Dispersion properties of energy-conserving discretizations for wave equations

Jason Frank
CWI, Amsterdam

Joint work with: Brian Moore, Sebastian Reich
Example 1: Non-monotone dispersion relation

Advection equation:

\[ u_t + u_x = 0 \]

2nd order central difference in space, exact in time:

\[ \frac{\Delta u_j}{\Delta x} = -\frac{u_{j+1} - u_{j-1}}{2\Delta x} \]

- under-resolved initial condition
  \[ \Delta x \gg 0 \]
- non-monotone dispersion relation does not conserve energy flow direction

Remedy: increase resolution
Example 2: Nonuniform grid

Wave equation:

\[ u_{tt} = u_{xx} \]

Staggered, 4th order central difference in space, exact in time.

- monotone dispersion relation
- energy transferred to left characteristic as the pulse crosses the interface

Remedy: *smooth grid transition*
Outline

• Wave equations: dispersion relation, energy flow
• Advection semi-discretizations: BEA, monotone dispersion relations
• Group velocity signature:
  – RK methods
  – FD methods
• Nonuniform grids
  – energy-conserving FD methods
  – energy exchange
• Higher order equations
  – first order form
  – general FD discretizations
• Conclusions
Wave equations

Consider Hamiltonian wave equations with smooth solutions and methods stressing energy conservation, as opposed to hyperbolic wave equations where the focus is on shocks and methods satisfying monotonicity.

Hamiltonian structure:

\[ u_t = \mathcal{J} \cdot \frac{\delta H}{\delta u}, \quad \mathcal{J} = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}, \quad \text{or} \quad \mathcal{J} = \partial_x \]

Multisymplectic structure: (Bridges ‘97, Marsden, Patrick & Shkoller, ‘99, Bridges & Reich ‘99)

\[ J u_t + L u_x = \nabla_u S(u), \quad J = -J^T, \quad L = -L^T \]

Examples: KdV, Nonlinear Schrödinger, geophysical fluids, electromagnetics

Energy conservation law:

\[ e = \frac{1}{2} (u^T L u_x) - S(u), \quad f = \frac{1}{2} u_t^T L u, \quad e_t + f_x = 0 \]

(i.e. \( \mathcal{H} = \int e(x, t) \, dx \).
Dispersion relation

The properties illustrated earlier can be understood in terms of the dispersion relation (e.g. Whitham ’74) – defined for a linearized PDE:

\[ Ju_t + Lu_x = Su, \quad u(x, t) \in \mathcal{R}^d \]

Look for a plane-wave solution with wave number \( \kappa \) and frequency \( \omega \)

\[ u(x, t) = e^{i(\kappa x - \omega t) \hat{a}} \]

Such a solution exists if \( (\omega, \kappa, \hat{a}) \) satisfy the generalized eigenvalue problem

\[ [-i\omega J + i\kappa L - S] \hat{a} = 0 \]

Dispersion relation is the functional relation between \( \kappa \) and \( \omega \)

\[ \mathcal{D}(\omega, \kappa) := \det[-i\omega J + i\kappa L - S] \]

\[ \mathcal{D}(\omega, \kappa) = 0 \]
Example: Korteweg-de Vries

The linearized KdV equation

\[ u_t = -u_x - \beta u_{xxx} \]

Identify:

\[ \partial_t \rightarrow -i\omega \]
\[ \partial_x \rightarrow i\kappa \]

Dispersion relation:

\[ \omega = \kappa - \beta \kappa^3 \]

Plot for \( \beta = 0.0015 \)
Phase and group velocities

- The slope $\omega/\kappa$ is the phase speed, the propagation speed of the wave front.

*Dispersion* if phase speed not constant.
Phase and group velocities

- The slope $\omega/\kappa$ is the *phase speed*, the propagation speed of the wave front.

