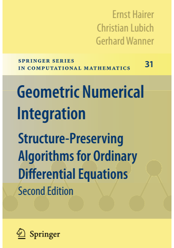
Designing conservative and accurately dissipative numerical integrators in time

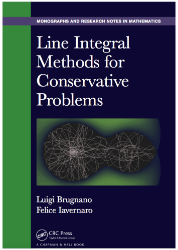
Patrick E. Farrell Boris Andrews


University of Oxford

July 30 2024

Structure preservation means different things in different contexts.





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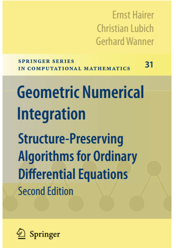

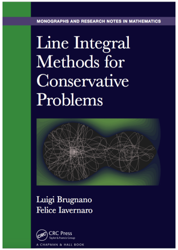

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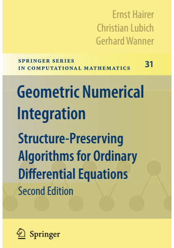

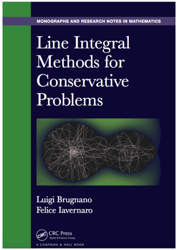

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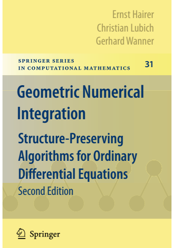

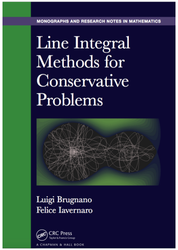

Symplecticity

The differential equation preserves the symplectic 2-form.

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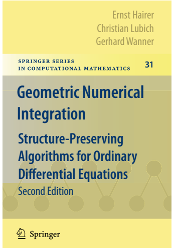

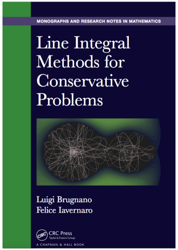

Reversibility

Negating the initial velocity only inverts the direction of motion.

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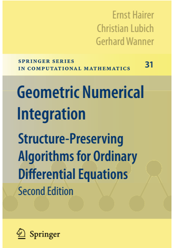

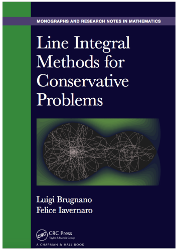

Conservation

The equation preserves invariants, like energy or angular momentum.

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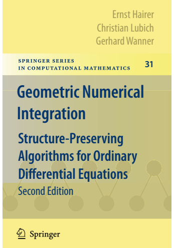

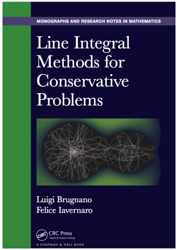

Dissipation

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

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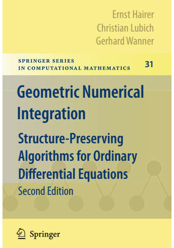
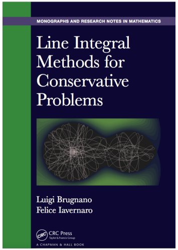




This talk

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

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

Section 2

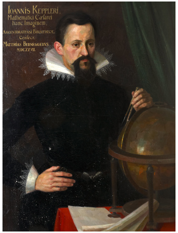
Examples

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

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



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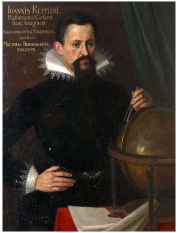

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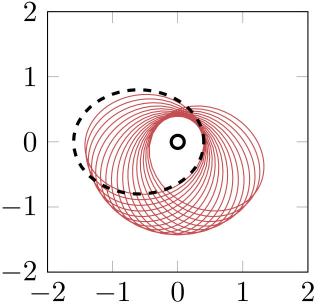

Implicit midpoint:

