

Symplectic-Hamiltonian Finite element methods for wave propagation

Bernardo Cockburn

School of Mathematics
University of Minnesota

Rome
Polytopal INdAM Workshop
May 19, 2021

Joint work with

- Manuel Sánchez, P.U.C., Santiago de Chile.
- N.-Cuong Nguyen, MIT.
- Jaime Peraire, MIT.

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The problem

We are interested in devising, as systematically as possible, fully discrete numerical schemes for hyperbolic problems which are **high-order accurate** and **preserve**, not only **the energy** of the system, but **as many as possible other physical quantities of interest** when **long-term** simulations are sought.

We are developing an approach to achieve this for hyperbolic problems with **Hamiltonian structure**. Here, we consider the case of **linear, wave-propagation** problems.

Three model wave equations

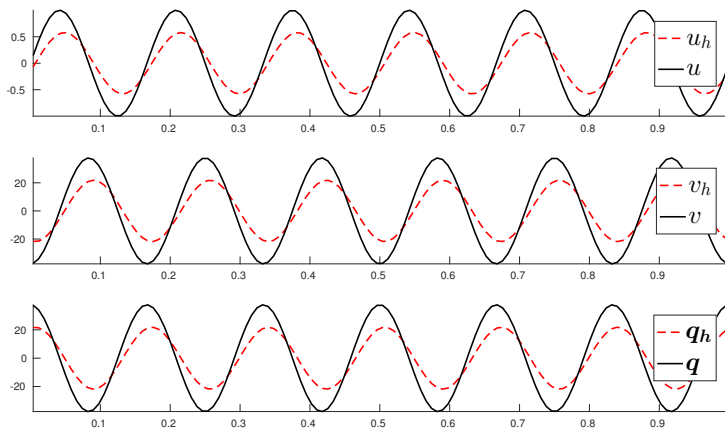
acoustic	elastic	electromagnetic
$\ddot{u} = \nabla \cdot (\kappa \nabla u) + f$	$\rho \ddot{\mathbf{u}} = \nabla \cdot (\mathbb{C} \underline{\boldsymbol{\varepsilon}}(\mathbf{u})) + \mathbf{f}$	$\varepsilon \ddot{\mathbf{E}} = -\nabla \times \frac{1}{\mu} \nabla \times \mathbf{E}$
$\begin{cases} \kappa^{-1} \dot{\mathbf{q}} = \nabla v \\ \dot{v} = \nabla \cdot \mathbf{q} + f \end{cases}$	$\begin{cases} \mathbb{C}^{-1} \dot{\boldsymbol{\sigma}} = \underline{\boldsymbol{\varepsilon}}(\mathbf{v}) \\ \rho \dot{\mathbf{v}} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} \end{cases}$	$\begin{cases} \varepsilon \dot{\mathbf{E}} = \nabla \times \mathbf{H} \\ \mu \dot{\mathbf{H}} = -\nabla \times \mathbf{E} \end{cases}$
$\begin{cases} \dot{\mathbf{u}} = \mathbf{v} \\ \varepsilon \dot{v} = \nabla \cdot (\kappa \nabla u) + f \end{cases}$	$\begin{cases} \dot{\mathbf{u}} = \mathbf{v} \\ \rho \dot{\mathbf{v}} = \nabla \cdot (\mathbb{C} \underline{\boldsymbol{\varepsilon}}(\mathbf{u})) + \mathbf{f} \end{cases}$	$\begin{cases} \dot{\mathbf{E}} = \mathbf{V} \\ \varepsilon \dot{\mathbf{V}} = -\nabla \times \frac{1}{\mu} \nabla \times \mathbf{E} \end{cases}$

Linear Symmetric hyperbolic or Hamiltonian systems?

- A DG discretization of each of the three wave equations, **written as hyperbolic, symmetric systems**, typically produces a dissipative scheme.
- A new DG discretization of each of the three wave equations, **written as Hamiltonian systems**, produces a non-dissipative scheme which can also provide non-drifting approximations to invariant functionals.

