i,j} - \frac{V\Delta t}{2\Delta x}(u_{i+1,j} - u_{i-1,j}) + \frac{D\Delta t}{\Delta x^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j})$$

Let's assume that the solution or at least part of the actual solution can be represented by a solution which oscillates from node to node with the amplitude of the oscillation increasing with x (a pretty reasonable assumption as we shall see later).



We will assume that we want these spatial oscillations to be damped out or at least that we do not want their absolute values to grow in time! Due to the linearity of the p.d.e. we are considering, we can examine the solution components due to the diffusion and convection terms separately.

(i) The time varying solution due to the diffusion term:

$$u_{i,j+1} = u_{i,j} + \frac{D\Delta t}{\Delta x^2}(u_{i+1,j} - 2u_{i,j} + u_{i-1,j})$$

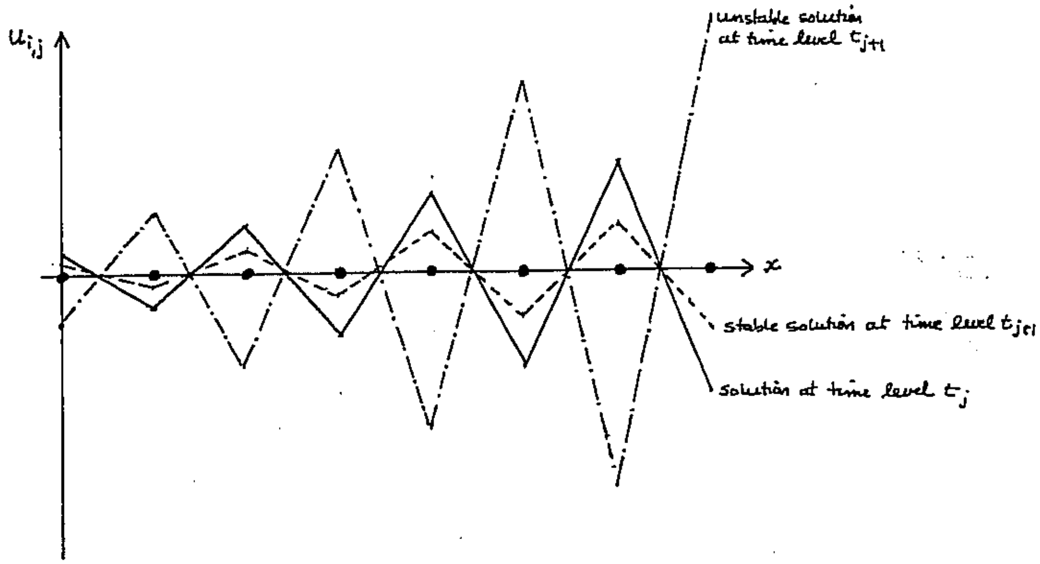
Since $u_{i,j} < 0$ $\quad u_{i+1,j} > 0$ and $u_{i-1,j} > 0$

$$\Rightarrow$$

$$u_{i+1,j} - 2u_{i,j} + u_{i-1,j} > 0 \quad \text{while} \quad u_{i,j} < 0$$

Thus $u_{i,j+1} > u_{i,j}$ and the diffusion term compensates (or corrects) $u_{i,j}$. However if $\frac{D\Delta t}{\Delta x^2}$ is too large, the correction ***overshoots*** and the absolute value of the solution grows. Thus the solution is no longer damped and:

$$|u_{i,j+1}| > |u_{i,j}|$$



This type of instability is known as a Dynamic Instability.

Thus we must have a ***constraint on*** Δt for stability which relates to $\dfrac{\Delta t D}{\Delta x^2}$. If this constraint is not satisfied, the solution grows and oscillates in time as well as in space.

(ii) The time varying solution due to the convection term:

$$u_{i,j+1} = u_{i,j} - \frac{V\Delta t}{2\Delta x}(u_{i+1,j} - u_{i-1,j})$$

Assume:

$$V > 0 \quad \text{and} \quad u_{i,j} < 0$$

$$u_{i+1,j} > 0 \quad \text{and} \quad u_{i-1,j} > 0 \quad \text{and} \quad u_{i+1,j} > u_{i-1,j}$$

Thus:

$$-(u_{i+1,j} - u_{i-1,j}) < 0 \quad \text{and} \quad u_{i,j} < 0$$

Thus we always have

$$|u_{i,j+1}| > |u_{i,j}|$$

Therefore the solution always grows monotonically. This is known as a static instability.

- Thus the unstable behavior of the convection (or advection) term is different from that of the diffusion term. We see steady growth.
- In reality both the convection and diffusion solutions are combined and stability will depend on the ratio of diffusion and convection.

<u>Fourier Analysis of the C-D Equation</u>

Let us examine the weighted implicit/explicit central space discretization to:

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = D\frac{\partial^2 u}{\partial x^2}$$

$$\Rightarrow$$

$$u_{p,q+1} - u_{p,q} = -\frac{\mathbf{C}_{\#}}{2}\left[\theta\left(u_{p+1,q+1} - u_{p-1,q+1}\right) + (1-\theta)\left(u_{p+1,q} - u_{p-1,q}\right)\right]$$

$$+\rho\left[\theta\left(u_{p+1,q+1} - 2u_{p,q+1} + u_{p-1,q+1}\right) + (1-\theta)\left(u_{p+1,q} - 2u_{p,q} + u_{p-1,q}\right)\right]$$

where

$$\rho = \frac{D\Delta t}{\Delta x^2}$$

$$\mathbf{C}_{\#} = \frac{V\Delta t}{\Delta x} = \text{Courant Number}$$

and recall that:

θ = the implicit fraction

θ = 0 fully explicit (FTCS)

θ = 0.5 Crank-Nicolson (central time)

θ = 1.0 fully implicit (BTCS)

We assume that the solution may be represented by a Fourier series in time and space:

$$u(x, t) = \sum_{n=-\infty}^{+\infty} U_n exp\,(\hat{i}\alpha_n t + \hat{i}\beta_n x)$$

where

$$\alpha_n = \text{frequency}$$

$$\beta_n = \text{wave number} = \frac{2\pi}{\lambda_n}$$

Due to linearity we need only consider 1 component:

$$u(x, t) = U_n e^{\hat{i}\alpha_n t} e^{\hat{i}\beta_n x}$$

Since $x = p\Delta x$ and $t = q\Delta t$:

$$u_{p,q} = U_n e^{\hat{i}\alpha_n q\Delta t} e^{\hat{i}\beta_n p\Delta x}$$

We define the amplification factor in time as:

$$\xi_n = e^{\hat{\imath}\alpha_n \Delta t}$$

Thus

$$u_{p,q} = U_n \xi_n^q e^{\hat{\imath}\beta_n p \Delta x}$$

Recall that ξ_n equals the amplification factor in time for component n such that:

$$u_{t+\Delta t} = \xi_n u_t$$

Substituting into the FD equation:

$$e^{\hat{\imath}\beta_n p\Delta x}\xi_n^{q+1} - e^{\hat{\imath}\beta_n p\Delta x}\xi_n^{q} = -\frac{C_\#}{2}(\theta(e^{\hat{\imath}\beta_n (p+1)\Delta x}\xi_n^{q+1}$$

$$-e^{\hat{\imath}\beta_n (p-1)\Delta x}\xi_n^{q+1}) + (1-\theta)(e^{\hat{\imath}\beta_n (p+1)\Delta x}\xi_n^{q} - e^{\hat{\imath}\beta_n (p-1)\Delta x}\xi_n^{q}))$$

$$+\rho\Big[\theta(e^{\hat{\imath}\beta_n (p+1)\Delta x}\xi_n^{q+1} - 2e^{\hat{\imath}\beta_n p\Delta x}\xi_n^{q+1} + e^{\hat{\imath}\beta_n (p-1)\Delta x}\xi_n^{q+1})$$

$$+(1-\theta)(e^{\hat{\imath}\beta_n (p+1)\Delta x}\xi_n^{q} - 2e^{\hat{\imath}\beta_n p\Delta x}\xi_n^{q} + e^{\hat{\imath}\beta_n (p-1)\Delta x}\xi_n^{q})\Big]$$

$$\Rightarrow$$

$$\xi_n - 1 = -\frac{C_\#}{2}\Big[\theta(e^{\hat{\imath}\beta_n\Delta x} - e^{-\hat{\imath}\beta_n\Delta x})\xi_n + (1-\theta)(e^{\hat{\imath}\beta_n\Delta x} - e^{-\hat{\imath}\beta_n\Delta x})\Big]$$

$$+\rho\Big[\theta(e^{\hat{\imath}\beta_n\Delta x} + e^{-\hat{\imath}\beta_n\Delta x} - 2)\xi_n + (1-\theta)(e^{\hat{\imath}\beta_n\Delta x} + e^{-\hat{\imath}\beta_n\Delta x} - 2)\Big]$$

However recall that:

$$e^{\hat{i}\beta_n\Delta x} + e^{-\hat{i}\beta_n\Delta x} = 2\cos\beta_n\Delta x$$

$$e^{\hat{i}\beta_n\Delta x} - e^{-\hat{i}\beta_n\Delta x} = 2\hat{i}\sin\beta_n\Delta x$$

thus

$$\xi_n - 1 = -\frac{\mathbf{C}_\#}{2}\left[\theta\,(2\hat{i}\sin\beta_n\Delta x)\,\xi_n + (1-\theta)\,(2\hat{i}\sin\beta_n\Delta x)\right]$$

$$+\rho\left[\theta\,(2\cos\beta_n\Delta x - 2)\,\xi_n + (1-\theta)\,(2\cos\beta_n\Delta x - 2)\right]$$

$$\Rightarrow$$

$$\xi_n\{1 + \theta\,[\mathbf{C}_\#\hat{i}\sin\beta_n\Delta x + 2\rho\,(1-\cos\beta_n\Delta x)]\} =$$

$$\{1 - (1-\theta)\,[\mathbf{C}_\#\hat{i}\sin\beta_n\Delta x + 2\rho\,(1-\cos\beta_n\Delta x)]\}$$

$$\Rightarrow$$

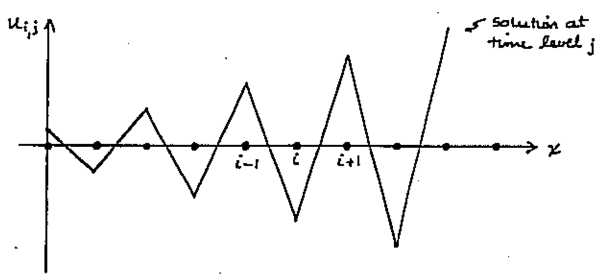
$$\xi_n = \frac{1 - (1-\theta)\,[\mathbf{C}_\#\hat{i}\sin\beta_n\Delta x + 2\rho\,(1-\cos\beta_n\Delta x)]}{1 + \theta\,[\mathbf{C}_\#\hat{i}\sin\beta_n\Delta x + 2\rho\,(1-\cos\beta_n\Delta x)]}$$

Let's examine cases $\theta = 0$, $\theta = 0.5$ and $\theta = 1.0$.

Fully Explicit Solution to the C-D Equation: $\theta = 0$

$$\xi_n = 1 - 2\rho\,(1 - \cos\beta_n \Delta x) - \hat{i} C_{\#} \sin\beta_n \Delta x$$

- Note that the amplification factor is now complex. ***This relates to the phase of propagation.***
- If $C_{\#} = 0$ (i.e. $V = 0$) then the amplification factor will reduce down to that of the pure diffusion equation (i.e. there is no complex component in ξ). The phase component of ξ is always zero since there's no propagation.
- Therefore we only have a phase component if $|V| > 0$ and there is propagation.
- If we have a phase, this numerically computed phase may differ from the analytical phase. ***This leads to PHASE ERRORS which creates wiggles or perturbations on the solution which look like those assumed in the Heuristic approach.***



- Stability still requires that

$$|\xi| \le 1$$

To satisfy the stability condition, we must compute the amplitude of the complex amplification factor.

