Discretization of wave equations and grid-induced reflections

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Outline

- Physical reflections due to inhomogeneity

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- Grid-induced reflections: $u_t = -cu_x$
- Grid-induced reflections: $u_{tt} = c^2 u_{xx}$
- Extensions

Reflection due to inhomogeneity, $u_{tt} = c^2 u_{xx}$

Consider the second order wave equation in the form

$$\begin{aligned} u_t &= v_x \\ v_t &= c^2 u_x \end{aligned}$$

with solution

$$\begin{aligned} u(x,t) &= r(x-ct) + \ell(x+ct) \\ v(x,t) &= c[-r(x-ct) + \ell(x+ct)]. \end{aligned}$$

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Two regions

$$c(x) = \begin{cases} c_1, & x < 0 \\ c_2, & x \geq 0 \end{cases}$$

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Interface conditions:

$$\begin{aligned} u_1(0,t) = u_2(0,t) \quad &\Rightarrow \quad r_1 + \ell_1 = r_2 \\ v_1(0,t) = v_2(0,t) \quad &\Rightarrow \quad c_1(-r_1 + \ell_1) = c_2(-r_2) \end{aligned}$$

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Reflection ratio:

$$\rho = \frac{\ell_1}{r_1} = \frac{c_1 - c_2}{c_1 + c_2}$$

Reflection due to inhomogeneity, $u_{tt} = c^2 u_{xx}$, example

Experiment - 'Box scheme'

- 160 gridpoints on $[0, 1)$
- $t \in [0, 0.9]$
- $\Delta t = 0.01$
- $c(x) = \{1, x < 0.66; 1/2, x \geq 0.66\}$
- $u(x, t) = \exp(-20^2(x - t - 1/4)^2)$

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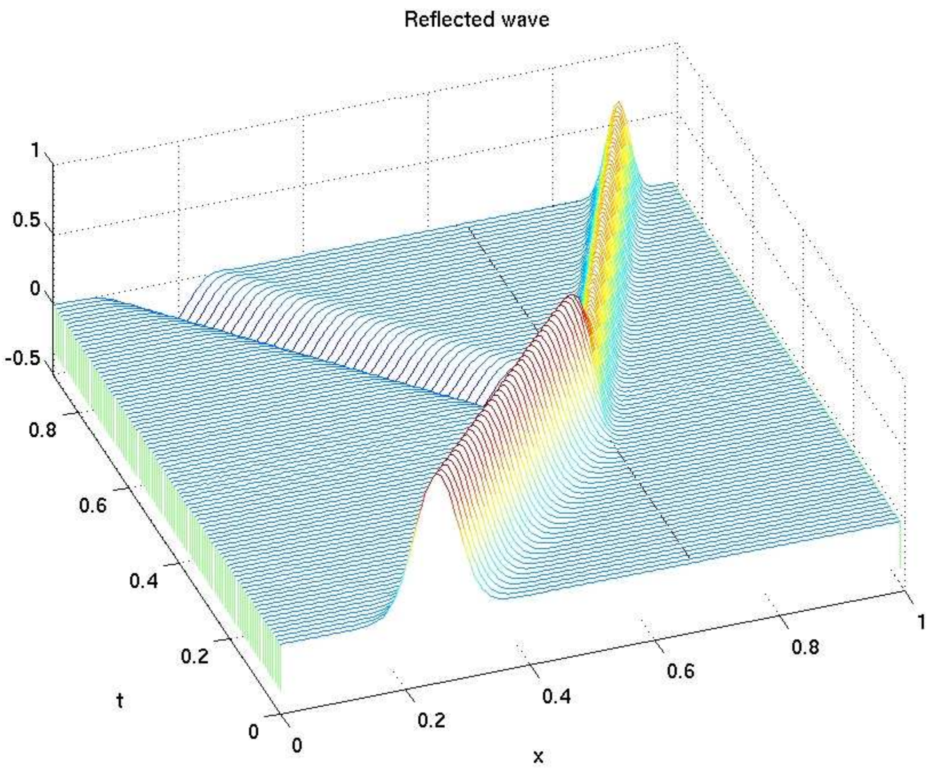
$$\rho = \frac{1/2}{1 + 1/2} = 1/3$$



Grid-induced reflections, $u_t = -cu_x$, example

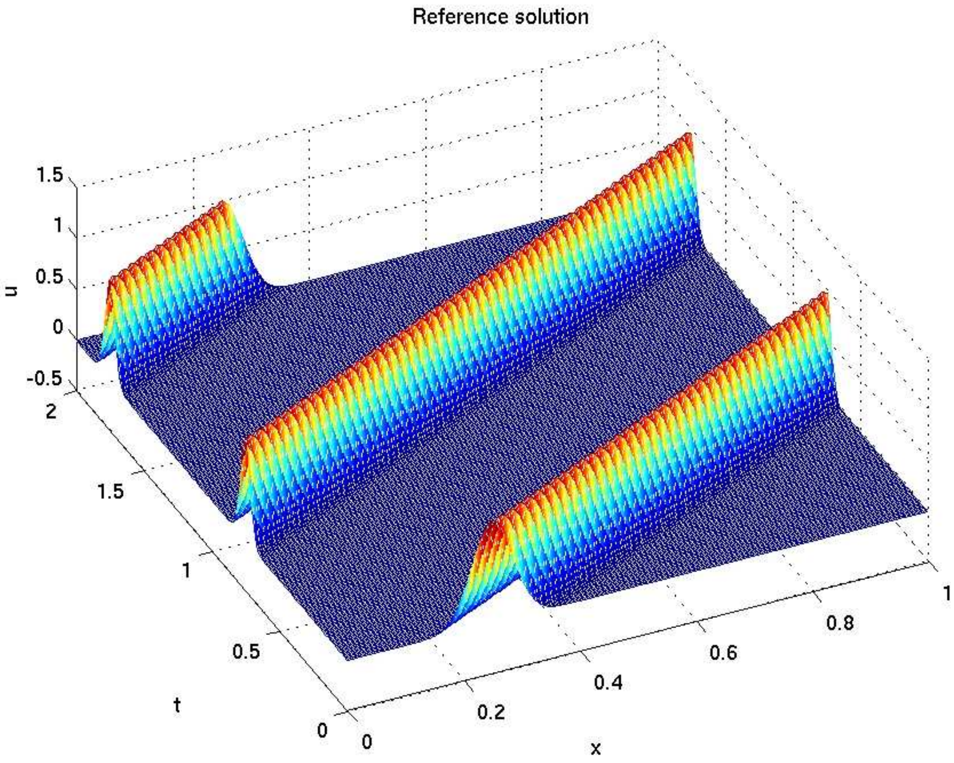
Consider the right-running wave equation
$u_t = -cu_x$.

