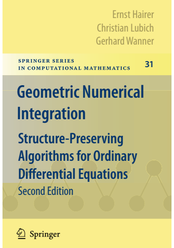
Enforcing conservation laws and dissipation inequalities numerically via auxiliary variables

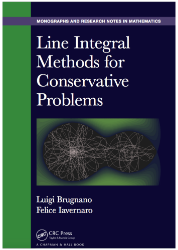
Patrick E. Farrell[1,2]   Boris Andrews[1]

[1]University of Oxford

[2]Charles University

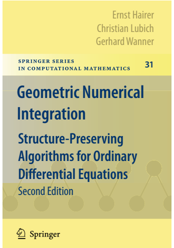
Here are four properties an initial value problem might have:

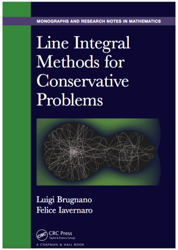




Here are four properties an initial value problem might have:

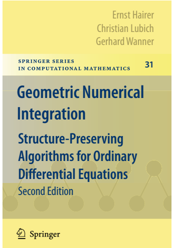
symplecticity	symmetry
conservation	dissipation

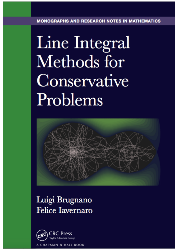




Here are four properties an initial value problem might have:

symplecticity	symmetry
conservation	dissipation



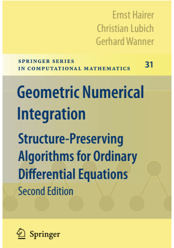


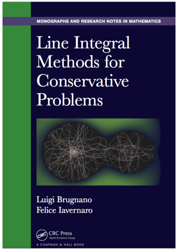
Symplecticity

The differential equation preserves the symplectic 2-form.

Here are four properties an initial value problem might have:

symplecticity	symmetry
conservation	dissipation



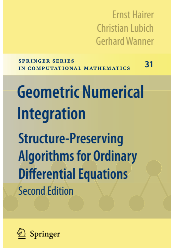


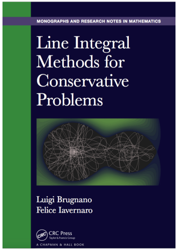
Symmetry

The system is invariant under e.g. translation, rotation, time reversal + momentum negation.

Here are four properties an initial value problem might have:

symplecticity	symmetry
conservation	dissipation



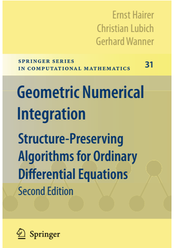


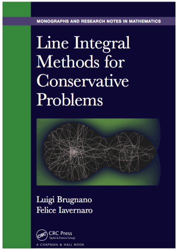
Conservation

The equation preserves invariants, like energy or angular momentum.

Here are four properties an initial value problem might have:

symplecticity	symmetry
conservation	dissipation



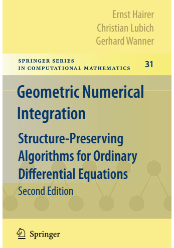


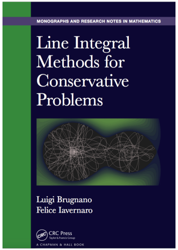
Dissipation

The equation dissipates certain quantities like entropy at a known, definite rate.

Here are four properties an initial value problem might have:

symplecticity	symmetry
conservation	**dissipation**





This talk

We aim to **preserve conservation laws and dissipation inequalities** on discretisation . . .

. . . in a symmetric way, without projections onto manifolds or Lagrange multipliers.

Section 2

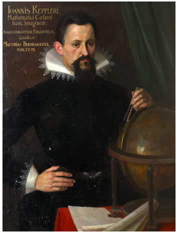
Examples

Consider the two-body Kepler problem with Hamiltonian

$$H(\mathbf{p},\mathbf{q}) = \frac{1}{2}\|\mathbf{p}\|^2 - \frac{1}{\|\mathbf{q}\|},$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p},\mathbf{q}].$$



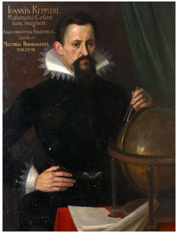
Johannes Kepler

Consider the two-body Kepler problem with Hamiltonian

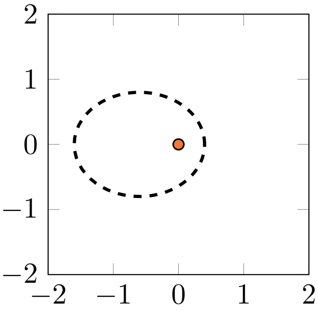
$$H(\mathbf{p},\mathbf{q}) = \frac{1}{2}\|\mathbf{p}\|^2 - \frac{1}{\|\mathbf{q}\|},$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p},\mathbf{q}].$$



Johannes Kepler



Keplerian orbits:

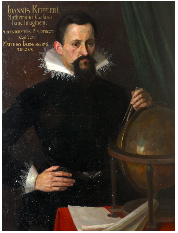
- ✓ symplecticity
- ✓ angular momentum
- ✓ energy
- ✓ orientation (LRL)

Consider the two-body Kepler problem with Hamiltonian

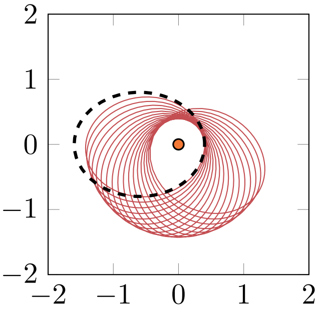
$$H(\mathbf{p}, \mathbf{q}) = \frac{1}{2}\|\mathbf{p}\|^2 - \frac{1}{\|\mathbf{q}\|},$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p}, \mathbf{q}].$$



Johannes Kepler



Implicit midpoint:

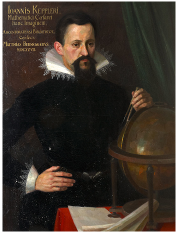
- ✓ symplecticity
- ✓ angular momentum
- ✓ energy
- ✗ orientation (LRL)

Consider the two-body Kepler problem with Hamiltonian

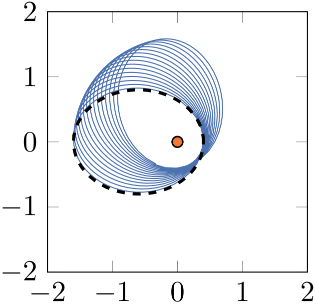
$$H(\mathbf{p},\mathbf{q}) = \frac{1}{2}\|\mathbf{p}\|^2 - \frac{1}{\|\mathbf{q}\|},$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p},\mathbf{q}].$$



Johannes Kepler



LaBudde–Greenspan:

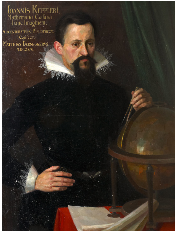
- ✗ symplecticity
- ✓ angular momentum
- ✓ energy
- ✗ orientation (LRL)

Consider the two-body Kepler problem with Hamiltonian

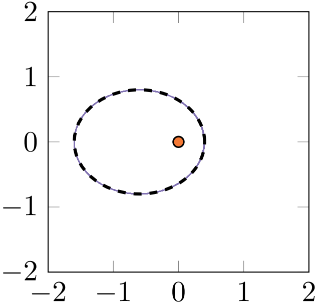
$$H(\mathbf{p},\mathbf{q}) = \frac{1}{2}\|\mathbf{p}\|^2 - \frac{1}{\|\mathbf{q}\|},$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p},\mathbf{q}].$$



Johannes Kepler



Our discretisation:

- ✗ symplecticity
- ✓ angular momentum
- ✓ energy
- ✓ orientation (LRL)

Can we do better? Can we have it all?

Jerrold Marsden

Ge Zhong

Can we do better? Can we have it all?

Theorem (Ge–Marsden, 1988)

Let H be a Hamiltonian which has no other conserved quantities in a given class, other than functions of H.

A symplectic integrator that conserves H exactly is the time advance map for the exact Hamiltonian system, up to a reparameterisation of time.

Jerrold Marsden

Ge Zhong

Can we do better? Can we have it all?

Theorem (Ge–Marsden, 1988)

Let H be a Hamiltonian which has no other conserved quantities in a given class, other than functions of H.

A symplectic integrator that conserves H exactly is the time advance map for the exact Hamiltonian system, up to a reparameterisation of time.

Jerrold Marsden

Bad news

Conservation or symplecticity, choose one.

Ge Zhong

Can we do better? Can we have it all?

Theorem (Ge–Marsden, 1988)

Let H be a Hamiltonian which has no other conserved quantities in a given class, other than functions of H.

A symplectic integrator that conserves H exactly is the time advance map for the exact Hamiltonian system, up to a reparameterisation of time.

Jerrold Marsden

Bad news

Conservation or symplecticity, choose one.

Comment

Both properties are useful in different situations!

The Kovalevskaya top is described by

$$H(\mathbf{l}, \mathbf{n}) = \frac{1}{2}\left(l_1^2 + l_2^2 + 2l_3^2\right) + n_1,$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & \mathrm{skew}(\mathbf{n}) \\ \mathrm{skew}(\mathbf{n}) & \mathrm{skew}(\mathbf{l}) \end{bmatrix}, \quad \mathbf{x} = [\mathbf{n}, \mathbf{l}].$$

Sofya Kovalevskaya

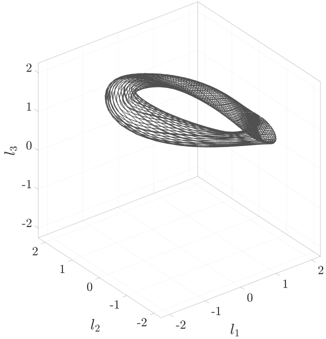
The Kovalevskaya top is described by

$$H(\mathbf{l}, \mathbf{n}) = \frac{1}{2}\left(l_1^2 + l_2^2 + 2l_3^2\right) + n_1,$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & \mathrm{skew}(\mathbf{n}) \\ \mathrm{skew}(\mathbf{n}) & \mathrm{skew}(\mathbf{l}) \end{bmatrix}, \quad \mathbf{x} = [\mathbf{n}, \mathbf{l}].$$

Sofya Kovalevskaya



Kovalevskaya trajectories:

- ✓ symplecticity
- ✓ angular momentum
- ✓ energy
- ✓ orientation
- ✓ Kovalevskaya invariant

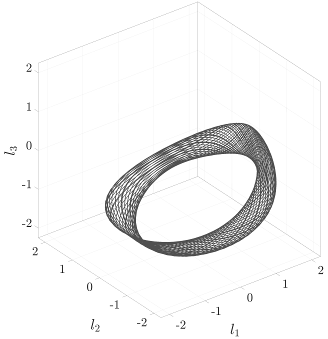
The Kovalevskaya top is described by

$$H(\mathbf{l}, \mathbf{n}) = \frac{1}{2}\left(l_1^2 + l_2^2 + 2l_3^2\right) + n_1,$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & \mathrm{skew}(\mathbf{n}) \\ \mathrm{skew}(\mathbf{n}) & \mathrm{skew}(\mathbf{l}) \end{bmatrix}, \quad \mathbf{x} = [\mathbf{n}, \mathbf{l}].$$

Sofya Kovalevskaya



Kovalevskaya trajectories:

- ✓ symplecticity
- ✓ angular momentum
- ✓ energy
- ✓ orientation
- ✓ Kovalevskaya invariant

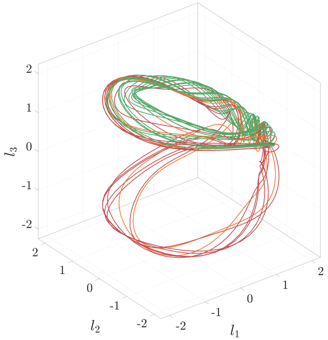
The Kovalevskaya top is described by

$$H(\mathbf{l},\mathbf{n}) = \frac{1}{2}\left(l_1^2 + l_2^2 + 2l_3^2\right) + n_1,$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & \mathrm{skew}(\mathbf{n}) \\ \mathrm{skew}(\mathbf{n}) & \mathrm{skew}(\mathbf{l}) \end{bmatrix}, \quad \mathbf{x} = [\mathbf{n}, \mathbf{l}].$$

Sofya Kovalevskaya



Implicit midpoint:

- ✓ symplecticity
- ✓ angular momentum
- ✓ energy
- ✓ orientation
- ✗ Kovalevskaya invariant

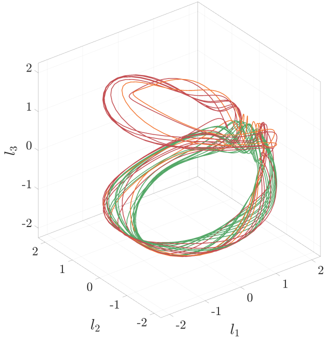
The Kovalevskaya top is described by

$$H(\mathbf{l}, \mathbf{n}) = \frac{1}{2}\left(l_1^2 + l_2^2 + 2l_3^2\right) + n_1,$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & \mathrm{skew}(\mathbf{n}) \\ \mathrm{skew}(\mathbf{n}) & \mathrm{skew}(\mathbf{l}) \end{bmatrix}, \quad \mathbf{x} = [\mathbf{n}, \mathbf{l}].$$

Sofya Kovalevskaya



Implicit midpoint:

- ✓ symplecticity
- ✓ angular momentum
- ✓ energy
- ✓ orientation
- ✗ Kovalevskaya invariant

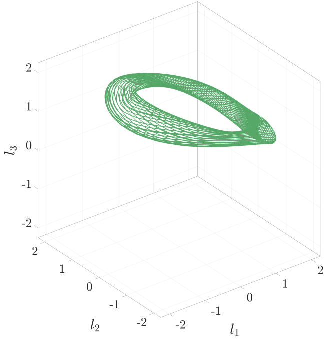
The Kovalevskaya top is described by

$$H(\mathbf{l}, \mathbf{n}) = \frac{1}{2}\left(l_1^2 + l_2^2 + 2l_3^2\right) + n_1,$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & \operatorname{skew}(\mathbf{n}) \\ \operatorname{skew}(\mathbf{n}) & \operatorname{skew}(\mathbf{l}) \end{bmatrix}, \quad \mathbf{x} = [\mathbf{n}, \mathbf{l}].$$

Sofya Kovalevskaya



Our discretisation:

- ✗ symplecticity
- ✓ angular momentum
- ✓ energy
- ✓ orientation
- ✓ Kovalevskaya invariant

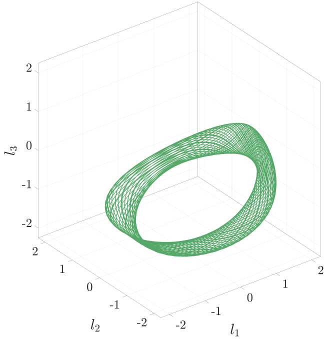
The Kovalevskaya top is described by

$$H(\mathbf{l},\mathbf{n}) = \frac{1}{2}\left(l_1^2 + l_2^2 + 2l_3^2\right) + n_1,$$

inducing the differential equations

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & \mathrm{skew}(\mathbf{n}) \\ \mathrm{skew}(\mathbf{n}) & \mathrm{skew}(\mathbf{l}) \end{bmatrix}, \quad \mathbf{x} = [\mathbf{n}, \mathbf{l}].$$

Sofya Kovalevskaya



Our discretisation:

- ✗ symplecticity
- ✓ angular momentum
- ✓ energy
- ✓ orientation
- ✓ Kovalevskaya invariant

This approach extends to more complicated problems.