We rewrite the equation for ξ_n as:

$$\xi_n = (1-2\rho) + (2\rho)\cos\beta_n\Delta x - \hat{i}C_{\#}\sin\beta_n\Delta x$$

In order for $|\xi_n|$ to fall within the unit circle. i.e. for $|\xi_n| \le 1$, we must satisfy:

$$\mathbf{C_{\#}} \le 1 \text{ and } \mathbf{C_{\#}}^2 \le 2\rho$$

These limits are plotted in Figure L10.1 in conjunction with the Peclet number, $\mathbf{P_e}$. We note that $\mathbf{P_e} = \dfrac{\mathbf{C_{\#}}}{\rho}$ and therefore:

$$\mathbf{C_{\#}}^2 \le \frac{2\mathbf{C_{\#}}}{\mathbf{P_e}} \qquad \Rightarrow$$

$$\mathbf{C_{\#}} \le \frac{2}{\mathbf{P_e}} \qquad \Rightarrow$$

$$\mathbf{P_e} \le \frac{2}{\mathbf{C_{\#}}}$$

Due to the constraints on $\mathbf{C_{\#}} \le 1$, we have a combined most restrictive limit:

$$\mathbf{P_e} \le 2 \quad \text{and} \quad \mathbf{C_{\#}} \le 1$$

- ***Note that for $D = 0$ (zero diffusion, pure convection), the explicit approach is <u>unconditionally unstable</u>. It will not work no matter how small we make Δt.***
- This case represents a static instability.

Fig L10.1

Stability range for FTCS (forward-time, central differencing) of T–D equations (after Leonard, 1979)

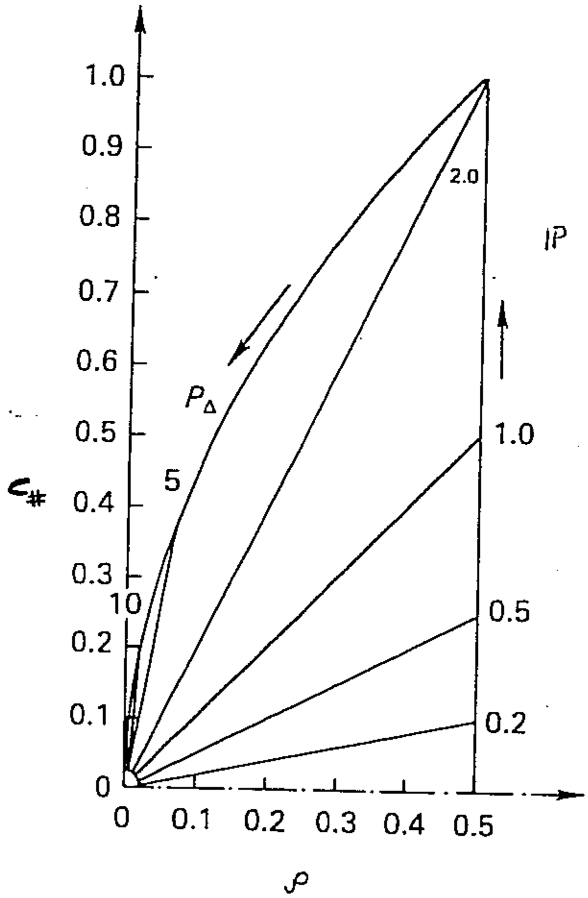
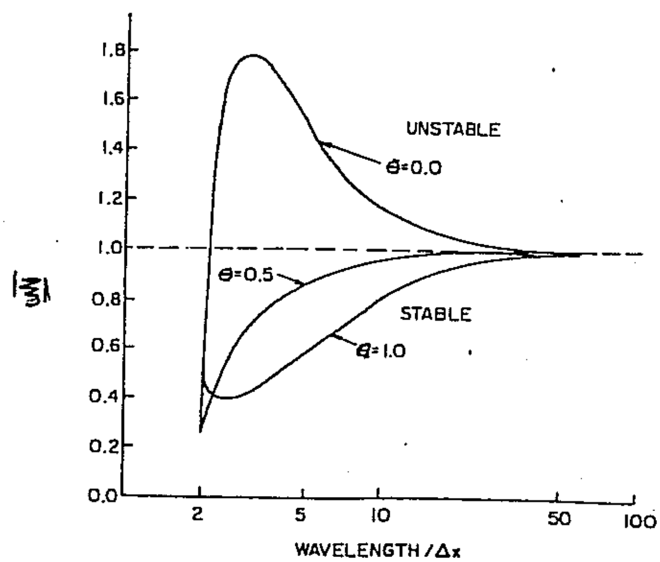


Figure L10.2



Amplification Factor of transport equation using a weighted implicit/explicit method (θ is time weighting factor)

$C_{\#} = 1.0$, $\rho = 0.1$, $P_\Delta = 10$; θ varies

Fully Implicit Solution to the C-D Equation: $\theta = 1$

$$\xi = \frac{1}{1 + \mathbf{C}_{\#}\hat{\imath}\sin(\beta_n \Delta x) + 2\rho[1 - \cos(\beta_n \Delta x)]}$$

Let

$$a = 1 + 2\rho[1 - \cos(\beta_n \Delta x)]$$

$$b = \mathbf{C}_{\#}\sin\beta_n \Delta x$$

Thus:

$$\xi = \frac{1}{a + ib}$$

$$\Rightarrow$$

$$\xi = \frac{a - ib}{a^2 + b^2}$$

$$\Rightarrow$$

$$|\xi|^2 = \frac{a^2 + b^2}{[a^2 + b^2]^2}$$

$$\Rightarrow$$

$$|\xi|^2 = \frac{1}{a^2 + b^2}$$

$$\Rightarrow$$

$$|\xi|^2 = \frac{1}{1 + 4\rho\,[1 - \cos(\beta_n \Delta x)] + 4\rho^2\,[1 - \cos(\beta_n \Delta x)]^2 + C_\#^{\,2}\sin^2(\beta_n \Delta x)}$$

However

$$1 - \cos(\beta_n \Delta x) = 2\sin^2\left(\cancel{2}\frac{\beta_n \Delta x}{2}\right)$$

Thus

$$|\xi|^2 = \frac{1}{1 + 8\rho\sin^2\left(\cancel{2}\frac{\beta_n \Delta x}{2}\right) + 8\rho^2\sin^2\left(\cancel{2}\frac{\beta_n \Delta x}{2}\right) + C_\#^{\,2}\sin^2(\beta_n \Delta x)}$$

However $\rho > 0$, $C_\#^2 > 0$ and $\sin^2 > 0$, therefore:

$$|\xi|^2 \leq 1$$

- ***Hence the implicit solution to the C-D equation is Unconditionally Stable.***

<u>Crank-Nicolson Solution to the C-D Equation:</u> $\theta = 0.5$

Crank-Nicolson solutions to the C-D equation can be shown to be unconditionally stable as well.

Notes on Stability:

Let us examine how stability varies with $\frac{\lambda_n}{\Delta x} = \frac{wavelength}{\Delta x}$, where $\lambda_n = \frac{2\pi}{\beta_n}$ and $\beta_n = wave\ number$. We have examined stability problems (using the Heuristic approach) associated with very short wavelength components of the solution.

The question which arises is how $|\xi_n|$ varies with different wavelength components. Let us examine Figure L10.2. Note that this plot is for a very specific selection of $\mathbf{C}_{\#}$ and $\mathbf{P}_{\mathbf{e}}$ values.

- The shortest possible wavelength is always $2 \cdot \Delta x$.
- For $\theta = 0$, the unstable behavior is particularly severe for the short near $2 \cdot \Delta x$ wavelengths while for long wavelengths the solution appears to approach stability. However the severe instabilities at the short wavelengths will always destroy the entire solution (since these always exist due to poor resolution of the i.c., roundoff error and/or nonlinear transfer of energy to high wavenumbers).
- For $\theta = 0.5, 1.0$, we note that the solution is stable for all wavelengths. In fact our analysis showed this to be true for all $\mathbf{C}_{\#}$ and $\mathbf{P}_{\mathbf{e}}$ values.

Lecture No. 11

References: Pinder and Gray, p. 150-169, Roache, p. 33-94, Peyret and Taylor, p 18-28; 37-65.

<u>Summary of the FD schemes examined:</u>

- Fully explicit, central space
  - Stability requires $\mathbf{P_e} \le 2$, $\mathbf{C_\#} \le 1.0$
  - accuracy $0(\Delta t, \Delta x^2)$
- Crank-Nicolson, central space
  - unconditionally stable
  - accuracy $0(\Delta t^2, \Delta x^2)$
- Fully implicit, central space
  - unconditionally stable
  - accuracy $0(\Delta t, \Delta x^2)$

<u>Numerical Experiments of 1-D FD Solutions to the C-D Equation</u>

Examine Figures L11.1a through L11.4c.

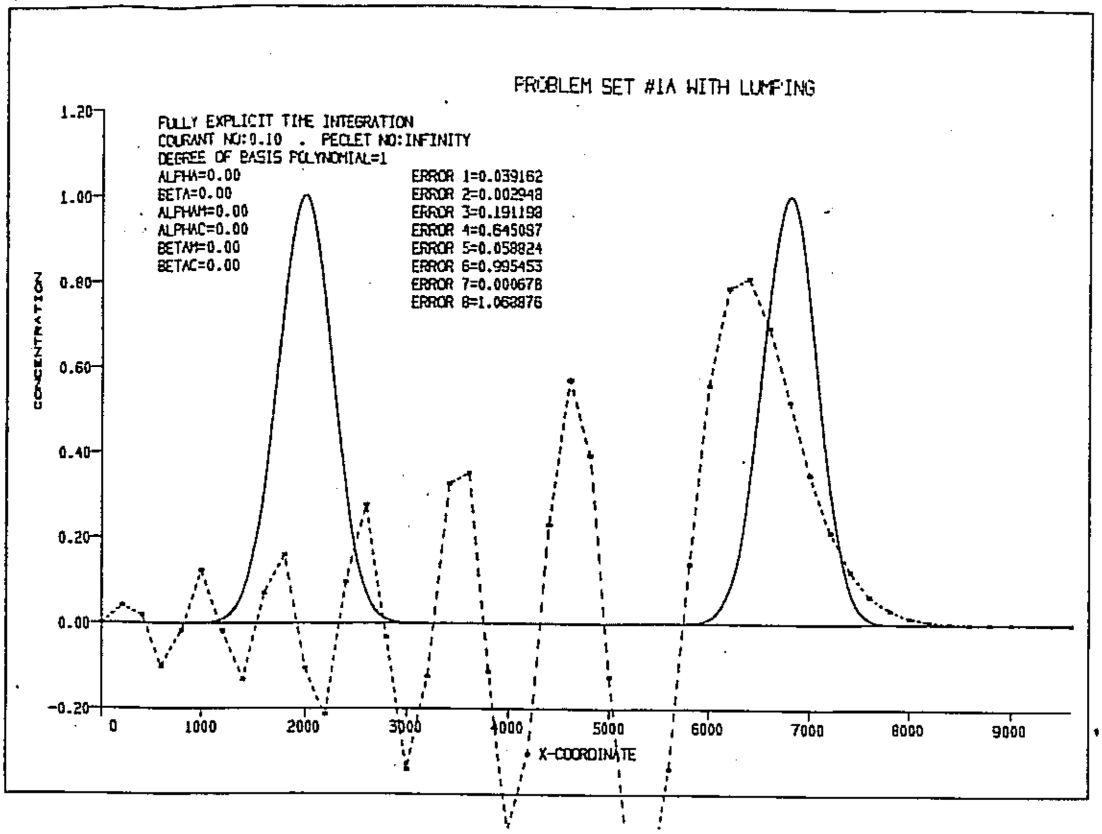
- Recall that $\mathbf{C_\#} = \dfrac{V\Delta t}{\Delta x}$, and that we vary Δt to vary $\mathbf{C_\#}$.
- $\mathbf{P_e} = \dfrac{V\Delta x}{D}$, and that we vary D to vary $\mathbf{P_e}$ (note that $D = 0$ leads to $\mathbf{P_e} = \infty$).