Central difference

$$\dot{u}_j = \frac{-c}{2h}(u_{j+1} - u_{j-1})$$

Numerical experiment

- 100 grid points on [0,1) periodic
- $h_1/h_2 = 1/3$
- $\tau = 0.02$
- $t \in [0, 2]$
- Same initial condition.



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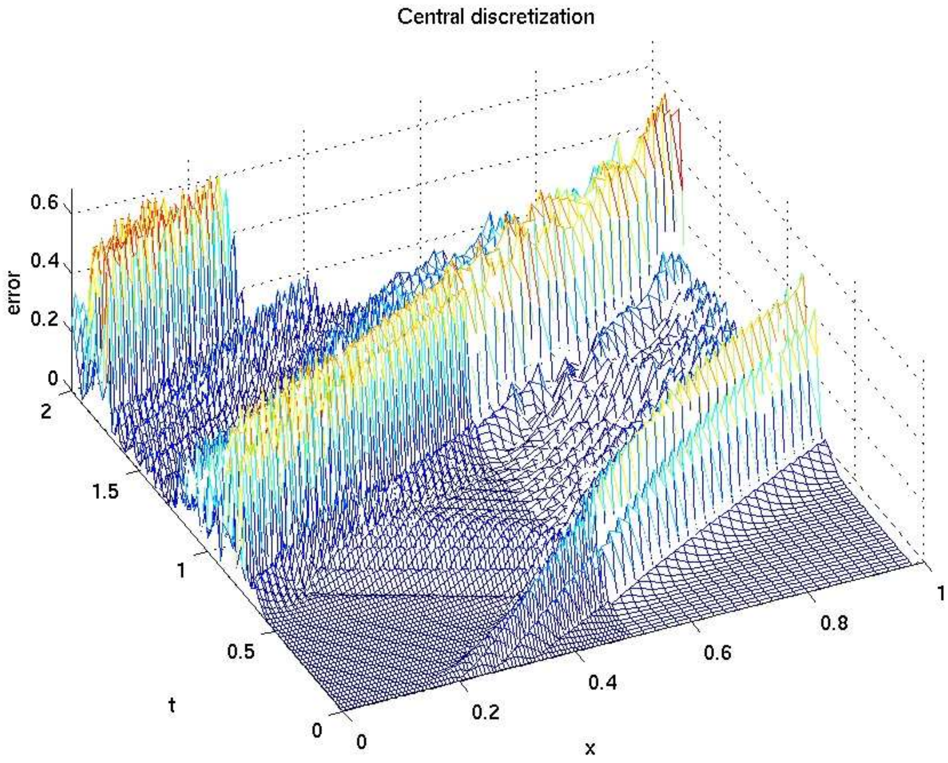

Vichnevetsky's analysis (1981)

Time Fourier transform:

$$u(t,x) = \int_{-\infty}^{\infty} \hat{u}(\omega,x)\mathrm{e}^{\mathrm{i}\omega t}\,d\omega$$

The right-running wave equation becomes

$$\mathrm{i}\omega\,\hat{u}(\omega,x) = -c\,\hat{u}_x(\omega,x)$$

with exact solution

$$\hat{u}(\omega,x+h) = \exp(\frac{-\mathrm{i}h\omega}{c})\,\hat{u}(\omega,x).$$

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Time-transformed central differences

$$\mathrm{i}\omega\hat{u}_j = \frac{-c}{2h}(\hat{u}_{j+1} - \hat{u}_{j-1})$$

Difference recursion

$$\hat{u}_{j+1} + \mathrm{i}2h\omega c\,\hat{u}_j - \hat{u}_{j-1} = 0$$

with roots

$$R, L = -\frac{\mathrm{i}h\omega}{c} \pm \sqrt{1 - \frac{h^2\omega^2}{c^2}} = \mathrm{e}^{\mathrm{i}\Theta_{R,L}}$$

and solution

$$\hat{u}_j = \hat{r}_j + \hat{\ell}_j, \quad \hat{r}_j = R^j\hat{r}_0, \quad \hat{\ell}_j = L^j\hat{\ell}_0.$$

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Central differences for the first order wave equation support both left- and right-running solutions.

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Central differences for the first order wave equation support both left- and right-running solutions.

For a uniform grid, these solutions are de-coupled.