For the compressible Navier–Stokes equations, we can devise timestepping schemes that:

- conserve mass;

This approach extends to more complicated problems.

For the compressible Navier–Stokes equations, we can devise timestepping schemes that:

- conserve mass;
- conserve momentum;

This approach extends to more complicated problems.

For the compressible Navier–Stokes equations, we can devise timestepping schemes that:

- conserve mass;
- conserve momentum;
- conserve energy;

This approach extends to more complicated problems.

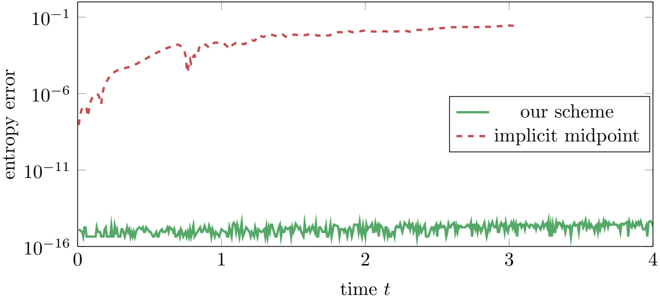
For the compressible Navier–Stokes equations, we can devise timestepping schemes that:

- conserve mass;
- conserve momentum;
- conserve energy;
- dissipate entropy.

This approach extends to more complicated problems.

For the compressible Navier–Stokes equations, we can devise timestepping schemes that:

- conserve mass;
- conserve momentum;
- conserve energy;
- dissipate entropy.



Error in the entropy for implicit midpoint and our scheme.

Section 3

How it works

Our approach is to take a variational formulation in time.

Our approach is to take a variational formulation in time.

Potential confusion

This does **not** require solving for all timesteps at once; we're still timestepping.

Our approach is to take a variational formulation in time.

Potential confusion

This does **not** require solving for all timesteps at once; we're still timestepping.

To understand this variational viewpoint, let's first study general methods for solving

$$\dot{u} = f(u).$$

We know $u = u_n$ at $t = t_n$. We want to compute u_{n+1} at $t = t_{n+1}$.

We know $u = u_n$ at $t = t_n$. We want to compute u_{n+1} at $t = t_{n+1}$.

General idea of many (single-step) schemes

Find $u \in P^s(t_n, t_{n+1})$, the space of degree-s polynomials on $[t_n, t_{n+1}]$, satisfying

$$u(t_n) = u_n,$$

and s other *test conditions*.

Set $u_{n+1} = u(t_{n+1})$.

We know $u = u_n$ at $t = t_n$. We want to compute u_{n+1} at $t = t_{n+1}$.

General idea of many (single-step) schemes

Find $u \in P^s(t_n, t_{n+1})$, the space of degree-s polynomials on $[t_n, t_{n+1}]$, satisfying

$$u(t_n) = u_n,$$

and s other *test conditions*.

Set $u_{n+1} = u(t_{n+1})$.

Forward Euler

For $s = 1$, demand that

$$\dot{u} = f(u)$$

at the test point $t = t_n$.

We know $u = u_n$ at $t = t_n$. We want to compute u_{n+1} at $t = t_{n+1}$.

General idea of many (single-step) schemes

Find $u \in P^s(t_n, t_{n+1})$, the space of degree-s polynomials on $[t_n, t_{n+1}]$, satisfying

$$u(t_n) = u_n,$$

and s other *test conditions*.

Set $u_{n+1} = u(t_{n+1})$.

Backward Euler

For $s = 1$, demand that

$$\dot{u} = f(u)$$

at the test point $t = t_{n+1}$.

We know $u = u_n$ at $t = t_n$. We want to compute u_{n+1} at $t = t_{n+1}$.

General idea of many (single-step) schemes

Find $u \in P^s(t_n, t_{n+1})$, the space of degree-s polynomials on $[t_n, t_{n+1}]$, satisfying

$$u(t_n) = u_n,$$

and s other *test conditions*.

Set $u_{n+1} = u(t_{n+1})$.

Implicit midpoint

For $s = 1$, demand that

$$\dot{u} = f(u)$$

at the $s = 1$ test point $t = \frac{1}{2}t_n + \frac{1}{2}t_{n+1}$.

Of course, not all schemes use $s = 1$:

Collocation Runge–Kutta, e.g. Gauss–Legendre/RadauIIA/LobattoIIIC

Demand that

$$\dot{u} = f(u)$$

at s test points $t = t_n + c_1\Delta t, t_n + c_2\Delta t, \ldots, t_n + c_s\Delta t$.

Of course, not all schemes use $s = 1$:

Collocation Runge–Kutta, e.g. Gauss–Legendre/RadauIIA/LobattoIIIC

Demand that

$$\dot{u} = f(u)$$

at s test points $t = t_n + c_1 \Delta t, t_n + c_2 \Delta t, \ldots, t_n + c_s \Delta t$.

The natural finite element in time scheme instead chooses another test set:

Continuous Petrov–Galerkin (cPG) test conditions

Demand that

$$\int_{t_n}^{t_{n+1}} \dot{u} v \ \mathrm{d}t = \int_{t_n}^{t_{n+1}} f(u) v \ \mathrm{d}t,$$

for all $v \in P^{s-1}(t_n, t_{n+1}) \quad (= \dot{P}_s)$.

Why is this variational viewpoint useful?

Why is this variational viewpoint useful?

Conservation laws

Conservation laws naturally arise from variational statements:

$$0 = J(u_{n+1}) - J(u_n)$$

Why is this variational viewpoint useful?

Conservation laws

Conservation laws naturally arise from variational statements:

$$
\begin{aligned}
0 &= J(u_{n+1}) - J(u_n) \\
&= \int_{t_n}^{t_{n+1}} \frac{\mathrm{d}J}{\mathrm{d}t} \, \mathrm{d}t
\end{aligned}
$$

Why is this variational viewpoint useful?

Conservation laws

Conservation laws naturally arise from variational statements:

$$
\begin{aligned}
0 &= J(u_{n+1}) - J(u_n) \\
&= \int_{t_n}^{t_{n+1}} \frac{\mathrm{d}J}{\mathrm{d}t} \, \mathrm{d}t \\
&= \int_{t_n}^{t_{n+1}} J'(u)\dot{u} \, \mathrm{d}t
\end{aligned}
$$

Why is this variational viewpoint useful?

Conservation laws

Conservation laws naturally arise from variational statements:

$$
\begin{aligned}
0 &= J(u_{n+1}) - J(u_n) \\
&= \int_{t_n}^{t_{n+1}} \frac{\mathrm{d}J}{\mathrm{d}t} \, \mathrm{d}t \\
&= \int_{t_n}^{t_{n+1}} J'(u)\dot{u} \, \mathrm{d}t \\
&= \int_{t_n}^{t_{n+1}} J'(u)f(u) \, \mathrm{d}t.
\end{aligned}
$$

Why is this variational viewpoint useful?

Conservation laws

Conservation laws naturally arise from variational statements:

$$\begin{aligned}
0 &= J(u_{n+1}) - J(u_n) \\
&= \int_{t_n}^{t_{n+1}} \frac{\mathrm{d}J}{\mathrm{d}t} \, \mathrm{d}t \\
&= \int_{t_n}^{t_{n+1}} J'(u)\dot{u} \, \mathrm{d}t \\
&= \int_{t_n}^{t_{n+1}} J'(u) f(u) \, \mathrm{d}t.
\end{aligned}$$

In other words, each conservation law has an

associated test function.

Why is this variational viewpoint useful?

Dissipation inequalities

Dissipation inequalities naturally arise from variational statements:

$$0 \leq J(u_{n+1}) - J(u_n)$$

Why is this variational viewpoint useful?

Dissipation inequalities

Dissipation inequalities naturally arise from variational statements:

$$
\begin{aligned}
0 \leq J(u_{n+1}) - J(u_n) \\
&= \int_{t_n}^{t_{n+1}} \frac{\mathrm{d}J}{\mathrm{d}t} \,\mathrm{d}t \\
&= \int_{t_n}^{t_{n+1}} J'(u)\dot{u} \,\mathrm{d}t \\
&= \int_{t_n}^{t_{n+1}} J'(u)f(u) \,\mathrm{d}t.
\end{aligned}
$$

In other words, each dissipation inequality has an

associated test function.

Good news!

If $J'(u)$ is in our test set, the cPG scheme also conserves/dissipates J.

Good news!

If $J'(u)$ is in our test set, the cPG scheme also conserves/dissipates J.

Bad news!

$J'(u)$ is rarely in our test set $P^{s-1}(t_n, t_{n+1})$.

Good news!

If $J'(u)$ is in our test set, the cPG scheme also conserves/dissipates J.

Bad news!

$J'(u)$ is rarely in our test set $P^{s-1}(t_n, t_{n+1})$.

Idea!

Compute an **approximation**

$$\widetilde{J'(u)} \approx J'(u), \quad \widetilde{J'(u)} \in P^{s-1}(t_n, t_{n+1}).$$

and modify the differential equation to use it.

Basic outline:

Basic outline:

A. Choose a base timestepping scheme.

Basic outline:

A. Choose a base timestepping scheme.

B. Identify the associated test functions for the structures to preserve.

Basic outline:

A. Choose a base timestepping scheme.

B. Identify the associated test functions for the structures to preserve.

C. Introduce corresponding auxiliary variables.

Basic outline:

A. Choose a base timestepping scheme.

B. Identify the associated test functions for the structures to preserve.

C. Introduce corresponding auxiliary variables.

D. Modify the right-hand side of the weak formulation to use them.

Section 4

Navier–Stokes equations

To fix ideas, consider the incompressible Navier–Stokes equations in Lamb form:

$$\begin{aligned} \dot{u} &= u \times (\nabla \times u) - \nabla p + \mathrm{Re}^{-1} \nabla^2 u, \\ 0 &= \nabla \cdot u, \end{aligned}$$

on a bounded Lipschitz domain $\Omega \subset \mathbb{R}^3$ with $u = 0$ on $\partial\Omega$.

Horace Lamb

To fix ideas, consider the incompressible Navier–Stokes equations in Lamb form:

$$\begin{aligned} \dot{u} &= u \times (\nabla \times u) - \nabla p + \mathrm{Re}^{-1} \nabla^2 u, \\ 0 &= \nabla \cdot u, \end{aligned}$$

on a bounded Lipschitz domain $\Omega \subset \mathbb{R}^3$ with $u = 0$ on $\partial\Omega$.

Horace Lamb

A. Define the cPG discretisation

For suitable space-time $\mathbb{X}$, the cPG discretisation is to find $u \in \mathbb{X}$ such that

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v) \ \mathrm{d}t = \int_{t_n}^{t_{n+1}} \left[(u \times (\nabla \times u), v) - \mathrm{Re}^{-1} (\nabla u, \nabla v) \right] \ \mathrm{d}t$$

for all $v \in \dot{\mathbb{X}}$.

To fix ideas, consider the incompressible Navier–Stokes equations in Lamb form:

$$\begin{aligned} \dot{u} &= u \times (\nabla \times u) - \nabla p + \mathrm{Re}^{-1}\nabla^2 u, \\ 0 &= \nabla \cdot u, \end{aligned}$$

on a bounded Lipschitz domain $\Omega \subset \mathbb{R}^3$ with $u = 0$ on $\partial\Omega$.

Horace Lamb

A. Define the cPG discretisation

For suitable space-time $\mathbb{X}$, the cPG discretisation is to find $u \in \mathbb{X}$ such that

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v) \ \mathrm{d}t = \int_{t_n}^{t_{n+1}} \left[(u \times (\nabla \times u), v) - \mathrm{Re}^{-1} (\nabla u, \nabla v) \right] \ \mathrm{d}t$$

for all $v \in \dot{\mathbb{X}}$.

Here $\mathbb{X}$ is continuous in time of degree s, while $\dot{\mathbb{X}}$ is discontinuous in time of degree $s - 1$.

Our next task is to identify the structures we wish to preserve.

