Multi-Symplectic Integration for Linear PDEs

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Symplectic methods for Hamiltonian ODEs

- Methods which define a symplectic mapping
- Preserve symplectic structure of the ODE
- Near conservation of energy
- Excellent long-time simulation

The plot shows numerical integration of the Kepler problem using forward Euler and symplectic Euler methods. The forward Euler method pumps energy into the system leading to unstable orbits, but the symplectic Euler method maintains a nearly constant energy resulting in excellent long-time simulation.
The great success of these methods has led to the consideration of analogous methods for Hamiltonian PDEs. Such methods have become known as \textit{multi-symplectic integrators}.

**Questions**

- What does it mean for a method to be multi-symplectic?
- When excellent long-time simulation is the purpose of symplectic integration, is it necessary to preserve the spatial symplectic structure of a Hamiltonian PDE?

**Multi-Symplectic PDEs**

\[
Kz_t + Lz_x = \nabla_z S(z)
\]

- \( K \) and \( L \) are skew-symmetric matrices
- \( z = z(x,t) \) is the vector of state variables
- \( \nabla_z S(z) \) is the gradient of a smooth function
Introduced in [2,3], this formulation exploits the symplectic structure regarding each independent variable. Examples include KdV, Boussinesq, nonlinear Schrödinger, nonlinear wave equations, etc.

We consider a linearized version

\[ K \frac{\partial z}{\partial t} + L \frac{\partial z}{\partial x} = Az, \]

where \( A \) is symmetric.

**Dispersion Relations**

Substituting the single mode solution

\[ z(x, t) = ae^{i(kx + \omega t)} \]

into \( K \frac{\partial z}{\partial t} + L \frac{\partial z}{\partial x} = Az \) gives

\[ [i\omega K + ikL - A]a = 0 \]

which implies the dispersion relation

\[ g(\omega, k) := \det[i\omega K + ikL - A] = 0, \]
and the group velocity is given by

$$v = \omega'(k) = -\frac{g_k}{g\omega}.$$ 

**Note:** The sign of the group velocity determines the direction of energy transport.

### Multi-Symplectic Methods

**Properties** of multi-symplectic methods

(A) Result of discrete variational mechanics

(B) Satisfy a multi-symplectic conservation law

(C) Real dispersion relations (no numerically induced diffusion)

(D) Preserve the sign of the group velocity

**Methods** considered here

(1) Gauss-Legendre Runge-Kutta Methods [8]

\[ K \frac{z^{n+1/2,i+1} - z^{n+1/2,i}}{\Delta t} + L \frac{z^{n+1,i+1/2} - z^{n,i+1/2}}{\Delta x} = A z^{n+1/2,i+1/2} \]
The Explicit Mid-Point Method

\[ \frac{z^n_{n,i+1} - z^n_{n,i-1}}{2\Delta t} + \frac{Lz^n_{n+1,i} - z^n_{n-1,i}}{2\Delta x} = Az^n_{n,i} \]

Methods (1) and (2) satisfy properties (A), (B), and (C). (See references [4,6,7].) Property (D) is the topic considered here.

**Numerical Dispersion Relations**

(1) and (2) satisfy a dispersion relation

\[ g(\omega, k) = 0 \quad \text{for} \quad \omega = \omega(\Omega) \quad \text{and} \quad k = k(K). \]

- Numerical frequency: \( \Omega \)
- Numerical wave number: \( K \)
- Numerical group velocity:

\[ V = -\frac{g_k k'(K)}{g_\omega \omega'(\Omega)} = \frac{v k'(K)}{\omega'(\Omega)} \]

**Note:** \( k'(K) > 0 \) and \( \omega'(\Omega) > 0 \) imply the sign of the group velocity is preserved by the method.
Important Results

**Theorem** [5] A GL-RK method (1) with stability function $R(z)$ satisfies the dispersion relation $g(\omega, k) = 0$ where $\omega$ and $k$ are defined implicitly by $e^{i\Omega \Delta t} = R(i\omega \Delta t)$ and $e^{iK \Delta x} = R(i k \Delta x)$

**Implications**: GL-RK methods have monotonic dispersion relations, meaning the method preserves the sign of the group velocity.