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Vichnevetsky's analysis (1981)

Consider a mesh

$$x_j = \begin{cases} jh_1, & j < 0 \\ jh_2, & j > 0 \end{cases}$$

Assume a right-running incident wave in $x < 0$, no left-running wave in $x > 0$. At $x = 0$, let $u_0^{(1)} = u_0^{(2)}$:

$$\hat{r}_0^{(1)} + \hat{\ell}_0^{(1)} = \hat{r}_0^{(2)}$$

Furthermore,

$$\begin{aligned} \hat{u}_{-1} &= R(h_1\omega)^{-1}\hat{r}_0^{(1)} + L(h_1\omega)^{-1}\hat{\ell}_0^{(1)} \\ \hat{u}_1 &= R(h_2\omega)\hat{r}_0^{(2)}. \end{aligned}$$

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Inserting these in the central difference formula for $\hat{u}_0$, the reflection ratio is

$$\rho = \frac{\hat{\ell}_0^{(1)}}{\hat{r}_0^{(1)}} = \frac{\nu_1 - \nu_2}{\nu_1 + \nu_2}$$

where

$$\nu_{1,2} = c\sqrt{1 - \left(\frac{h_{1,2}\,\omega}{c}\right)^2}$$

are the discrete group velocities in (x<0) and (x>0).

Grid-induced reflections, $u_t = -cu_x$, example

Instead consider

Box scheme

$$\frac{1}{2}(\dot{u}_{j+1} + \dot{u}_j) = \frac{-c}{\Delta x}(u_{j+1} - u_j)$$

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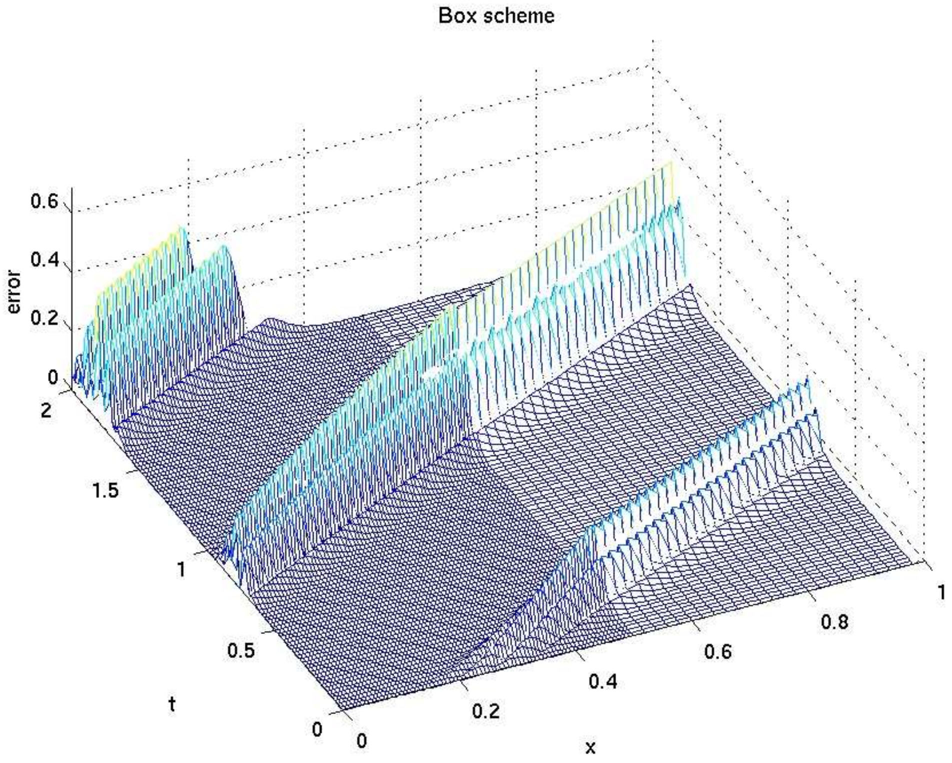

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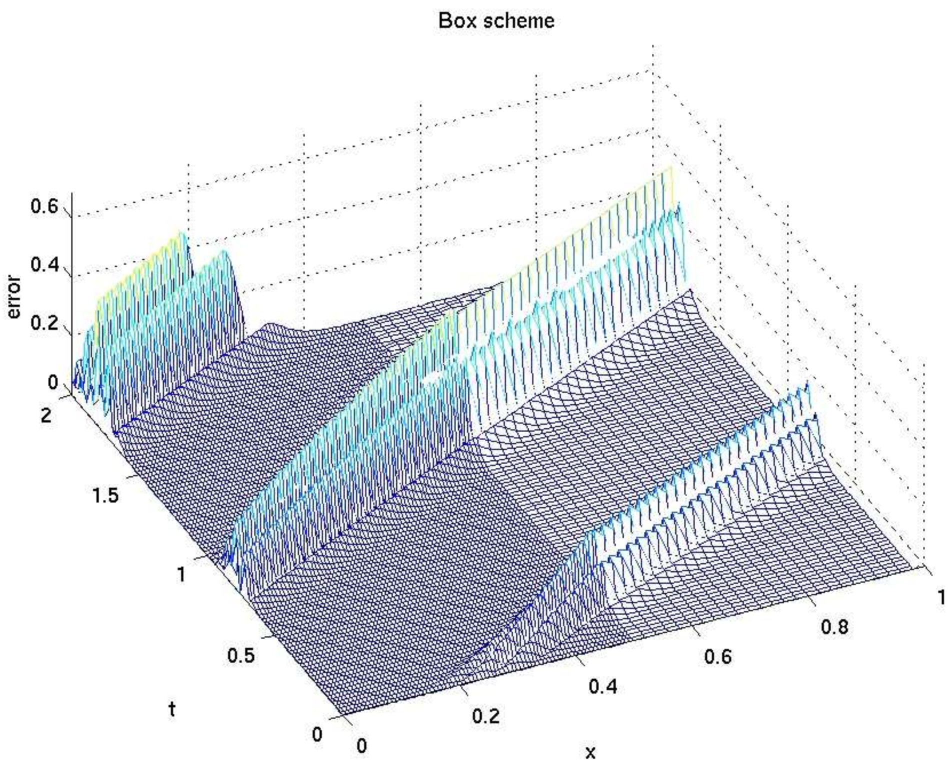