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

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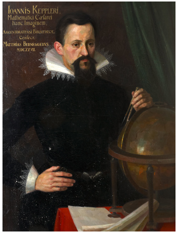

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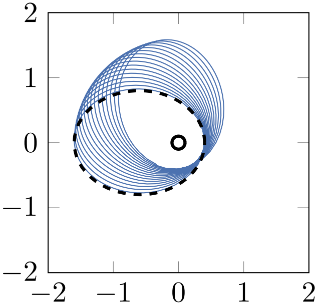

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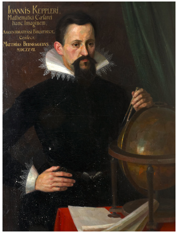

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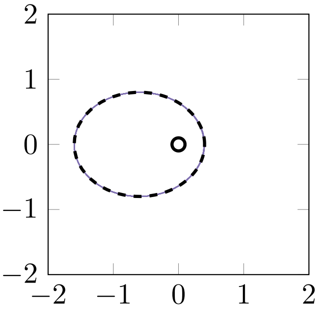

Our discretisation:

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The Kovalevskaya top is described by

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

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Sofya Kovalevskaya

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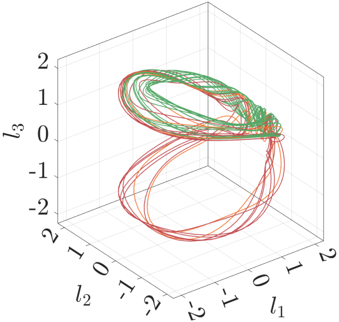

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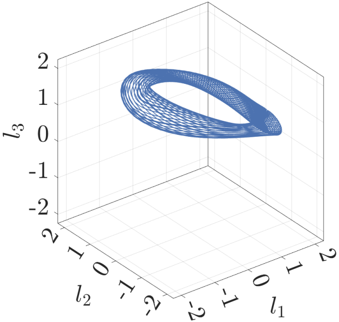

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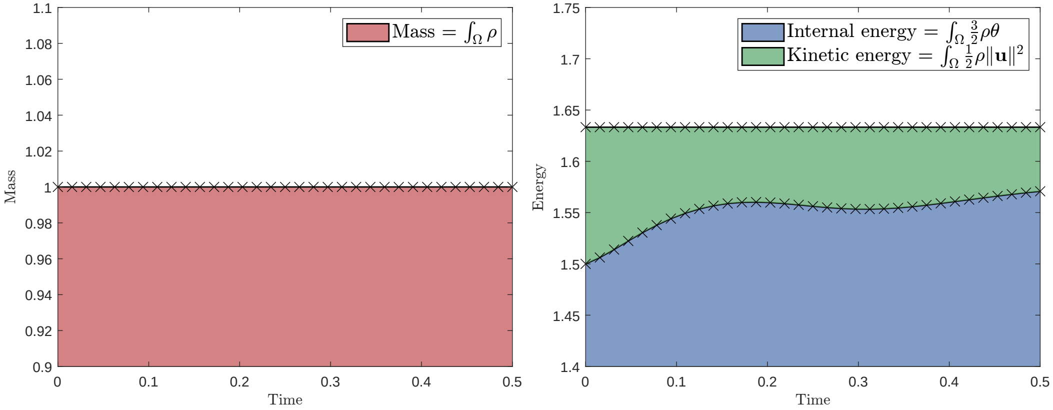
This approach extends to more complicated problems. The compressible Navier–Stokes equations conserve mass and energy:



Section 3

How it works

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To understand FET, let's first study collocation Runge–Kutta schemes for the ODE

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

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General idea

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

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Collocation Runge–Kutta test conditions

Demand that

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

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

We can rewrite the collocation Runge–Kutta test conditions:

Collocation Runge–Kutta test conditions, rephrased (I)

Demand that

$$\int_{t_n}^{t_{n+1}} \dot{u}\delta\left(t - (t_n + c_i \Delta t)\right) \, \mathrm{d}t = \int_{t_n}^{t_{n+1}} f(u)\delta\left(t - (t_n + c_i \Delta t)\right) \, \mathrm{d}t,$$

for $i = 1, \ldots, s$.