- The slope $d\omega/d\kappa$ of the dispersion relation is referred to as the *group velocity*.

$$G(\kappa) := \frac{d\omega}{d\kappa} = -\frac{\partial D/\partial \kappa}{\partial D/\partial \omega}$$

- The group velocity is the mean speed of propagation of a composite wave pattern.
Phase and group velocities

- The slope $\omega/\kappa$ is the \textit{phase speed}, the propagation speed of the wave front.

- The slope $d\omega/d\kappa$ of the dispersion relation is referred to as the \textit{group velocity}.

$$G(\kappa) := \frac{d\omega}{d\kappa} = -\frac{\partial D/\partial \kappa}{\partial D/\partial \omega}$$

- The group velocity is the mean speed of propagation of a composite wave pattern.

- For KdV it can have opposite sign to the phase speed.

(Wave numbers 19 & 21)
Group velocity and energy flow

- For a single mode solution, energy propagates at the group velocity:

\[ f = Ge, \quad e_t + (G(\kappa)e)_x = 0 \]

- Sign of group velocity = direction of energy flow at wavelength \( \kappa \).
- Numerical methods introduce dispersion.
Group velocity and energy flow

- For a single mode solution, energy propagates at the group velocity:
  \[ f = G e, \quad e_t + (G(\kappa)e)_x = 0 \]

- Sign of group velocity = direction of energy flow at wavelength \( \kappa \).
- Numerical methods introduce dispersion.
- More generally, energy density is conserved between group lines (Whitham 1974)
  \[ E(t) = \int_{G(\kappa_1)t}^{G(\kappa_2)t} e(x,t) \, dx = \text{const} \]
Advection equation semi-discretizations

Consider semi-discretizations of the advection equation

\[ u_x = -u_t, \quad \omega = \kappa \]

Runge-Kutta methods in space (e.g. BVPs (Ascher, Mattheij & Russell) and GLRK-box (Reich))

\[ U_k = u_j - \Delta x \sum_{\ell=1}^{s} a_{k\ell} \dot{U}_\ell, \quad k = 1, \ldots, s \]

\[ u_{j+1} = u_j - \Delta x \sum_{k=1}^{s} b_k \dot{U}_k \]

To determine the dispersion relation of the semi-discretization, insert the semi-discrete plane-wave

\[ u_j = e^{i(Kj \Delta x - \omega t)} \hat{\alpha} \]

The dispersion relation (symmetric RK) is:

\[ e^{iK \Delta x} = R(i\omega \Delta x) \]

(stability function)

Noting (\(\omega = \kappa\)), an equivalent approach via BEA for \(u_x = i\kappa u\):

\[ e^{iK \Delta x} = R(i\kappa \Delta x) \]
Monotonicity of RK methods

For symmetric RK methods, backward error analysis defines a modified wave number \( K(\kappa; \Delta x) \), i.e.

\[
e^{iK \Delta x} = R(i\kappa \Delta x)
\]

For symmetric, A-stable RK methods, Lemma 1 of Guglielmi & Hairer (1999) implies this relationship is monotone.

\[
dK/d\kappa > 0
\]

On a grid, \( K \Delta x \in (-\pi, \pi] \), and \( K(\kappa) \) is invertible, so the semi-discrete dispersion relation becomes

\[
D(\omega, \kappa(K; \Delta x)) = 0
\]

The sign of group velocity (energy flow direction) is preserved:

\[
\frac{d\omega}{dK} = \frac{\partial \omega}{\partial \kappa} \cdot \frac{d\kappa}{dK}
\]
Dispersion relation, RK methods, fully discretizations

In the more general linear wave equation \( Ju_t + Lu_x = Su \)

The dispersion relation is \( \mathcal{D}(\omega, \kappa) := \text{det}[-i\omega J + i\kappa L - S] = 0 \)

In the fully discrete case, BEA yields modified wave number \( K \) and frequency \( \Omega \)

\[ e^{iK \Delta x} = R_1(i\kappa \Delta x), \quad e^{i\Omega \Delta x} = R_0(i\omega \Delta x) \]