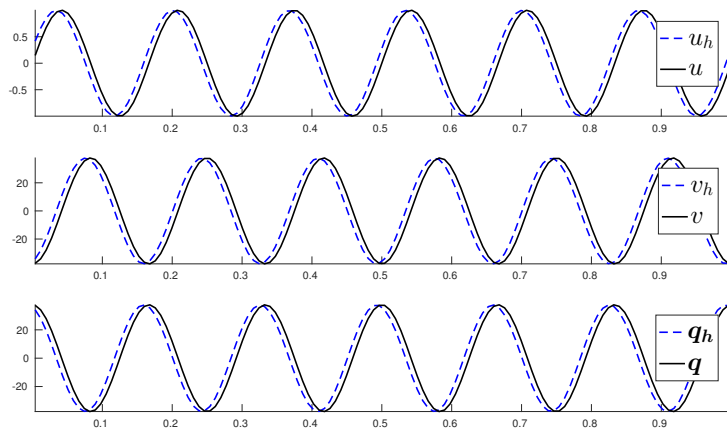
A numerical illustration

A Dissipative DG method for the acoustic wave equation



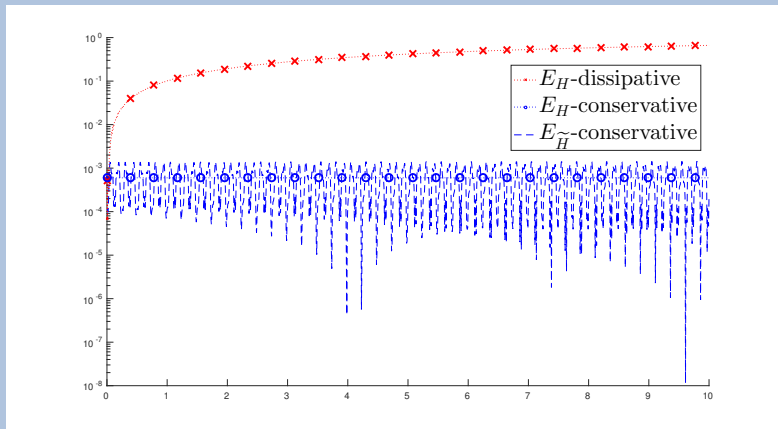
A numerical illustration

An S-H DG method for the acoustic wave equation



A numerical illustration

The total energy for the acoustic wave equation



The main idea and its two ingredients

To devise such schemes, the idea is to first discretize the **Hamiltonian** system in **space** so that the resulting system of ODEs is also **Hamiltonian**.

Then, an application of a **symplectic time-marching** scheme guarantees the **non-drifting** property of the Hamiltonian (and other first integrals of the system).

The first ingredient: Symplectic methods

The simplest Hamiltonian system

The simplest Hamiltonian system is the following:

$$\dot{p} = -\frac{\partial}{\partial q} H(p, q), \quad \dot{q} = \frac{\partial}{\partial p} H(p, q),$$

and $H(p, q)$ is called the Hamiltonian.

On the orbits of the system, $t \mapsto (p(t), q(t))$, the Hamiltonian remains **constant** because

$$\frac{d}{dt} H(p(t), q(t)) = \dot{p} \frac{\partial}{\partial p} H + \dot{q} \frac{\partial}{\partial q} H = 0.$$

Let us find what happens when this system is discretized by a symplectic method.

The first ingredient: Symplectic methods

The symplectic Euler method

We discretize our Hamiltonian system by the symplectic Euler method:

$$p_{n+1} = p_n - \Delta t \frac{\partial}{\partial q} H(p_{n+1}, q_n), \quad q_{n+1} = q_n + \Delta t \frac{\partial}{\partial p} H(p_{n+1}, q_n),$$

That the method is symplectic **means** that we have

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n,$$

and this **implies** that **there is** a discrete Hamiltonian $H_{\Delta t}$, close to H , such that

$$H_{\Delta t}(p_{n+1}, q_{n+1}) = H_{\Delta t}(p_n, q_n).$$

The first ingredient: Symplectic methods

The Harmonic oscillator

For the **harmonic oscillator**, $H(p, q) = q^2/2 + p^2/2$, we can easily find that

$$H_{\Delta t}(p_{n+1}, q_{n+1}) = H_{\Delta t}(p_n, q_n)$$

where

$$H_{\Delta t}(p, q) = H(p, q) - \Delta t p q.$$

This shows that all the discrete orbits of the Symplectic Euler method stay on the ellipse $H_{\Delta t}(p, q) = H(p_0, q_0) - \Delta t p_0 q_0$, and that the approximate energy **does not drift** from the exact one for all time.