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for $i=1,\dots,s$.

Or we could write them as:

Collocation Runge–Kutta test conditions, rephrased (II)

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 $v \in \mathrm{span}(\delta_{c_1},\dots,\delta_{c_s})$.

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The natural FET scheme instead chooses another test set:

Continuous Petrov–Galerkin (cPG) test conditions

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In other words, each conservation law has an

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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. Define the 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.

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 $\partial\Omega$.

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A. Define the cPG discretisation

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

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

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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 $s - 1$.

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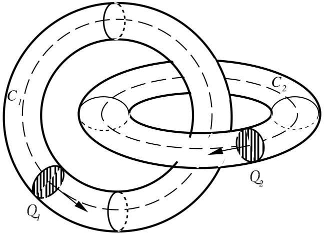
and the change in *helicity*, a topological measure of the knottedness of the flow,

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



From Arnold & Khesin (1998).

At the continuous level, we derive a dissipation law for the energy by testing our weak formulation with $v = u$, the velocity itself:

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

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&= -\mathrm{Re}^{-1} \int_{t_n}^{t_{n+1}} \|\nabla u\|^2\ \mathrm{d}t \le 0.
\end{aligned}
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Similarly, we derive a law for the helicity by testing our weak formulation with $v = \nabla \times u$, the vorticity:

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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}
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Similarly, we derive a law for the helicity by testing our weak formulation with $v = \nabla \times u$, the vorticity:

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&= -\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.

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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.

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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!

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

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We therefore recover a conservation law in the ideal limit.

Good news

The auxiliary velocity can be computed explicitly.

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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.

Leo Rebholz

For the compressible Navier–Stokes equations,

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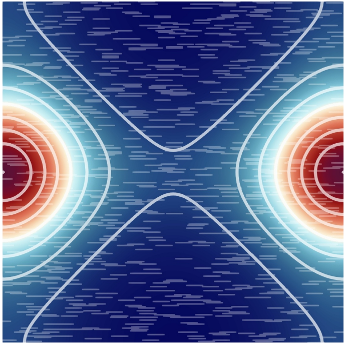
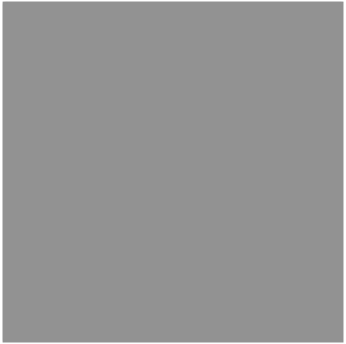
\end{aligned}$$

there are four structures one might wish to preserve:

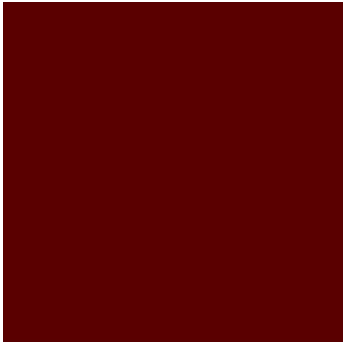
- mass conservation;
- momentum conservation;
- energy conservation;
- entropy dissipation.



