Chapter 2 The One-Dimensional Scalar Wave Equation

2.1 – examine simplest differential equation describing wave propagation ?

2.2

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \qquad (2.1)$$

has as general solutions functions of form

$$u(x,t) = F(x+ct) + G(x-ct) \qquad (2.2)$$

some functions that satisfy (2.1)

Take $\frac{\partial}{\partial t}$ partial

$$\frac{\partial u}{\partial t} = \underbrace{\frac{dF(x+ct)}{d(x+ct)}}_{\text{call this } F'(x+ct)} \underbrace{\frac{\partial(\cancel{x}+ct)}{\partial t}}_{c} + \underbrace{\frac{dG(x-ct)}{d(x-ct)}}_{\text{call this } G'(x-ct)} \underbrace{\frac{\partial(\cancel{x}-ct)}{\partial t}}_{-c}$$

$$= c\,F'(x+ct) - c\,G'(x-ct) \qquad (2.3a)$$

Repeat process

$$\frac{\partial^2 u}{\partial t^2} = c^2 F''(x+ct) + c^2 G''(x-ct) \qquad (2.3b)$$

2.2 cont.

$$\frac{\partial u}{\partial x} = \frac{dF(x+ct)}{d(x+ct)} \underbrace{\frac{\partial(x+ct)}{\partial x}}_{1} + \frac{dG(x-ct)}{d(x-ct)} \underbrace{\frac{\partial(x-ct)}{\partial x}}_{1}$$

$$= F'(x+ct) + G'(x-ct) \qquad (2.4a)$$

Repeat process

$$\frac{\partial^2 u}{\partial x^2} = F''(x+ct) + G''(x-ct) \qquad (2.4b)$$

Now substitute back into (2.1)

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}$$

$$c^2 F''(x+ct) + c^2 G''(x-ct) = c^2 \left[F''(x+ct) + G''(x-ct)\right] \qquad (2.5)$$

↳ Proves that (2.2) satisfies (2.1)

2.3 Dispersion Relation

→ how does wavelength λ change w/ frequency f?

Start by examining one solution to the 1D wave eqn (2.1)

$$u(x,t) = e^{j(\omega t - kx)} \qquad (2.6)$$

← fwd traveling sol'n $G(x-ct)$

where the wavenumber $k = \frac{2\pi}{\lambda} = \frac{\omega}{v_p}$ and the angular frequency $\omega = 2\pi f$

$$\frac{\partial u}{\partial t} = j\omega e^{j(\omega t - kx)} \qquad \frac{\partial u}{\partial x} = -jk e^{j(\omega t - kx)}$$

$$\frac{\partial^2 u}{\partial t^2} = (j\omega)^2 e^{j(\omega t - kx)} \qquad \frac{\partial^2 u}{\partial x^2} = (-jk)^2 e^{j(\omega t - kx)}$$

sub. into (2.1)

$$(j\omega)^2 e^{j(\omega t - kx)} = c^2 (-jk)^2 e^{j(\omega t - kx)}$$

divide out common terms

$$\omega^2 = c^2 k^2$$

$$k = \pm \omega/c$$

dispersion relation (2.7b)

OR $$\underline{v_p = \frac{\omega}{k} = \pm c} \qquad (2.8)$$

phase velocity

* Since v_p is constant wrt frequency, this solution is <u>dispersionless</u>.

2.3 cont.

* group velocity $v_g = \frac{d\omega}{dK}$

* In this case, start w/ $\omega^2 = c^2 K^2$ to get v_g

$$\frac{d(\omega^2)}{dK} = \frac{d(c^2K^2)}{dK}$$

$$2\omega \frac{d\omega}{dK} = c^2(2K)$$

$$v_g = \frac{d\omega}{dK} = \frac{c^2(2K)}{2\omega} = \frac{c^2(\pm \omega/c)}{\omega}$$

$$\underline{v_g = \pm c} \qquad (2.9)$$

(group velocity is also a constant (no frequency dependence)

2.4 Finite Differences

Do a Taylor's series expansion of $u(x,t)$

Def'n of Taylor's series expansion of $f(x)$ about point $x=a$

$$f(x) = f(a) + (x-a)\left.\frac{\partial f(x)}{\partial x}\right|_{x=a} + \frac{(x-a)^2}{2!}\left.\frac{\partial^2 f(x)}{\partial x^2}\right|_{x=a}$$

$$+ \dots \frac{(x-a)^{n-1}}{(n-1)!}\frac{\partial^{n-1} f(x)}{\partial x^{n-1}} + R_n$$ ~ Remainder term

Where

$$R_n = \frac{(x-a)^n}{n!}\left.\frac{\partial^n f(x)}{\partial x^n}\right|_{x=\xi} \quad a<\xi<x$$ (Lagrange's form)

lowercase Xi

For our Taylor's series expansion of $u(x,t)$, we'll select a fixed time point t_n and expand about spatial point x_i to evaluate $u(x,t)$ at $x_i+\Delta x$ yielding

$$u(x_i+\Delta x, t_n) = u(x_i,t_n) + \frac{\overbrace{(x_i+\Delta x - x_i)}^{\Delta x}}{1!}\left.\frac{\partial u}{\partial x}\right|_{x_i,t_n} + \frac{(\Delta x)^2}{2!}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i,t_n}$$

$$+ \frac{(\Delta x)^3}{3!}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i,t_n} + \frac{(\Delta x)^4}{4!}\left.\frac{\partial^4 u}{\partial x^4}\right|_{\xi_1,t_n}$$

$$u(x_i+\Delta x, t_n) = u(x_i,t_n) + \Delta x\left.\frac{\partial u}{\partial x}\right|_{x_i,t_n} + \frac{\Delta x^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i,t_n}$$

$$+ \frac{\Delta x^3}{6}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i,t_n} + \frac{\Delta x^4}{24}\left.\frac{\partial^4 u}{\partial x^4}\right|_{\xi_1,t_n} \qquad (2.10a)$$

error/remainder term

2.4 cont.

Repeat process for $(x_i - \Delta x, t_n)$ to get

$$u(x_i-\Delta x, t_n) = u(x_i, t_n) + \frac{\overbrace{(x_i - \Delta x - x_i)}^{-\Delta x}}{1!} \left.\frac{\partial u}{\partial x}\right|_{x_i, t_n} + \frac{(-\Delta x)^2}{2!} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i, t_n}$$

$$+ \frac{(-\Delta x)^3}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i, t_n} + \frac{(-\Delta x)^4}{4!} \left.\frac{\partial^4 u}{\partial x^4}\right|_{\xi_2, t_n}$$

$$= u(x_i, t_n) - \Delta x \left.\frac{\partial u}{\partial x}\right|_{x_i, t_n} + \frac{\Delta x^2}{2} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i, t_n}$$

$$- \frac{\Delta x^3}{6} \left.\frac{\partial^3 u}{\partial x^2}\right|_{x_i, t_n} + \frac{\Delta x^4}{24} \left.\frac{\partial^4 u}{\partial x^4}\right|_{\xi_2, t_n} \qquad (2.10b)$$

$$x_i - \Delta x < \xi_2 < x_i$$

Now add (2.10a) to (2.10b)

$$u(x_i+\Delta x, t_n) + u(x_i - \Delta x, t_n) = 2u(x_i, t_n) + 0 + \Delta x^2 \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i, t_n}$$

$$+ 0 + \underbrace{\frac{\Delta x^4}{24}\left(\left.\frac{\partial^4 u}{\partial x^4}\right|_{\xi_1, t_n} + \left.\frac{\partial^4 u}{\partial x^4}\right|_{\xi_2, t_n} \right)}_{\text{combine}}$$

$$(2.11) \quad u(x_i+\Delta x, t) + u(x_i - \Delta x, t_n) = 2u(x_i, t_n) + \Delta x^2 \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i, t_n} + \frac{\Delta x^4}{12} \left.\frac{\partial^4 u}{\partial x^4}\right|_{\xi_3, t_n}$$

where $x_i - \Delta x < \xi_3 < x_i + \Delta x$

Now, solve (2.11) for $\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i, t_n}$

2.4 cont.

$$(2.12)\quad \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i,t_n} = \frac{u(x_i+\Delta x,t_n) - 2u(x_i,t_n) + u(x_i-\Delta x,t_n)}{\Delta x^2} - \underbrace{\frac{\Delta x^4}{12\Delta x^2}\left.\frac{\partial^4 u}{\partial x^4}\right|_{\xi_3,t_n}}_{\text{Remainder term} \;\longrightarrow\; O[(\Delta x)^2]}$$

Using the standard FDTD notation where

$x_i = i\Delta x$ and $t_n = n\Delta t$ and $u(x_i,t_n) = u_i^n$

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i,t_n} = \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} + O[(\Delta x)^2] \quad (2.13)$$

Similarly, we can do a Taylor's series expansion of $u(x,t)$ for a fixed spatial point x_i and expand about the time point t_n both forward $(t_n+\Delta t)$ and backward $(t_n-\Delta t)$ in time to get

$$\left.\frac{\partial^2 u}{\partial t^2}\right|_{x_i,t_n} = \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} + O[(\Delta t)^2] \quad (2.14)$$

* (2.13) and (2.14) are second-order accurate $(\Delta x^2, \Delta t^2)$, central-difference approximations to $\frac{\partial^2 u}{\partial x^2}$ and $\frac{\partial^2 u}{\partial t^2}$.