Summary of observations

- Fully explicit scheme is statically unstable when $\mathbf{P_e} > 2$ and dynamically unstable when $\mathbf{C_\#} \ge 1.0$.
- $C-N$ scheme is unconditionally stable. ***However the solutions do exhibit wiggles for*** $\mathbf{P_e} > 2$.

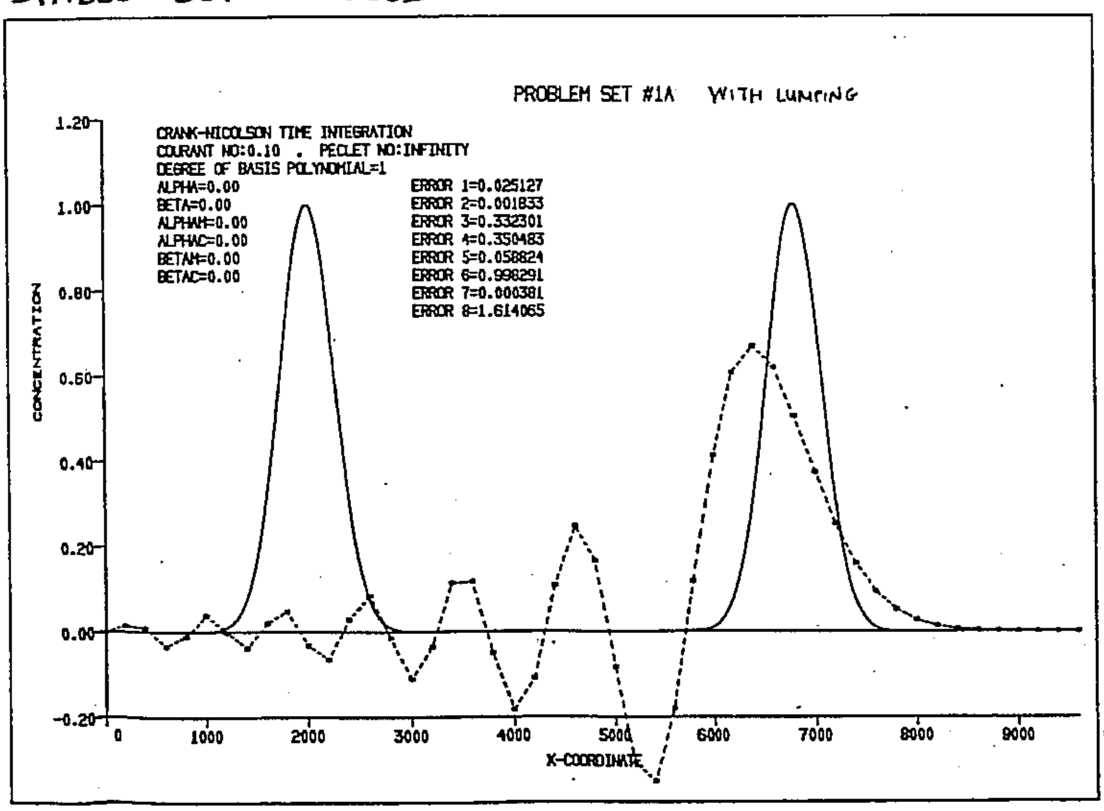
F.D. $\theta = 0$ $C_x = 0.1$ $P_e = \infty$ Fig L11-1a

STATICALLY UNSTABLE



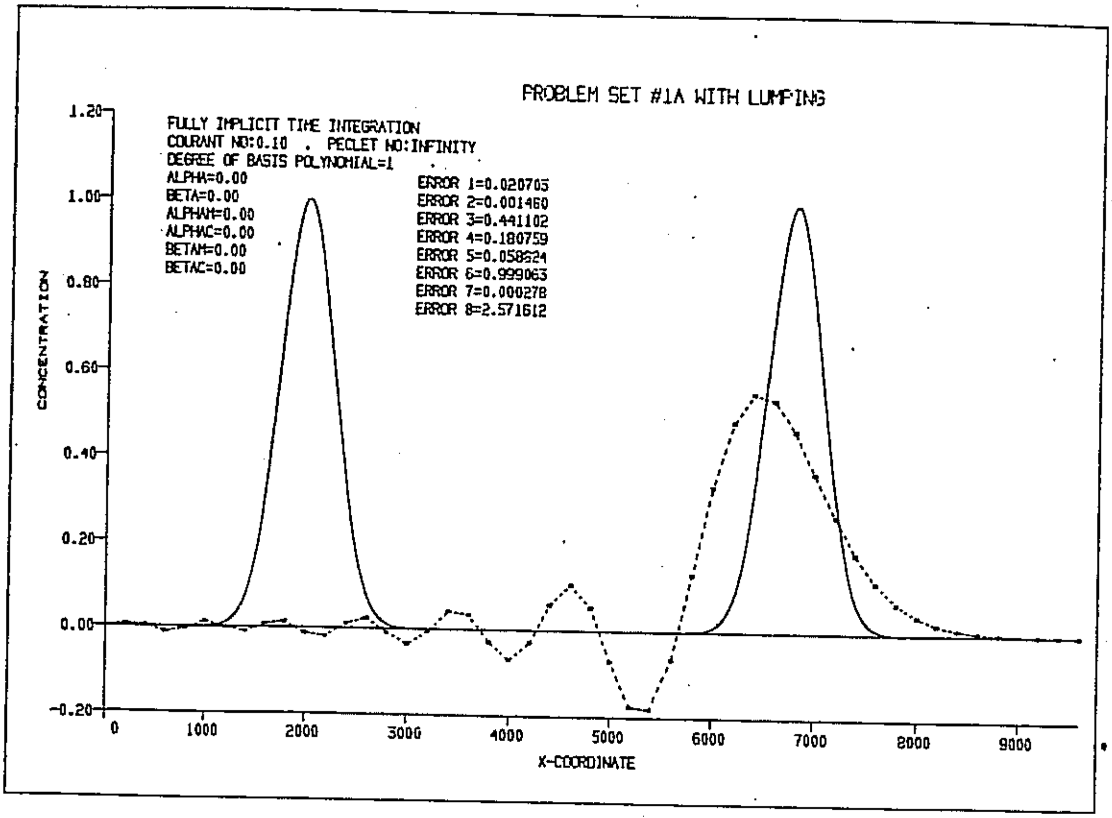
F.D. $\Theta = 0.5$ $C_x = 0.1$ $P_e = \infty$ Fig L11-1b

STABLE BUT WIGGLES



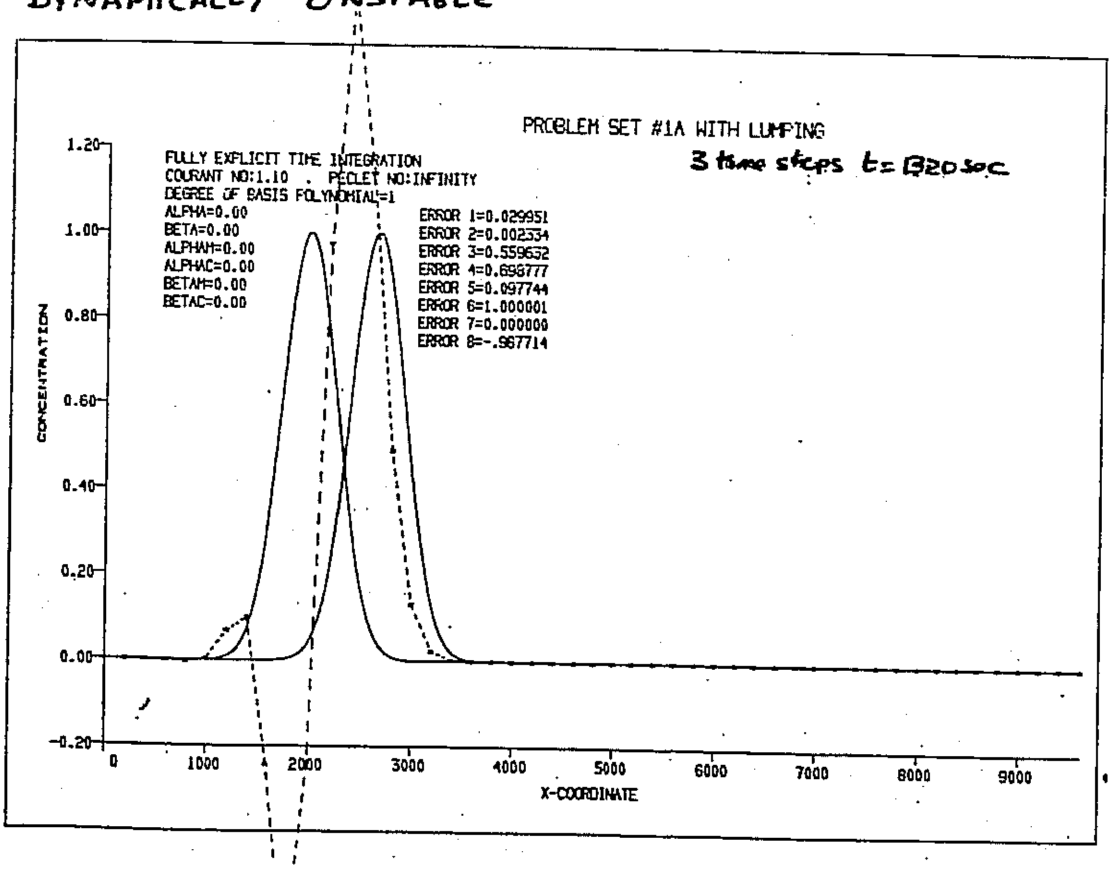
F.D. $\theta = 1.0$ $C_{\#} = 0.1$ $P_e = \infty$ Fig L11-1c

STABLE BUT WIGGLES (LESS THAN $\theta = 0.5$)