Discretization admits a plane-wave \( u^n_j = e^{i(jK \Delta x - n\Omega \Delta t)} \hat{a} = R_1(i\kappa \Delta x)^j R_0(i\omega \Delta t)^n \hat{a} \)

As long as \( K(\kappa) \) and \( \Omega(\omega) \) are invertible, the numerical dispersion relation is

\[ \mathcal{D}(\Omega, K) := \mathcal{D}(\omega(\Omega), \kappa(K)) \]

For symmetric, A-stable RK methods, the group velocity signature is preserved:

\[ \frac{d\Omega}{dK} = -\frac{\partial \mathcal{D}/\partial \kappa}{\partial \mathcal{D}/\partial \omega \frac{d\omega}{d\Omega}} = \mathcal{G}(\kappa) \frac{d\kappa/dK}{d\omega/d\Omega} \]

(Ascher & McLachlan, 2004; Frank, Moore & Reich 2005).
Finite difference methods for advection

Similar analysis for symmetric finite difference semi-discretizations. Using notation of linear multistep methods \( (u_x = -u_t) \)

\[
\sum_{\ell=0}^{k} \alpha_{\ell} u_{j+\ell} = -\Delta x \sum_{\ell=0}^{k} \beta_{\ell} u_{j+\ell}, \quad \alpha_{\ell} = -\alpha_{k-\ell}, \quad \beta_{\ell} = \beta_{k-\ell}
\]

Associated polynomials \( \rho(z) = \sum_{\ell=0}^{k} \alpha_{\ell} z^{\ell}, \quad \sigma(z) = \sum_{\ell=0}^{k} \beta_{\ell} z^{\ell} \)

Insert plane-wave solution \( u_j = e^{i(jK\Delta x - \omega t)\tilde{\alpha}} \)

Dispersion relation \( i\omega \Delta x = \frac{\rho(e^{iK\Delta x})}{\sigma(e^{iK\Delta x})} \)

Roots: \( \rho(z) - i\omega\sigma(z) = 0 \Rightarrow \rho(1/\tilde{z}) - i\omega\sigma(1/\tilde{z}) = 0 \)

\( \rho(z) = 0 \Rightarrow \rho(1/z) = 0, \quad \sigma(z) = 0 \Rightarrow \sigma(1/z) = 0, \quad (\cup\{\tilde{z}, 1/\tilde{z}\}) \)

Rational function is \textit{good} if no poles on \( |K\Delta x| < \pi \) \cite{IserlesNørsett91, \leq}
Node-centered finite difference methods

Node-centered FD methods (k even)
(include all explicit methods)

\[
\dot{u}_j = -\frac{u_{j+1} - u_{j-1}}{2\Delta x}
\]

\[
\dot{u}_j = -\frac{-u_{j+2} + 8u_{j+1} - 8u_{j-1} + u_{j-2}}{12\Delta x}
\]

Consider \(\omega = 0 = \rho(z)/\sigma(z)\). For consistency,

\[\rho(1) = 0 \quad (K \Delta x = 0)\]
(simple). Even number of roots, another must satisfy \(z = 1/z \neq 1\), so must be at -1

\[\rho(-1) = 0 \quad (K \Delta x = \pm \pi)\]

Non-monotone dispersion relation

In particular no explicit monotone FD method.
Cell-centered finite difference methods

Cell-centered FD methods ( $k$ odd )
(necessarily implicit)

\[ \frac{u_{j+1} - u_j}{2} = -\frac{u_{j+1} - u_j}{\Delta x} \]

\[ \begin{bmatrix} -\frac{1}{16} & \frac{9}{16} & -\frac{9}{16} & \frac{1}{16} \end{bmatrix} \hat{u} = -\frac{1}{\Delta x} \begin{bmatrix} \frac{1}{24} & -\frac{27}{24} & \frac{27}{24} & -\frac{1}{24} \end{bmatrix} u \]

Odd number of poles; for goodness’ sake

$\sigma(1) \neq 0$

so there must be a pole at -1

$\omega(K \Delta x = \pm \pi) \to \infty$

(Strictly only pretty good.)