velocity

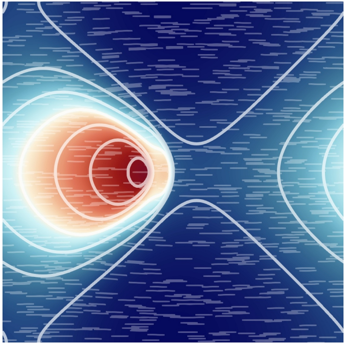


density

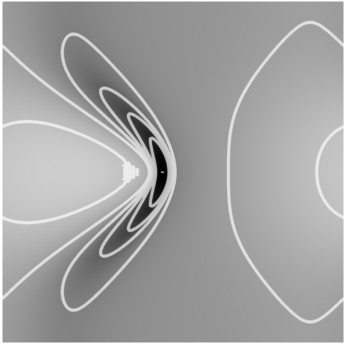


temperature

Supersonic compressible Navier–Stokes simulation



velocity



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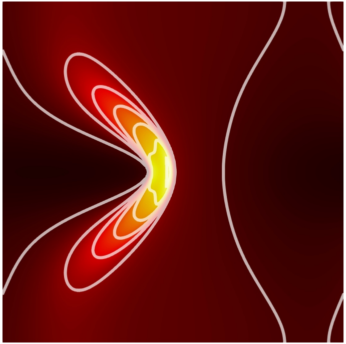

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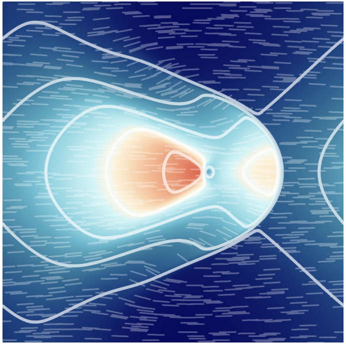
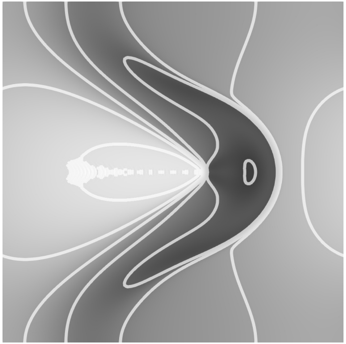


velocity



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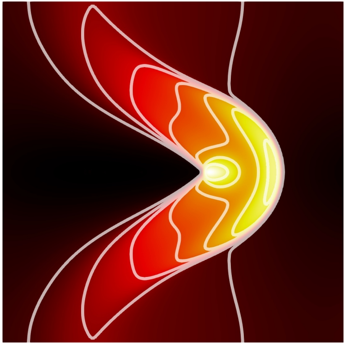

temperature

Supersonic compressible Navier–Stokes simulation

The associated test function for mass conservation is

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

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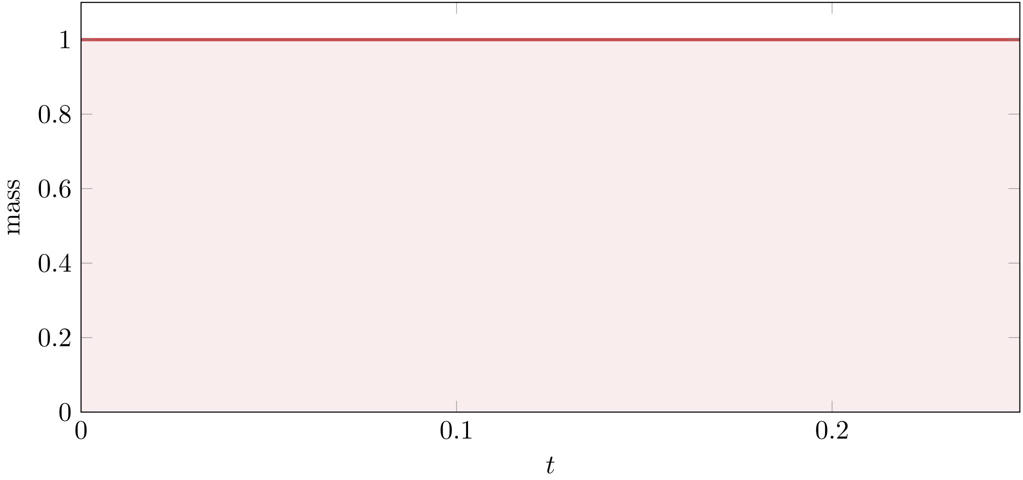