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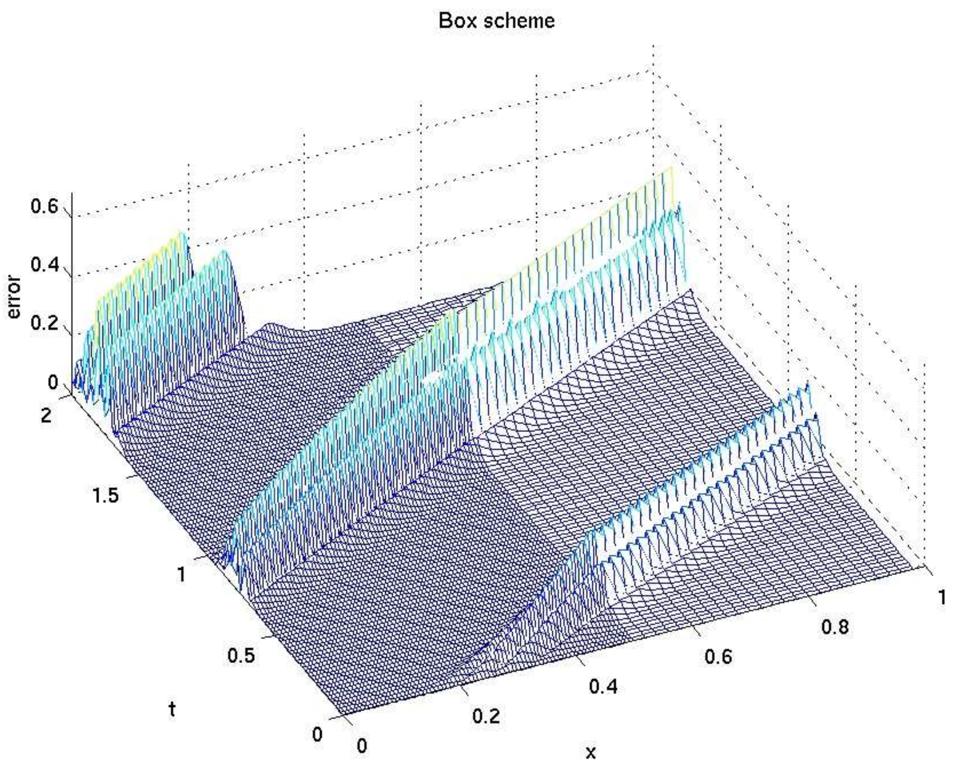

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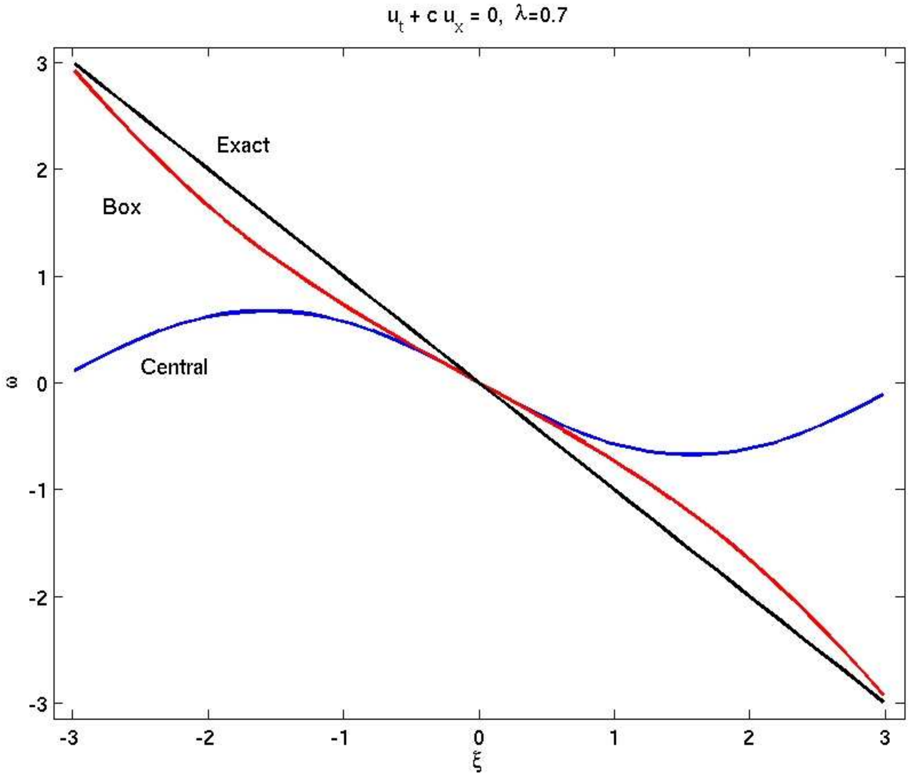
A similar analysis proves this is so, following from a scalar propagation function (single root).

However, it is also immediate from the dispersion relation . . .

Grid-induced reflections, $u_t = -cu_x$, dispersion relation

Dispersion relations, central and box schemes

Ascher & McLachlan (2003) showed that the box scheme has a dispersion relation which is conjugate to that the true dispersion relation for any first order PDE. In particular this implies that group velocity always has the proper sign.