2.5 Finite-Difference Approximation of the Scalar Wave Equation

Now, substitute (2.13) and (2.14) into the 1D wave equation (2.1) to get

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} + O\left[(\Delta t)^2\right] = c^2 \left\{ \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} + O\left[(\Delta x)^2\right] \right\}$$

Dropping the error/remainder terms and solving for u_i^{n+1} (step forward in time) yields

$$u_i^{n+1} \simeq \underbrace{\left(\frac{c\Delta t}{\Delta x}\right)^2 \left[u_{i+1}^n - 2u_i^n + u_{i-1}^n\right] + 2u_i^n - u_i^{n-1}}_{\text{all these terms are known at time } t_n} \quad (2.16)$$

calculate future values using information from current + past time steps

If we choose our time interval Δt such that $\underline{c\Delta t = \Delta x}$ (magic time-step)

$$\underline{u_i^{n+1} = u_{i+1}^n + u_{i-1}^n - u_i^{n-1}} \quad (2.17)$$

$\uparrow$ **Not** approximation anymore

2.5 cont'

Proof

Going back to $u(x,t) = F(x+ct) + G(x-ct)$, and evaluating at (x_i, t_n) gives

$$U_i^n = F(x_i + ct_n) + G(x_i - ct_n).$$

Next, substitute this into (2.17) to get

$$\begin{bmatrix} F(x_i + ct_{n+1}) \\ + G(x_i - ct_{n+1}) \end{bmatrix} = \underbrace{\begin{bmatrix} F(x_{i+1} + ct_n) \\ + G(x_{i+1} - ct_n) \end{bmatrix} + \begin{bmatrix} F(x_{i-1} + ct_n) \\ + G(x_{i-1} - ct_n) \end{bmatrix} - \begin{bmatrix} F(x_i + ct_{n-1}) \\ + G(x_i - ct_{n-1}) \end{bmatrix}}_{RHS} \quad (2.18a)$$

$$RHS = \begin{Bmatrix} F[(i+1)\Delta x + cn\Delta t] \\ + G[(i+1)\Delta x - cn\Delta t] \end{Bmatrix} + \begin{Bmatrix} F[(i-1)\Delta x + cn\Delta t] \\ + G[(i-1)\Delta x - cn\Delta t] \end{Bmatrix} - \begin{Bmatrix} F(i\Delta x + c(n-1)\Delta t) \\ + G(i\Delta x - c(n-1)\Delta t) \end{Bmatrix} \quad (2.18b)$$

Substitute in the magic time-step $c\Delta t = \Delta x$, to get

cancel

$$RHS = \begin{Bmatrix} F[(i+1)\cancel{\Delta x} + n\Delta x] \\ + G[(i+1)\cancel{\Delta x} - n\Delta x] \end{Bmatrix} + \begin{Bmatrix} F[(i-1)\cancel{\Delta x} + n\Delta x] \\ + G[(i-1)\Delta x - n\Delta x] \end{Bmatrix} - \begin{Bmatrix} F(i\Delta x \cancel{+} (n-1)\Delta x) \\ + G(i\Delta x \cancel{-} (n-1)\Delta x) \end{Bmatrix} \quad (2.18c)$$

cancel

$$RHS = F[(i+1+n)\Delta x] + G[(i-1-n)\Delta x] \quad (2.18d)$$

original term moved to right by Δx ↑ ↖ original term moved left Δx

2.5 cont.

How can we prove this?

$$u_i^{n+1} = F(x_i + ct_{n+1}) + G(x_i - ct_{n+1})$$

$$= F[i\Delta x + c(n+1)\Delta t] + G[i\Delta x - c(n+1)\Delta t] \qquad (2.19a)$$

Again, substitute in the magic time-step $(c\Delta t = \Delta x)$

$$\underline{u_i^{n+1} = F[(i+n+1)\Delta x] + G[(i-n-1)\Delta x]} \qquad (2.19b)$$

same as (2.18d)

$\Rightarrow$ Approximation errors/remainders cancel out at magic time-step.

2.6 Numerical Dispersion Relation

→ want to characterize dispersion due to the finite-difference solution/approximation to the 1D scalar wave equation

Again, consider $u(x,t) = e^{j(\omega t - kx)}$ (2.6)

as represented numerically w/ k replaced with $\tilde{k} = \tilde{k}_{real} + j\,\tilde{k}_{imag}$ (numerical wave number).

This gives

$$u_i^n = e^{j(\omega n\Delta t - \tilde{k} i\Delta x)} = e^{\tilde{k}_{imag} i\Delta x}\, e^{j(\omega n\Delta t - \tilde{k}_{real} i\Delta x)} \quad (2.20)$$

Ideally, $\tilde{k}_{imag} = 0$ and $\tilde{k}_{real} = k$.

Next, substitute (2.20) into the finite-difference approximation of (2.16) to get

$$e^{j[\omega(n+1)\Delta t - \tilde{k} i\Delta x]} = \left(\frac{c\Delta t}{\Delta x}\right)^2 \left\{ e^{j[\omega n\Delta t - \tilde{k}(i+1)\Delta x]} - 2e^{j[\omega n\Delta t - \tilde{k} i\Delta x]} + e^{j[\omega n\Delta t - \tilde{k}(i-1)\Delta x]} \right\}$$
$$+ 2e^{j[\omega n\Delta t - \tilde{k} i\Delta x]} - e^{j[\omega(n-1)\Delta t - \tilde{k} i\Delta x]} \quad (2.21a)$$

divide out common $e^{j[\omega n\Delta t - \tilde{k} i\Delta x]}$ terms, to get

2.6 cont

$$e^{j\omega\Delta t} = \left(\frac{c\Delta t}{\Delta x}\right)^2 \left[e^{-j\tilde{k}\Delta x} - 2 + e^{j\tilde{k}\Delta x}\right] + 2 - e^{-j\omega\Delta t} \quad (2.21b)$$

Do a little algebra to allow Euler's ID for cosine terms (i.e., $\cos A = \frac{e^{jA} + e^{-jA}}{2}$) to be applied

$$\frac{e^{j\omega\Delta t} + e^{-j\omega\Delta t}}{2} = \left(\frac{c\Delta t}{\Delta x}\right)^2 \left[\frac{e^{j\tilde{k}\Delta x} + e^{-j\tilde{k}\Delta x}}{2} - 1\right] + 1 \quad (2.21c)$$

This gives

$$\cos(\omega\Delta t) = \left(\frac{c\Delta t}{\Delta x}\right)^2 \left[\cos(\tilde{k}\Delta x) - 1\right] + 1 \quad (2.22)$$

and

$$\tilde{k} = \frac{1}{\Delta x} \cos^{-1}\left\{1 + \left(\frac{\Delta x}{c\Delta t}\right)^2 \left[\cos(\omega\Delta t) - 1\right]\right\} \quad (2.23)$$

{Now we can find how choices of Δx and Δt will cause $\tilde{k}$ to be different than $k = \pm \omega/c$ (2.7b)

2.6.1 Case 1: Very Fine Sampling in Time + Space

→ assume Δt + Δx are very small wrt T and λ respectively

→ can truncate the Taylor's Series expansion of the cosine function to two terms, e.g.

$$\cos x = 1 - \frac{x^2}{2!} + \underbrace{\frac{x^4}{4!} - \frac{x^6}{6!} + \ldots}_{\text{neglect}}$$

So (2.23) becomes

$$\tilde{k} = \frac{1}{\Delta x} \cos^{-1}\left\{ 1 + \left(\frac{\Delta x}{c\Delta t}\right)^2 \left[\overbrace{\cos(\omega \Delta t)}^{1-\frac{(\omega\Delta t)^2}{2}} - 1 \right] \right\}$$

$$\simeq \frac{1}{\Delta x} \cos^{-1}\left\{ 1 + \left(\frac{\Delta x}{c\Delta t}\right)^2 \left(- \frac{(\omega \Delta t)^2}{2} \right) \right\}$$

$$\simeq \frac{1}{\Delta x} \cos^{-1}\left[1 - \underbrace{\left(\frac{\omega}{c}\right)^2}_{k^2} \Delta x^2 / 2 \right]$$

$$\tilde{k} \simeq \frac{1}{\Delta x} \cos^{-1}\left[1 - \frac{(k\Delta x)^2}{2} \right] \qquad (2.24a)$$

Again use $\cos x \simeq 1 - \frac{x^2}{2}$ for $|x| \ll 1$

$$\cos^{-1}(\cos x) = x \simeq \cos^{-1}\left(1 - \frac{x^2}{2}\right)$$

to get

$$\underline{\underline{\tilde{k} \simeq \frac{1}{\Delta x}(k\Delta x) = k}} \qquad (2.24b)$$

2.6.1 cont.