Our next task is to identify the structures we wish to preserve.

In this example, we care about the dissipation of energy

$$E(u) = \frac{1}{2}(u, u)$$

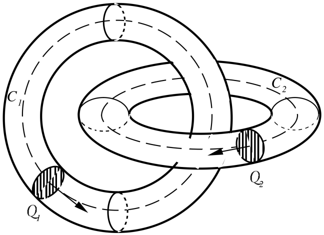
Our next task is to identify the structures we wish to preserve.

In this example, we care about the dissipation of energy

$$E(u) = \frac{1}{2}(u, u)$$

and the change in *helicity*, a topological measure of the knottedness of the flow,

$$H(u) = \frac{1}{2}(u, \nabla \times u).$$



From Arnold & Khesin (1998).

Vladimir Arnold

The energy is given by

$$E(u) = \frac{1}{2}(u, u),$$

so its associated test function is the L^2 Riesz representative of its Fréchet derivative

$$E_u(u; z) = (u, z),$$

i.e. the special test function is the velocity u itself:

The energy is given by

$$E(u) = \frac{1}{2}(u, u),$$

so its associated test function is the L^2 Riesz representative of its Fréchet derivative

$$E_u(u; z) = (u, z),$$

i.e. the special test function is the velocity u itself:

$$E(u_{n+1}) - E(u_n) = \int_{t_n}^{t_{n+1}} (\dot{u}, u) \, \mathrm{d}t$$

The energy is given by

$$E(u) = \frac{1}{2}(u, u),$$

so its associated test function is the L^2 Riesz representative of its Fréchet derivative

$$E_u(u; z) = (u, z),$$

i.e. the special test function is the velocity u itself:

$$\begin{aligned} E(u_{n+1}) - E(u_n) &= \int_{t_n}^{t_{n+1}} (\dot{u}, u) \ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \left[(u \times (\nabla \times u), u) - \mathrm{Re}^{-1}(\nabla u, \nabla u)\right] \ \mathrm{d}t, \end{aligned}$$

The energy is given by

$$E(u) = \frac{1}{2}(u, u),$$

so its associated test function is the L^2 Riesz representative of its Fréchet derivative

$$E_u(u; z) = (u, z),$$

i.e. the special test function is the velocity u itself:

$$\begin{aligned} E(u_{n+1}) - E(u_n) &= \int_{t_n}^{t_{n+1}} (\dot{u}, u)\ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \left[(u \times (\nabla \times u), u) - \mathrm{Re}^{-1}(\nabla u, \nabla u)\right]\ \mathrm{d}t, \\ &= -\mathrm{Re}^{-1} \int_{t_n}^{t_{n+1}} \|\nabla u\|^2\ \mathrm{d}t \leq 0. \end{aligned}$$

Similarly, we derive a law for the helicity

$$H(u) = \frac{1}{2}(u, \nabla \times u)$$

by testing our weak formulation with the L^2 Riesz representative of its Fréchet derivative

$$H_u(u; z) = (\nabla \times u, z),$$

i.e. the special test function is the vorticity $\nabla \times u$:

Similarly, we derive a law for the helicity

$$H(u) = \frac{1}{2}(u, \nabla \times u)$$

by testing our weak formulation with the L^2 Riesz representative of its Fréchet derivative

$$H_u(u; z) = (\nabla \times u, z),$$

i.e. the special test function is the vorticity $\nabla \times u$:

$$H(u_{n+1}) - H(u_n) = \int_{t_n}^{t_{n+1}} (\dot{u}, \nabla \times u) \, \mathrm{d}t$$

Similarly, we derive a law for the helicity

$$H(u) = \frac{1}{2}(u, \nabla \times u)$$

by testing our weak formulation with the L^2 Riesz representative of its Fréchet derivative

$$H_u(u; z) = (\nabla \times u, z),$$

i.e. the special test function is the vorticity $\nabla \times u$:

$$\begin{aligned} H(u_{n+1}) - H(u_n) &= \int_{t_n}^{t_{n+1}} (\dot{u}, \nabla \times u) \, \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \left[(u \times (\nabla \times u), \nabla \times u) - \mathrm{Re}^{-1}(\nabla u, \nabla \nabla \times u) \right] \, \mathrm{d}t, \end{aligned}$$

Similarly, we derive a law for the helicity

$$H(u) = \frac{1}{2}(u, \nabla \times u)$$

by testing our weak formulation with the L^2 Riesz representative of its Fréchet derivative

$$H_u(u; z) = (\nabla \times u, z),$$

i.e. the special test function is the vorticity $\nabla \times u$:

$$\begin{aligned} H(u_{n+1}) - H(u_n) &= \int_{t_n}^{t_{n+1}} (\dot{u}, \nabla \times u) \,\mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \left[(u \times (\nabla \times u), \nabla \times u) - \mathrm{Re}^{-1}(\nabla u, \nabla\nabla \times u)\right] \,\mathrm{d}t, \\ &= -\mathrm{Re}^{-1} \int_{t_n}^{t_{n+1}} (\nabla u, \nabla\nabla \times u) \,\mathrm{d}t. \end{aligned}$$

B. Identify test functions

To replicate these laws discretely, we need approximations of

$$u \text{ and } \nabla \times u$$

in our discrete test space $\dot{\mathbb{X}}$.

Our next step is to introduce variables approximating these associated test functions.

Our next step is to introduce variables approximating these associated test functions.

C. Introduce auxiliary variables

Find $(u, w_1, w_2) \in \mathbb{X} \times \dot{\mathbb{X}} \times \dot{\mathbb{X}}$ such that

$$\begin{aligned}
\int_{t_n}^{t_{n+1}} (\dot{u}, v) \ \mathrm{d}t &= \int_{t_n}^{t_{n+1}} \left[(u \times (\nabla \times u), v) - \mathrm{Re}^{-1}(\nabla u, \nabla v)\right] \ \mathrm{d}t, \\
\int_{t_n}^{t_{n+1}} (w_1, v_1) \ \mathrm{d}t &= \int_{t_n}^{t_{n+1}} (u, v_1) \ \mathrm{d}t, \\
\int_{t_n}^{t_{n+1}} (w_2, v_2) \ \mathrm{d}t &= \int_{t_n}^{t_{n+1}} (\nabla \times u, v_2) \ \mathrm{d}t,
\end{aligned}$$

for all $(v, v_1, v_2) \in \dot{\mathbb{X}} \times \dot{\mathbb{X}} \times \dot{\mathbb{X}}$.

In order to derive a discrete version of the laws for energy and helicity, we must modify the right-hand side of our problem to use w_1 and w_2.

In order to derive a discrete version of the laws for energy and helicity, we must modify the right-hand side of our problem to use w_1 and w_2.

D. Final time discretisation

Find $(u, w_1, w_2) \in \mathbb{X} \times \dot{\mathbb{X}} \times \dot{\mathbb{X}}$ such that

$$\begin{aligned}
\int_{t_n}^{t_{n+1}} (\dot{u}, v) \, \mathrm{d}t &= \int_{t_n}^{t_{n+1}} \left[(\underline{w_1 \times w_2}, v) - \mathrm{Re}^{-1} (\nabla \underline{w_1}, \nabla v) \right] \, \mathrm{d}t, \\
\int_{t_n}^{t_{n+1}} (w_1, v_1) \, \mathrm{d}t &= \int_{t_n}^{t_{n+1}} (u, v_1) \, \mathrm{d}t, \\
\int_{t_n}^{t_{n+1}} (w_2, v_2) \, \mathrm{d}t &= \int_{t_n}^{t_{n+1}} (\nabla \times u, v_2) \, \mathrm{d}t,
\end{aligned}$$

for all $(v, v_1, v_2) \in \dot{\mathbb{X}} \times \dot{\mathbb{X}} \times \dot{\mathbb{X}}$.

This allows us to replicate the energy and helicity laws discretely!

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\begin{aligned}
\int_{t_n}^{t_{n+1}} (\dot{u}, v) \, \mathrm{d}t &= \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1} (\nabla w_1, \nabla v) \right] \, \mathrm{d}t, \\
\int_{t_n}^{t_{n+1}} (w_1, v_1) \, \mathrm{d}t &= \int_{t_n}^{t_{n+1}} (u, v_1) \, \mathrm{d}t.
\end{aligned}$$

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v) \ \mathrm{d}t = \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right] \ \mathrm{d}t,$$

$$\int_{t_n}^{t_{n+1}} (w_1, v_1) \ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (u, v_1) \ \mathrm{d}t.$$

$$E(u_{n+1}) - E(u_n) = \int_{t_n}^{t_{n+1}} (\dot{u}, u) \ \mathrm{d}t$$

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v)\ \mathrm{d}t \ = \ \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right]\ \mathrm{d}t,$$

$$\int_{t_n}^{t_{n+1}} (w_1, v_1)\ \mathrm{d}t \ = \ \int_{t_n}^{t_{n+1}} (u, v_1)\ \mathrm{d}t.$$

$$E(u_{n+1}) - E(u_n) = \int_{t_n}^{t_{n+1}} (\dot{u}, u)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (\dot{u}, w_1)\ \mathrm{d}t$$

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v) \ \mathrm{d}t \ = \ \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right] \ \mathrm{d}t,$$

$$\int_{t_n}^{t_{n+1}} (w_1, v_1) \ \mathrm{d}t \ = \ \int_{t_n}^{t_{n+1}} (u, v_1) \ \mathrm{d}t.$$

$$\begin{aligned} E(u_{n+1}) - E(u_n) &= \int_{t_n}^{t_{n+1}} (\dot{u}, u) \ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (\dot{u}, w_1) \ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, w_1) - \mathrm{Re}^{-1}(\nabla w_1, \nabla w_1)\right] \ \mathrm{d}t, \end{aligned}$$

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\begin{aligned}
\int_{t_n}^{t_{n+1}} (\dot{u}, v) \,\mathrm{d}t &= \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right] \,\mathrm{d}t, \\
\int_{t_n}^{t_{n+1}} (w_1, v_1) \,\mathrm{d}t &= \int_{t_n}^{t_{n+1}} (u, v_1) \,\mathrm{d}t.
\end{aligned}$$

$$\begin{aligned}
E(u_{n+1}) - E(u_n) &= \int_{t_n}^{t_{n+1}} (\dot{u}, u) \,\mathrm{d}t = \int_{t_n}^{t_{n+1}} (\dot{u}, w_1) \,\mathrm{d}t \\
&= \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, w_1) - \mathrm{Re}^{-1}(\nabla w_1, \nabla w_1)\right] \,\mathrm{d}t, \\
&= -\mathrm{Re}^{-1} \int_{t_n}^{t_{n+1}} \|\nabla w_1\|^2 \,\mathrm{d}t \leq 0.
\end{aligned}$$

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right]\ \mathrm{d}t,$$
$$\int_{t_n}^{t_{n+1}} (w_1, v_1)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (u, v_1)\ \mathrm{d}t.$$

$$\begin{aligned} E(u_{n+1}) - E(u_n) &= \int_{t_n}^{t_{n+1}} (\dot{u}, u)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (\dot{u}, w_1)\ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, w_1) - \mathrm{Re}^{-1}(\nabla w_1, \nabla w_1)\right]\ \mathrm{d}t, \\ &= -\ \mathrm{Re}^{-1} \int_{t_n}^{t_{n+1}} \|\nabla w_1\|^2\ \mathrm{d}t \le 0. \end{aligned}$$

We therefore recover a conservation law in the ideal limit.

This allows us to replicate the energy and helicity laws discretely!

,

,

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right]\ \mathrm{d}t,$$

$$\int_{t_n}^{t_{n+1}} (w_2, v_2)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (\nabla \times u, v_2)\ \mathrm{d}t.$$

,

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\begin{aligned}
\int_{t_n}^{t_{n+1}} (\dot{u}, v)\ \mathrm{d}t &= \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right]\ \mathrm{d}t, \\
\int_{t_n}^{t_{n+1}} (w_2, v_2)\ \mathrm{d}t &= \int_{t_n}^{t_{n+1}} (\nabla \times u, v_2)\ \mathrm{d}t.
\end{aligned}$$

$$H(u_{n+1}) - H(u_n) = \int_{t_n}^{t_{n+1}} (\dot{u}, \nabla \times u)\ \mathrm{d}t$$

,

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v)\ \mathrm{d}t \ = \ \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right]\ \mathrm{d}t,$$

$$\int_{t_n}^{t_{n+1}} (w_2, v_2)\ \mathrm{d}t \ = \ \int_{t_n}^{t_{n+1}} (\nabla \times u, v_2)\ \mathrm{d}t.$$

$$H(u_{n+1}) - H(u_n) = \int_{t_n}^{t_{n+1}} (\dot{u}, \nabla \times u)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (\dot{u}, w_2)\ \mathrm{d}t$$

,

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right]\ \mathrm{d}t,$$

$$\int_{t_n}^{t_{n+1}} (w_2, v_2)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (\nabla \times u, v_2)\ \mathrm{d}t.$$

$$\begin{aligned} H(u_{n+1}) - H(u_n) &= \int_{t_n}^{t_{n+1}} (\dot{u}, \nabla \times u)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (\dot{u}, w_2)\ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, w_2) - \mathrm{Re}^{-1}(\nabla w_1, \nabla w_2)\right]\ \mathrm{d}t, \end{aligned}$$

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right]\ \mathrm{d}t,$$

$$\int_{t_n}^{t_{n+1}} (w_2, v_2)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (\nabla \times u, v_2)\ \mathrm{d}t.$$

$$\begin{aligned} H(u_{n+1}) - H(u_n) &= \int_{t_n}^{t_{n+1}} (\dot{u}, \nabla \times u)\ \mathrm{d}t = \int_{t_n}^{t_{n+1}} (\dot{u}, w_2)\ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, w_2) - \mathrm{Re}^{-1}(\nabla w_1, \nabla w_2)\right]\ \mathrm{d}t, \\ &= -\mathrm{Re}^{-1} \int_{t_n}^{t_{n+1}} (\nabla w_1, \nabla w_2)\ \mathrm{d}t. \end{aligned}$$

This allows us to replicate the energy and helicity laws discretely!