F.D. $\theta = 0.0$ $C_{\#} = 1.1$ $P_e = \infty$ Fig L11-2a

DYNAMICALLY UNSTABLE



F.D. $\theta = 0.5$ $C_{\#} = 1.1$ $P_e = \infty$ Fig LII-2b

STABLE BUT WIGGLES

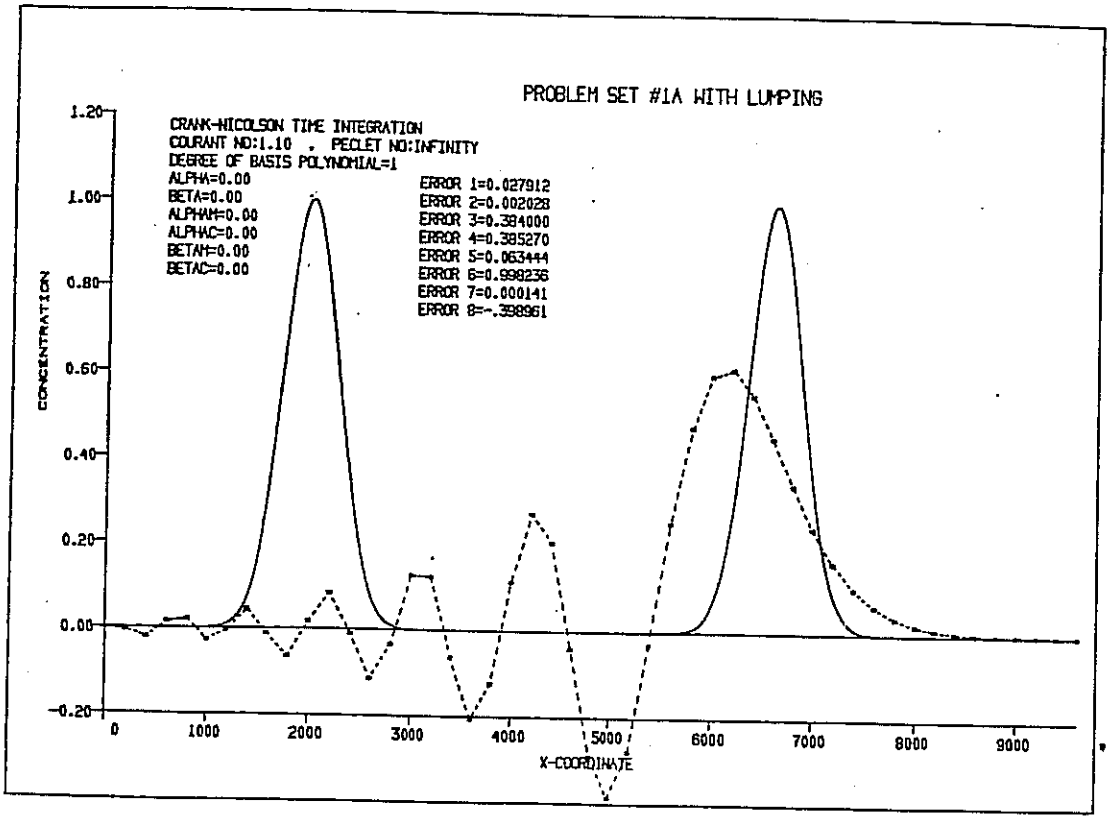
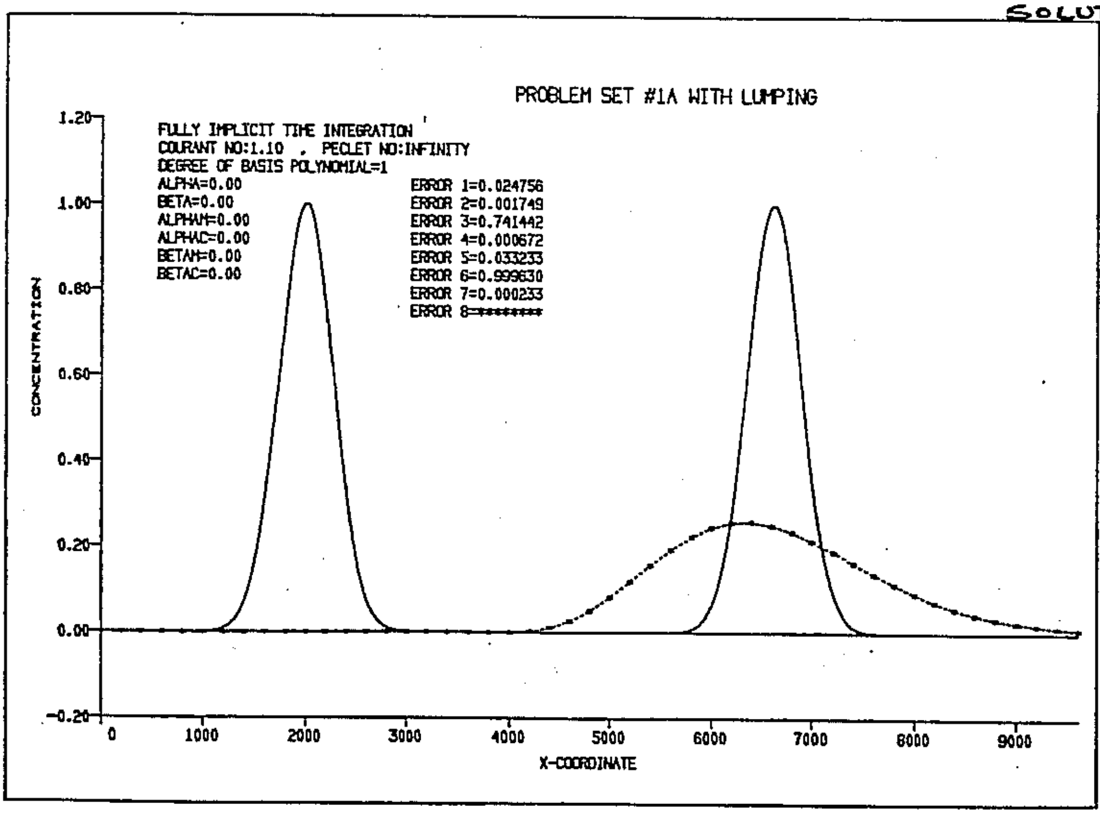


Fig LII-2c

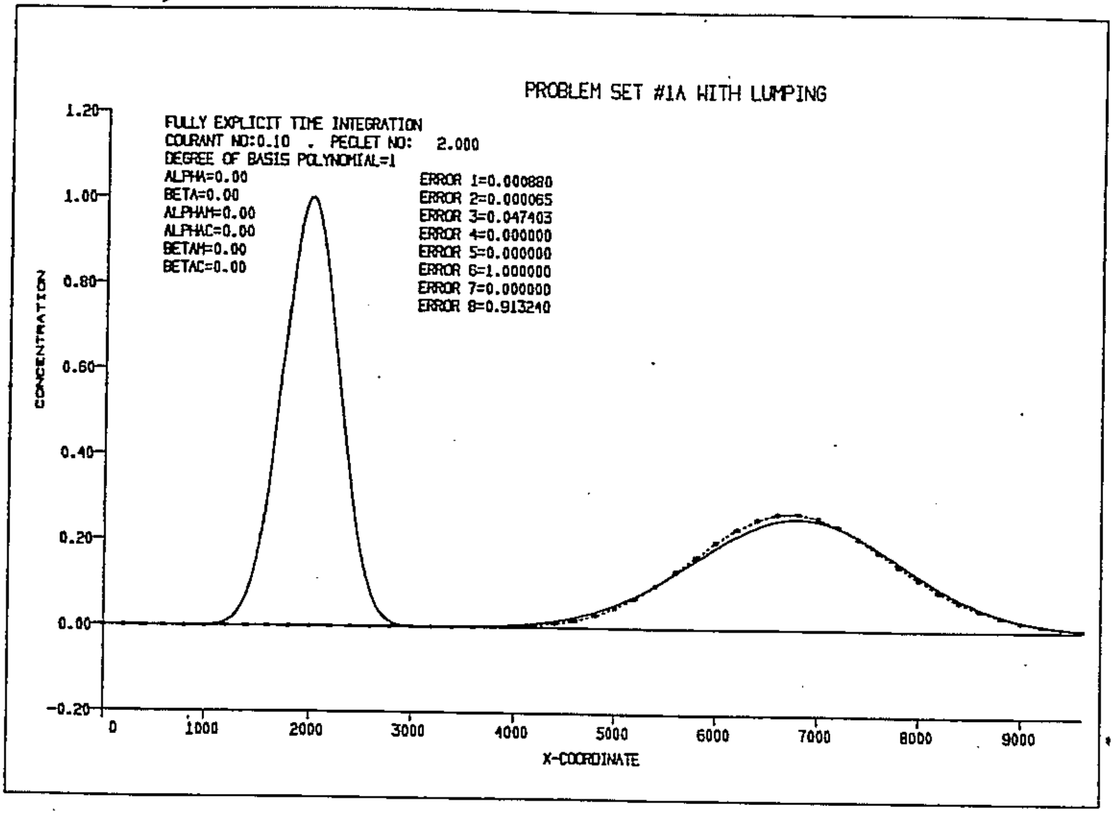
F.D. $\theta = 1.0$ $C_{*} = 1.1$ $P_e = \infty$

STABLE ; NO WIGGLES ; EXCESSIVE DAMPING OF FUNDAMENTAL SOLUTION



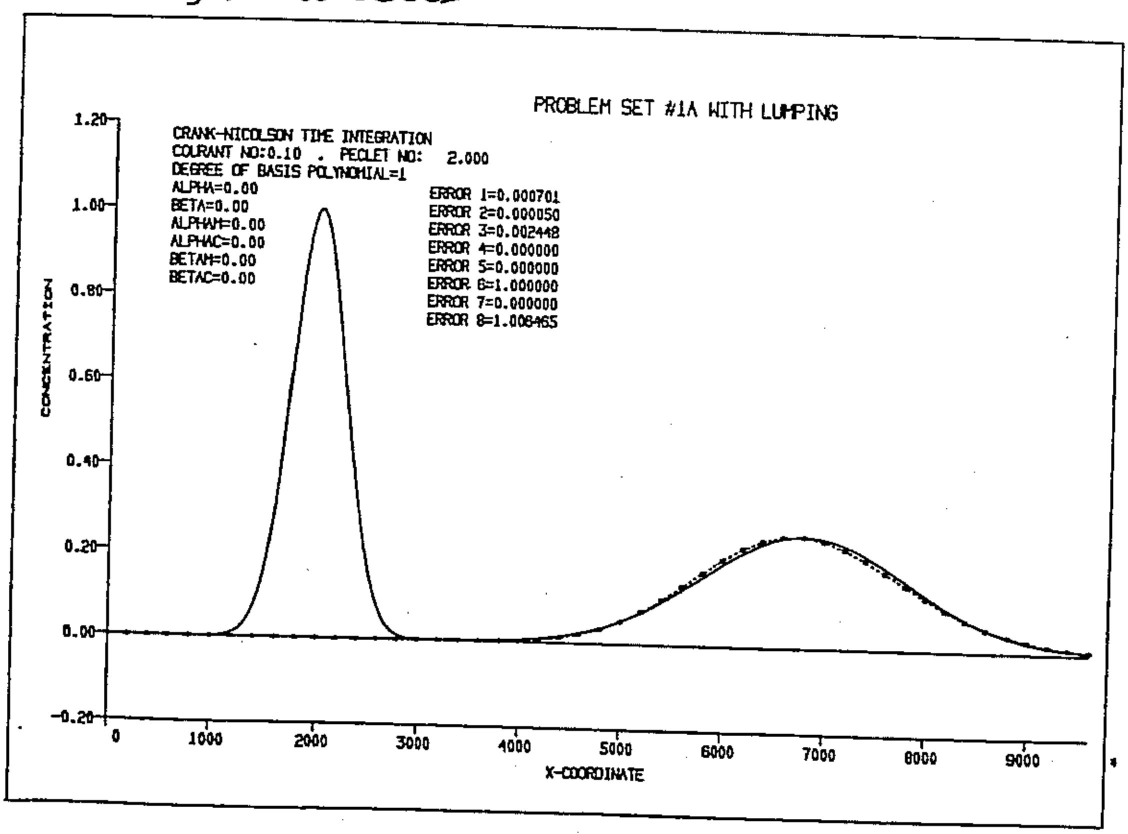
F.D. $\theta = 0.0$ $\quad C_{\#}=0.1$ $\quad P_e = 2.0$ Fig. L11-3a