→ As might be expected, for very fine sampling, the numerical solution converges w/ the continuous solution (i.e., No Dispersion!)

2.6.2 Case 2: Magic Time-Step

→ let $\Delta x = c\Delta t$ in (2.23)

$$\tilde{k} = \frac{1}{\underbrace{\Delta x}_{c\Delta t}} \cos^{-1}\left\{ 1 + \left(\frac{\cancel{\Delta x}}{\cancel{c\Delta t}}\right)^{2}\left[\cos(\omega\Delta t) - 1\right]\right\} \quad (2.25a)$$

$$= \frac{1}{c\Delta t} \cos^{-1}\left\{\cos(\omega\Delta t)\right\} = \frac{\omega\Delta t}{c\Delta t}$$

$$\underline{\underline{\tilde{k} = \omega/c = k}} \quad (2.25b)$$

→ Again, No Dispersion! However, there are no restrictions on Δx + Δt other than they obey $\Delta x = c\Delta t$.

2.6.3 Case 3: Dispersive Wave Propagation

→ What happens if Δx + Δt don't satisfy case 1 or 2?

ex. let $\Delta x = \lambda_0/10$ and choose $c\Delta t = \Delta x/2$

$\left(\frac{\Delta x}{c\Delta t} = 2 \rightarrow \text{two time steps to travel } \Delta x \right)$

$$\tilde{k} = \frac{1}{\Delta x} \cos^{-1}\left\{ 1 + \Big(\underbrace{\frac{\Delta x}{c\Delta t}}_{2}\Big)^2 \Big[\cos\big(\omega \overbrace{\Delta t}^{\frac{\Delta x}{2c}}\big) - 1 \Big] \right\}$$

$$= \frac{1}{\Delta x} \cos^{-1}\left\{ 1 + 4\left[\cos\left(\frac{\omega \Delta x}{2c} \right) - 1 \right] \right\}$$

$k = \omega/c = 2\pi/\lambda_0$

$$= \frac{1}{\Delta x} \cos^{-1}\left\{ 1 + 4\left[\cos\left(\frac{2\pi}{\lambda_0} \frac{\overbrace{\Delta x}^{\lambda_0/10}}{2} \right) - 1 \right] \right\}$$

$$= \frac{1}{\Delta x} \cos^{-1}\left\{ 1 + 4\left[\cos\left(\pi/10 \right) - 1 \right] \right\}$$

$$= \frac{1}{\Delta x} \cos^{-1}\left\{ 0.804226 \right\} = \frac{0.636424}{\underbrace{\Delta x}_{\lambda_0/10}} \qquad (2.265)$$

$$\tilde{k} = \frac{6.364242196}{\lambda_0}$$

1.29% larger than k!

$$k = \frac{2\pi}{\lambda_0} = \frac{6.2831853}{\lambda_0}$$

2.6.3 cont.

ex. cont.

looking at the numerical phase velocity $\tilde{v}_p$

$$\tilde{v}_p = \frac{\omega}{\tilde{k}} = \frac{2\pi f^{\nearrow c/\lambda_0}}{\left(\frac{6.364242196}{\lambda_0}\right)} = \underline{\underline{0.98726c}} \quad (2.276)$$

↳ wave propagates slower than speed of light in the numerical grid (1.27% slower)

ex. let $\Delta x = \lambda_0/20$ w/ $c\Delta t = \Delta x/2$ again

$$\tilde{k} = \frac{1}{\underbrace{\Delta x}_{\lambda_0/20}} \cos^{-1}\left\{1 + 4\left[\cos\left(\frac{2\pi}{\lambda_0}\frac{\overset{\lambda_0/20}{\Delta x}}{2}\right) - 1\right]\right\}$$

$$= \frac{20}{\lambda_0} \cos^{-1}\{0.950753362\}$$

$$\underline{\underline{\tilde{k} = \frac{6.302776}{\lambda_0}}}$$ ← only 0.312% larger than $k = 2\pi/\lambda_0$

$$\tilde{v}_p = \frac{2\pi \, c/\lambda_0}{(6.303/\lambda_0)} = \underline{\underline{0.99689c}}$$ ← much better match (0.31% slower)

2.6.3 cont.

Now, let's consider the general case. Start by defining a numerical stability factor or

$$\underline{\text{Courant number} \equiv S = \frac{c\Delta t}{\Delta x}} \qquad (2.28a)$$

and the grid sampling resolution

$$\underline{N_\lambda = \frac{\lambda_o}{\Delta x}} \qquad (2.28b)$$

With these the numerical wavenumber can be written

$$\tilde{k} = \frac{1}{\Delta x}\cos^{-1}\left\{1 + \left(\frac{1}{S}\right)^2\left[\cos\left(\frac{2\pi S}{N_\lambda}\right) - 1\right]\right\}$$

$$= \frac{1}{\Delta x}\cos^{-1}\{\zeta\} = \frac{1}{\Delta x}\left[\pi/2 - \sin^{-1}(\zeta)\right] \qquad (2.29a)$$

zeta

where $\zeta = 1 + (1/S)^2\left[\cos\left(\frac{2\pi S}{N_\lambda}\right) - 1\right]$

If $\zeta < -1$, $\tilde{k}$ becomes complex

This translates to

$$N_\lambda\Big|_{\text{transition}} = \frac{2\pi S}{\cos^{-1}(1 - 2S^2)} \qquad (2.30)$$

2.6.3 cont.

If $N_\lambda > N_\lambda\big|_{trans}$, $\tilde{k}$ is real. Conversely, if $N_\lambda < N_\lambda\big|_{trans}$, $\tilde{k}$ is imaginary.

ex. In the previous example, $c\Delta t = \frac{\Delta x}{2}$.

Therefore, $S = \frac{c\Delta t}{\Delta x} = 0.5$

$$N_\lambda\big|_{trans} = \frac{2\pi(0.5)}{\cos^{-1}(1-2(0.5)^2)} = 3$$

Let's choose $N_\lambda = 2.5$ w/ $S = 0.5$, and calculate $\tilde{k}$

$$\zeta = 1 + \left(\frac{1}{0.5}\right)^2\left[\cos\left(\frac{2\pi(0.5)}{2.5}\right) - 1\right]$$
$$= -1.763932$$

$$\tilde{k} = \frac{1}{\Delta x}\cos^{-1}\{-1.763932\} = \frac{\pi - j1.16845}{\Delta x \to \lambda_0/2.5}$$

$$\tilde{k} = \frac{2.5\pi - j2.921}{\lambda_0}$$ ← Nowhere close to $k = 2\pi/\lambda_0$

2.6.3 cont.