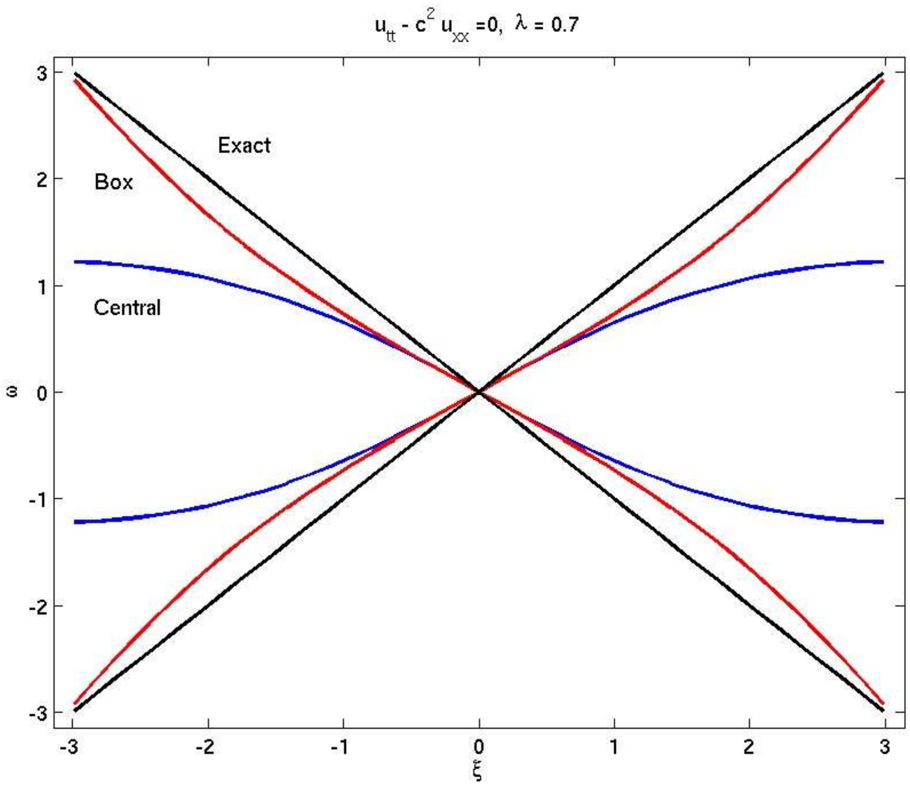
Grid-induced reflections, $u_{tt} = c^2 u_{xx}$, dispersion relation

But that is not the end of the story...

For the second order wave equation, both left- and right-running waves are admissible.

Both central (3 pt.) and the box schemes have monotone branches.

Yet. . .



Grid-induced reflections, $u_{tt} = c^2 u_{xx}$, example

Numerical experiment

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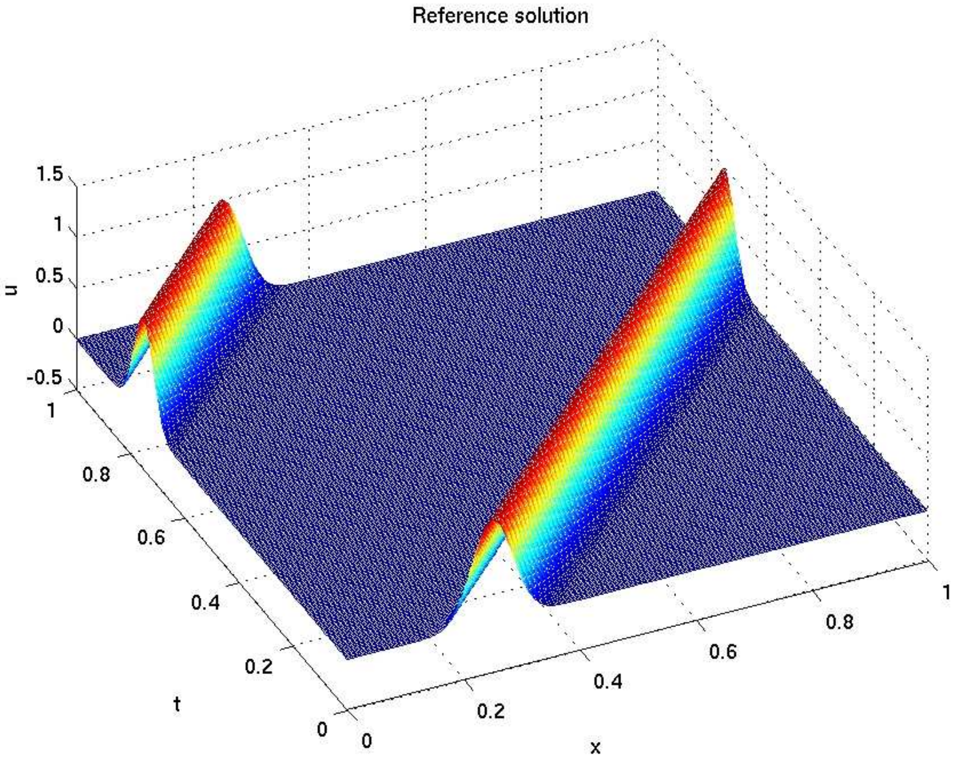