STABLE, NO WIGGLES



F.D. $\theta = 0.5$ $\quad C_{\#}=0.1$ $\quad P_e = 2.0$ Fig L11-3b

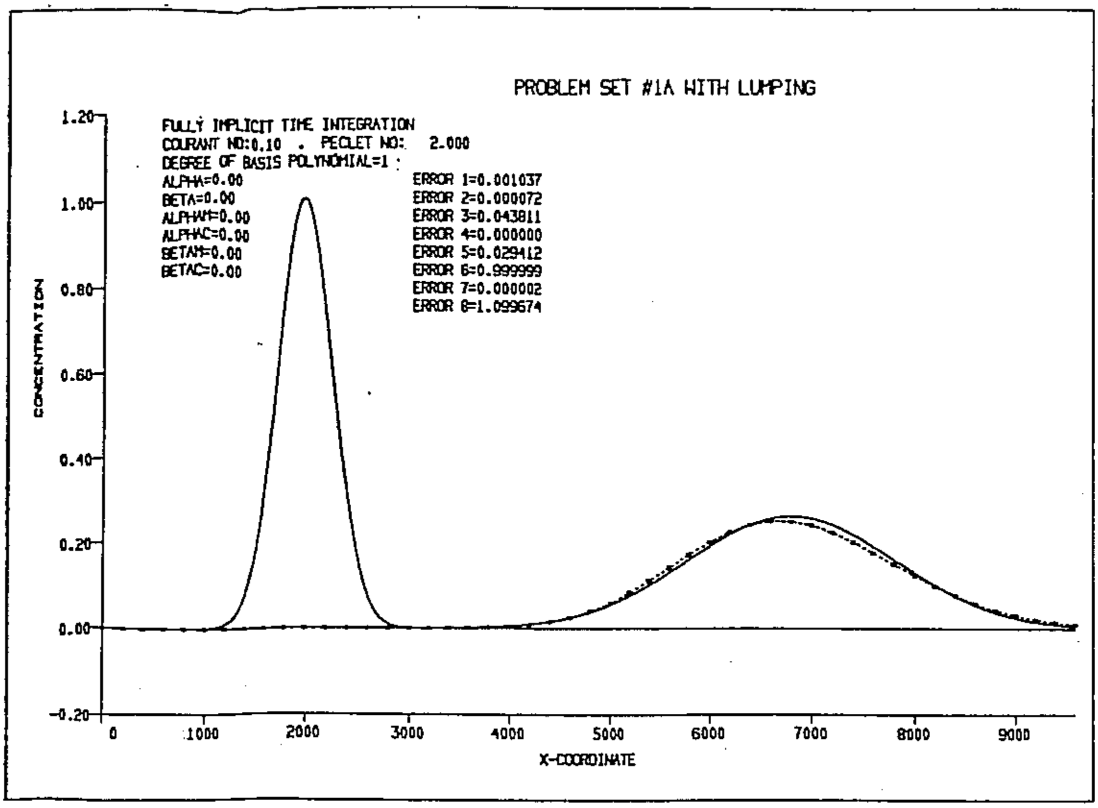
STABLE, NO WIGGLES



FD $\theta=1.0$ $C_{\#}=0.1$ $\mathbb{P}_e=2.0$

Fig L11-3c

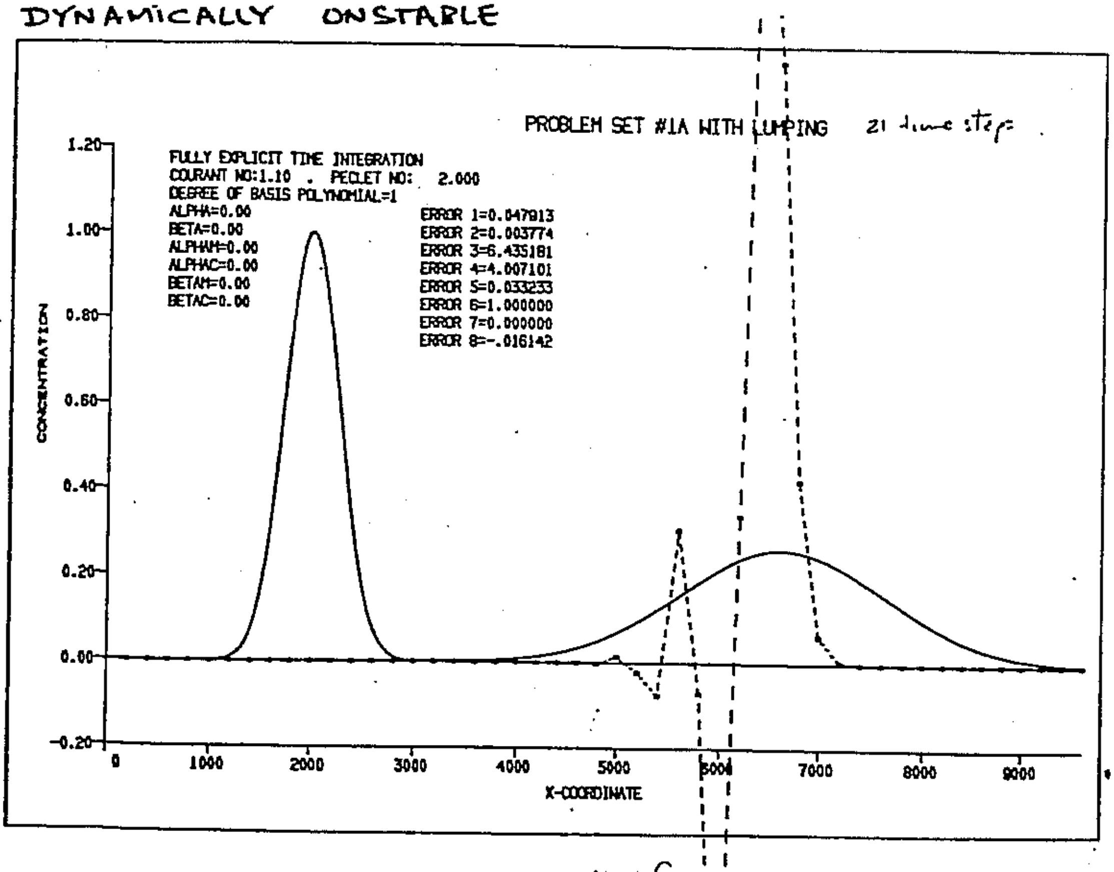
STABLE , NO WIGGLES



F.D. $\theta=0$ $C_{\#}=1.1$ $\mathbb{P}_e=2.0$

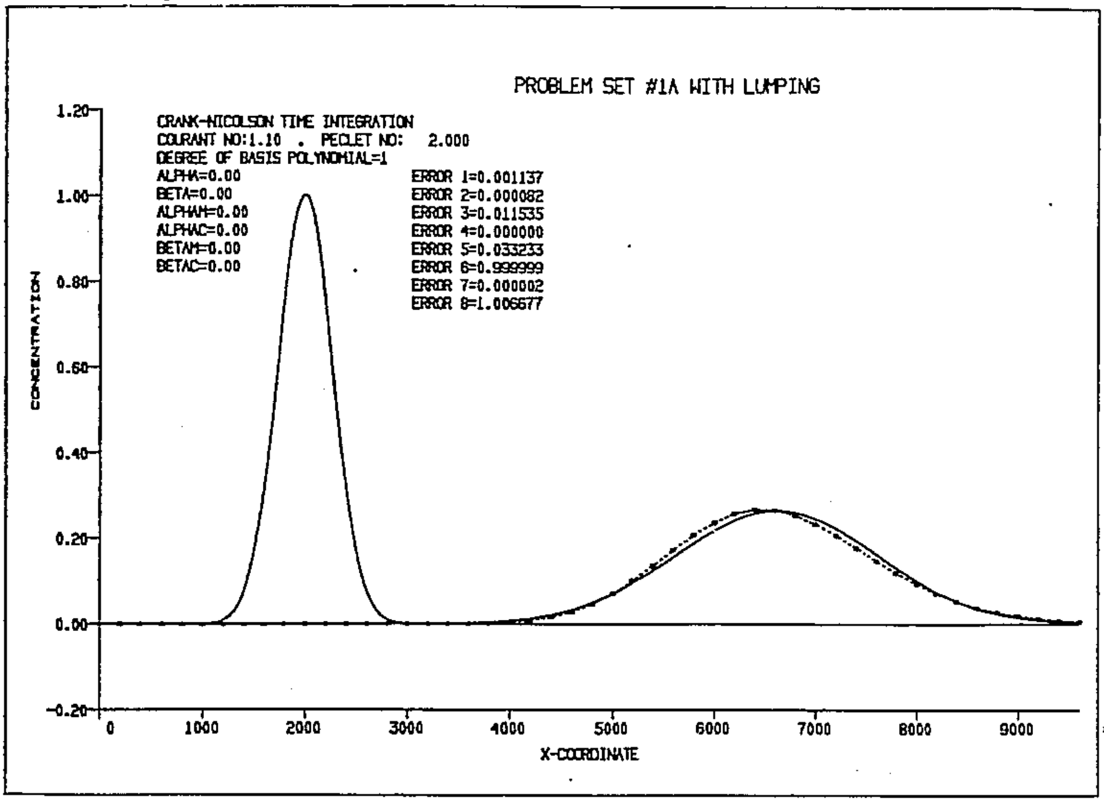
Fig L11-4a

DYNAMICALLY UNSTABLE



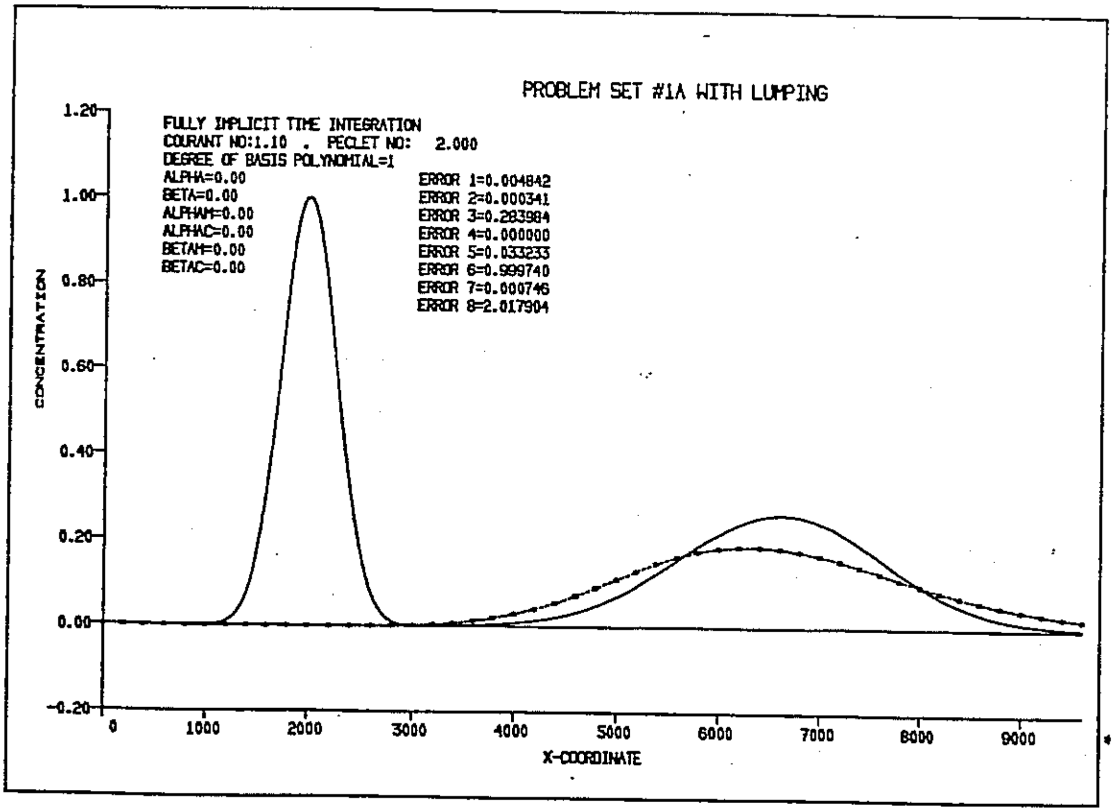
F.D. $\theta = 0.5$ $\mathbb{C}_{\#} = 1.1$ $\mathbb{P}_e = 2.0$ Fig L11-4b

STABLE, NO WIGGLES



F.D. $\theta = 1.0$ $\mathbb{C}_{\#} = 1.1$ $\mathbb{P}_e = 2.0$ Fig L11-4c

STABLE, NO WIGGLES, EXCESSIVE DAMPING



- Fully implicit scheme is unconditionally stable. ***The solution has wiggles for*** $\mathbf{P_e > 2}$ ***at low*** $\mathbf{C_\#}$ ***but does not at high*** $\mathbf{C_\#}$ ***where the solution is excessively damped.***

Fourier Analysis to Analyze the Behavior of Numerical Solutions

- So far Fourier analysis has only indicated whether a solution or a component of a solution will experience unstable growth.
- Typically the short wavelength components of the solution are the features which lead to stability problems (see Figure L10.1).
- ***Fourier Analysis can also be used to investigate the accuracy of a numerical solution!***
- ***By comparing the results of a Fourier analysis of the exact p.d.e., with those of the difference equation, we can get a handle on how our scheme performs.***
- Therefore we examine the Fourier components of a solution as they are propagated analytically and numerically. This gives substantial information regarding the accuracy of a numerical scheme.