Real $\tilde{K}$ $\left(N_\lambda > N_\lambda\big|_{transition}\right)$

$$\tilde{K} = \tilde{K}_{real} = \frac{1}{\Delta X}\cos^{-1}\left\{1 + (1/S)^2\left[\cos\left(\frac{2\pi S}{N_\lambda}\right) - 1\right]\right\}$$

$\tilde{K}_{imag} = 0$ ← No numerical wave amplification or attenuation $\left(e^{\tilde{K}_{imag}\Delta X} = e^0 = 1\right)$

$\tilde{K}$ complex $\left(N_\lambda < N_\lambda\big|_{transition}\right)$

$$\boxed{\begin{aligned} \tilde{K}_{real} &= \frac{\pi}{\Delta X} \\ \tilde{K}_{imag} &= \frac{1}{\Delta X}\ln\left(-\zeta - \sqrt{\zeta^2 - 1}\right) \end{aligned}} \qquad (2.36)$$

$$\tilde{V}_p = \frac{\omega}{\tilde{K}_{real}} = \frac{\omega}{(\pi/\Delta X)} = \frac{2 f \lambda_0}{N_\lambda} = \underline{\underline{\frac{2}{N_\lambda} c}} \qquad (2.37a)$$

and wave-amplitude multiplier per ΔX

$$e^{\tilde{K}_{imag}\Delta X} \equiv e^{-\alpha \Delta X} = e^{\ln\left(-\zeta - \sqrt{\zeta^2 - 1}\right)} = \underline{\underline{-\zeta - \sqrt{\zeta^2 - 1}}} \qquad (2.37b)$$

Note: If $N_\lambda < 2$, $\tilde{V}_p > c$!

(Remember Nyquist Sampling Rate $\quad f_{max} = \frac{1}{2\Delta t} = \frac{f_{sample}}{2}$?)

2.6.3 cont.

Applying this observation

$$\lambda_{0,min} = c/f_{max} = 2c\Delta t$$

which leads to

$$N_{\lambda,min} = \frac{\lambda_{0,min}}{\Delta x} = \frac{2c\Delta t}{\Delta x} = 2S \quad (2.38b)$$

For stability $S \leq 1$, this leads to

$$N_{\lambda,min} = 2S \leq 2 \quad (2.38c)$$

and

$$\tilde{v}_{p,max} = \frac{2}{N_{\lambda,min}} c = \frac{1}{S} c \geq c \quad (2.39a)$$

$$\tilde{v}_{p,max} = \frac{\Delta x}{\Delta t} \quad (2.39b)$$

* Tells us wave can go no more than $1\,\Delta x$ per time increment Δt.

* Also, $\tilde{v}_{p,max}$ doesn't depend on material properties

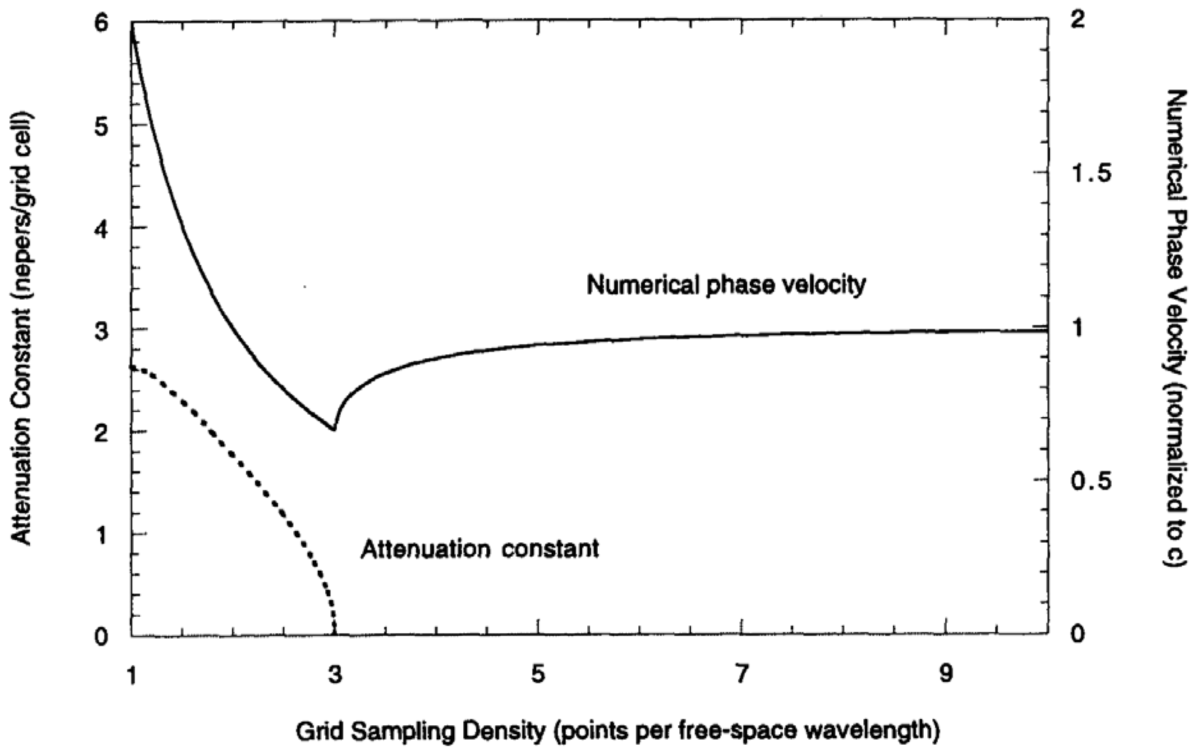


Fig. 2.1 Variation of the normalized numerical phase velocity $\tilde{v}_p/c$ and attenuation per grid cell $\alpha\Delta x$ as a function of the grid sampling density $(1 \le N_\lambda \le 10)$ for a Courant stability factor $S = 0.5$.

Comments:

- In this case, $N_\lambda\big|_{\text{transition}} = 3$.
- Note how the attenuation constant disappears for $N_\lambda > N_\lambda\big|_{\text{transition}} = 3$.
- Note how the attenuation constant approaches 2.639 as $N_\lambda \to 1$.
- Note how the numerical phase velocity is greater than the speed of light for $N_\lambda < 2$.
- Note how the numerical phase velocity is less than the speed of light for $N_\lambda < 2$.
- Note how the numerical phase velocity approaches the speed of light as $N_\lambda \to \infty$.

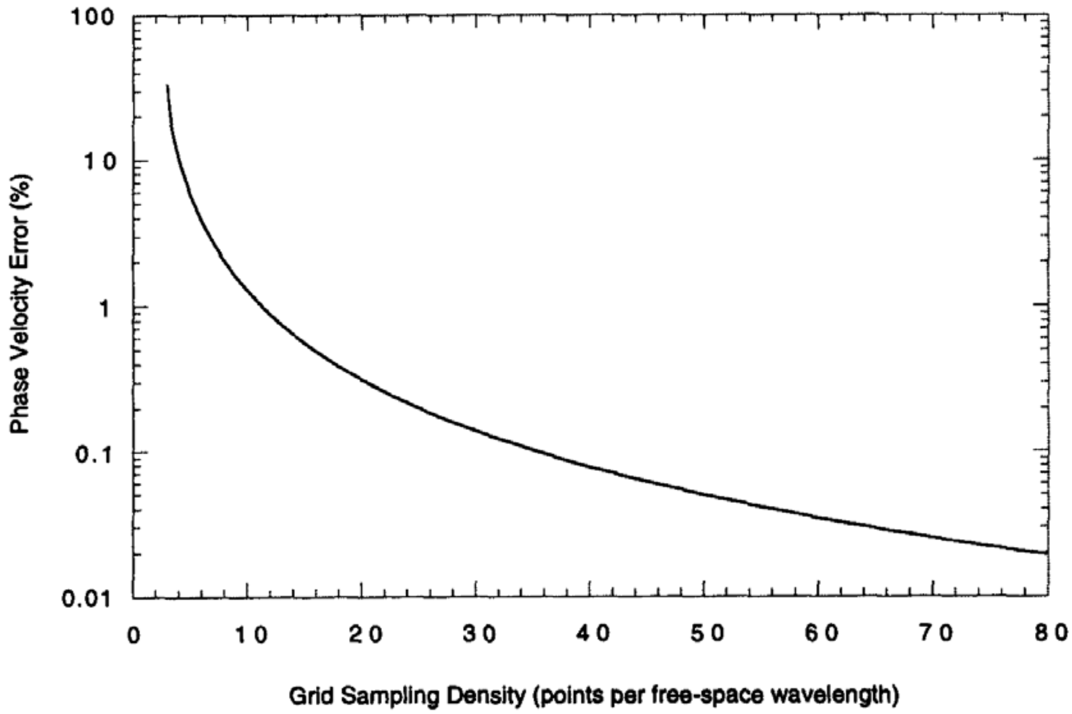
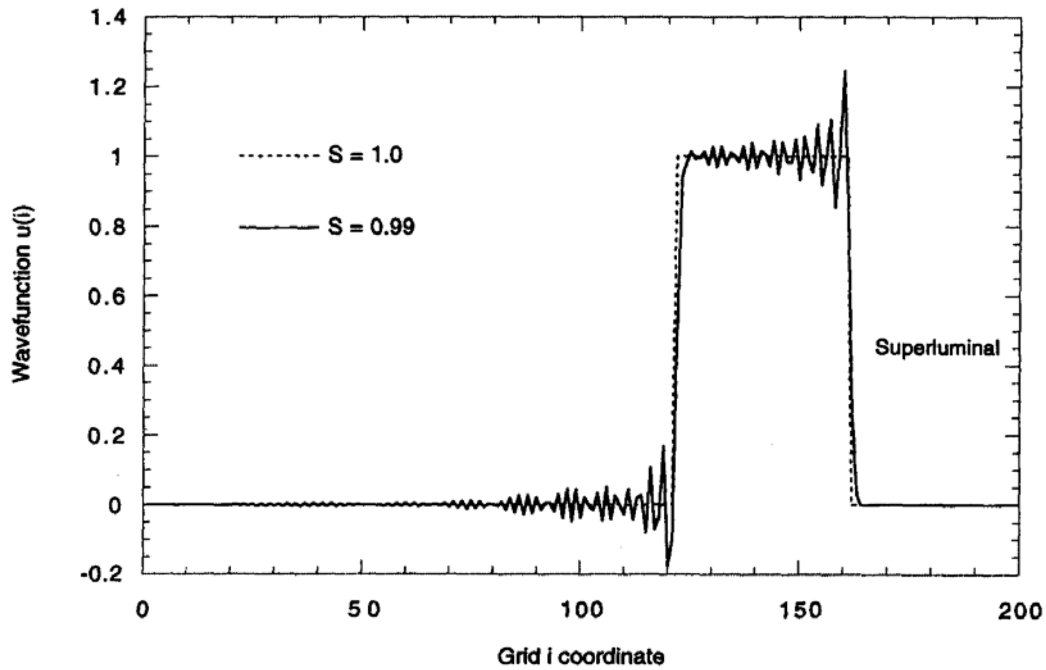