The first ingredient: Symplectic methods

References for symplectic methods

- There is a **vast literature** on symplectic methods: see the 92 review by J.M. Sanz-Serna in [Acta Numerica](#).
- Of particular interest to us are the **symplectic Runge-Kutta** methods characterized in 94 by P.B. Bochev and C. Scovel in [BIT](#).
- For separable Hamiltonians, the **Explicit Partitioned Runge-Kutta** methods can be very efficiently implemented and are symplectic, see the 93 paper by L. Abia and J.M. Sanz-Serna in [Math. Comp.](#).

The second ingredient: The Hamiltonian machinery

The initial-boundary value problem

$$\begin{aligned} \dot{\mathbf{u}} &= \mathbf{v} && \text{in } \Omega \times (0, T], \\ \rho \dot{\mathbf{v}} &= \nabla \cdot (\mathcal{C}\underline{\boldsymbol{\varepsilon}}(\mathbf{u})) + \mathbf{f} && \text{in } \Omega \times (0, T], \\ \mathbf{u} &= \mathbf{u}_D && \text{on } \Gamma_D \times (0, T], \\ \mathcal{C}\underline{\boldsymbol{\varepsilon}}(\mathbf{u})\mathbf{n} &= \boldsymbol{\sigma}_N && \text{on } \Gamma_N \times (0, T]. \end{aligned}$$

The second ingredient: The Hamiltonian machinery

The Hamiltonian formulation

The mappings $t \mapsto (\mathbf{u}(t), \mathbf{v}(t))$ are orbits on a smooth manifold \mathcal{M} defining a dynamical system which is **Hamiltonian** if we can rewrite it as

$$\dot{C} = \{C, H\},$$

for the **coordinates** functionals C , defined on the **phase space** \mathcal{M} and identified with a space of **test functions** \mathcal{T} . Here H is the **Hamiltonian** and $\{\cdot, \cdot\}$ is the **Poisson bracket**. The triple $(\mathcal{M}, \{\cdot, \cdot\}, H)$ is called a **Hamiltonian dynamical system**.

The second ingredient: The Hamiltonian machinery

The Hamiltonian formulation

The **Hamiltonian** is

$$H(\mathbf{u}(t), \mathbf{v}(t)) = \frac{1}{2} \int_{\Omega} (\rho \mathbf{v}(t) \cdot \mathbf{v}(t) + \mathcal{C} \underline{\boldsymbol{\varepsilon}}(\mathbf{u}(t)) : \underline{\boldsymbol{\varepsilon}}(\mathbf{u}(t))) \\ - \int_{\Omega} \mathbf{f} \cdot \mathbf{u}(t) - \int_{\Gamma_N} \boldsymbol{\sigma}_N \cdot \mathbf{u}(t).$$

The **Poisson bracket** is

$$\{F, G\} = \int_{\Omega} \rho^{-1} \left(\frac{\delta F}{\delta \mathbf{u}} \cdot \frac{\delta G}{\delta \mathbf{v}} - \frac{\delta F}{\delta \mathbf{v}} \cdot \frac{\delta G}{\delta \mathbf{u}} \right),$$

for $F = F(\mathbf{u}, \mathbf{v})$ and $G = G(\mathbf{u}, \mathbf{v})$ functionals on \mathcal{M} , where $\frac{\delta F}{\delta \mathbf{u}}$ and $\frac{\delta F}{\delta \mathbf{v}}$ denote the functional derivatives of the functional F .

The second ingredient: The Hamiltonian machinery

The Hamiltonian formulation

The **phase manifold** is

$$\mathcal{M} = \{ \boldsymbol{\omega} \in L^2(\Omega)^d : \nabla \cdot (\mathcal{C}\boldsymbol{\varepsilon}(\boldsymbol{\omega})) \in L^2(\Omega)^d, \boldsymbol{\omega} = \boldsymbol{u}_D \text{ on } \Gamma_D \} \times L^2(\Omega)^d,$$