Fourier Analysis of the Analytical Solution

$$\frac{\partial u}{\partial t} + V\frac{\partial u}{\partial x} = D\frac{\partial^2 u}{\partial x^2}$$

Let the general solution be represented by the Fourier Series:

$$u = \sum_{n=-\infty}^{+\infty} U_n exp\,[\hat{i}\alpha_n t + \hat{i}\beta_n x]$$

where

α_n = frequency of the n^{th} component

β_n = spatial frequency or wave number

$\hat{i}$ = $\sqrt{-1}$

Since the p.d.e. is linear we need only examine 1 component of the Fourier series. Therefore:

$$u \approx U_n exp\,[\hat{i}\alpha_n t + \hat{i}\beta_n x]$$

Now we can determine the relationship between wave number β_n and frequency α_n in addition to the analytical amplification factor, ξ_n, by substituting into the p.d.e.:

$$U_n \hat{i}\alpha_n exp\,[\hat{i}\alpha_n t + \hat{i}\beta_n x] + VU_n \hat{i}\beta_n exp\,[\hat{i}\alpha_n t + \hat{i}\beta_n x]$$

$$= D\hat{i}^2\beta_n^2 U_n exp\,[\hat{i}\alpha_n t + \hat{i}\beta_n x]$$

$$\Rightarrow$$

$$\alpha_n = \beta_n(\hat{i}D\beta_n - V)$$

Dispersion relationship of analytical eq. !!
freq $\leftrightarrow$ wave no.

- Thus frequency is a function of wave number.

Substituting α_n back into the solution for u, we have:

$$u \approx U_n exp\,[\hat{i}\beta_n(x - Vt)]\,exp\,[-\beta_n^2 Dt]$$

- The first portion of this solution represents translation of a Fourier component.
- The second portion represents the amplitude modification of a Fourier component.
- ***The amplitude and phase of a numerical solution component with wavenumber β_n, <u>do not necessarily coincide</u> with these analytical values.***

Let's relate the expression for u to the amplification factor ξ.

- Recall that $u_{t+\Delta t} = \xi_n u_t$ ←
- and that $\xi_n = e^{\hat{\imath}\alpha_n \Delta t}$
- However we found that $\alpha_n = \beta_n (\hat{\imath} D \beta_n - V)$

Therefore the analytical amplification factor for solution component n with wavenumber β_n:

$$\xi_n = e^{\hat{\imath}\beta_n (\hat{\imath} D \beta_n - V)\Delta t}$$

$$\Rightarrow$$

$$\xi_n = e^{-D\beta_n^2 \Delta t} e^{-\hat{\imath} V \beta_n \Delta t}$$

$$\Rightarrow$$

$$\xi_n = [\cos(\beta_n V \Delta t) - \hat{\imath} \sin(\beta_n V \Delta t)]\, e^{-D\beta_n^2 \Delta t}$$

Thus the amplitude of the analytical amplification factor is:

$$|\xi_n|^2 = \cos^2(\beta_n V\Delta t)\, e^{-2D\beta_n^2\Delta t} + \sin^2(\beta_n V\Delta t)\, e^{-2D\beta_n^2\Delta t}$$

$$\Rightarrow$$

$$|\xi_n|^2 = e^{-2D\beta_n^2\Delta t}$$

- $|\xi_n|$ represents the ratio of the magnitude of the analytical wave after one time step to its magnitude at the beginning of that time step.
- Note on complex numbers:

$$z = u + iv$$

$$\Rightarrow$$

$$z = r(\cos\phi + i\sin\phi) = re^{i\phi}$$

where

$$r = \sqrt{u^2 + v^2} \qquad \text{and} \qquad \phi = \tan^{-1}\left(\frac{v}{u}\right)$$

The phase of analytical amplification factor is:

$$e^{\hat{i}\phi_n} = \frac{\xi_n}{|\xi_n|} = \frac{e^{-D\beta_n^2\Delta t}\, e^{-iV\beta_n\Delta t}}{e^{-\beta_n^2 D\Delta t}} = e^{-\hat{i}V\beta_n\Delta t}$$

$$\Rightarrow$$

$$\phi_n = -V\beta_n\Delta t$$

Fourier Analysis of the Numerical Solution

We use an identical procedure as was used in the analysis of the amplification factor for the weighted implicit/explicit solution (previously used to study stability).

$$u_{p,q+1} - u_{p,q} + \frac{C_\#}{2}[\theta(u_{p+1,q+1} - u_{p-1,q+1}) + (1-\theta)(u_{p+1,q} - u_{p-1,q})]$$

$$-\rho[\theta(u_{p+1,q+1} - 2u_{p,q+1} + u_{p-1,q+1}) + (1-\theta)(u_{p+1,q} - 2u_{p,q} + u_{p-1,q})]$$

We assume that the solution can be represented by

$$u(x,t) = \sum_{n=-\infty}^{+\infty} U_n exp(\hat{i}\alpha'_n t + \hat{i}\beta_n x)$$

- We note that the frequency α'_n obtained in the numerical solution does not necessarily equal to that obtained in the analytical solution.

Again due to linearity considerations we need only consider 1 component of the solution series:

$$u(x,t) = U_n e^{\hat{i}\alpha'_n t} e^{\hat{i}\beta_n x}$$

$$\Rightarrow$$

$$u_{p,q} = U_n e^{\hat{i}\alpha'_n q\Delta t} e^{\hat{i}\beta_n p\Delta x}$$

We again define the amplification factor (for the numerical solution) as:

$$\xi'_n = e^{\hat{i}\alpha'_n \Delta t}$$

- We note that ξ'_n equals the amplification factor for the numerical solution in time such that:

$$u_{p,\,q+1} = \xi'_n u_{p,\,q}$$

Therefore

$$u_{p,\,q} = U_n \xi'^{q}_{n} e^{\hat{i}\beta_n p\Delta x}$$

We substitute $u_{p,\,q}$ into our FD equation to find:

$$\xi'_n = \frac{1-(1-\theta)\,\{\mathbf{C}_{\#}\hat{i}\sin(\beta_n\Delta x) + 2\rho\,[1-\cos(\beta_n\Delta x)]\,\}}{1+\theta\,\{\mathbf{C}_{\#}\hat{i}\sin(\beta_n\Delta x) + 2\rho\,[1-\cos(\beta_n\Delta x)]\,\}}$$

- For stability we must have $|\xi'_n| \le 1.0$

Comparison of the Analytical and the Numerical Amplification Factors

- We must examine both the ratio of the amplitudes and of the phases.
- We normalize the comparisons by comparing the amplification factors for each wave component after that component has propagated its full wavelength.

$$\lambda_n = VN_n\Delta t$$

where N_n = the number of required time steps required for λ_n to propagate 1 wavelength:

$$N_n = \frac{\lambda_n}{V\Delta t} = \left(\frac{\lambda_n}{\Delta x}\right)\left(\frac{\Delta x}{V\Delta t}\right)$$

$$\Rightarrow$$

$$N_n = \left(\frac{\lambda_n}{\Delta x}\right)\left(\frac{1}{\mathbf{C}_{\#}}\right)$$

- Recall that wavelength $\lambda_n = \dfrac{2\pi}{\beta_n}$

<u>Ratio of the Computed to Actual (Analytical) Amplitude After Propagating 1 Wavelength</u>

$$R_A = \frac{\textit{computed amplitude}}{\textit{actual amplitude}} = \left[\frac{|\xi'_n|}{|\xi_n|}\right]^{N_n}$$

$$\Rightarrow$$

$$R_A = \left[\frac{|\xi'_n|}{exp\,(-\beta_n^2 D\Delta t)}\right]^{N_n}$$

$$\Rightarrow$$

$$R_A = \left[\frac{|\xi'_n|}{exp\,(-4\pi^2\rho\,(\Delta x/\lambda_n)^2)}\right]^{\frac{\lambda_n}{\Delta x}\frac{1}{\mathbf{C}_{\#}}}$$

Now substitute in $|\xi'_n|$ from the amplification factor analysis completed for the numerical solution.

See the plots for the amplitude ratio, R_A, in Figures L11.5 and L11.6.

- The amplitude ratio, R_A, may be greater or smaller than 1.0.
- Ratio = 1.0 for all $\frac{\lambda_n}{\Delta x}$, indicates that the amplitude of the numerical solution is perfect for all wavelengths.
- Ratio < 1.0, indicates that the numerical solution is damped more than the analytical solution.
- Ratio << 1, indicates an excessively damped numerical solution.
- Ratio > 1.0, numerical solution damps less than the analytical solution. However the solution is not necessarily unstable since this is only the ratio. We must check $|\xi'_n|$ for stability (e.g. see Figure L10.2).
- For the case shown in Figure L11.6, we note that the fully implicit solution $(\theta = 1.0)$ exhibits greater damping than the $C-N$ case $(\theta = 0.5)$. This is especially true when $\mathbf{C}_\#$ gets larger (i.e. closer to unity). We found this to be the case for the fully implicit solutions in our numerical experiments. Let's compare ratio's, R_A, at $\theta = 1.0$ for different $\mathbf{C}_\#$ values. Examining Figure L11.6.

  - Shows that for $\theta = 1$, $\mathbf{P_e} = \infty$ and $\mathbf{C}_\# = 0.1$, the ratio is $R_A \cong 1$ Therefore neither short wavelengths (wiggles) nor longer wavelength components of the solution are significantly damped.

  - Shows that for $\theta = 1$, $\mathbf{P_e} = \infty$ and $\mathbf{C}_\# = 1.1$, the ratio $R_A << 1$ for a very large range of $\lambda_n / \Delta x$. Therefore both short (wiggles) and long wavelength components of the solution will be excessively damped.

  - Shows that for $\theta = 0.5$, $\mathbf{P_e} = \infty$ and $\mathbf{C}_\# = 0.1$ and 1.1, the ratio $R_A = 1$ for all $\lambda_n / \Delta x$. Therefore we expect no damping greater than the analytical solution for all wavelengths (thus wiggles are not eliminated).

Fig L11-5

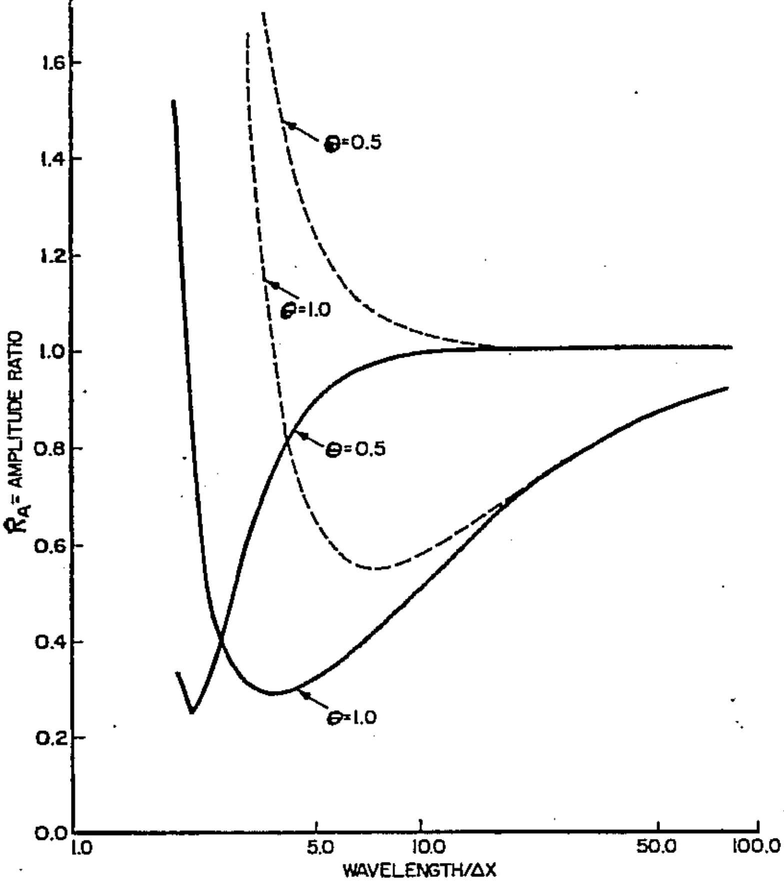
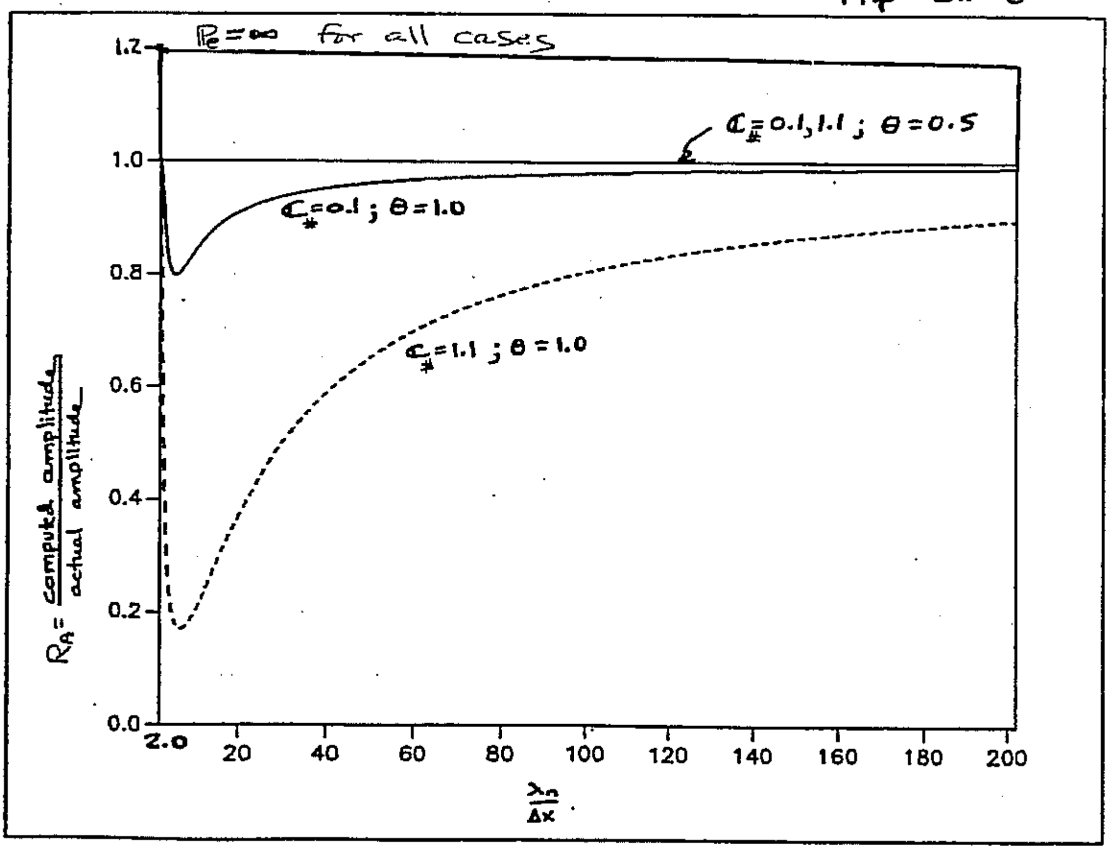