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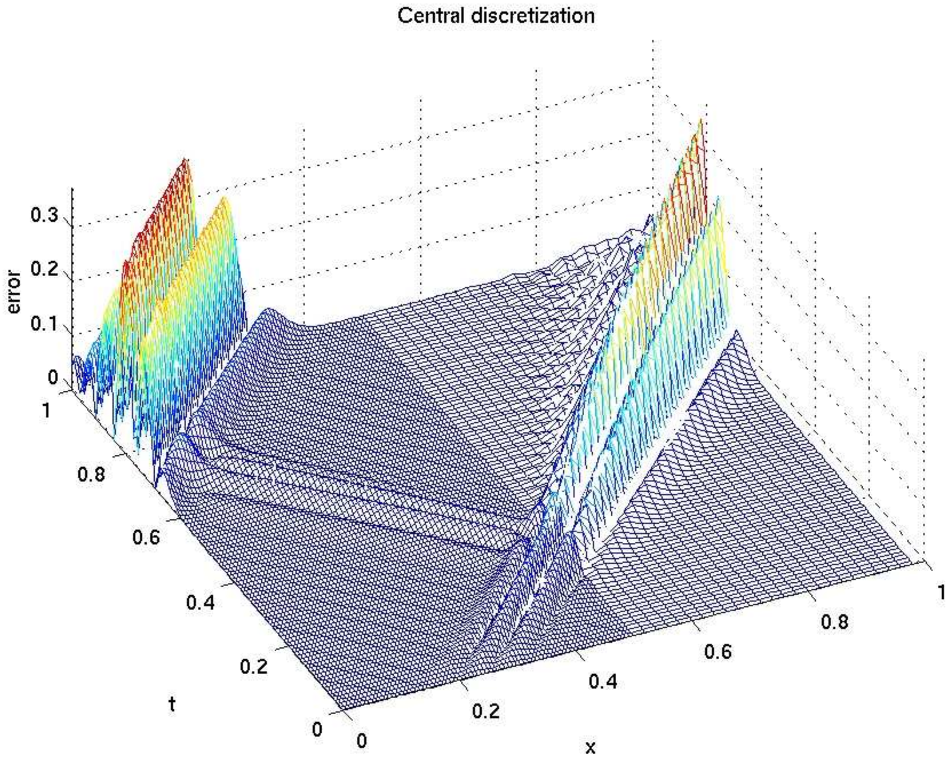

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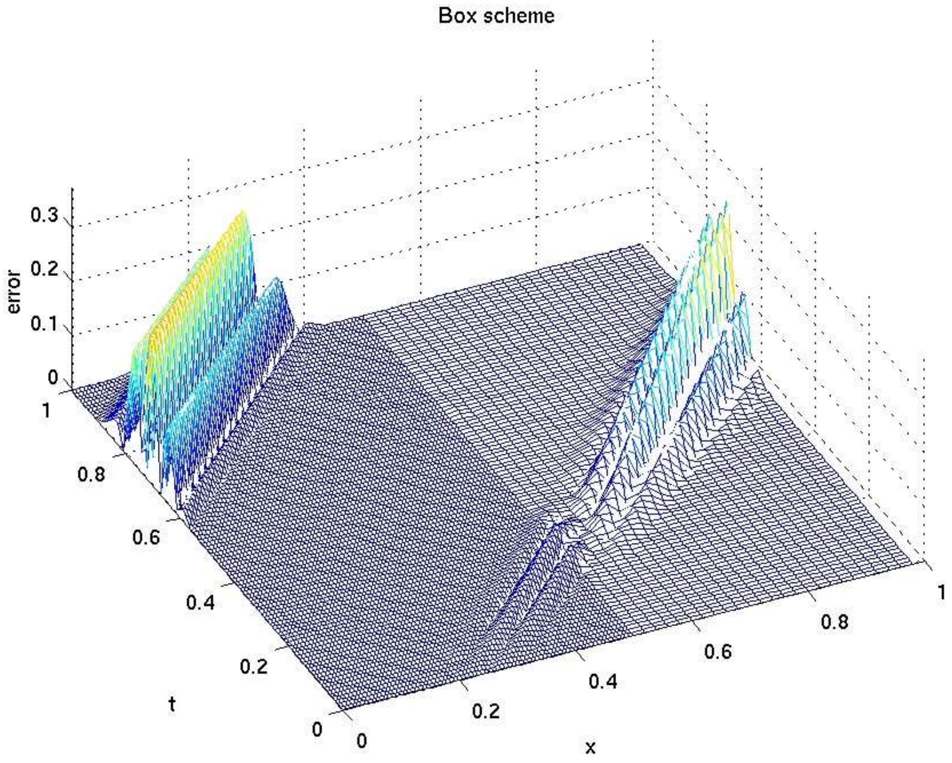

Box scheme analysis, $u_{tt} = c^2 u_{xx}$

Wave equation as a first order system

$$\begin{aligned} u_t &= v \\ u_x &= w \\ v_t &= c^2 w_x \end{aligned}$$

Box scheme semi-discretization

$$\begin{aligned} (\dot{u}_{j+1} + \dot{u}_j)/2 &= (v_{j+1} + v_j)/2 \\ (u_{j+1} - u_j)/h &= (w_{j+1} + w_j)/2 \\ (\dot{v}_{j+1} + \dot{v}_j)/2 &= c^2 (w_{j+1} - w_j)/h \end{aligned}$$

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Properties (Reich):

- Discrete conservation laws for energy and momentum
- Multisymplectic

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Properties (Reich):

- Discrete conservation laws for energy and momentum
- Multisymplectic

Generalizing Vichnevetsky's analysis to this case:
Time-transformation, eliminate $\hat{v}_j$ and solve for $\hat{u}_{j+1}$, $\hat{w}_{j+1}$

$$\begin{pmatrix} \hat{u}_{j+1} \\ \hat{w}_{j+1} \end{pmatrix} = \Phi(h\omega) \begin{pmatrix} \hat{u}_j \\ \hat{w}_j \end{pmatrix}, \qquad \Phi(h\omega) = \begin{bmatrix} \frac{1-h^2\omega^2/4}{1+h^2\omega^2/4} & \frac{h\omega^2}{1+h^2\omega^2/4} \\ \frac{h}{1+h^2\omega^2/4} & \frac{1-h^2\omega^2/4}{1+h^2\omega^2/4} \end{bmatrix}$$