D. Final time discretisation

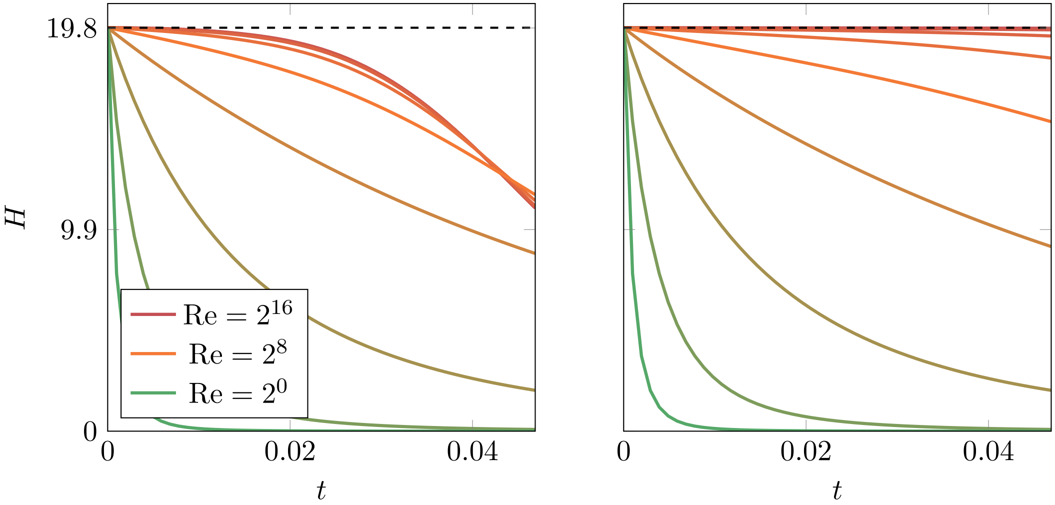
$$\begin{aligned}
\int_{t_n}^{t_{n+1}} (\dot{u}, v)\ \mathrm{d}t &= \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, v) - \mathrm{Re}^{-1}(\nabla w_1, \nabla v)\right]\ \mathrm{d}t, \\
\int_{t_n}^{t_{n+1}} (w_2, v_2)\ \mathrm{d}t &= \int_{t_n}^{t_{n+1}} (\nabla \times u, v_2)\ \mathrm{d}t.
\end{aligned}$$

$$\begin{aligned}
H(u_{n+1}) - H(u_n) = \int_{t_n}^{t_{n+1}} (\dot{u}, \nabla \times u)\ \mathrm{d}t &= \int_{t_n}^{t_{n+1}} (\dot{u}, w_2)\ \mathrm{d}t \\
&= \int_{t_n}^{t_{n+1}} \left[(w_1 \times w_2, w_2) - \mathrm{Re}^{-1}(\nabla w_1, \nabla w_2)\right]\ \mathrm{d}t, \\
&= -\mathrm{Re}^{-1} \int_{t_n}^{t_{n+1}} (\nabla w_1, \nabla w_2)\ \mathrm{d}t.
\end{aligned}$$

We again recover a conservation law in the ideal limit.

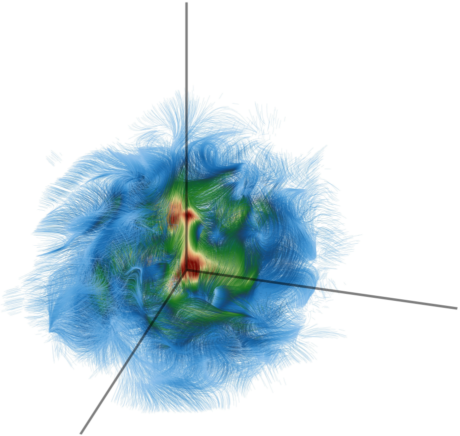
Does helicity preservation matter?

Does helicity preservation matter?

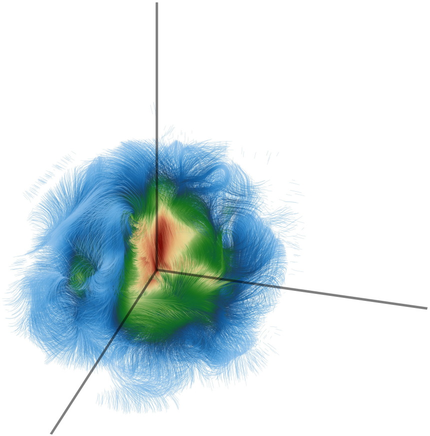


preserving E | preserving E, H

Does helicity preservation matter?



preserving E



preserving E, H

Streamlines of velocity at final time, coloured by $\|u\|$.

Good news

The auxiliary velocity can be computed explicitly.

Good news

The auxiliary velocity can be computed explicitly.

Leo Rebholz

This analysis gives an arbitrary-order generalisation of

L. G. Rebholz. "An energy- and helicity-conserving finite element scheme for the Navier–Stokes equations". In: *SIAM Journal on Numerical Analysis* 45.4 (2007), pp. 1622–1638. DOI: 10.1137/060651227.

In fact, our scheme generalises . . .

French & Schaeffer (1990)

cPG sometimes conservative; proposes auxiliary variable for energy conservation in KdV.

Continuous Finite Element Methods Which Preserve Energy Properties for Nonlinear Problems

Donald A. French* and Jack W. Schaeffer†

Department of Mathematics
Carnegie Mellon University
Pittsburgh, Pennsylvania 15213-3890

Transmitted by Melvin R. Scott

In fact, our scheme generalises . . .

Simo & Armero (1994)

Energy-dissipating timestepping schemes for Navier–Stokes.

Unconditional stability and long-term behavior of transient algorithms for the incompressible Navier–Stokes and Euler equations*

J.C. Simo and F. Armero

Division of Applied Mechanics, Department of Mechanical Engineering, Stanford University, Stanford, CA 94305, USA

Received 8 October 1992
Revised manuscript received 14 April 1993

In fact, our scheme generalises . . .

McLachlan, Quispel & Robidoux (1999)

Lowest-order energy-conserving discrete gradient schemes.

Geometric integration using discrete gradients

By Robert I. McLachlan[1], G. R. W. Quispel[2] and Nicolas Robidoux[1]

[1] *Mathematics Department, Massey University, Palmerston North, New Zealand*
[2] *Faculty of Science, LaTrobe University, Bundoora, Melbourne 3083, Australia*

This paper discusses the discrete analogue of the gradient of a function and shows how discrete gradients can be used in the numerical integration of ordinary differential equations (ODEs). Given an ODE and one or more first integrals (i.e. constants of the motion) and/or Lyapunov functions, it is shown that the ODE can be rewritten as a 'linear-gradient system'. Discrete gradients are used to construct discrete approximations to the ODE which preserve the first integrals and Lyapunov functions exactly. The method applies to all Hamiltonian, Poisson and gradient systems, and also to many dissipative systems (those with a known first integral or Lyapunov function).

In fact, our scheme generalises . . .

Betsch & Steinmann (2000)

cPG is energy-conservative for Hamiltonian ODEs in canonical coordinates.

Inherently Energy Conserving Time Finite Elements for Classical Mechanics

P. Betsch* and P. Steinmann†

Department of Mechanical Engineering, University of Kaiserslautern, Postfach 3049, 67653 Kaiserslautern, Germany

E-mail: *pbetsch@rhrk.uni-kl.de and †ps@rhrk.uni-kl.de

Received October 27, 1998; revised November 24, 1999

In fact, our scheme generalises . . .

Cohen & Hairer (2011)

Higher-order energy-conserving discrete gradient schemes.

Linear energy-preserving integrators for Poisson systems

David Cohen · Ernst Hairer

Received: 25 April 2010 / Accepted: 6 January 2011 / Published online: 20 January 2011

In fact, our scheme generalises . . .

Egger, Habrich & Shashkov (2021)

cPG is energy-conservative for a particular formulation of Hamiltonian PDEs.

DE GRUYTER Comput. Methods Appl. Math. 2021; 21(2): 335–349

Research Article

Herbert Egger*, Oliver Habrich and Vsevolod Shashkov

On the Energy Stable Approximation of Hamiltonian and Gradient Systems

https://doi.org/10.1515/cmam-2020-0025
Received February 29, 2020; revised August 27, 2020; accepted November 16, 2020

In fact, our scheme generalises . . .

. . . and many more besides.

For the compressible Navier–Stokes equations,

$$
\begin{aligned}
\dot{\rho} &= -\mathrm{div}[\rho u], \\
\rho \dot{u} &= -\rho u \cdot \nabla u - \nabla[\rho\theta] + \frac{2}{\mathrm{Re}_\mu}\mathrm{div}[\rho\varepsilon[u]] + \frac{1}{\mathrm{Re}_\zeta}\nabla[\rho \mathrm{div} u], \\
C\rho\dot{\theta} &= -C\rho u \cdot \nabla\theta - \rho\theta \mathrm{div} u + \frac{1}{\mathrm{Pe}}\mathrm{div}[\rho\nabla\theta] + \frac{2}{\mathrm{Re}_\mu}\rho\|\varepsilon[u]\|^2 + \frac{1}{\mathrm{Re}_\zeta}\rho(\mathrm{div} u)^2,
\end{aligned}
$$

For the compressible Navier–Stokes equations,

$$\begin{aligned}
\dot{\rho} &= -\mathrm{div}[\rho u], \\
\rho\dot{u} &= -\rho u \cdot \nabla u - \nabla[\rho\theta] + \frac{2}{\mathrm{Re}_\mu}\mathrm{div}[\rho\varepsilon[u]] + \frac{1}{\mathrm{Re}_\zeta}\nabla[\rho\mathrm{div}u], \\
C\rho\dot{\theta} &= -C\rho u \cdot \nabla\theta - \rho\theta\mathrm{div}u + \frac{1}{\mathrm{Pe}}\mathrm{div}[\rho\nabla\theta] + \frac{2}{\mathrm{Re}_\mu}\rho\|\varepsilon[u]\|^2 + \frac{1}{\mathrm{Re}_\zeta}\rho(\mathrm{div}u)^2,
\end{aligned}$$

we agreed to preserve four structures:

- mass conservation;

For the compressible Navier–Stokes equations,

$$
\begin{aligned}
\dot{\rho} &= -\mathrm{div}[\rho u], \\
\rho \dot{u} &= -\rho u \cdot \nabla u - \nabla[\rho\theta] + \frac{2}{\mathrm{Re}_\mu}\mathrm{div}[\rho\varepsilon[u]] + \frac{1}{\mathrm{Re}_\zeta}\nabla[\rho \mathrm{div} u], \\
C\rho\dot{\theta} &= -C\rho u \cdot \nabla\theta - \rho\theta \mathrm{div} u + \frac{1}{\mathrm{Pe}}\mathrm{div}[\rho\nabla\theta] + \frac{2}{\mathrm{Re}_\mu}\rho\|\varepsilon[u]\|^2 + \frac{1}{\mathrm{Re}_\zeta}\rho(\mathrm{div} u)^2,
\end{aligned}
$$

we agreed to preserve four structures:

- mass conservation;
- momentum conservation;

For the compressible Navier–Stokes equations,

$$
\begin{aligned}
\dot{\rho} &= -\mathrm{div}[\rho u],\\
\rho\dot{u} &= -\rho u\cdot\nabla u - \nabla[\rho\theta] + \frac{2}{\mathrm{Re}_\mu}\mathrm{div}[\rho\varepsilon[u]] + \frac{1}{\mathrm{Re}_\zeta}\nabla[\rho\mathrm{div}u],\\
C\rho\dot{\theta} &= -C\rho u\cdot\nabla\theta - \rho\theta\mathrm{div}u + \frac{1}{\mathrm{Pe}}\mathrm{div}[\rho\nabla\theta] + \frac{2}{\mathrm{Re}_\mu}\rho\|\varepsilon[u]\|^2 + \frac{1}{\mathrm{Re}_\zeta}\rho(\mathrm{div}u)^2,
\end{aligned}
$$

we agreed to preserve four structures:

- mass conservation;
- momentum conservation;
- energy conservation;

For the compressible Navier–Stokes equations,

$$
\begin{aligned}
\dot{\rho} &= -\mathrm{div}[\rho u], \\
\rho\dot{u} &= -\rho u \cdot \nabla u - \nabla[\rho\theta] + \frac{2}{\mathrm{Re}_\mu}\mathrm{div}[\rho\varepsilon[u]] + \frac{1}{\mathrm{Re}_\zeta}\nabla[\rho\,\mathrm{div}u], \\
C\rho\dot{\theta} &= -C\rho u \cdot \nabla\theta - \rho\theta\,\mathrm{div}u + \frac{1}{\mathrm{Pe}}\mathrm{div}[\rho\nabla\theta] + \frac{2}{\mathrm{Re}_\mu}\rho\|\varepsilon[u]\|^2 + \frac{1}{\mathrm{Re}_\zeta}\rho(\mathrm{div}u)^2,
\end{aligned}
$$

we agreed to preserve four structures:

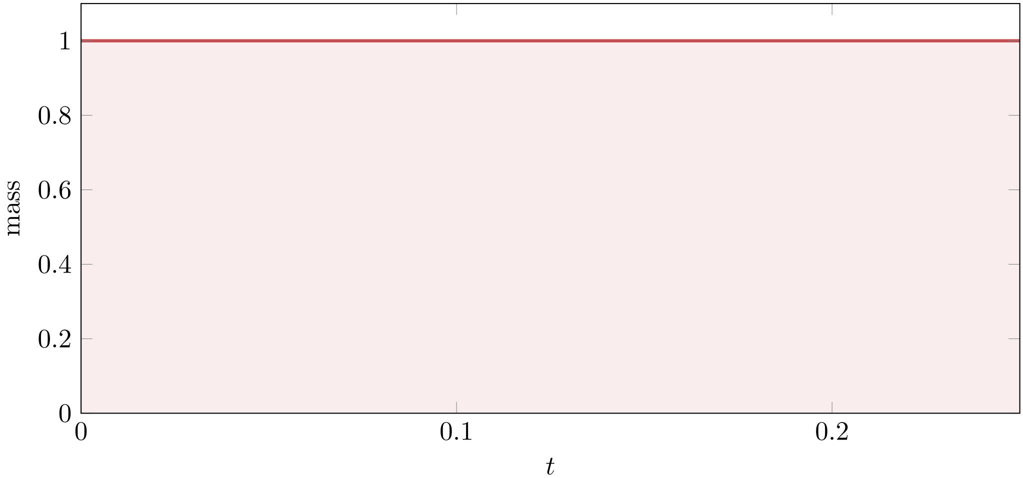
- mass conservation;
- momentum conservation;
- energy conservation;
- entropy dissipation.