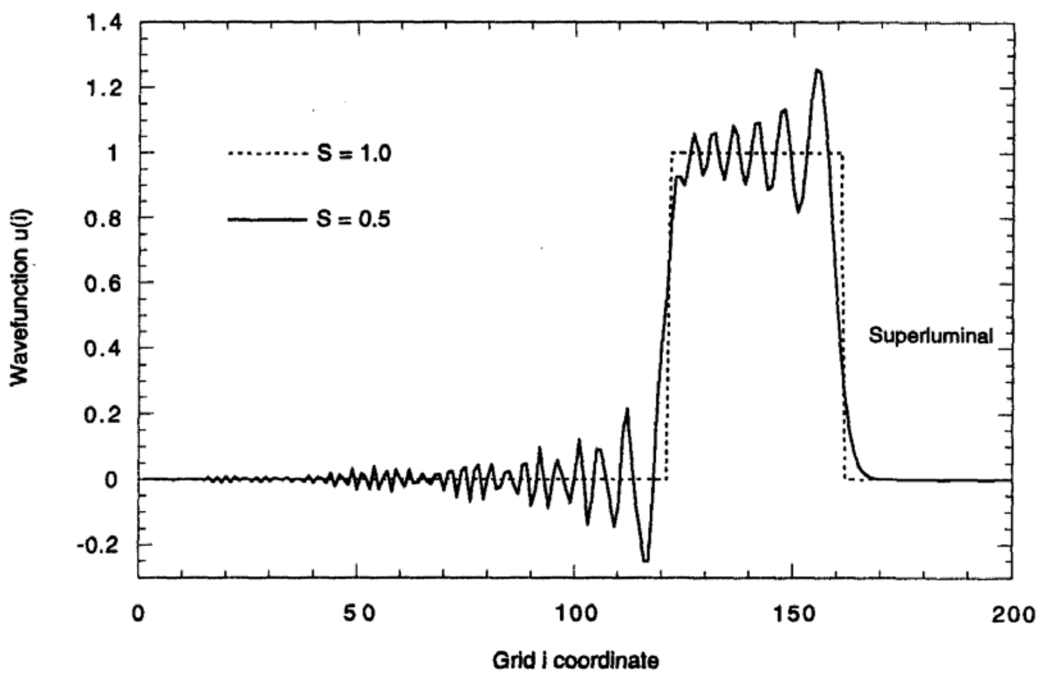
Fig. 2.2 Percent numerical phase-velocity error relative to the free-space speed of light as a function of the grid sampling density $(3 \le N_\lambda \le 80)$ for a Courant stability factor $S = 0.5$.

Comments:

- Note how the % error between the numerical phase velocity and free-space phase velocity approaches 0 as $N_\lambda \to \infty$.
- Decrease is proportional to $1/N_\lambda^2$ due to second-order accuracy of finite-difference approximation.



(a) Comparison of calculated pulse propagation for $S = 1$ and $S = 0.99$.



(b) Comparison of calculated pulse propagation for $S = 1$ and $S = 0.5$.

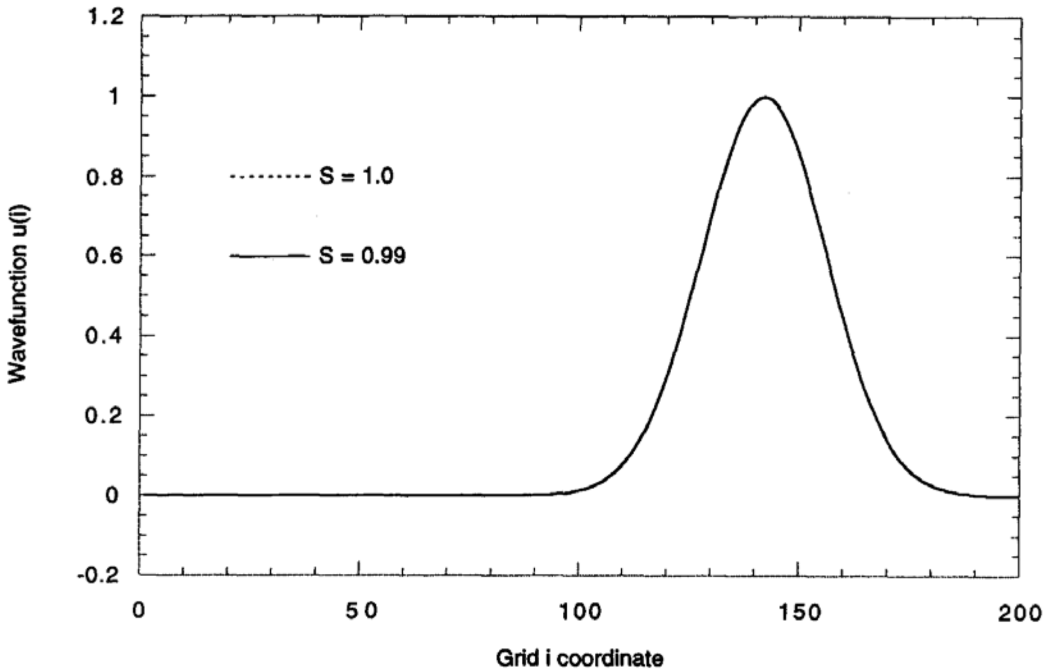
Fig. 2.3 Effect of numerical dispersion upon a rectangular pulse propagating in free space for different Courant stability factors: (a) $S = 1$ (Δt equal to the magic time-step) and $S = 0.99$ (Δt just 1% below the magic time-step); (b) $S = 1$ and $S = 0.5$ (Δt 50% below the magic time-step).