Box scheme analysis

Diagonalizing Φ gives

$$\begin{pmatrix} \hat{u}_{j+1} \\ \hat{w}_{j+1} \end{pmatrix} = \Phi(h\omega) \begin{pmatrix} \hat{u}_j \\ \hat{w}_j \end{pmatrix}, \qquad \Phi(h\omega) = X(\omega)D(h\omega)X(\omega)^{-1}$$

where

$$D(h\omega) = \text{diag}\,(L(h\omega), R(h\omega))\,, \quad L(h\omega), R(h\omega) = \frac{1 - h^2\omega^2/4 \pm \mathrm{i}h\omega}{1 + h^2\omega^2/4}$$

and

$$X = \begin{bmatrix} i\omega & -i\omega \\ 1 & 1 \end{bmatrix} = X(\omega), \quad \text{independent of } h \text{ (the eigenspace of the PDE)}$$

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Left and right moving solutions are given by

$$\begin{pmatrix}\hat{\ell}_{j+1}\\ \hat{r}_{j+1}\end{pmatrix} = X(\omega)^{-1}\begin{pmatrix}\hat{u}_{j+1}\\ \hat{w}_{j+1}\end{pmatrix} = \begin{pmatrix}L(h\omega)^{j+1}\hat{\ell}_0\\ R(h\omega)^{j+1}\hat{r}_0\end{pmatrix}$$

Box scheme analysis

Across a jump in grid spacing from h_1 to h_2 at x_0, we have, for the box scheme

$$\begin{pmatrix} \hat{u}_1 \\ \hat{w}_1 \end{pmatrix} = \Phi(h_2\omega)\Phi(h_1\omega) \begin{pmatrix} \hat{u}_{-1} \\ \hat{w}_{-1} \end{pmatrix} = X(\omega)D(h_2\omega)D(h_1\omega)X(\omega)^{-1} \begin{pmatrix} \hat{u}_{-1} \\ \hat{w}_{-1} \end{pmatrix},$$

that is

$$\hat{\ell}_1 = L(h_2\omega)L(h_1\omega)\hat{\ell}_{-1}, \qquad \hat{r}_1 = R(h_2\omega)R(h_1\omega)\hat{r}_{-1}$$

Left- and right-running waves remain decoupled.

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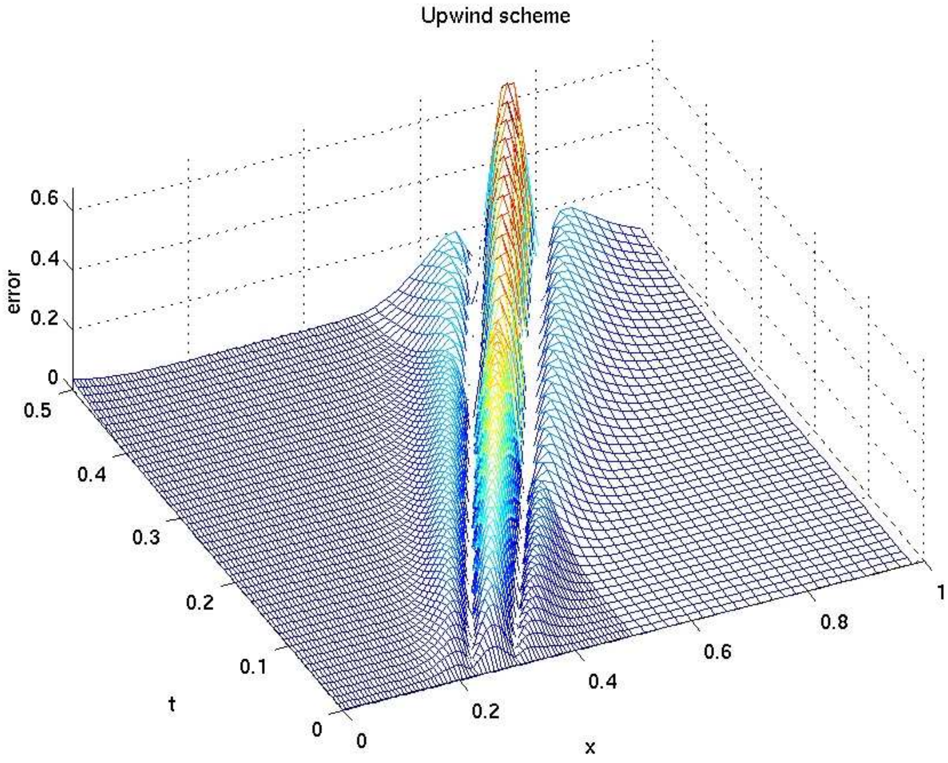
Note that the group velocities in the two domains are *not* equal, so Vichnevetsky's formula for the reflection ratio does not apply here.

Runge-Kutta space discretizations

The absence of grid-induced reflections for the Box scheme is due to the commutativity of diagonalization and discretization, which holds for any Runge-Kutta method (but not for partitioned R-K methods).

Thus, any Runge-Kutta spatial discretization of a system of linear first-order wave equations will be free of grid-induced reflections.

For example, upwind differencing . . .