The associated test function for mass conservation is

$$\tilde{\rho} = 1, \quad \tilde{u} = 0, \quad \tilde{\theta} = 0.$$

The associated test function for mass conservation is

$$\tilde{\rho} = 1, \quad \tilde{u} = 0, \quad \tilde{\theta} = 0.$$

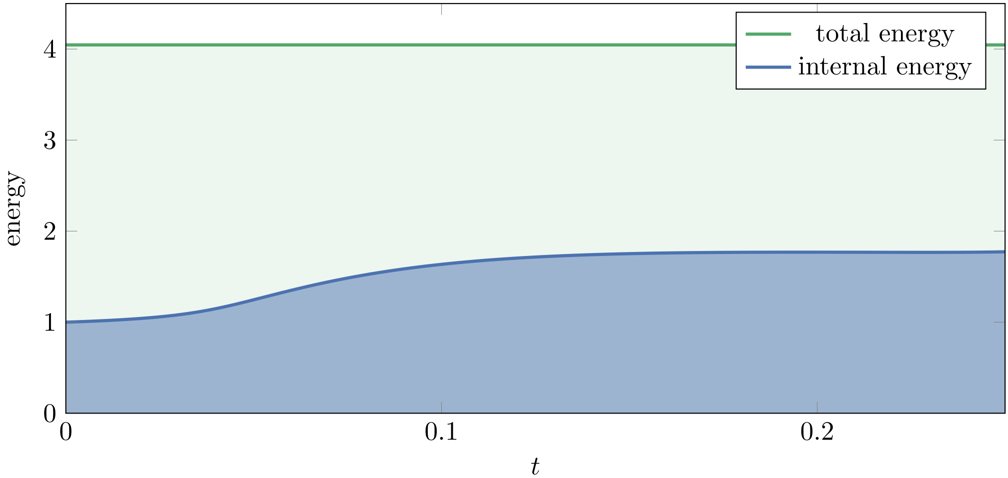


The associated test function for energy conservation is

$$\tilde{\rho} = 0, \quad \tilde{u} = u, \quad \tilde{\theta} = 1.$$

The associated test function for energy conservation is

$$\tilde{\rho} = 0, \quad \tilde{u} = u, \quad \tilde{\theta} = 1.$$



The associated test function for entropy dissipation is

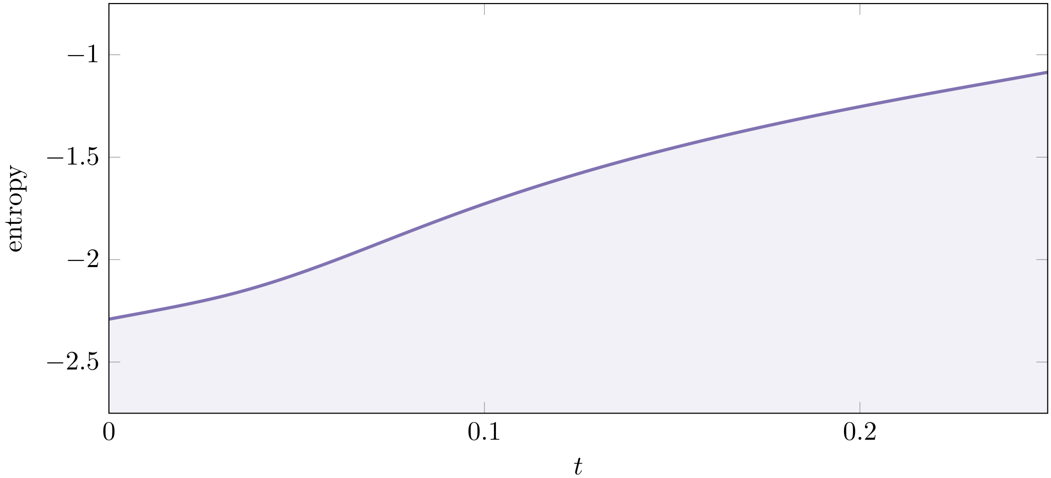
$$\tilde{\rho} = g, \quad \tilde{u} = 0, \quad \tilde{\theta} = \theta^{-1},$$

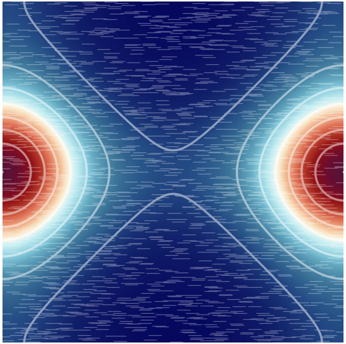
where $-g$ is the Gibbs free energy per unit mass per unit temperature.

The associated test function for entropy dissipation is

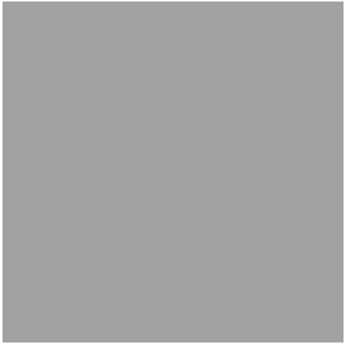
$$\tilde{\rho} = g, \quad \tilde{u} = 0, \quad \tilde{\theta} = \theta^{-1},$$

where $-g$ is the Gibbs free energy per unit mass per unit temperature.

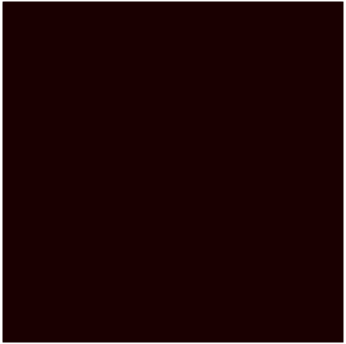




velocity

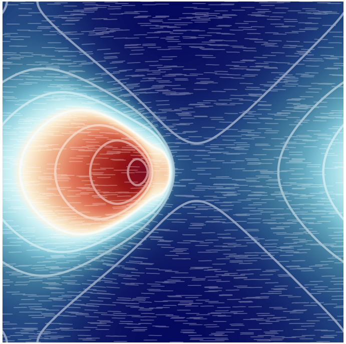


density

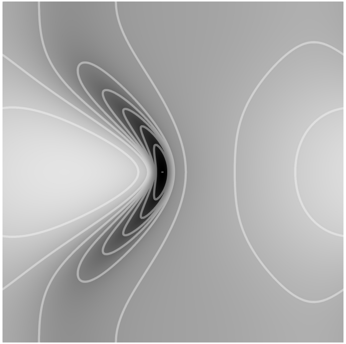


temperature

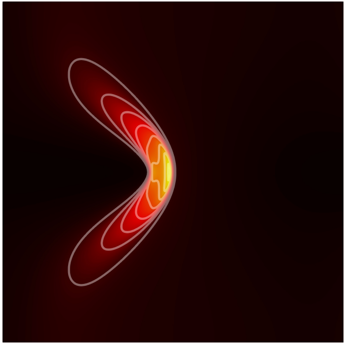
Supersonic compressible Navier–Stokes simulation at $\mathrm{Pr} = 0.71, \mathrm{Re} = 128$



velocity

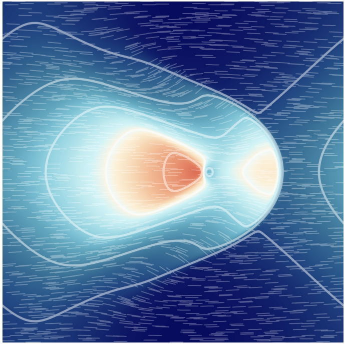


density

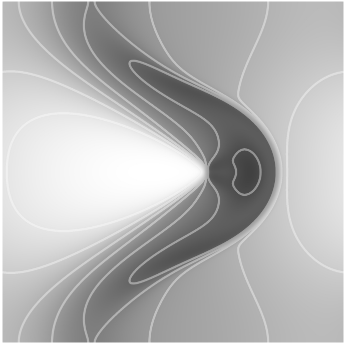


temperature

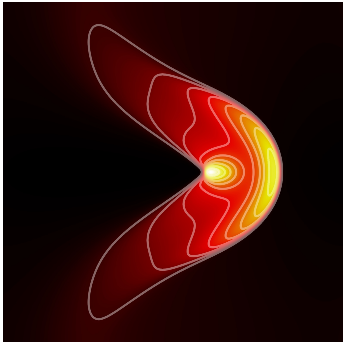
Supersonic compressible Navier–Stokes simulation at $\mathrm{Pr} = 0.71, \mathrm{Re} = 128$



velocity

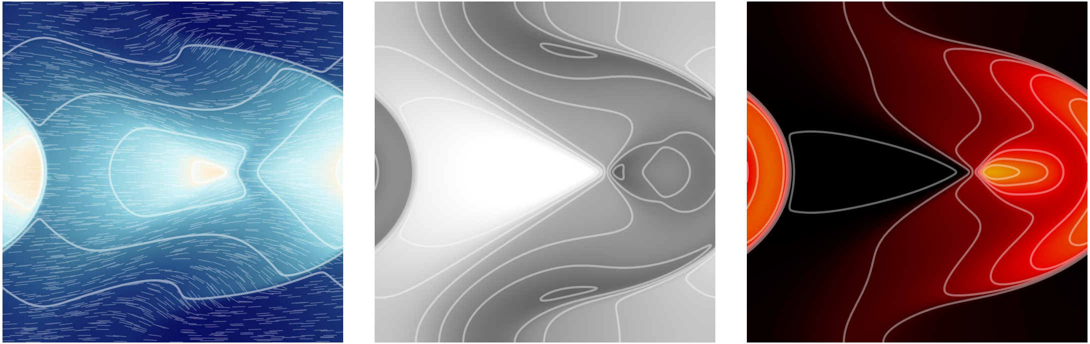


density



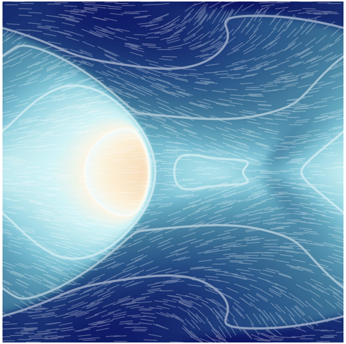
temperature

Supersonic compressible Navier–Stokes simulation at $\mathrm{Pr} = 0.71, \mathrm{Re} = 128$

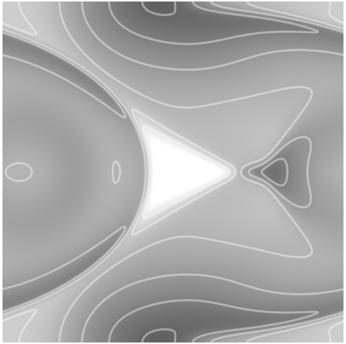


velocity density temperature

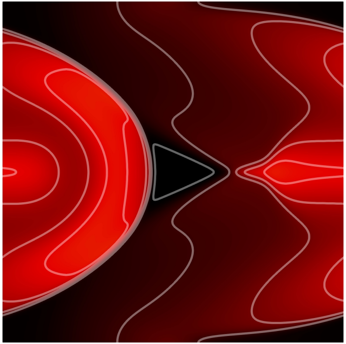
Supersonic compressible Navier–Stokes simulation at $\mathrm{Pr} = 0.71, \mathrm{Re} = 128$



velocity



density



temperature

Supersonic compressible Navier–Stokes simulation at $\mathrm{Pr} = 0.71, \mathrm{Re} = 128$

Section 7

The Kepler problem

The two-body Kepler problem has three invariants: the energy,

$$H(\mathbf{p}, \mathbf{q}) = \frac{1}{2}\|\mathbf{p}\|^2 - \frac{1}{\|\mathbf{q}\|},$$

The two-body Kepler problem has three invariants: the energy,

$$H(\mathbf{p}, \mathbf{q}) = \frac{1}{2}\|\mathbf{p}\|^2 - \frac{1}{\|\mathbf{q}\|},$$

the angular momentum,

$$\mathbf{L}(\mathbf{p}, \mathbf{q}) = \mathbf{q} \times \mathbf{p}$$

The two-body Kepler problem has three invariants: the energy,

$$H(\mathbf{p},\mathbf{q}) = \frac{1}{2}\|\mathbf{p}\|^2 - \frac{1}{\|\mathbf{q}\|},$$

the angular momentum,

$$\mathbf{L}(\mathbf{p},\mathbf{q}) = \mathbf{q} \times \mathbf{p}$$

and the Laplace–Runge–Lenz vector,

$$\mathbf{A}(\mathbf{p},\mathbf{q}) = \mathbf{p} \times \mathbf{L} - \frac{\mathbf{q}}{\|\mathbf{q}\|}.$$

The two-body Kepler problem has three invariants: the energy,

$$H(\mathbf{p}, \mathbf{q}) = \frac{1}{2}\|\mathbf{p}\|^2 - \frac{1}{\|\mathbf{q}\|},$$

the angular momentum,

$$\mathbf{L}(\mathbf{p}, \mathbf{q}) = \mathbf{q} \times \mathbf{p}$$

and the Laplace–Runge–Lenz vector,

$$\mathbf{A}(\mathbf{p}, \mathbf{q}) = \mathbf{p} \times \mathbf{L} - \frac{\mathbf{q}}{\|\mathbf{q}\|}.$$

These invariants are related to each other, so in two dimensions it is enough to conserve H and $\mathbf{A}$ to conserve all three.

