Symplectic-Hamiltonian Finite element methods for wave propagation

Bernardo Cockburn

School of Mathematics
University of Minnesota

Montpellier
NEw generation MEthods for numerical SImulationS
June 21, 2021

Joint work with

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

Table of Contents I

1. The problem
   - Three model wave equations
   - Linear Symmetric hyperbolic or Hamiltonian systems?
   - The main idea and its two ingredients
2. The first ingredient: Symplectic methods
   - The simplest Hamiltonian system
   - The symplectic Euler method
   - The harmonic oscillator
3. The second ingredient: The Hamiltonian machinery
   - The initial-boundary value problem
   - The Hamiltonian formulation
   - Conservation laws
4. Combining the two ingredients
5. Previous and related work
6. Ongoing work

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

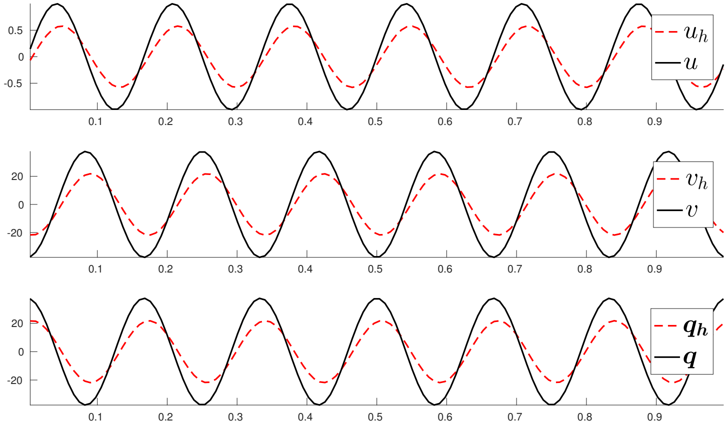
Linear Symmetric hyperbolic or Hamiltonian systems?

• 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.

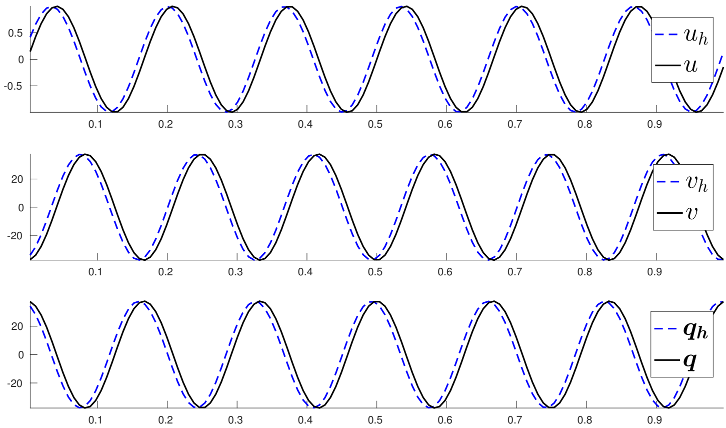
A numerical illustration

A Dissipative DG method for the acoustic wave equation



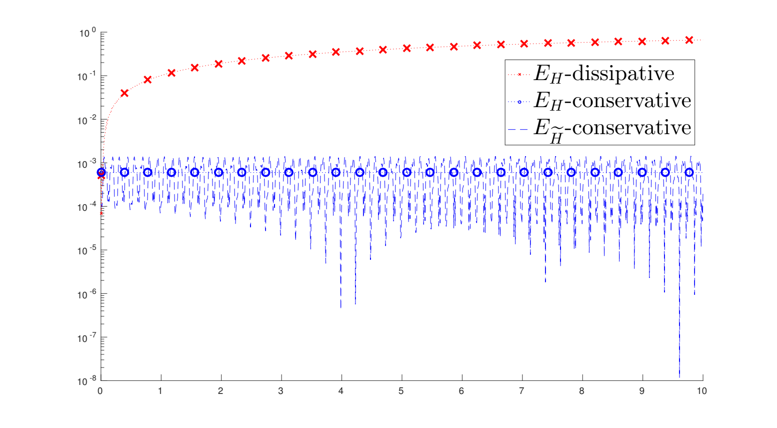
A numerical illustration

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 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

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

The mappings $t \mapsto (\boldsymbol{u}(t), \boldsymbol{v}(t))$ 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 Hamiltonian is

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

The Poisson bracket is

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

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

The phase manifold is

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

The coordinates functionals are

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

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

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

Taking $C := C_{\boldsymbol{u}}(\boldsymbol{\phi})$ and $C := C_{\boldsymbol{v}}(\boldsymbol{\psi})$, we get

$$\int_\Omega \rho\, \dot{\boldsymbol{u}} \cdot \boldsymbol{\phi} = \dot{C}_{\boldsymbol{u}}(\boldsymbol{\phi}) = \{C_{\boldsymbol{u}}(\boldsymbol{\phi}), H\} = \int_\Omega \rho^{-1} \frac{\delta C_{\boldsymbol{u}}(\boldsymbol{\phi})}{\delta \boldsymbol{u}} \cdot \frac{\delta H}{\delta \boldsymbol{v}} = \int_\Omega \rho\, \boldsymbol{v} \cdot \boldsymbol{\phi},$$

$$\begin{aligned} \int_\Omega \rho\, \dot{\boldsymbol{v}} \cdot \boldsymbol{\psi} = \dot{C}_{\boldsymbol{v}}(\boldsymbol{\psi}) = \{C_{\boldsymbol{v}}(\boldsymbol{\psi}), H\} &= -\int_\Omega \rho^{-1} \frac{\delta C_{\boldsymbol{v}}(\boldsymbol{\psi})}{\delta \boldsymbol{v}} \cdot \frac{\delta H}{\delta \boldsymbol{u}} \\ &= -\int_\Omega \mathcal{C}\underline{\boldsymbol{\varepsilon}}(\boldsymbol{u}) : \underline{\boldsymbol{\varepsilon}}(\boldsymbol{\psi}) + \int_\Omega \boldsymbol{f} \cdot \boldsymbol{\psi} + \int_{\Gamma_N} \boldsymbol{\sigma}_N \cdot \boldsymbol{\psi}, \end{aligned}$$

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

Assume that $\Gamma_D = \emptyset$, $\boldsymbol{f} = 0$ and $\boldsymbol{\sigma}_N = 0$.