**Theorem** [5] The explicit midpoint method (2) satisfies the dispersion relation $g(\omega, k) = 0$ with

$$
\omega = \frac{\sin(\Omega \Delta t)}{\Delta t} \quad \text{and} \quad k = \frac{\sin(K \Delta x)}{\Delta x}
$$

for $-\pi < \Omega \Delta t < \pi$ and $-\pi < K \Delta x < \pi$.

**Implications**: The midpoint method has dispersion relations that are not monotonic and do not preserve the sign of the group velocity.
A Simple Example

The wave equation $u_{tt} = u_{xx}$ is equivalent to

$$v_t + w_x = 0, \quad u_t = v, \quad u_x = -w,$$

which can be stated explicitly in multi-symplectic form $Kz_t + Lz_x = Az$, as

$$
\begin{bmatrix}
0 & -1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
u_t \\
v_t \\
w_t
\end{bmatrix}
+ 
\begin{bmatrix}
0 & 0 & -1 \\
0 & 0 & 0 \\
1 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
u_x \\
v_x \\
w_x
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
v \\
-w
\end{bmatrix}.
$$

Exact Dispersion Relation: $\omega^2 = k^2$

Numerical Dispersion Relation: $\omega(\Omega)^2 = k(K)^2$

(1) Index 2 GL-RK Method [1]

$$\omega(\Omega) = \frac{\tan(\Omega \Delta t/2)}{\Delta t/2} \quad \text{and} \quad k(K) = \frac{\tan(K \Delta x/2)}{\Delta x/2}$$

Notice $\omega(\Omega)$ and $k(K)$ are monotonic and invertible for $-\pi < \Omega \Delta t < \pi$ and $-\pi < K \Delta x < \pi$. 
(2) Explicit Midpoint Scheme

\[ \omega(\Omega) = \frac{\sin(\Omega \Delta t)}{\Delta t} \quad \text{and} \quad k(K) = \frac{\sin(K \Delta x)}{\Delta x} \]

Here, \( \omega(\Omega) \) and \( k(K) \) are not monotonic for \(-\pi < \Omega \Delta t, K \Delta x < \pi\), and are not defined if \(|\omega \Delta t|, |k \Delta x| > 1\) (instability of the method).
Here we plot snapshots of an EMP numerical solution of \( u_{tt} = u_{xx} \). The exact solution is a wave packet traveling to the right. The small wave packet traveling to the left is a numerical artifact resulting from a nonmonotonic dispersion relation.

The remaining plots compare various numerical (red lines) and exact (blue crosses) dispersion relations. The parameter \( \beta = \Delta t / \Delta x \) refers to a CFL condition.
The left of the previous plot shows dispersion relations for a 4th-order GL-RK space-time discretization. A CFL type condition (\( \beta < 1 \)) must be satisfied to avoid intersecting branches, and to guarantee the sign of the group velocity is preserved. On the right are dispersion relations for a 4th-order composition method based on the implicit midpoint scheme, showing that intersecting branches are not present regardless of the size of \( \beta \).

Numerical dispersion relations for explicit midpoint discretization (EMP) in space and implicit midpoint discretization (IMP) in time, showing that non-monotonicity of the dispersion relation results purely from a 'bad' discretization in space.
On the left is the numerical dispersion relation for EMP in time and symplectic Störmer-Verlet discretization (SV) in space. The spurious branches are due to the EMP discretization in time. On the right, the discretizations are reversed, and the non-monotonicity is due to the EMP discretization in space, demonstrating the importance of discretizing both space and time with preserving schemes.

**Summary**

We have considered Gauss-Legendre Runge-Kutta and explicit midpoint methods for solving linear Hamiltonian PDEs. We showed that GL-RK methods preserve the sign of the group
velocity (the direction in which the energy is transported), but EMP methods do not. This is a result of preserving the symplectic structure of the PDE in space, and shows why it may be important to use multi-symplectic methods for long-time simulation. GL-RK methods are truly multi-symplectic, but EMP methods are not, in spite of the fact that they satisfy a multi-symplectic conservation law and can be derived from a discrete variational principle.

References