The associated test function for energy conservation is

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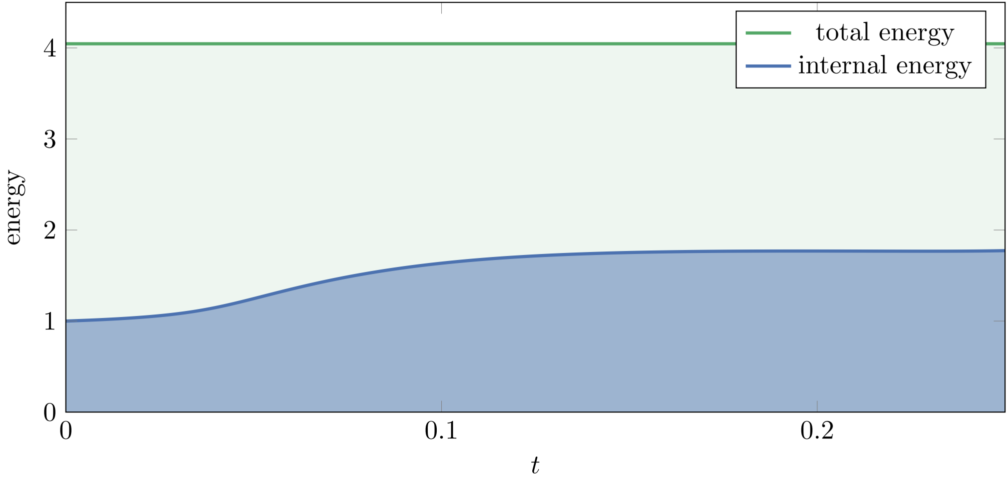

The associated test function for entropy dissipation is

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

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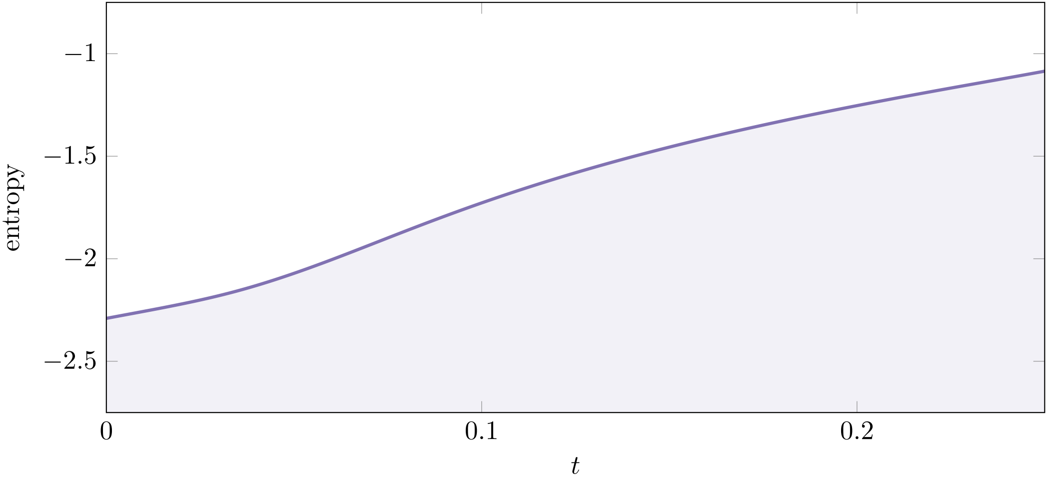

Section 7

The Kepler problem

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

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

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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