Fig. 5.13. Amplitude ratio for the single equation finite element (——) and finite difference (---) methods, where $D = 0.069$ and $C_{\#} = 0.369$. $\mathbb{P}_e = \frac{C}{D} = \frac{\frac{V\Delta t}{\Delta x}}{\frac{D\Delta t}{\Delta x^2}} = \frac{V\Delta x}{D} = 5.35$

Fig L11-6



- A perfect numerical solution would have the ratio $R_A = 1$ for all $\lambda_n / \Delta x$.
- ***Ideally we would like a scheme such that the ratio $R_A << 1$ only for small $\lambda_n / \Delta x$ and $R_A \cong 1$ for all other $\lambda_n / \Delta x$. Reasons for this include the computation of gradients of a solution as well as nonlinear energy transfer.***

Comparison of Analytical and Numerical Phase (Phase Lag)

Phase lag equals phase of the computed solution relative to the actual solution after that wave has propagated one complete wavelength:

$$\Phi = -\phi'_n N_n + \phi_n N_n$$

where

ϕ'_n = the phase of the numerical solution

ϕ_n = the phase of the analytical solution

N_n = the number of time steps to propagate 1 wavelength

Φ = phase lag

Recall that

$$N_n = \frac{\lambda_n}{\Delta x} \frac{\Delta x}{V \Delta t}$$

and

$$\phi_n = -V\beta_n \Delta t = -V\frac{2\pi}{\lambda_n}\Delta t$$

Thus

$$\Phi = -\phi'_n N_n - \left(V\frac{2\pi}{\lambda_n}\Delta t\right)\left(\frac{\lambda_n}{\Delta x}\frac{\Delta x}{V\Delta t}\right)$$

$$\Rightarrow$$

$$\Phi = -\phi'_n N_n - 2\pi$$

Φ relates to numerical dispersion. Certain wavelength components of the solution don't have the correct frequency and therefore do not propagate at the correct speed. Therefore incorrect phase of various wavelength components of the solution causes wiggles which trail the solution.

Note that the solution can still be stable (i.e., these short wavelength perturbations may be still damped or even neutrally stable, however we will see them trail our solution).

Let us examine the Phase Lag Plots shown in Figures L11.7.

- Characteristically the shorter wavelengths are propagated poorly while there is relatively little phase lag for the longer wavelengths.
- The $C-N$ (centered-time) $\theta = 0.5$ solutions exhibit slightly less phase lag than the fully implicit $\theta = 1.0$ solution. Therefore for $C-N$ we don't expect to see as much numerical dispersion, i.e., the wiggles won't be as bad.
- A perfect solution would have $\Phi = 0$ for all $\lambda_n/\Delta x$.

Fig L11-7

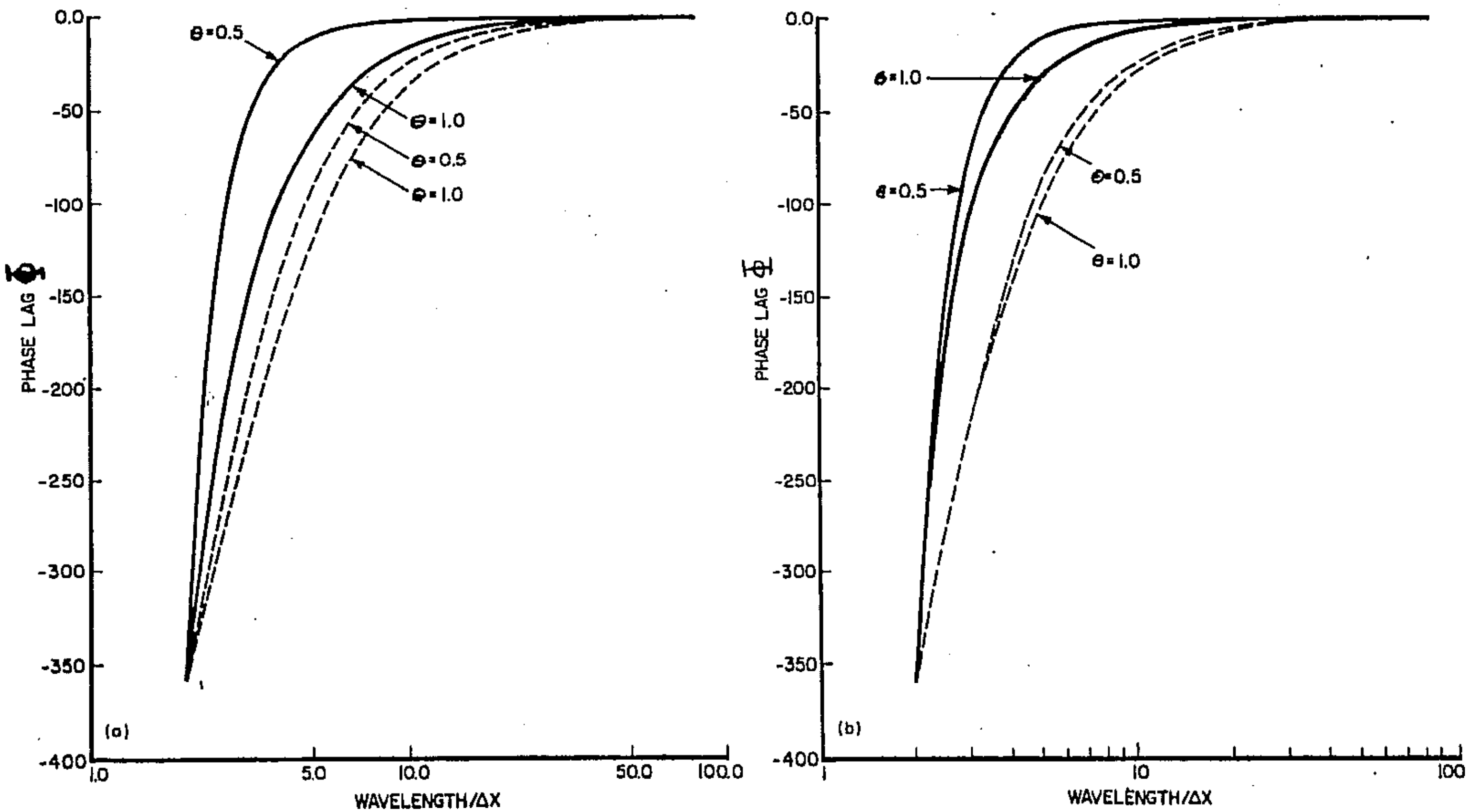


Fig. 5.12. Phase lag Φ_a for the single equation finite element (——) and finite difference (---) methods. (a) $\rho = 0.069$ and $C_{\#} = 0.369$; (b) $\rho = 0.0069$ and $C_{\#} = 0.369$.

Conclusion

- Fourier analysis helps understand accuracy of a numerical scheme (both amplitude and phase propagation characteristics). However we still don't have information regarding b.c.'s which may be very important. Furthermore the applicability of this approach is practically limited to linear problems.
- Ideally you want to design a numerical scheme which minimizes "numerical dispersion" or phase lag and which has a damping ratio $R_A \cong 1$ except for very short wavelengths.

Summary of Fourier Analysis

- for determining stability characteristics
- for determining accuracy characteristics

Fourier series solution to continuum p.d.e

$$U(x,t) = \sum_{n=-\infty}^{+\infty} A_n e^{i\alpha_n t} e^{i\beta_n x}$$

- α_n = freq. β_n = wave no. of constituent n
- time-space seperable form
- general solution has unknown coef.'s A_n
- we only need to consider 1 generic component n.

$$\boxed{U(x,t) = A_n e^{i\alpha_n t} e^{i\beta_n x}}$$

- Substitute for u into p.d.e and determine a relationship b/w α_n and β_n $\Rightarrow$

frequency <-> waveno. relationship => dispersion relationship

- Amplification factor describes how analytical solution component n changes during a time Δt

$$U(x, t+\Delta t) \equiv \xi_n U(x,t)$$

$$\Rightarrow$$

$$\xi_n = \frac{U(x,t+\Delta t)}{U(x,t)}$$

$$= \frac{A_n e^{i\alpha_n (t+\Delta t)} e^{i\beta_n x}}{A_n e^{i\alpha_n t} e^{i\beta_n x}}$$

$$\boxed{\xi_n = e^{i\alpha_n \Delta t}}$$ Analytical Amplification factor

∴ substitute into above eq. for α_n in terms of β_n (dispersion relationship)

- ξ_n is in general complex → has an amplitude and phase

$$|\xi_n|^2 = \text{Real}^2 + \text{Im}^2 \qquad e^{i\phi_n} = \frac{\xi_n}{|\xi_n|}$$

Fourier Series Solution to discrete equation

$$u(x,t) = \sum_{n=-\infty}^{+\infty} A_n e^{i\alpha_n' t} e^{i\beta_n x}$$

- same general form as analytical solution
- α_n' freq. and β_n' waveno. again related. However not necessarily same relationship as for analytical solution.