There do exist monotone methods, but all such methods are implicit.
Summary 1: dispersion relations

• A semi-discretization of a PDE in 1st order form preserves the sign of group velocity (direction of energy flow) if the discretization has a monotone dispersion relation for the advection equation.

• Symmetric, A-stable RK methods have monotone dispersion relations

• Node-centered FD methods have non-monotone dispersion relations

• Cell-centered FD methods can have monotone dispersion relations

• In particular, all explicit finite difference methods have non-monotone dispersion relations. Conversely all methods having monotone dispersion relations are implicit.
Conservative FD schemes on nonuniform meshes

Kitson, McLachlan & Robidoux (2003) investigated energy-conserving FD schemes on nonuniform meshes: (1) if a scheme is to be exact on polynomials of a given order, the stencil is globally dependent on the mesh (2) methods based on a smooth grid mapping suffer loss of order

Smooth grid mapping \( x_j = x(\xi_j) = x(j \Delta \xi) \)

Pull the derivative back to uniform grid \( u_x = \frac{u_\xi}{x_\xi} \approx \frac{\Delta u/\Delta \xi}{\Delta x/\Delta \xi} \)

Just a diagonal scaling of the difference matrix: (advection eqn. \( M = (\beta_j), D = (\alpha_j) \))

\[ M \dot{u} = \frac{1}{\Delta x} D u \quad \rightarrow \quad M \dot{u} = H^{-1} D u \]

where \( H = \text{diag}(h_j) \)

e.g. node centered: \( h_j = \frac{x_{j+1} - x_j - 1}{2} \), cell-centered: \( h_j = x_{j+1} - x_j \)

Conserves energy \( E = \frac{1}{2} (Mu)^T H (Mu) \)
Reflections in the advection case

(Following Vichnevetsky, 1981) Time-Fourier transform the semi-discretization

\[ \hat{u}_j(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} u_j(t) e^{i\omega t} \, dt \]

The FD scheme becomes

\[ \sum_{\ell=0}^{k} (\alpha_\ell - i\omega h_j \beta_\ell) \hat{u}_{j+\ell} = 0 \]

Written as a one-step recursion

\[
\begin{pmatrix}
\hat{u}_{j+k} \\
\hat{u}_{j+k-1} \\
\vdots \\
\hat{u}_{j+1}
\end{pmatrix}
= \begin{bmatrix}
\gamma_{k-1} & \gamma_{k-2} & \cdots & \gamma_0 \\
1 & 0 & & \\
& \ddots & \ddots & \\
& & 1 & 0
\end{bmatrix}
\begin{pmatrix}
\hat{u}_{j+k-1} \\
\hat{u}_{j+k-2} \\
\vdots \\
\hat{u}_j
\end{pmatrix} \quad \iff \quad \hat{U}_{j+1} = S_j \hat{U}_j
\]

\[ \gamma_\ell := - (\alpha_\ell - i\omega h_j \beta_\ell) / (\alpha_k - i\omega h_j \beta_k) \]

\[ S_j = S(\omega h_j) \]
Diagonalization

Diagonalizing the grid recursion \( \tilde{U}_{j+1} = S_j \tilde{U}_j = X_j \Lambda_j X_j^{-1} \tilde{U}_j \)

where

\[ \Lambda_j = \text{diag}(\lambda_1, \ldots, \lambda_k), \quad X_j = \begin{bmatrix} \lambda_1^{k-1} & \cdots & \lambda_k^{k-1} \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{bmatrix} \]

The \( \lambda_i \) are ‘wave numbers’ satisfying \( i \omega h_i = \rho(\lambda_i)/\sigma(\lambda_i) \).