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

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

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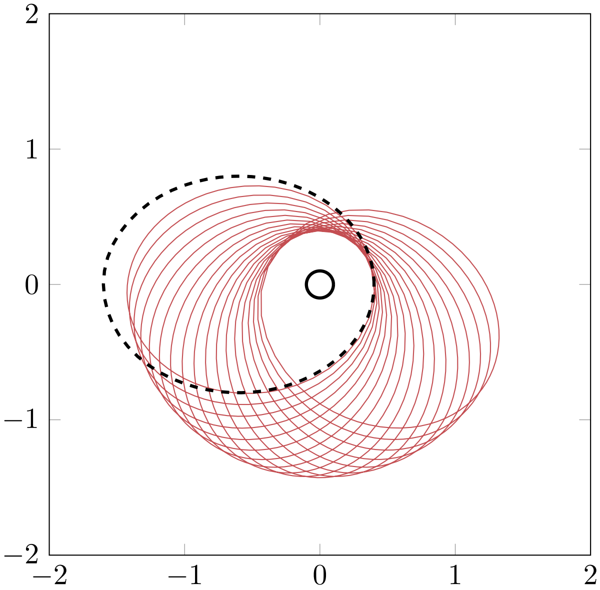
Setting $s = 1$ and approximating the integrals with a one-point Gauss–Legendre quadrature rule yields the familiar implicit midpoint scheme.



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 $\widetilde{\nabla H} \in \dot{\mathbb{X}}$;
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Energy-conserving discretisation (formal)

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

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

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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

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

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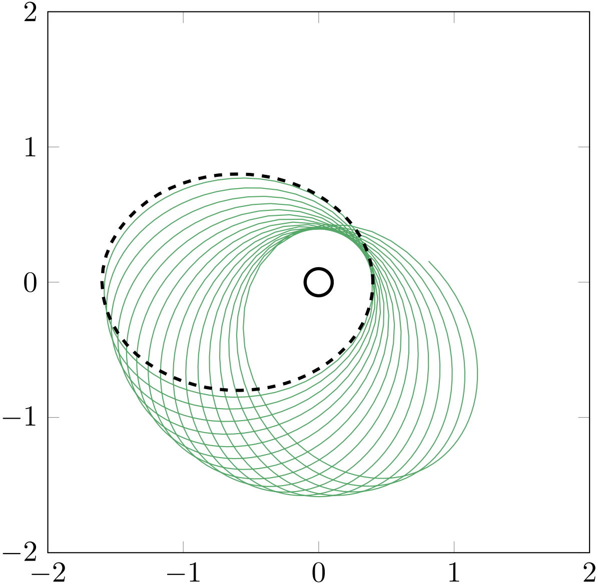
for all $\mathbf{y} \in \dot{\mathbb{X}}$.

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 $\widetilde{\nabla A_1}, \widetilde{\nabla A_2} \in \dot{\mathbb{X}}$;
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We compute δB by minimising its Frobenius norm subject to skew-symmetry and the orthogonality above. It requires solving an independent 2×2 linear system at each quadrature point.

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

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

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

$$\int_{t_n}^{t_{n+1}} \mathbf{y}_2^\top \widetilde{\nabla A_1} \ \mathrm{d}t = \int_{t_n}^{t_{n+1}} \mathbf{y}_2^\top \nabla A_1 \ \mathrm{d}t$$

$$\int_{t_n}^{t_{n+1}} \mathbf{y}_3^\top \widetilde{\nabla A_2} \ \mathrm{d}t = \int_{t_n}^{t_{n+1}} \mathbf{y}_3^\top \nabla A_2 \ \mathrm{d}t$$

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

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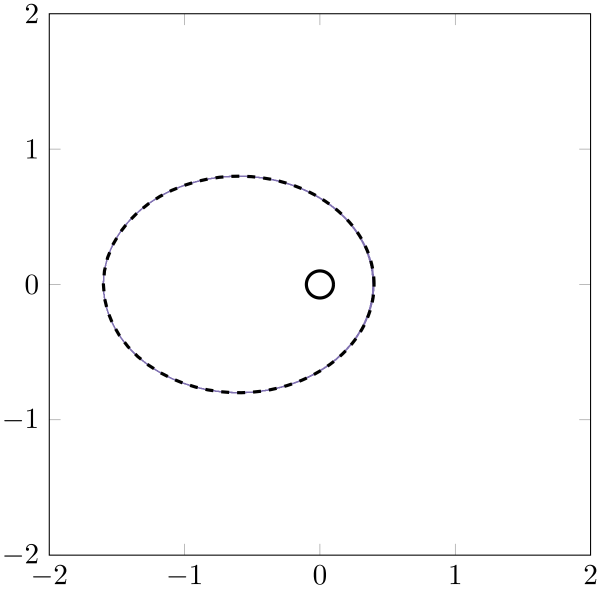
Again, this can be rewritten purely as a problem in $\mathbf{x}$.