- In discrete solution

$\beta_n = \frac{\pi}{\Delta x}$ $(\lambda_n = 2 \cdot \Delta x)$ shortest resolvable wave

$\beta_n = 0$ $(\lambda_n = \infty)$ longest wave

- Again due to linearity only need consider one component for generic waveno. β_n

$$u(x,t) = A_n e^{i\alpha_n' t} e^{i\beta_n x}$$

- In discrete form $x = p\Delta x$ $t = q\Delta t$

$$u_{p,q} = A_n e^{i\alpha_n' q\Delta t} e^{i\beta_n p\Delta x}$$

- Again amplification factor describes how the discrete solution for component n changes during a time Δt

$$u_{p,q+1} = \xi_n' u_{p,q}$$

$$\Rightarrow$$

$$\xi_n' = \frac{u_{p,q+\Delta t}}{u_{p,q}}$$

$$= \frac{A_n e^{i\alpha_n'(q+1)\Delta t} e^{i\beta_n p\Delta x}}{A_n e^{i\alpha_n' q\Delta t} e^{i\beta_n p\Delta x}}$$

$$\xi_n' = e^{i\alpha_n' \Delta t}$$

- Algebra is simpler to substitute for $e^{i\alpha_n'\Delta t}$ into generic form of $u_{p,q}$ (could solve for α_n' in terms of β_n and then substitute into above relationship)

$$\boxed{u_{p,q} = A_n \xi_n'^{\,q} e^{i\beta_n p \Delta x}}$$

- Substitute into discrete form of p.d.e. and develop relationship b/w β_n and ξ_n'

□ Stability requires that

$$|\xi_n'| \le 1$$

□ Accuracy Comparisons – Amplitude Ratio

Consider the ratio of the numerical and analytical solutions at future time level

$$\frac{|u_{p,q+1}|}{|U(x,t+\Delta t)|} = ?$$

recall that

$$u_{p,q+1} = \xi_n' u_{p,q}$$

$$U(x,t+\Delta t) = \xi_n U(x,t)$$

Thus

$$\frac{|u_{p,q+1}|}{|U(x,t+\Delta t)|} = \frac{|\xi_n'|}{|\xi_n|} \frac{|u_{p,q}|}{|U(x,t)|}$$

$\therefore$ If $\dfrac{|\xi_n'|}{|\xi_n|} = 1$ $\Rightarrow$ numerical and analytical solution damp at same rate

$\dfrac{|\xi_n'|}{|\xi_n|} < 1$ $\Rightarrow$ numerical solution damps more than analytical solution

$\dfrac{|\xi_n'|}{|\xi_n|} > 1$ $\Rightarrow$ numerical solution damps less than analytical solution

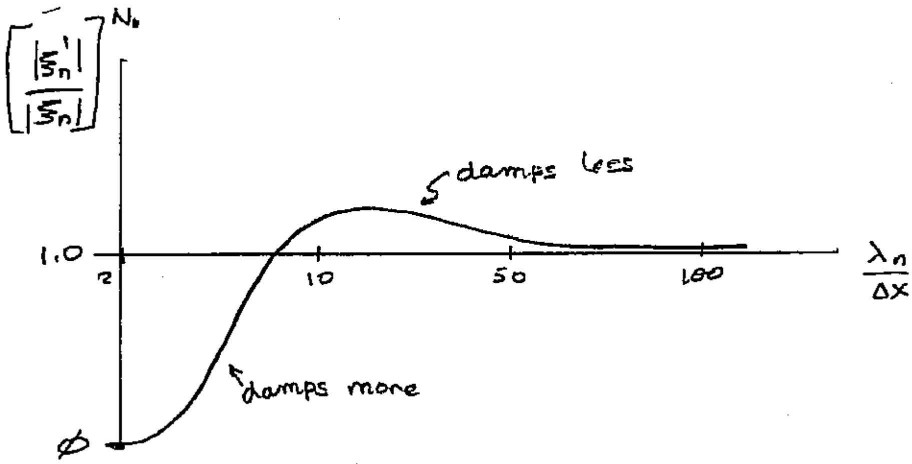
To make comparisons uniform for all different waveno.'s (ie. to normalize), we raise ratio to N_n = # of time steps required to propagate 1 wavelength, λ_n

$$\left[\frac{|\xi_n'|}{|\xi_n|}\right]^{N_n}$$

$$N_n = \frac{\lambda_n}{V\Delta t}$$ ← distance info. propagates per time step

$$= \frac{\lambda_n}{\Delta x} \cdot \frac{\Delta x}{V\Delta t}$$

$$N_n = \frac{\lambda_n}{\Delta x} \cdot \frac{1}{C_{\#}}$$



□ <u>Accuracy Comparisons – Phase</u>

Can look at phase behavior of solutions by comparing phase of the discrete solution to the phase of the analytical solution (normalized for one complete wave)

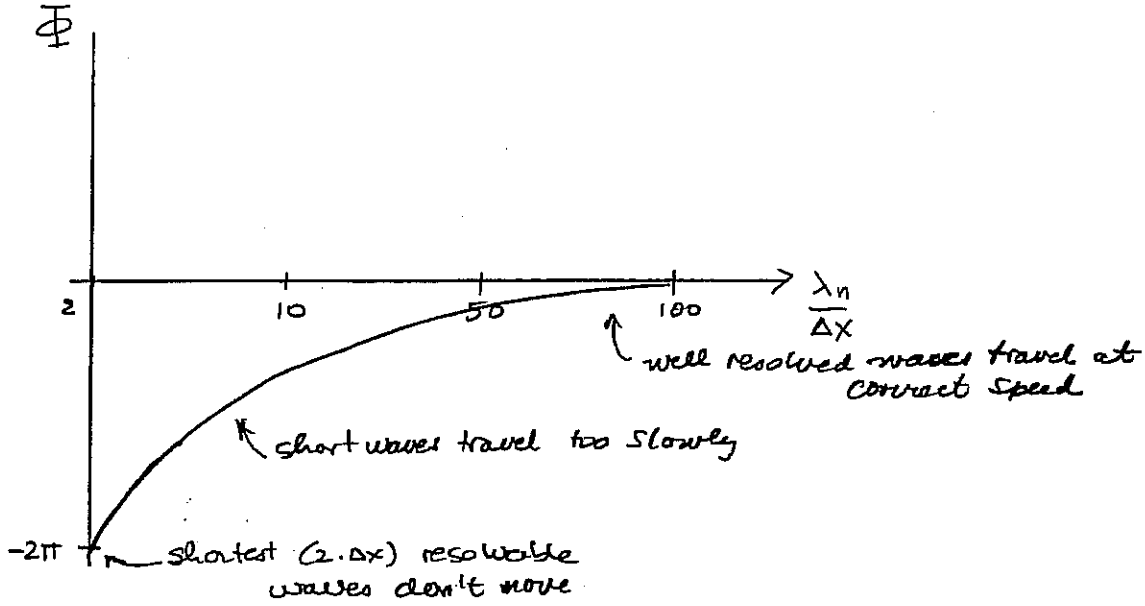
$$\Phi = -\phi_n' N_n + \phi_n N_n$$

$$\Phi = -\phi_n' N_n - 2\pi$$

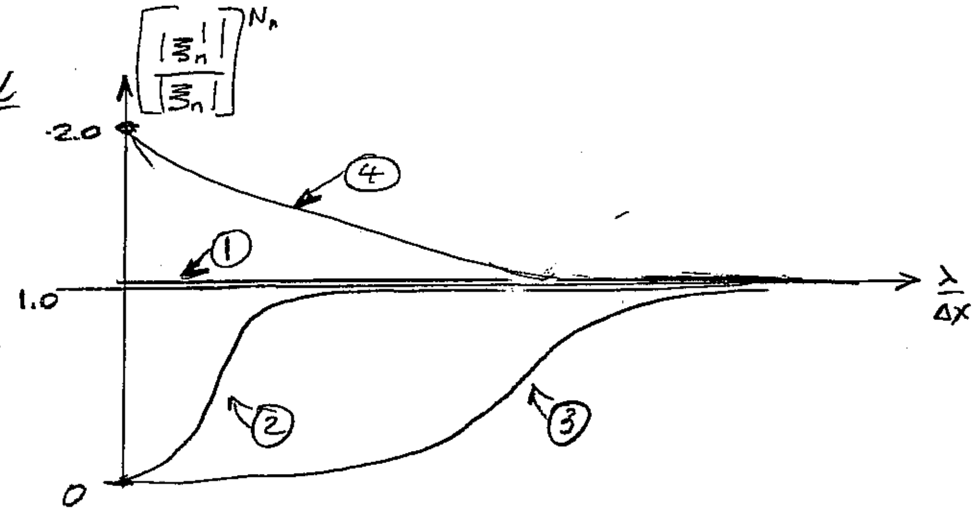
$\Phi = 0$ perfect phase

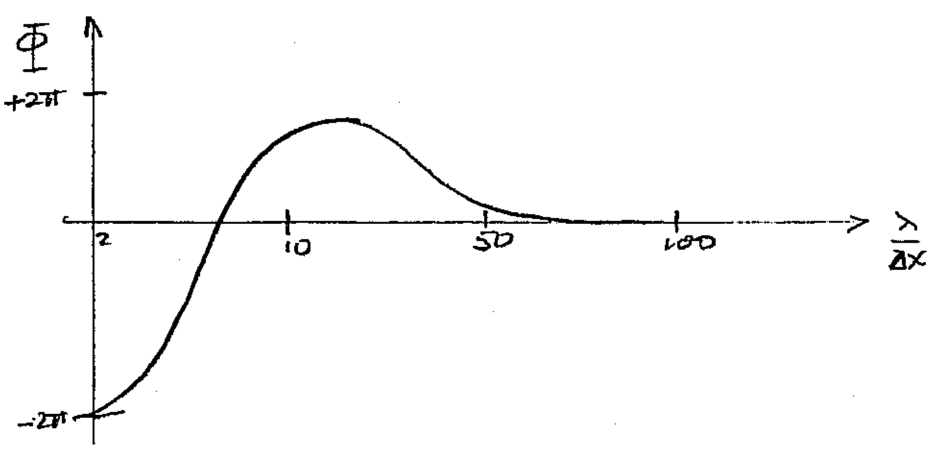
$\Phi < 0$ computed solution lags analytical solution

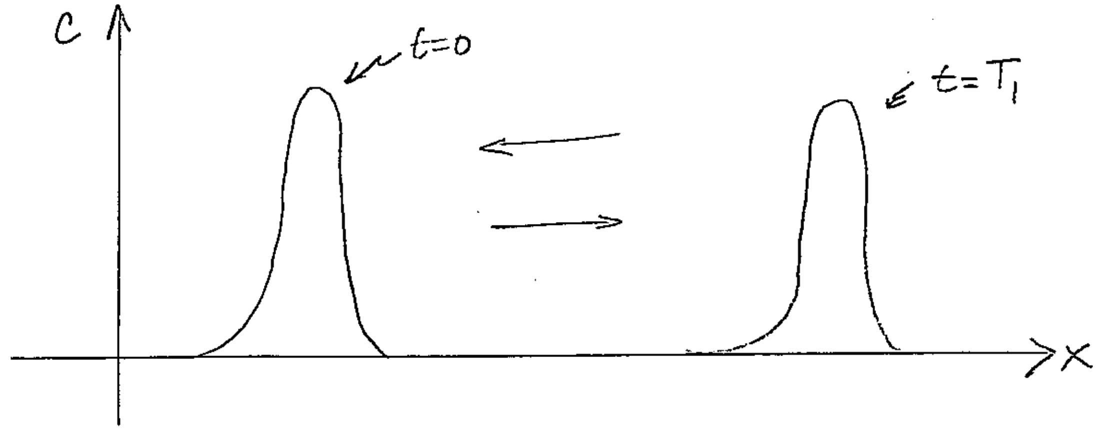
$\Phi > 0$ " " leads " "


Φ
2
10
50
100
λn / Δx
well resolved waves travel at correct speed
short waves travel too slowly
−2π
shortest (2·Δx) resolvable waves don't move

Ex


$\left[\frac{|\xi_n'|}{|\xi_n|}\right]^{N_n}$
2.0
4
1
1.0
λ / Δx
2
3
0


Φ
+2π
2
10
50
100
λ / Δx
−2π



Consider $P_e = \infty$ case with ratio and phase curves presented
$C = 0.5$

let plume go forward the backward $\left\{ \begin{array}{ll} V_x = +V_1 & \text{for } 0<t<T_1 \\ V = -V_1 & \text{for } T_1<t<2T_1 \end{array} \right.$

Draw results for cases 1, 2, 3, 4 at $t=T_1$ and $t=2T_1$