• Take $J := \boldsymbol{\eta} \cdot \int_\Omega \rho \boldsymbol{v} = C_{\boldsymbol{v}}(\boldsymbol{\psi})$ where $\boldsymbol{\psi} = \boldsymbol{\eta}$ because $\Gamma_D = \emptyset$. Then

$$\dot{J} = \{J, H\} = \{C_{\boldsymbol{v}}(\boldsymbol{\psi}), H\} = -\int_\Omega \mathcal{C}\underline{\boldsymbol{\varepsilon}}(\boldsymbol{u}) : \underline{\boldsymbol{\varepsilon}}(\boldsymbol{\eta}) = 0,$$

because $\boldsymbol{f} = 0$ and $\boldsymbol{\sigma}_N = 0$. This proves the conservation of the linear momentum.

• Take $J := \boldsymbol{\eta} \cdot \int_\Omega \boldsymbol{x} \times \rho \boldsymbol{v}$. Then, by a similar argument, we see that $J = C_{\boldsymbol{v}}(\boldsymbol{\psi})$ where $\boldsymbol{\psi} = \boldsymbol{\eta} \times \boldsymbol{x}$. As a consequence,

$$\{J, H\} = -\int_\Omega \mathcal{C}\underline{\boldsymbol{\varepsilon}}(\boldsymbol{u}) : \underline{\boldsymbol{\varepsilon}}(\boldsymbol{\eta} \times \boldsymbol{x}) = 0$$

This proves the conservation of angular momentum.

• For $J := H$, the conservation in time of H follows from the fact that $\{H, H\} = 0$, by the antisymmetry of the Poisson bracket.

We now discretize the equations of elastodynamics by using weak formulations of the original equations with mixed, DG or HDG methods. The resulting mappings $t \mapsto (\boldsymbol{u}_h(t), \boldsymbol{v}_h(t))$ 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.

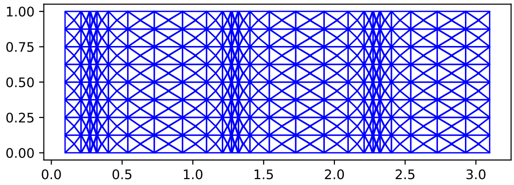
Combining the two ingredients: Elastic waves

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.

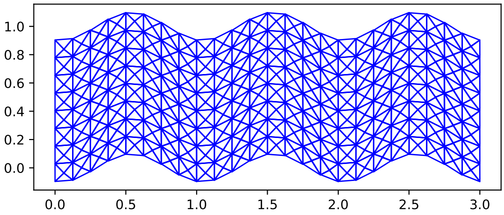
Combining the two ingredients: Elastic waves

Numerical illustration. P-wave



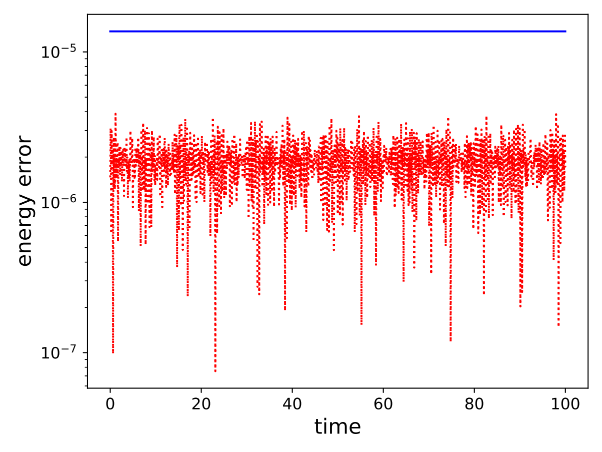
Combining the two ingredients: Elastic waves

Numerical illustration. S-wave



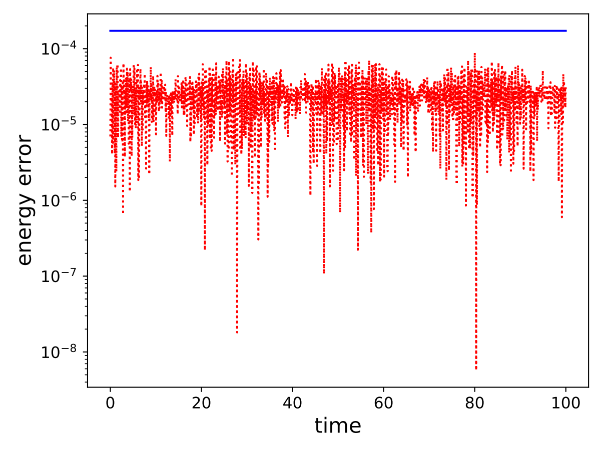
Combining the two ingredients: Elastic waves

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, 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, with Shukai Du, U. of Wisconsin-Madison.
- Large deformations.
- Nonlinear water waves.