The **coordinates functionals** are

$$C_u(\boldsymbol{\phi}) = \int_{\Omega} \rho \boldsymbol{u} \cdot \boldsymbol{\phi}, \quad C_v(\boldsymbol{\psi}) = \int_{\Omega} \rho \boldsymbol{v} \cdot \boldsymbol{\psi},$$

for $(\boldsymbol{\phi}, \boldsymbol{\psi})$ in the space of **test functions**

$$\mathcal{T} = \mathcal{C}^\infty(\Omega)^d \times \{ \boldsymbol{\eta} \in \mathcal{C}^\infty(\Omega)^d : \boldsymbol{\eta} = 0 \text{ on } \Gamma_D \},$$

The second ingredient: The Hamiltonian machinery

The Hamiltonian formulation

Taking $C := C_u(\phi)$ and $C := C_v(\psi)$, we get

$$\begin{aligned}\int_{\Omega} \rho \dot{\mathbf{u}} \cdot \boldsymbol{\phi} &= \dot{C}_u(\boldsymbol{\phi}) = \{C_u(\boldsymbol{\phi}), H\} = \int_{\Omega} \rho^{-1} \frac{\delta C_u(\boldsymbol{\phi})}{\delta \mathbf{u}} \cdot \frac{\delta H}{\delta \mathbf{v}} = \int_{\Omega} \rho \mathbf{v} \cdot \boldsymbol{\phi}, \\ \int_{\Omega} \rho \dot{\mathbf{v}} \cdot \boldsymbol{\psi} &= \dot{C}_v(\boldsymbol{\psi}) = \{C_v(\boldsymbol{\psi}), H\} = - \int_{\Omega} \rho^{-1} \frac{\delta C_v(\boldsymbol{\psi})}{\delta \mathbf{v}} \cdot \frac{\delta H}{\delta \mathbf{u}} \\ &= - \int_{\Omega} \mathbb{C} \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\boldsymbol{\psi}) + \int_{\Omega} \mathbf{f} \cdot \boldsymbol{\psi} + \int_{\Gamma_N} \boldsymbol{\sigma}_N \cdot \boldsymbol{\psi},\end{aligned}$$

for all $(\boldsymbol{\phi}, \boldsymbol{\psi}) \in \mathcal{T}$. This means that the equations of linear elastodynamics define a **Hamiltonian dynamical system**.

The second ingredient: The Hamiltonian machinery

Conservation Laws

- Take $J := \boldsymbol{\eta} \cdot \int_{\Omega} \rho \mathbf{v}$. Then, since $\Gamma_D = \emptyset$, we have that $\mathcal{T} = \mathcal{C}^\infty(\Omega) \times \mathcal{C}^\infty(\Omega)$ and we can write that $J = C_{\mathbf{v}}(\boldsymbol{\psi})$ where $\boldsymbol{\psi} = \boldsymbol{\eta}$. As a consequence, $\{J, H\} = 0$. This proves the conservation of the linear momentum in time.
- Take $J := \boldsymbol{\eta} \cdot \int_{\Omega} \mathbf{x} \times \rho \mathbf{v}$. Then, by a similar argument, we see that $J = C_{\mathbf{v}}(\boldsymbol{\psi})$ where $\boldsymbol{\psi} = \boldsymbol{\eta} \times \mathbf{x}$. As a consequence, $\{J, H\} = 0$. This proves the conservation of angular momentum.
- For $J := E$, the conservation in time follows from the fact that, when \mathbf{f} and $\boldsymbol{\sigma}_N$ are zero, $E = H$ and from the fact that $\{H, H\} = 0$, by the antisymmetry of the Poisson bracket.

The second ingredient: The Hamiltonian machinery

The space discretization

We now discretize the equations of elastodynamics by using weak formulations of the original equations with mixed, DG or HDG methods. The resulting mappings $t \mapsto (\mathbf{u}_h(t), \mathbf{v}_h(t))$ are now orbits on a smooth manifold \mathcal{M}_h defining a dynamical system which can be shown to be **Hamiltonian**. This means we can rewrite the equations defining the method as

$$\dot{C}_h = \{C_h, H_h\}_h,$$

for some discrete **coordinates** functionals C_h , defined on the finite-dimensional **phase space** \mathcal{M}_h and identified with a space of **test functions** in the finite-dimensional space \mathcal{T}_h . Here H_h is the discrete **Hamiltonian** and $\{\cdot, \cdot\}_h$ is the discrete **Poisson bracket**. The triple $(\mathcal{M}_h, \{\cdot, \cdot\}_h, H_h)$ is then a **Hamiltonian dynamical system**.