The equations of motion are

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p}, \mathbf{q}].$$

The equations of motion are

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p}, \mathbf{q}].$$

The conservation of energy may be straightforwardly deduced by

$$H(\mathbf{x}_{n+1}) - H(\mathbf{x}_n) = \int_{t_n}^{t_{n+1}} \dot{H} \; \mathrm{d}t$$

The equations of motion are

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p}, \mathbf{q}].$$

The conservation of energy may be straightforwardly deduced by

$$\begin{aligned} H(\mathbf{x}_{n+1}) - H(\mathbf{x}_n) &= \int_{t_n}^{t_{n+1}} \dot{H} \; \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \nabla H^\top \dot{\mathbf{x}} \; \mathrm{d}t \end{aligned}$$

The equations of motion are

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p}, \mathbf{q}].$$

The conservation of energy may be straightforwardly deduced by

$$\begin{aligned} H(\mathbf{x}_{n+1}) - H(\mathbf{x}_n) &= \int_{t_n}^{t_{n+1}} \dot{H} \, \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \nabla H^\top \dot{\mathbf{x}} \, \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \nabla H^\top B \nabla H \, \mathrm{d}t \end{aligned}$$

The equations of motion are

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p}, \mathbf{q}].$$

The conservation of energy may be straightforwardly deduced by

$$\begin{aligned} H(\mathbf{x}_{n+1}) - H(\mathbf{x}_n) &= \int_{t_n}^{t_{n+1}} \dot{H} \ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \nabla H^\top \dot{\mathbf{x}} \ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \nabla H^\top B \nabla H \ \mathrm{d}t \\ &= 0. \end{aligned}$$

The equations of motion are

$$\dot{\mathbf{x}} = B\nabla H(\mathbf{x}), \quad B = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad \mathbf{x} = [\mathbf{p}, \mathbf{q}].$$

The conservation of energy may be straightforwardly deduced by

$$\begin{aligned} H(\mathbf{x}_{n+1}) - H(\mathbf{x}_n) &= \int_{t_n}^{t_{n+1}} \dot{H} \; \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \nabla H^\top \dot{\mathbf{x}} \; \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \nabla H^\top B \nabla H \; \mathrm{d}t \\ &= 0. \end{aligned}$$

The other invariants $Q(\mathbf{x})$ also have $\nabla Q^\top B \nabla H = 0$.

First consider a standard cPG discretisation of the Kepler problem:

Base cPG discretisation

Find $\mathbf{x} \in \mathbb{X} := \{\mathbf{y} \in P^s([t_n, t_{n+1}], \mathbb{R}^4) : \mathbf{y}(t_n) = \mathbf{x}_n\}$ such that

$$\int_{t_n}^{t_{n+1}} \mathbf{y}^\top \dot{\mathbf{x}} \, \mathrm{d}t = \int_{t_n}^{t_{n+1}} \mathbf{y}^\top B \nabla H(\mathbf{x}) \, \mathrm{d}t$$

for all $\mathbf{y} \in \dot{\mathbb{X}} := P^{s-1}([t_n, t_{n+1}], \mathbb{R}^4)$.

First consider a standard cPG discretisation of the Kepler problem:

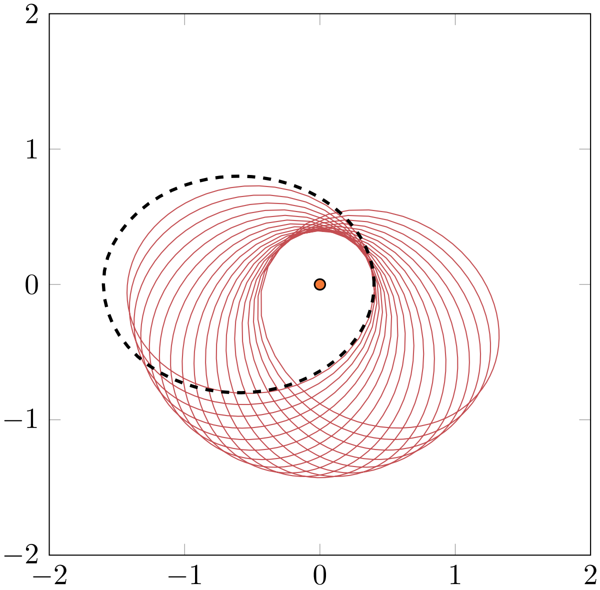
Base cPG discretisation

Find $\mathbf{x} \in \mathbb{X} := \{\mathbf{y} \in P^s([t_n, t_{n+1}], \mathbb{R}^4) : \mathbf{y}(t_n) = \mathbf{x}_n\}$ such that

$$\int_{t_n}^{t_{n+1}} \mathbf{y}^\top \dot{\mathbf{x}} \; \mathrm{d}t = \int_{t_n}^{t_{n+1}} \mathbf{y}^\top B \nabla H(\mathbf{x}) \; \mathrm{d}t$$

for all $\mathbf{y} \in \dot{\mathbb{X}} := P^{s-1}([t_n, t_{n+1}], \mathbb{R}^4)$.

Setting $s = 1$ and approximating the integrals with a one-point Gauss–Legendre quadrature rule yields the familiar implicit midpoint scheme.



Carl Friedrich Gauss

Implicit midpoint:

- ✓ symplecticity
- ✓ angular momentum
- ✓ energy
- ✗ orientation (LRL)

Let us first consider how to modify the scheme to conserve energy. We

- compute an approximate $\widetilde{\nabla H} \in \dot{\mathbb{X}}$;
- use it in the right-hand side of the ODE.

Let us first consider how to modify the scheme to conserve energy. We

- compute an approximate $\widetilde{\nabla H} \in \dot{\mathbb{X}}$;
- use it in the right-hand side of the ODE.

Energy-conserving discretisation (formal)

Find $(\mathbf{x}, \widetilde{\nabla H}) \in \mathbb{X} \times \dot{\mathbb{X}}$ such that

$$\int_{t_n}^{t_{n+1}} \mathbf{y}^\top \dot{\mathbf{x}} \, \mathrm{d}t = \int_{t_n}^{t_{n+1}} \mathbf{y}^\top B \widetilde{\nabla H} \, \mathrm{d}t$$
$$\int_{t_n}^{t_{n+1}} \mathbf{y}_1^\top \widetilde{\nabla H} \, \mathrm{d}t = \int_{t_n}^{t_{n+1}} \mathbf{y}_1^\top \nabla H \, \mathrm{d}t$$

for all $(\mathbf{y}, \mathbf{y}_1) \in \dot{\mathbb{X}} \times \dot{\mathbb{X}}$.

Let us first consider how to modify the scheme to conserve energy. We

- compute an approximate $\widetilde{\nabla H} \in \dot{\mathbb{X}}$;
- use it in the right-hand side of the ODE.

Energy-conserving discretisation (formal)

Find $(\mathbf{x}, \widetilde{\nabla H}) \in \mathbb{X} \times \dot{\mathbb{X}}$ such that

$$\int_{t_n}^{t_{n+1}} \mathbf{y}^\top \dot{\mathbf{x}} \, \mathrm{d}t = \int_{t_n}^{t_{n+1}} \mathbf{y}^\top B \widetilde{\nabla H} \, \mathrm{d}t$$
$$\int_{t_n}^{t_{n+1}} \mathbf{y}_1^\top \widetilde{\nabla H} \, \mathrm{d}t = \int_{t_n}^{t_{n+1}} \mathbf{y}_1^\top \nabla H \, \mathrm{d}t$$

for all $(\mathbf{y}, \mathbf{y}_1) \in \dot{\mathbb{X}} \times \dot{\mathbb{X}}$.

This is more expensive than necessary. The second equation states that $\widetilde{\nabla H}$ is the projection onto $\dot{\mathbb{X}}$ of ∇H; in the discrete case, this can be evaluated exactly.

Using the explicit projection $\mathbb{P}$, we can write:

Energy-conserving discretisation (practical)

Find $\mathbf{x} \in \mathbb{X}$ such that

$$\int_{t_n}^{t_{n+1}} \mathbf{y}^\top \dot{\mathbf{x}} \; \mathrm{d}t = \int_{t_n}^{t_{n+1}} \mathbf{y}^\top B \mathbb{P}[\nabla H(\mathbf{x})] \; \mathrm{d}t$$

for all $\mathbf{y} \in \dot{\mathbb{X}}$.

Using the explicit projection $\mathbb{P}$, we can write:

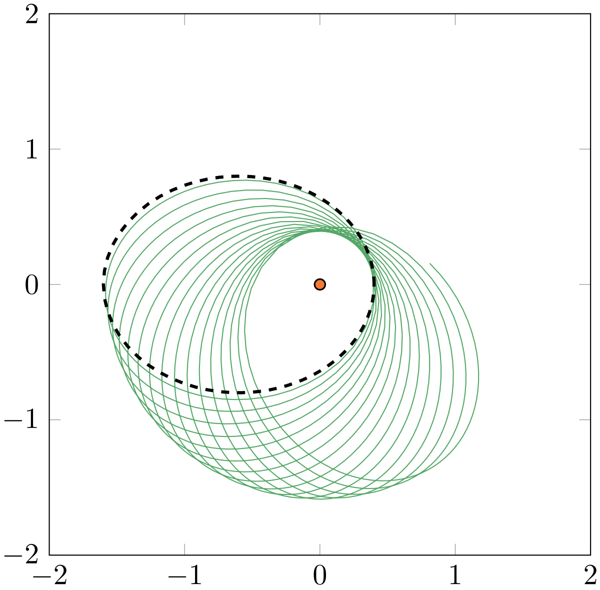
Energy-conserving discretisation (practical)

Find $\mathbf{x} \in \mathbb{X}$ such that

$$\int_{t_n}^{t_{n+1}} \mathbf{y}^\top \dot{\mathbf{x}} \, \mathrm{d}t = \int_{t_n}^{t_{n+1}} \mathbf{y}^\top B \mathbb{P}[\nabla H(\mathbf{x})] \, \mathrm{d}t$$

for all $\mathbf{y} \in \dot{\mathbb{X}}$.

This is an alternative derivation of the energy-preserving scheme of Cohen & Hairer (2011) (when certain quadrature rules are used).



David Cohen

Ernst Hairer

Cohen & Hairer (2011):

- ✗ symplecticity
- ✗ angular momentum
- ✓ energy
- ✗ orientation (LRL)

Now let us modify the scheme to also preserve $\mathbf{A}$ (and hence $\mathbf{L}$):

- compute approximate $\widetilde{\nabla A_1}, \widetilde{\nabla A_2} \in \dot{\mathbb{X}}$;
- modify the right-hand side.

Now let us modify the scheme to also preserve $\mathbf{A}$ (and hence $\mathbf{L}$):

- compute approximate $\widetilde{\nabla A_1}, \widetilde{\nabla A_2} \in \dot{\mathbb{X}}$;
- modify the right-hand side.

How can we modify the right-hand side, though? It seems ∇A_1 and ∇A_2 don't appear.

It turns out we can rewrite the right-hand side to expose them:

Alternating form

There exists a scalar function $\lambda(\mathbf{x})$ such that

$$\mathbf{y}^\top B \nabla H(x) = \lambda(\mathbf{x}) \det \begin{pmatrix} \nabla H & \nabla A_1 & \nabla A_2 & \mathbf{y} \end{pmatrix}.$$

It turns out we can rewrite the right-hand side to expose them:

Alternating form

There exists a scalar function $\lambda(\mathbf{x})$ such that

$$\mathbf{y}^\top B \nabla H(x) = \lambda(\mathbf{x}) \det \begin{pmatrix} \nabla H & \nabla A_1 & \nabla A_2 & \mathbf{y} \end{pmatrix}.$$

Theorem

For finite-dimensional Hamiltonian/Poisson systems, the right-hand side can be written as an alternating form of the test function and gradients of conserved quantities.

Energy- and orientation-conserving discretisation (formal)

Find $(\mathbf{x}, \widetilde{\nabla H}, (\widetilde{\nabla A_1}, \widetilde{\nabla A_2})) \in \mathbb{X} \times \dot{\mathbb{X}} \times \dot{\mathbb{X}}^2$ such that

$$
\begin{aligned}
\int_{t_n}^{t_{n+1}} \mathbf{y}^\top \dot{\mathbf{x}} \, \mathrm{d}t &= \int_{t_n}^{t_{n+1}} \lambda(\mathbf{x}) \det \begin{pmatrix} \widetilde{\nabla H} & \widetilde{\nabla A_1} & \widetilde{\nabla A_2} & \mathbf{y} \end{pmatrix} \mathrm{d}t \\
\int_{t_n}^{t_{n+1}} \mathbf{y}_1^\top \widetilde{\nabla H} \, \mathrm{d}t &= \int_{t_n}^{t_{n+1}} \mathbf{y}_1^\top \nabla H \, \mathrm{d}t \\
\int_{t_n}^{t_{n+1}} \mathbf{y}_2^\top \widetilde{\nabla A_1} \, \mathrm{d}t &= \int_{t_n}^{t_{n+1}} \mathbf{y}_2^\top \nabla A_1 \, \mathrm{d}t \\
\int_{t_n}^{t_{n+1}} \mathbf{y}_3^\top \widetilde{\nabla A_2} \, \mathrm{d}t &= \int_{t_n}^{t_{n+1}} \mathbf{y}_3^\top \nabla A_2 \, \mathrm{d}t
\end{aligned}
$$

for all $(\mathbf{y}, \mathbf{y}_1, (\mathbf{y}_2, \mathbf{y}_3)) \in \dot{\mathbb{X}} \times \dot{\mathbb{X}} \times \dot{\mathbb{X}}^2$.