Extensions, Nonlinear problems

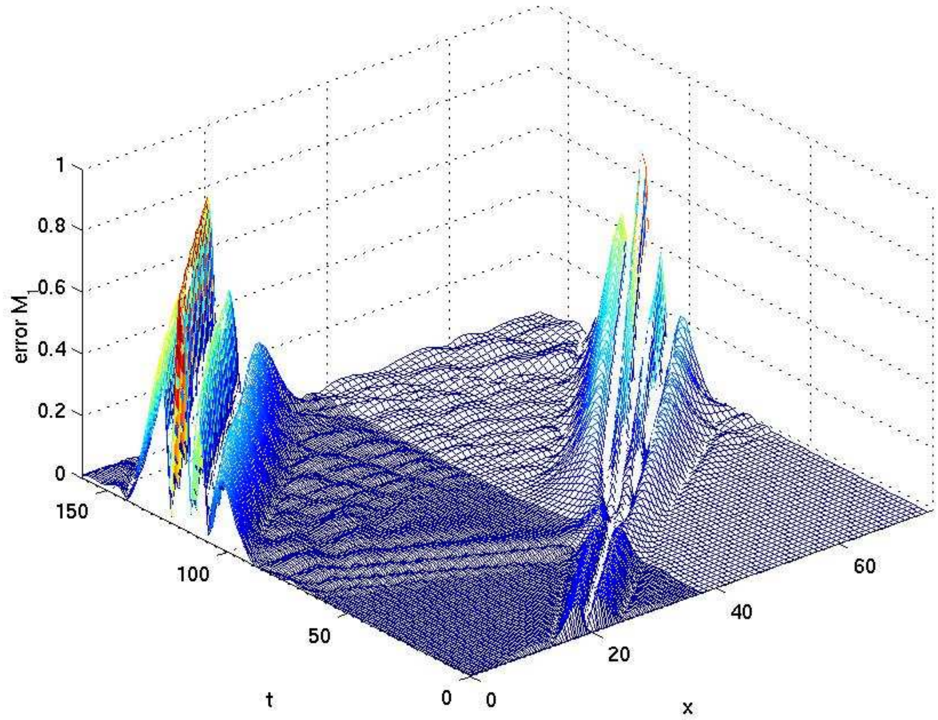
The Landau-Lifshitz equation:

$$\mathbf{m}_t = \mathbf{m} \times (\mathbf{m}_{xx} + \mathbf{\Omega}_0), \quad \mathbf{m}(x,t) \in \mathbf{R}^3.$$

Numerical experiment

- 160 grid points on $[0, 1)$, periodic
- $h_1/h_2 = 1/3$
- $\tau = 0.2$
- [Soliton solution] (Tjon & Wright 1977), m^1 component

Central



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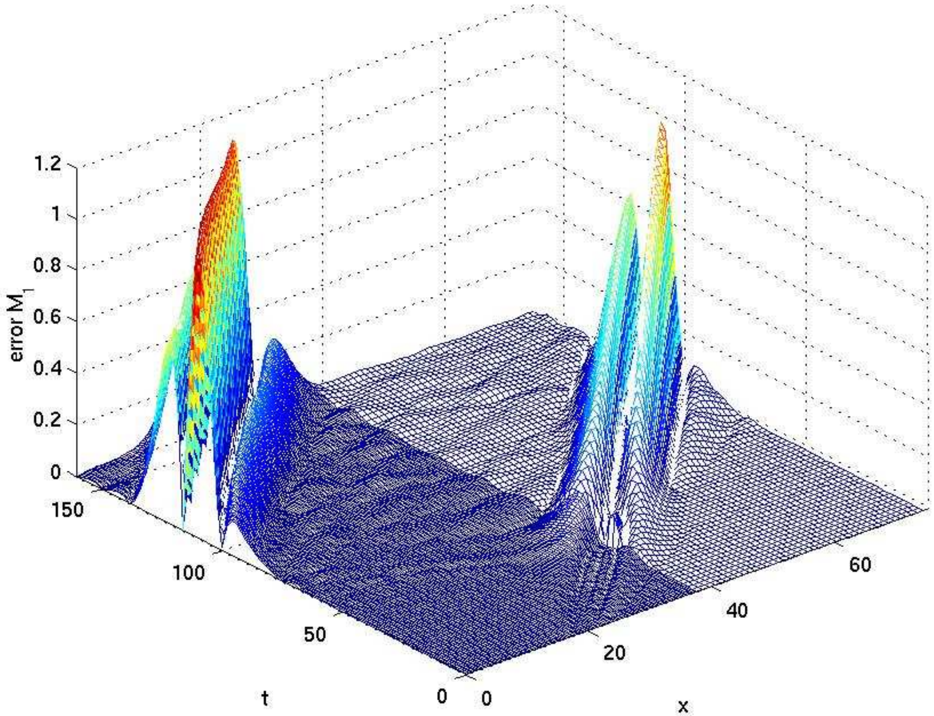
Box



Extensions, Higher spatial dimensions

2D wave equation $u_{tt} = c^2(u_{xx} + u_{yy})$.
Numerical experiment

- 80×80 grid points on $[0, 1)^2$, double periodic
- $h_1/h_2 = 1/7$ in each dimension
- $\tau = 0.02$
- $t \in [0, \sqrt{2}]$
- Plane wave with velocity $(-1/\sqrt{2}, -1/\sqrt{2})$ with Gaussian profile

[Central differences] [Box Scheme] [Error Box Scheme]

Extensions, Non-reflecting boundary conditions in 2D

2D wave equation $u_t = -c(u_x + u_y)$.
Numerical experiment

- 50×50 grid points on $[0, 1)^2$
- Dirichlet conditions on $x = 0$ and $y = 0$
- $\tau = 0.03$
- $t \in [0, 3.6]$
- Plane wave with velocity $(1/3, 2/3)$ with Gaussian profile

[Evolution] [Error propagation]

Summary

We have shown that in particular the box scheme and in general Runge-Kutta spatial discretizations for first order linear wave equations avoid the spurious reflections due to variations in grid spacing that plague multistep spatial discretizations.

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The End