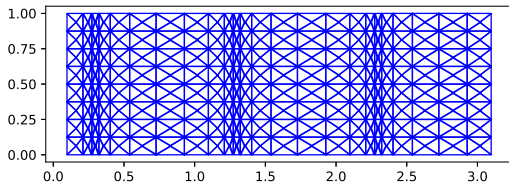
Combining the two ingredients: Elastic waves

The fully discrete method

By applying a symplectic scheme to the Hamiltonian system of ODEs defined by the space discretization, we obtain a fully discrete scheme. As a consequence, non-drifting approximations to the conserved quantities are immediately obtained.

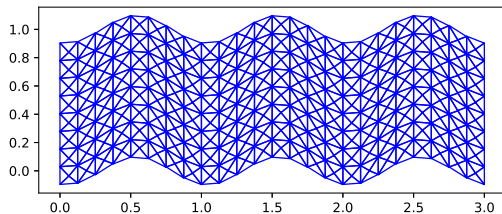
Combining the two ingredients: Elastic waves

Numerical illustration. P-wave



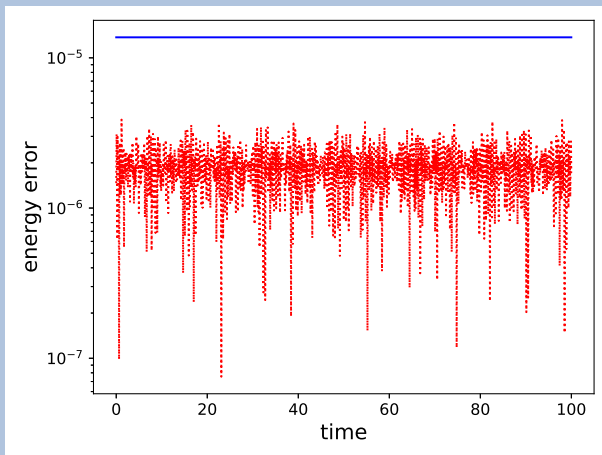
Combining the two ingredients: Elastic waves

Numerical illustration. S-wave



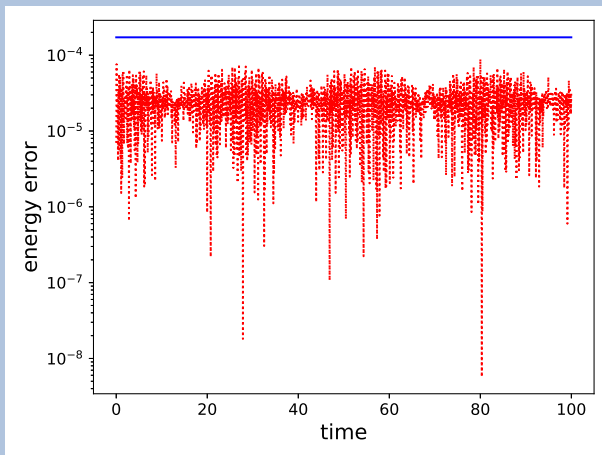
Combining the two ingredients: Elastic waves

Numerical illustration. P-wave



Combining the two ingredients: Elastic waves

Numerical illustration. S-wave



Previous and related work

- The idea of using Symplectic-Hamiltonian methods with finite-difference and finite volume methods is very old. Yee's 1966 famous scheme for electromagnetism uses the Symplectic Euler method which is fully explicit for Maxwell equations.
- The interest in using finite element methods for S-H methods is more recent: first in 2008 by Y. Xu et al. (DG), then in 2015 by Kirby and Kieu (mixed method).
- S-H HDG methods for the acoustic wave equation, JCP, 2017, also with C. Ciuca. First work using HDG methods. Canonical formulation.
- New DG methods for symmetric, hyperbolic systems, JCP, 2019, by G. Fu and C.-W. Shu.
- S-H HDG methods for linear elastodynamics, CMAME, 2021. The Poisson bracket formulation and the incorporation of test functions.

Ongoing work

- Electromagnetism, also with [Shukai Du](#), U. of Wisconsin-Madison.
- Large deformations.
- Nonlinear water waves.