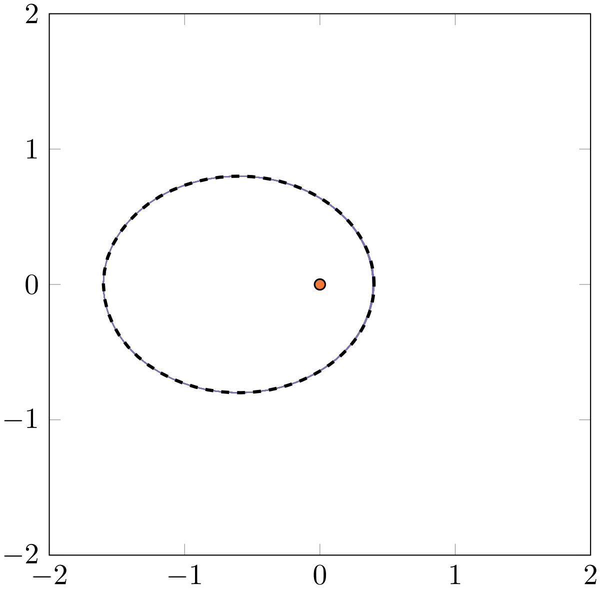
Energy- and orientation-conserving discretisation (formal)

Find $(\mathbf{x}, \widetilde{\nabla H}, (\widetilde{\nabla A_1}, \widetilde{\nabla A_2})) \in \mathbb{X} \times \dot{\mathbb{X}} \times \dot{\mathbb{X}}^2$ such that

$$
\begin{aligned}
\int_{t_n}^{t_{n+1}} \mathbf{y}^\top \dot{\mathbf{x}} \,\mathrm{d}t &= \int_{t_n}^{t_{n+1}} \lambda(\mathbf{x}) \det \begin{pmatrix} \widetilde{\nabla H} & \widetilde{\nabla A_1} & \widetilde{\nabla A_2} & \mathbf{y} \end{pmatrix} \mathrm{d}t \\
\int_{t_n}^{t_{n+1}} \mathbf{y}_1^\top \widetilde{\nabla H} \,\mathrm{d}t &= \int_{t_n}^{t_{n+1}} \mathbf{y}_1^\top \nabla H \,\mathrm{d}t \\
\int_{t_n}^{t_{n+1}} \mathbf{y}_2^\top \widetilde{\nabla A_1} \,\mathrm{d}t &= \int_{t_n}^{t_{n+1}} \mathbf{y}_2^\top \nabla A_1 \,\mathrm{d}t \\
\int_{t_n}^{t_{n+1}} \mathbf{y}_3^\top \widetilde{\nabla A_2} \,\mathrm{d}t &= \int_{t_n}^{t_{n+1}} \mathbf{y}_3^\top \nabla A_2 \,\mathrm{d}t
\end{aligned}
$$

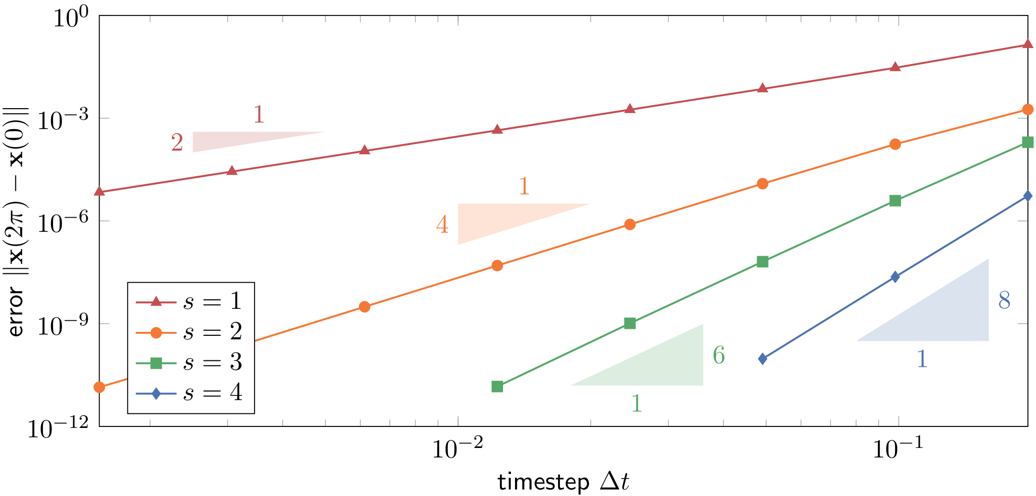
for all $(\mathbf{y}, \mathbf{y}_1, (\mathbf{y}_2, \mathbf{y}_3)) \in \dot{\mathbb{X}} \times \dot{\mathbb{X}} \times \dot{\mathbb{X}}^2$.

Again, this can be rewritten purely as a problem in $\mathbf{x}$.



Our scheme:

- ✗ symplecticity
- ✓ angular momentum
- ✓ energy
- ✓ orientation (LRL)


10^0
10^{-3}
10^{-6}
10^{-9}
10^{-12}
error $\|\mathbf{x}(2\pi) - \mathbf{x}(0)\|$
10^{-2}
10^{-1}
timestep Δt
$s = 1$
$s = 2$
$s = 3$
$s = 4$
1
2
1
4
6
1
8
1

Section 8

Hamiltonian PDE

The Benjamin–Bona–Mahony equation

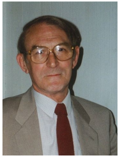
$$u_t + u_x + u u_x - u_{xxt} = 0, \quad u(-50) = u(50),$$

has a Hamiltonian structure:

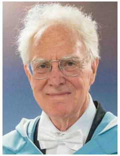
$$\left(\mathrm{id} - \partial_x^2\right) \dot{u} = -\partial_x H'(u),$$

with Hamiltonian

$$H(u) = \int_\Omega \frac{1}{2} u^2 + \frac{1}{6} u^3 \, \mathrm{d}x.$$



T. Brooke Benjamin



Jerry Bona

John Joseph Mahony

The Benjamin–Bona–Mahony equation

$$u_t + u_x + u u_x - u_{xxt} = 0, \quad u(-50) = u(50),$$

has a Hamiltonian structure:

$$\left(\mathrm{id} - \partial_x^2\right) \dot{u} = -\partial_x H'(u),$$

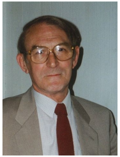
with Hamiltonian

$$H(u) = \int_\Omega \frac{1}{2} u^2 + \frac{1}{6} u^3 \, \mathrm{d}x.$$

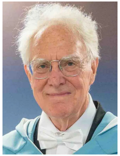
The equation has exactly two other invariants:

$$I_1(u) = \int_\Omega u \, \mathrm{d}x,$$

$$I_2(u) = \int_\Omega u^2 + u_x^2 \, \mathrm{d}x.$$



T. Brooke Benjamin



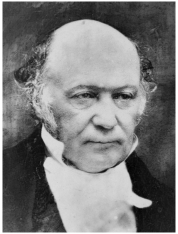
Jerry Bona

John Joseph Mahony

Our general formulation is

$$M[\dot{u}] = B[H'(u)],$$

where $M^{-1}B$ is skew-symmetric.



William Rowan Hamilton

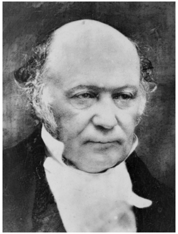
Our general formulation is

$$M[\dot{u}] = B[H'(u)],$$

where $M^{-1}B$ is skew-symmetric.

This conserves the Hamiltonian, by the usual argument:

$$H(u(t_{n+1})) - H(u(t_n)) = \int_{t_n}^{t_{n+1}} \dot{H}\ \mathrm{d}t$$



William Rowan Hamilton

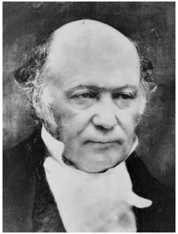
Our general formulation is

$$M[\dot{u}] = B[H'(u)],$$

where $M^{-1}B$ is skew-symmetric.

This conserves the Hamiltonian, by the usual argument:

$$\begin{aligned} H(u(t_{n+1})) - H(u(t_n)) &= \int_{t_n}^{t_{n+1}} \dot{H} \ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} H'(u)\dot{u} \ \mathrm{d}t \end{aligned}$$



William Rowan Hamilton

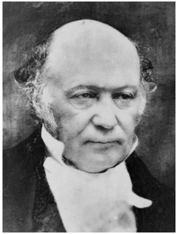
Our general formulation is

$$M[\dot{u}] = B[H'(u)],$$

where $M^{-1}B$ is skew-symmetric.

This conserves the Hamiltonian, by the usual argument:

$$\begin{aligned} H(u(t_{n+1})) - H(u(t_n)) &= \int_{t_n}^{t_{n+1}} \dot{H} \ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} H'(u)\dot{u} \ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} H'(u)M^{-1}BH'(u) \ \mathrm{d}t \end{aligned}$$



William Rowan Hamilton

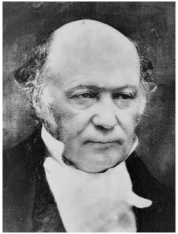
Our general formulation is

$$M[\dot{u}] = B[H'(u)],$$

where $M^{-1}B$ is skew-symmetric.

This conserves the Hamiltonian, by the usual argument:

$$\begin{aligned} H(u(t_{n+1})) - H(u(t_n)) &= \int_{t_n}^{t_{n+1}} \dot{H} \ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} H'(u)\dot{u} \ \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} H'(u)M^{-1}BH'(u) \ \mathrm{d}t \\ &= 0. \end{aligned}$$



William Rowan Hamilton

Following a similar analysis, it turns out that the right auxiliary variable to use is

$$w_1 \approx M^{-*}[H'(u)],$$

which is not obvious (to me).

Following a similar analysis, it turns out that the right auxiliary variable to use is

$$w_1 \approx M^{-*}[H'(u)],$$

which is not obvious (to me).

Energy-conserving discretisation

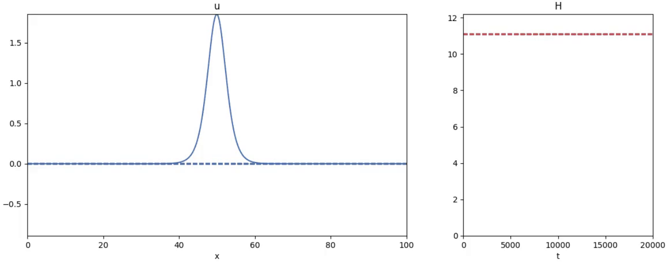
Find $(u, w_1) \in \mathbb{X} \times \dot{\mathbb{X}}$ such that

$$\int_{t_n}^{t_{n+1}} vM[\dot{u}] \, \mathrm{d}t = \int_{t_n}^{t_{n+1}} vBM^*[w_1] \, \mathrm{d}t$$

$$\int_{t_n}^{t_{n+1}} w_1 M[v_1] \, \mathrm{d}t = \int_{t_n}^{t_{n+1}} H'[u]v_1 \, \mathrm{d}t$$

for all $(v, v_1) \in \dot{\mathbb{X}} \times \dot{\mathbb{X}}$.

We simulate a soliton that travels rightwards at constant speed with a fourth-order scheme ($s = 2$).



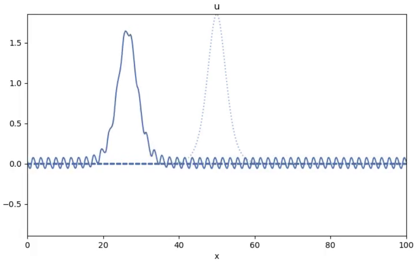
Simulation near $t = 0$.

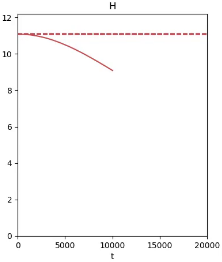
Carl Friedrich Gauss

Gauss method:

- ✓ symplecticity
- ✓ integral
- ✓ H^1-norm
- ✓ energy

We simulate a soliton that travels rightwards at constant speed with a fourth-order scheme ($s = 2$).





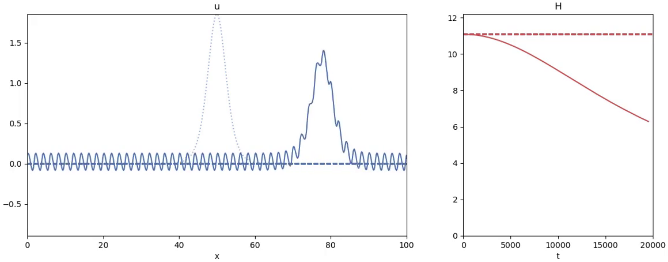
Simulation near $t = 10000$.

Carl Friedrich Gauss

Gauss method:

- ✓ symplecticity
- ✓ integral
- ✓ H^1-norm
- ✓ energy

We simulate a soliton that travels rightwards at constant speed with a fourth-order scheme ($s = 2$).