Fig. 2.3a) comments:

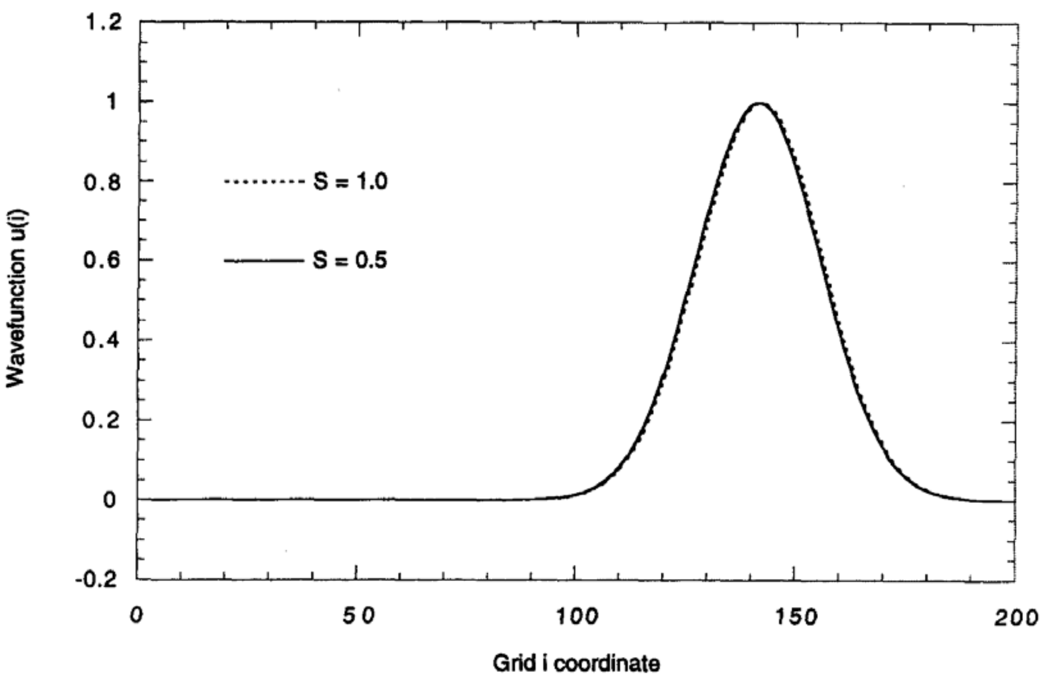
- In this case, the input signal is a rectangular pulse which is 40 spatial cells wide. From Fourier transform theory we know that this signal has infinite frequency content that does not damp out quickly, e.g., $p_\tau(t) \quad \leftrightarrow \quad \tau\,\mathrm{sinc}\left(\frac{\tau\omega}{2\pi}\right)$.
- For the magic time-step ($S = 1 = c\Delta t / \Delta x$), the pulse is perfectly recreated since $\tilde{v}_p \equiv c$ is constant at all frequencies (no dispersion).
- However, when S = 0.99, $\tilde{v}_p$ is NOT constant at all frequencies (dispersion) and we see delayed ringing at the edges of the pulse (high frequency content is not adequately sampled).
- Also, when S = 0.99, we see some superluminal signal content **before** the leading edge of the pulse (i.e., $\tilde{v}_p > c$).

Fig. 2.3b) comments:

- Here, we see what happens when S = 0.5.
- Much worse ringing with S = 0.5.
- More superluminal signal content with S = 0.5.



(a) Comparison of calculated pulse propagation for $S = 1$ and $S = 0.99$.



(b) Comparison of calculated pulse propagation for $S = 1$ and $S = 0.5$.

Fig. 2.4 Effect of numerical dispersion upon a Gaussian pulse propagating in free space for different Courant stability factors: (a) $S = 1$ (Δt equal to the magic time-step) and $S = 0.99$ (Δt just 1% below the magic time-step); (b) $S = 1$ and $S = 0.5$ (Δt 50% below the magic time-step).

Fig. 2.4a) comments:

- In this case, the input signal is a Gaussian pulse which is 40 spatial cells wide at the 1/*e* = 0.368 points. From Fourier transform theory, we know that this signal has infinite frequency content, e.g., $e^{-\left(\frac{t^2}{2\tau_p^2}\right)} \leftrightarrow \sqrt{2\pi}\,\tau_p\, e^{-\left(\frac{\omega^2\tau_p^2}{2}\right)}$. However, it falls off exponentially.
- For the magic time-step ($S = 1 = c\Delta t / \Delta x$), the pulse is perfectly recreated since $\tilde{v}_p \equiv c$ is constant at all frequencies (no dispersion).
- When S = 0.99, $\tilde{v}_p$ is NOT constant at all frequencies (dispersion possible). However, since this signal has much less high frequency content, we see no visible difference with the S = 1 case.

Fig. 2.4b) comments:

- Here, we see what happens to the Gaussian pulse when S = 0.5.
- Still no visible ringing with S = 0.5.
- Some dispersion visible in that the S = 0.5 pulse lags the S = 1 pulse slightly (i.e., $\tilde{v}_p < c$)
- No visible superluminal signal content with S = 0.5.

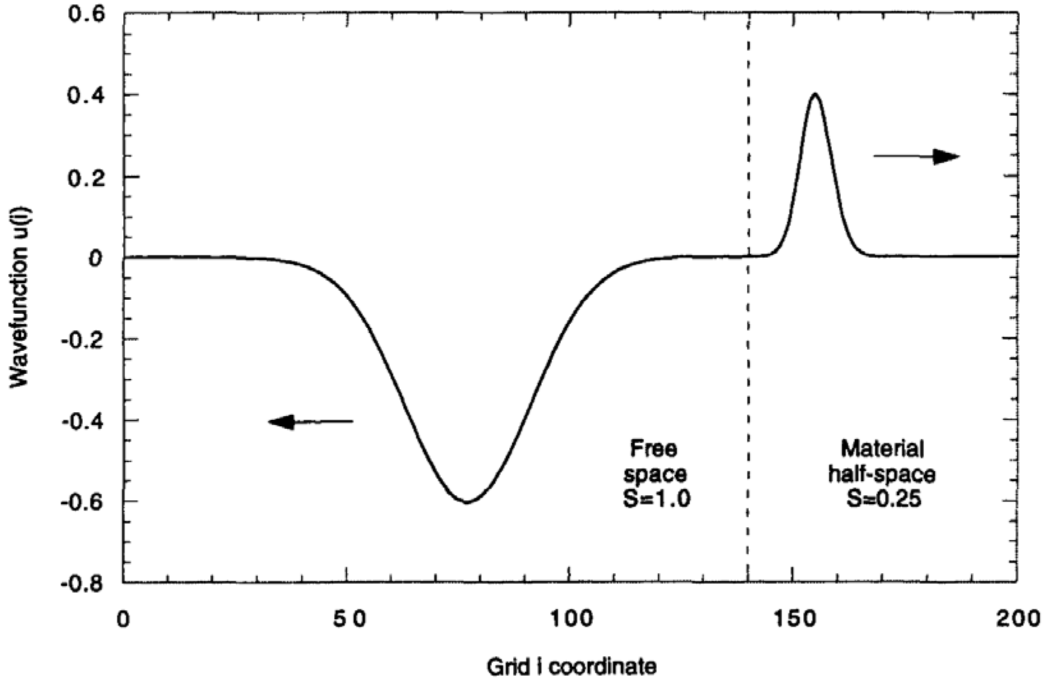


Fig. 2.5 Example of the calculated reflection and transmission of a Gaussian pulse at an interface between free space and a lossless material half-space having $v_p = c/4$.

Fig. 2.5 comments:

- In this case, the input signal was a Gaussian pulse 40 spatial cells wide at the $1/e$ = 0.368 points that is incident from free space on a lossless material where $v_p = c/4$ at spatial index i = 140. The pulse is partially reflected (Γ = -0.6) and partially transmitted (τ = 0.4). The grid Δx and Δt are held constant, causing the free space $S = 1$ to change to $S = 0.25$ in the other material.
- As can be seen, the results are very good (e.g., $\Gamma \approx$ -0.603, pulse width is approximately 10, a fourth of the original, in the new material, …)

2.7 Numerical Stability

→ Want to ensure that a bounded input results in bounded results.

→ Numerical solution is unstable if a bounded input yields unbounded results.

2.7.1 Complex-Frequency Analysis

→ assume a forward traveling sinusoidal wave in a finite-difference grid (Δx & Δt)

(2.6) $u(x,t) = e^{j(\omega t - kx)}$ where $k \rightarrow \tilde{k}$ and $\omega \rightarrow \tilde{\omega}$.

→ In standard notation

$$u_i^n = e^{j(\tilde{\omega} n \Delta t - \tilde{k} i \Delta x)} = e^{j\left[(\tilde{\omega}_{real} + j\tilde{\omega}_{imag}) n \Delta t - \tilde{k} i \Delta x\right]}$$

$$= e^{-\tilde{\omega}_{imag} n \Delta t} e^{j(\tilde{\omega}_{real} n \Delta t - \tilde{k} i \Delta x)} \qquad (2.40)$$

→ If $\tilde{\omega}_{imag} > 0$, wave decays exponentially w/ time.

→ If $\tilde{\omega}_{imag} < 0$, the wave grows exponentially w/ time.