Define the fundamental (characteristic) modes \( \tilde{C}_j = X_j^{-1} \tilde{U}_j \)

On a uniform grid, \( S_j \) \( S \), and the characteristics decouple globally \( \tilde{C}_{j+1} = \Lambda \tilde{C}_j \)

On a nonuniform mesh, we have \( \tilde{C}_{j+1} = X_{j+1}^{-1} X_j \Lambda_j \tilde{C}_j = B \Lambda_j \tilde{C}_j \)

But B consists of the Lagrange interpolating polynomials through the roots of \( S_{j+1} \), evaluated at the roots of \( S_j \)

\[
B_{k\ell} = e_k^T X_{j+1}^{-1} X_j e_\ell = (X_{j+1}^{-T} e_k)^T X_j e_\ell
\]

\[
B_{k\ell} = p_{k}^{(j+1)}(\lambda^{(j)}_\ell)
\]

which will be nonzero in general.
Summary 2: reflections

- So in general there will be an exchange of energy between all fundamental modes at a grid nonuniformity.
- If the numerical dispersion relation is monotone, there is only one $\lambda_i$ of modulus one (oscillatory mode), and reflections cannot occur.
- If the numerical dispersion relation is non-monotone, then there will be at least two $\lambda_i$ of modulus one. Reflections will be generated in those with negative group velocity.
Considerations for higher order wave equations

Wave equations with higher order derivatives can be written in 1st order form by introducing additional variables (multisymplectic).
If the 1st order form discretization is applied uniformly, then the fundamental mode coupling is preserved.

**Example:**
The wave equation \( u_{tt} = u_{xx} \) written in first order form \( u_t = v_x, \; v_t = u_x \)

Semi-discretize both using the same FD method

\[
Mu_t = H^{-1}Dv, \quad Mv_t = H^{-1}Du
\]

Introduce characteristic variables \( r = u - v, \; \ell = u + v \)
and these decouple and inherit the underlying dispersion properties of advection

\[
Mr_t = -H^{-1}Dr, \quad M\ell_t = H^{-1}D\ell
\]

**However,** direct discretizations of higher order derivatives (or staggering, PRK, mimetic) usually leads to coupling on nonuniform grids. *Even if the dispersion relation is monotone.*
Considerations for higher order wave equations

Wave equations with higher order derivatives can be written in 1st order form by introducing additional variables (multisymplectic). If the 1st order form discretization is applied uniformly, then the fundamental mode coupling is preserved.

**Example:**
The wave equation $u_{tt} = u_{xx}$ written in first order form

Semi-discretize both using the same FD method

$$M u_t = H^{-1} D v, \quad M v_t = H^{-1} D u$$

Introduce characteristic variables $r = u - v$, and these decouple and inherit the underlying dispersion properties of advection

$$M r_t = -H^{-1} D r, \quad M \ell_t = H^{-1} D \ell$$

**However,** direct discretizations of higher order derivatives (or staggering, PRK, mimetic) usually leads to coupling on nonuniform grids. *Even if the dispersion relation is monotone.*
Conclusions

• Group velocity signature is conserved by discretizations with monotone dispersion relations for the advection equation: symmetric, A-stable RK methods and some (implicit) cell-centered FD schemes.

• Explicit FD schemes do not have monotone dispersion for the advection equation. These have spurious modes with opposite group velocity.

• Energy is exchanged between fundamental modes at a grid nonuniformity. Reflections will occur if the dispersion relation is not monotone.

• For higher order waves, discretizations based on a reduction to first order form (e.g. multisymplectic form) retain the fundamental mode coupling and inherit the dispersion properties of the underlying advection discretization.

• In particular, symmetric Runge-Kutta schemes are attractive because they give no reflections, preserve the sign of group velocity, and maintain their order on arbitrary grids.

The End