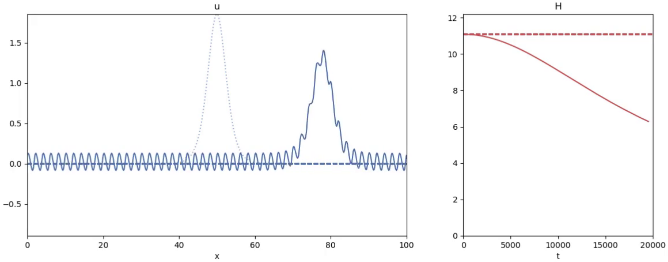
Simulation near $t = 20000$.

Carl Friedrich Gauss

Gauss method:

- ✓ symplecticity
- ✓ integral
- ✓ H^1-norm
- ✓ energy

We simulate a soliton that travels rightwards at constant speed with a fourth-order scheme ($s = 2$).



Simulation near $t = 20000$.

Carl Friedrich Gauss

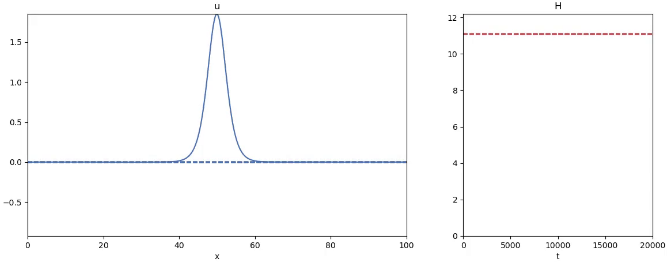
Gauss method:

- ✓ symplecticity
- ✓ integral
- ✓ H^1-norm
- ✓ energy

Spurious oscillations

H^1 norm conserved but L^2 norm decreases $\to$ oscillation.

The same soliton, again:



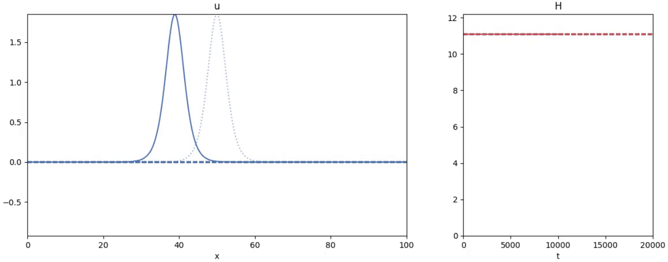
Simulation near $t = 0$.

Boris Andrews

Our method:

- ✗ symplecticity
- ✓ integral
- ✓ H^1-norm
- ✓ energy

The same soliton, again:



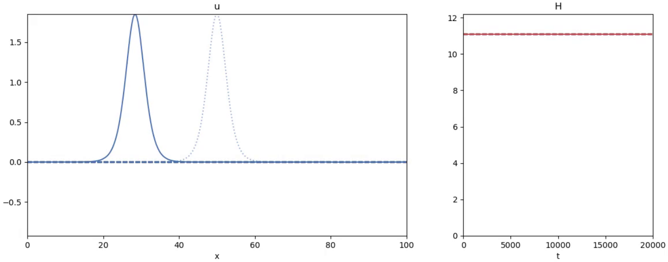
Simulation near $t = 10000$.

Boris Andrews

Our method:

- ✗ symplecticity
- ✓ integral
- ✓ H^1-norm
- ✓ energy

The same soliton, again:



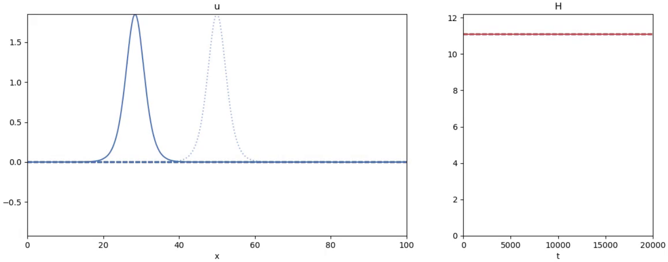
Simulation near $t = 20000$.

Boris Andrews

Our method:

- ✗ symplecticity
- ✓ integral
- ✓ H^1-norm
- ✓ energy

The same soliton, again:



Simulation near $t = 20000$.

Boris Andrews

Our method:

- ✗ symplecticity
- ✓ integral
- ✓ H^1-norm
- ✓ energy

Good news

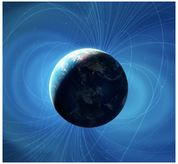
Soliton character is preserved even over very long timescales.

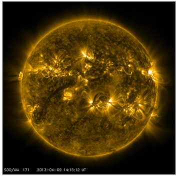
Section 9

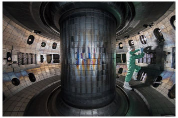
The Parker problem

Ideal magnetohydrodynamics

$$
\begin{aligned}
u_t - \operatorname{div}(2\nu\varepsilon(u)) + \operatorname{div}(u \otimes u) + \operatorname{grad} p + SB \times (E + u \times B) &= f \quad \text{in } \Omega,\\
\operatorname{div} u &= 0 \quad \text{in } \Omega,\\
B_t + \operatorname{curl} E &= 0 \quad \text{in } \Omega,\\
E + u \times B &= 0 \quad \text{in } \Omega.
\end{aligned}
$$

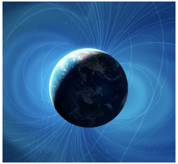


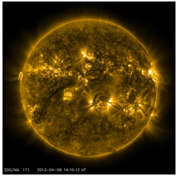




Ideal magnetohydrodynamics

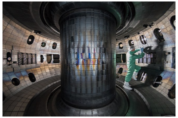
$$
\begin{aligned}
u_t - \operatorname{div}(2\nu\varepsilon(u)) + \operatorname{div}(u \otimes u) + \operatorname{grad} p + SB \times (E + u \times B) &= f \quad \text{in } \Omega, \\
\operatorname{div} u &= 0 \quad \text{in } \Omega, \\
B_t + \operatorname{curl} E &= 0 \quad \text{in } \Omega, \\
E + u \times B &= 0 \quad \text{in } \Omega.
\end{aligned}
$$





Two structures to preserve:

- energy $E = \|u\|^2 + \|B\|^2$ is dissipated;
- helicity $H = (A, B)_{L^2}$ is conserved, for any A s.t. $\operatorname{curl} A = B$.



The Parker conjecture (1972)

For almost all initial conditions, the magnetic field develops tangential discontinuities during ideal magnetic relaxation to a force-free equilibrium.

Eugene N. Parker

The Parker conjecture (1972)

For almost all initial conditions, the magnetic field develops tangential discontinuities during ideal magnetic relaxation to a force-free equilibrium.

Parker conjectured the existence of the solar wind. The shape of the magnetic field in the outer solar system is now called a Parker spiral.

Eugene N. Parker

The Parker conjecture (1972)

For almost all initial conditions, the magnetic field develops tangential discontinuities during ideal magnetic relaxation to a force-free equilibrium.

Eugene N. Parker

Parker conjectured the existence of the solar wind. The shape of the magnetic field in the outer solar system is now called a Parker spiral.

This conjecture has many important consequences in solar physics, including for the coronal heating problem (why is the corona millions of degrees hotter than the surface?).

There is a crucal relationship between helicity H and energy E:

The Arnold inequality

$$|H| \lesssim \|B\|_{L^2}.$$

Vladimir Arnold

There is a crucal relationship between helicity H and energy E:

The Arnold inequality

$$|H| \lesssim \|B\|_{L^2}.$$

This means that, while the system is dissipative, initial data with nonzero helicity cannot relax to the zero state.

Vladimir Arnold

There is a crucal relationship between helicity H and energy E:

The Arnold inequality

$$|H| \lesssim \|B\|_{L^2}.$$

This means that, while the system is dissipative, initial data with nonzero helicity cannot relax to the zero state.

The helicity provides a *topological barrier* that is crucial for the physics of the problem.

Vladimir Arnold

The Parker conjecture can be investigated with the magneto-frictional equations:

$$
\begin{aligned}
\frac{\partial \boldsymbol{B}}{\partial t} + \nabla \times \boldsymbol{E} &= \boldsymbol{0}, \\
\boldsymbol{E} + \boldsymbol{u} \times \boldsymbol{B} &= \boldsymbol{0}, \\
\boldsymbol{j} &= \nabla \times \boldsymbol{B}, \\
\boldsymbol{u} &= \tau \boldsymbol{j} \times \boldsymbol{B}, \\
\operatorname{div} \boldsymbol{B} &= 0.
\end{aligned}
$$

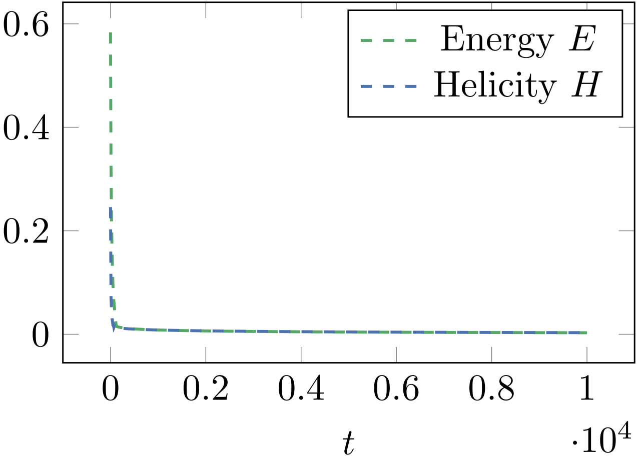
The Parker conjecture can be investigated with the magneto-frictional equations:

$$
\begin{aligned}
\frac{\partial \boldsymbol{B}}{\partial t} + \nabla \times \boldsymbol{E} &= \boldsymbol{0}, \\
\boldsymbol{E} + \boldsymbol{u} \times \boldsymbol{B} &= \boldsymbol{0}, \\
\boldsymbol{j} &= \nabla \times \boldsymbol{B}, \\
\boldsymbol{u} &= \tau \boldsymbol{j} \times \boldsymbol{B}, \\
\operatorname{div} \boldsymbol{B} &= 0.
\end{aligned}
$$

This system also dissipates energy, conserves helicity, satisfies the Arnold inequality, and has the same equilibria as the original MHD system.

We have devised a structure-preserving discretisation of these equations.

It requires both the ideas in this talk and finite element exterior calculus.

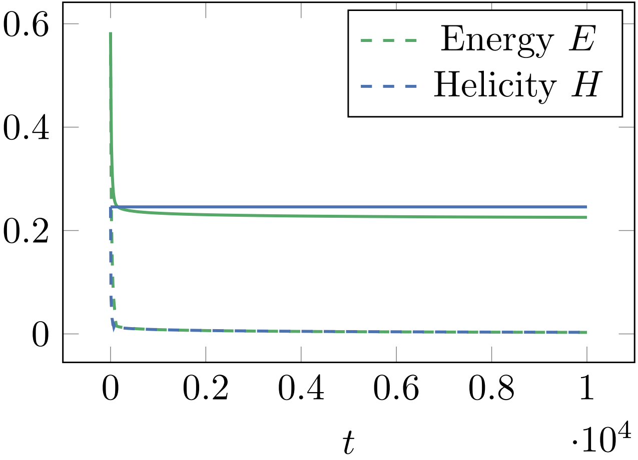


Kaibo Hu

Mingdong He

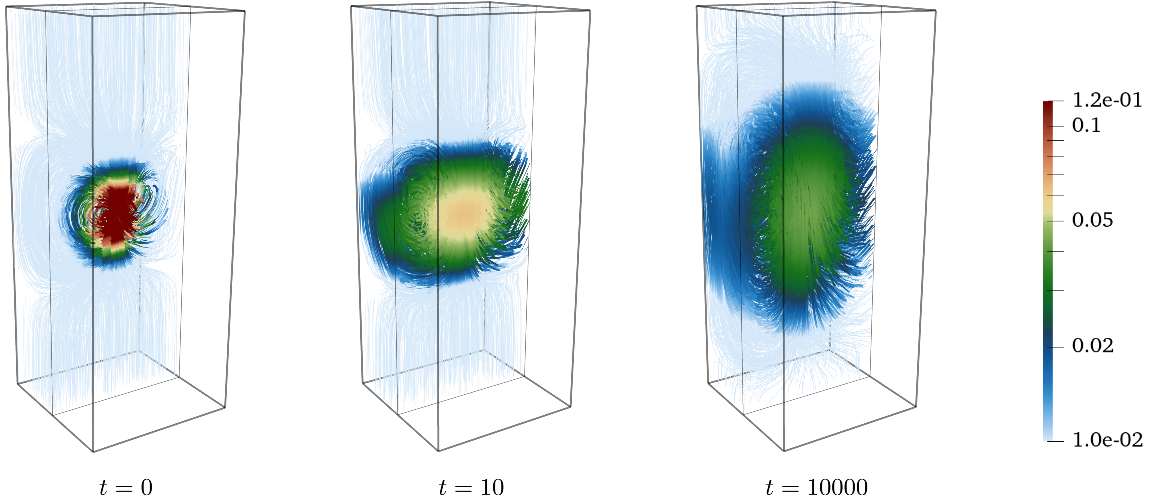
We have devised a structure-preserving discretisation of these equations.

It requires both the ideas in this talk and finite element exterior calculus.



Kaibo Hu

Mingdong He



Magnetic field lines for a large-scale simulation on ARCHER2, coloured by magnetic field strength $\|B\|$.

Section 10

Conclusions

Good news

We can now (with work) discretely replicate many conservation/dissipation laws.

Good news

We can now (with work) discretely replicate many conservation/dissipation laws.

Potential applications

magnetohydrodynamics, multicomponent flows, viscoelastic fluids, geometric PDE, Hamiltonian systems, the Lorentz system, hyperelasticity, gradient flows . . . .