2.7.1 cont.

→ Going back to the numerical dispersion relation of (2.22), we have

$$\cos(\tilde{\omega}\Delta t) = \left(\frac{c\Delta t}{\Delta x}\right)^2\left[\cos(\tilde{k}\Delta x) - 1\right] + 1 \qquad (2.41)$$

Substituting in $S = c\Delta t/\Delta x$ (Courant stability factor) and solving for $\tilde{\omega}$, yields

$$\tilde{\omega} = \frac{1}{\Delta t}\cos^{-1}\left\{S^2\left[\cos(\tilde{k}\Delta x) - 1\right] + 1\right\}$$

$$= \frac{1}{\Delta t}\cos^{-1}(\xi) = \frac{1}{\Delta t}\left[\pi/2 - \sin^{-1}(\xi)\right] \qquad (2.42a)$$

where
$$\xi = S^2\left[\cos(\tilde{k}\Delta x) - 1\right] + 1 \qquad (2.42b)$$

→ If $\tilde{k}$ is real, $1 - 2S^2 \leq \xi \leq 1$.
(no attenuation due to $\tilde{k}$)

a) when $0 \leq S \leq 1$, $\underset{@\,S=1}{-1} \leq \xi \leq \underset{@\,S=0}{1}$ and $\tilde{\omega}$ is real ⇒ STABLE.

b) when $S > 1$, $1 - 2S^2 \leq \xi < \underset{@\,S=1}{-1}$ ⇒ $\tilde{\omega}$ is complex since $\sin^{-1}(\xi)$ will be complex.

2.7.1 cont.

b) cont.

* The most negative ξ occurs when the $\cos(\tilde{k}\Delta x)$ term of (2.42b) is -1, i.e. $\tilde{k}\Delta x = \pi$ or $\tilde{\lambda} = 2\Delta x$. So,

$$\xi_{\substack{lower\\bound}} = 1 - 2S^2 \quad \text{for } \tilde{k}\Delta x = \pi$$

* Also, in this case,

$$\sin^{-1}(\xi) = -j \ln\left(j\xi + \sqrt{1-\xi^2}\right) \qquad (2.44)$$

Using (2.44) in (2.42a) gives

$$\tilde{\omega} = \frac{1}{\Delta t}\left[\pi/2 + j\ln\left(j\xi + \sqrt{1-\xi^2}\right)\right]$$

$$= \frac{1}{\Delta t}\left[\pi/2 + j\ln\left(j\xi + j\sqrt{\xi^2-1}\right)\right] \qquad (2.45a)$$

Using $j = e^{j\pi/2}$, we can show that

$$\tilde{\omega} = \frac{1}{\Delta t}\left\{\pi + j\ln\left(-\xi - \sqrt{\xi^2-1}\right)\right\} \qquad (2.45c)$$

$$= \tilde{\omega}_{real} + j\,\tilde{\omega}_{imag}$$

2.7.1 cont. Case b) cont.

Comparing terms

$$\tilde{\omega}_{real} = \pi/\Delta t \quad \text{and} \quad \tilde{\omega}_{imag} = \frac{1}{\Delta t} \ln\left(-\xi - \sqrt{\xi^2 - 1}\right) \tag{2.46}$$

Putting this back into our u_i^n expression yields

$$u_i^n = e^{-n \ln\left(-\xi - \sqrt{\xi^2 - 1}\right)} e^{j\left[\frac{\pi}{\Delta t}(n\Delta t) - \tilde{K} i \Delta x\right]}$$

$$u_i^n = \left(\frac{1}{-\xi - \sqrt{\xi^2 - 1}}\right)^n e^{j\left[\frac{\pi}{\Delta t}(n\Delta t) - \tilde{K} i \Delta x\right]} \tag{2.47}$$

Define a multiplicative factor g_{growth}

$$g_{growth} \equiv \frac{1}{-\xi - \sqrt{\xi^2 - 1}} = -\xi + \sqrt{\xi^2 - 1} \tag{2.48}$$

Remember $\xi < -1$ for case b), so

$g_{growth} > 1 \Rightarrow$ exponential growth w/ n!

2.7.1 cont.

Case b) cont.

Looking at the worst case $\xi_{\substack{lower\\bound}} = 1-2S^2$ where $\tilde{k}\Delta x = \pi$ or $\tilde{\lambda} = 2\Delta x$, we get

$$
\begin{aligned}
g_{\substack{growth\\max}} &= -(1-2S^2) + \sqrt{(1-2S^2)^2 - 1} \\
&= \left(S + \sqrt{S^2-1}\right)^2 \qquad (2.49)
\end{aligned}
$$

→ If $S = 1$, $(g_{growth})_{max} = 0$

→ If $S = 1.0005$, $g_{growth} = 1.0653$

$(1.0653)^{10} = 1.8822$

$(1.0653)^{100} = 558.7$ ↓ explodes!

⋮

→ The corresponding frequency f_0 to $\tilde{\omega}_{real} = \pi/\Delta t$ is

$$f_0 = \frac{\tilde{\omega}_{real}}{2\pi} = \frac{\pi/\Delta t}{2\pi} = \frac{1}{2\Delta t} \quad \leftarrow \text{freq. of instability!} \qquad (2.50)$$

2.7.1 cont.

case b) cont.

→ corresponding numerical wave velocity is

$$\tilde{v}_p = \frac{\tilde{\omega}_{real}}{\tilde{k}} = \frac{(\pi/\Delta t)}{(\pi/\Delta x)} = \frac{\Delta x}{\Delta t} = c/S \qquad (2.51)$$

Since $S > 1$ in this case, $\tilde{v}_p < c$ for the instability.

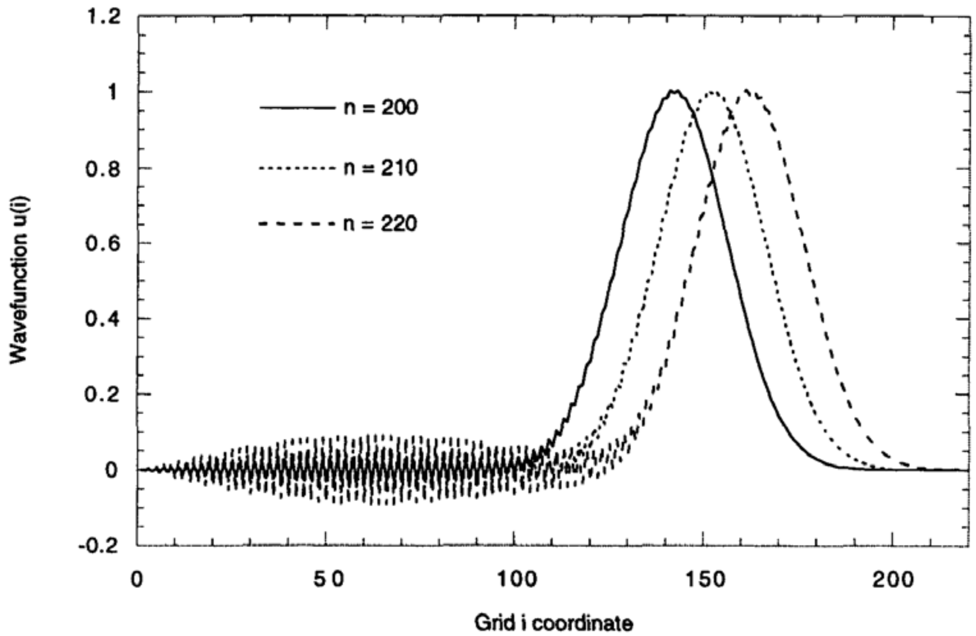
For Stability, $\underline{\underline{S \leq 1}}$ or $\underline{\Delta t \leq \frac{\Delta x}{c}}$ (2.52)

Usually, choose Δx + S then

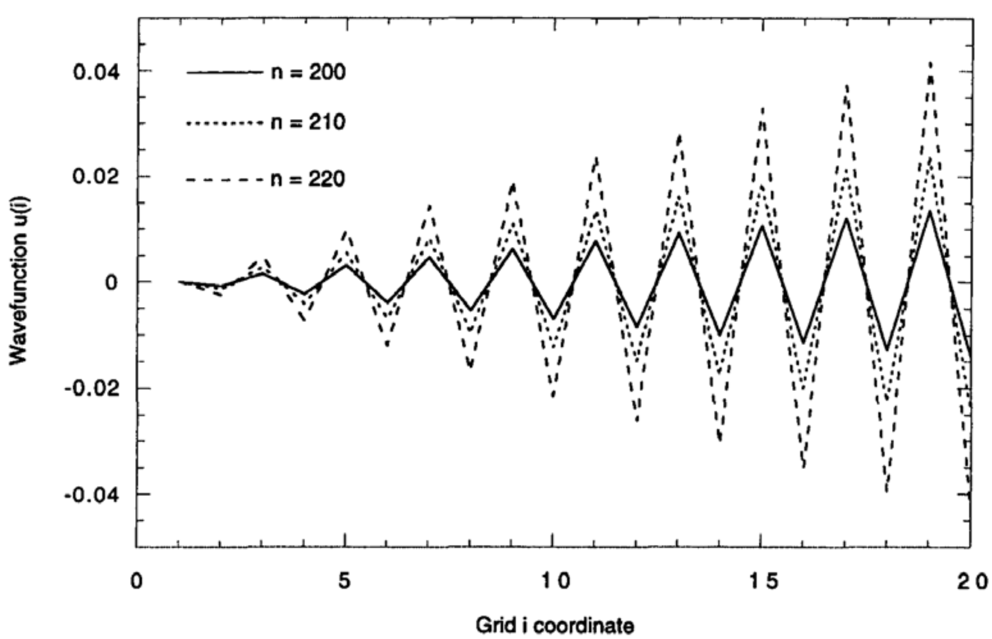
$$\Delta t = \frac{S\,\Delta x}{c} \quad \text{or} \quad \Delta t \leq \frac{\Delta x}{c} \text{ for stability}$$

* Careful choosing $S = 1$, any numerical round-off upward results in instability.

2.7.2 Examples of Calculations Involving Numerical Instability



(a) Comparison of calculated pulse propagation at $n = 200$, 210, and 220 time-steps over grid coordinates $i = 1$ through $i = 220$.



(b) Expanded view of (a) over grid coordinates $i = 1$ through $i = 20$.

Fig. 2.6 The beginning of numerical instability for a Gaussian pulse propagating in free space. The Courant stability factor is $S = 1.0005$ at each gridpoint.

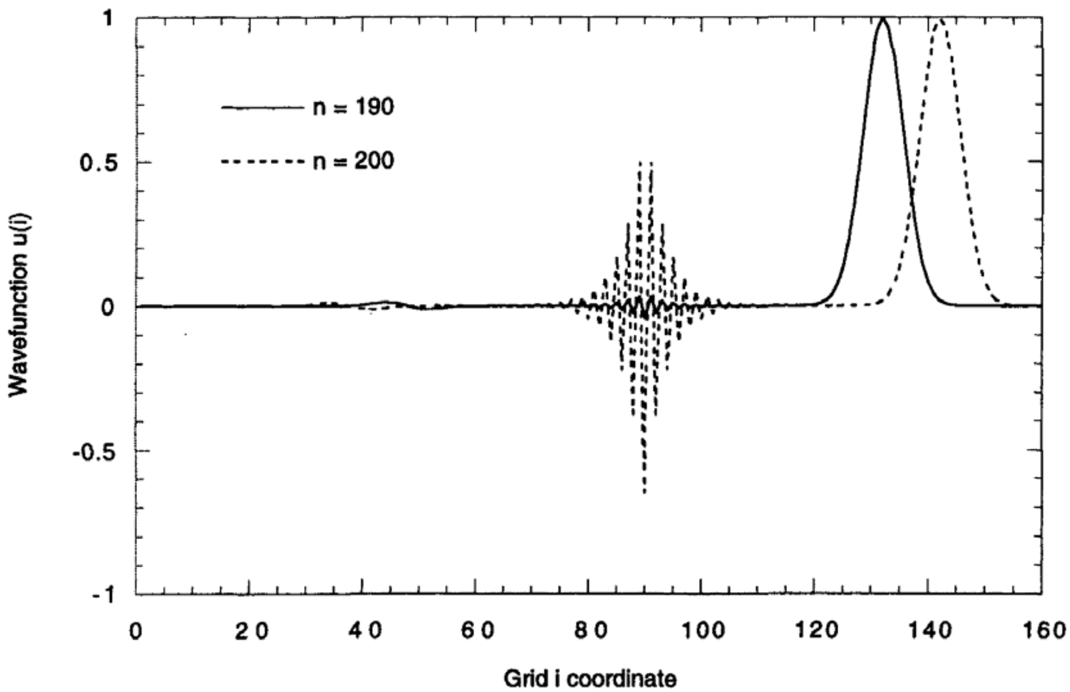
2.7.2 cont.

Fig. 2.6a) comments:

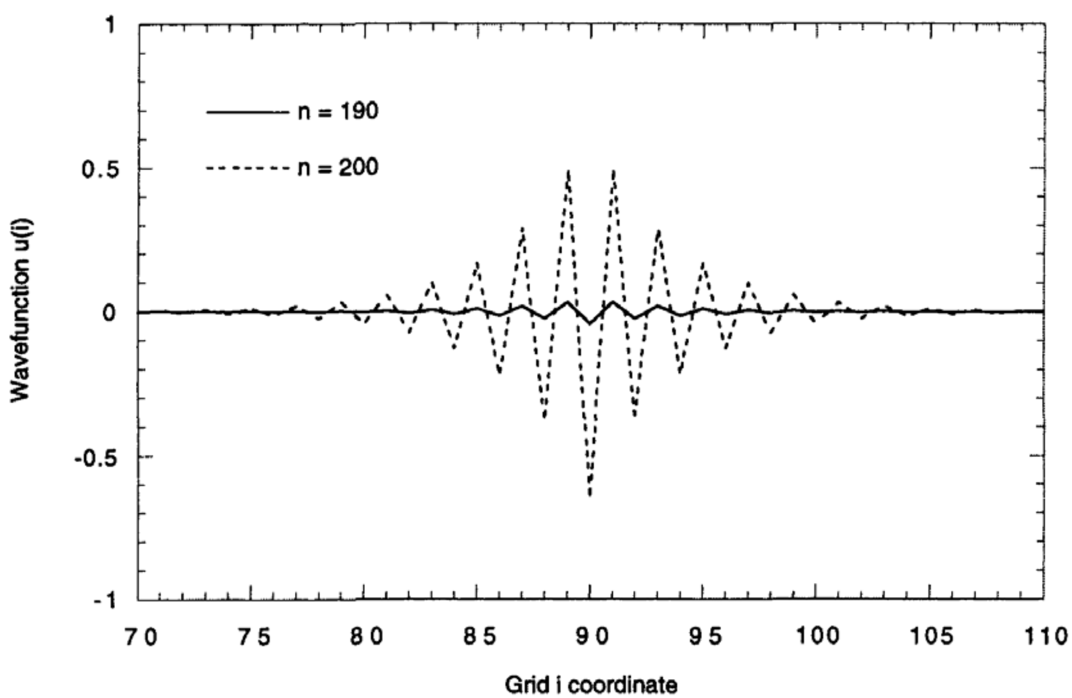
- Let $S = 1.0005$ at all points in the grid for a Gaussian pulse input signal which is 40 temporal cells wide at the $1/e = 0.368$ points.
- Look at several snapshots in time and see instability growing on the trailing edge of the signal.

Fig. 2.6b) comments:

- Here, we zoom in on the small i signal components.
- Exponential growth with respect to n is evident and near the predicted rate.
- Wavelength of instability is $2\Delta x$ as predicted.



(a) Comparison of calculated pulse propagation at $n = 190$ and $n = 200$ time-steps over grid coordinates $i = 1$ through $i = 160$.



(b) Expanded view of (a) over grid coordinates $i = 70$ through $i = 110$.

Fig. 2.7 The beginning of numerical instability for a Gaussian pulse propagating in free space. Unlike Fig. 2.6, the Courant stability factor is $S = 1$ at all gridpoints but $i = 90$, where $S = 1.075$.

<u>Fig. 2.7a) comments:</u>

- Let S = 1.075 at a single point (i =90) in the grid for a Gaussian pulse input signal which is 40 temporal cells wide at the 1/e = 0.368 points. S = 1 elsewhere in the grid.
- Look at several snapshots in time and see instability growing, centered on i =90, at the trailing edge of the signal.

<u>Fig. 2.7b) comments:</u>

- Here, we zoom in on the signal components near i = 90.
- Exponential growth with respect to n is evident, but is slower than predicted rate for global grid.
- Wavelength of instability is $2\Delta x$ as predicted.