Our scheme:

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

Section 8

Hamiltonian PDE

The Benjamin–Bona–Mahony equation

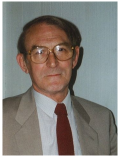
$$u_t + u_x + uu_x - u_{xxt} = 0, \quad u(-50) = u(50),$$

has a Hamiltonian structure:

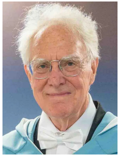
$$\left(\mathrm{id} - \partial_x^2\right) \dot{u} = -\partial_x H'(u),$$

with Hamiltonian

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



T. Brooke Benjamin



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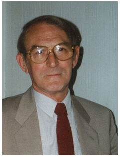
The equation has exactly two other invariants:

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

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



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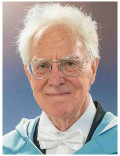

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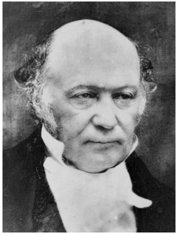
John Joseph Mahony

Our general formulation is

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

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



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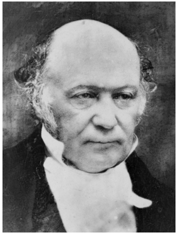
This conserves the Hamiltonian, by the usual argument:

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



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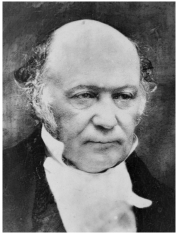

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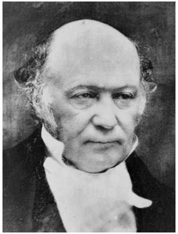

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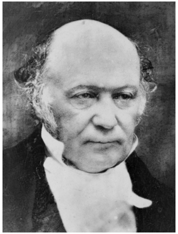

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Following a similar analysis, it turns out that the right auxiliary variable to use is

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

which is not obvious (to me).

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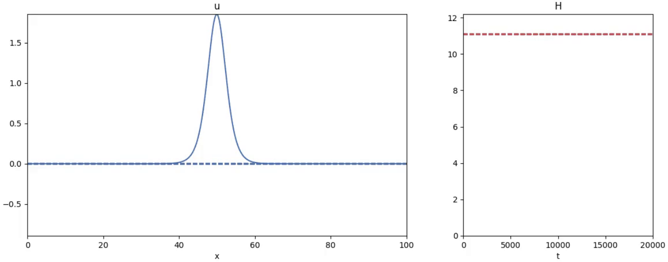
Energy-conserving discretisation

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.



Simulation near $t = 0$.

Carl Friedrich Gauss

Gauss method:

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

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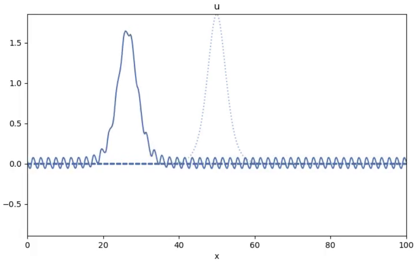

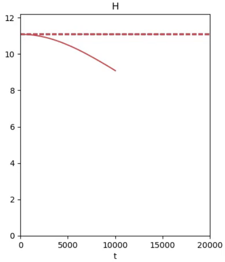

Simulation near $t = 10000$.

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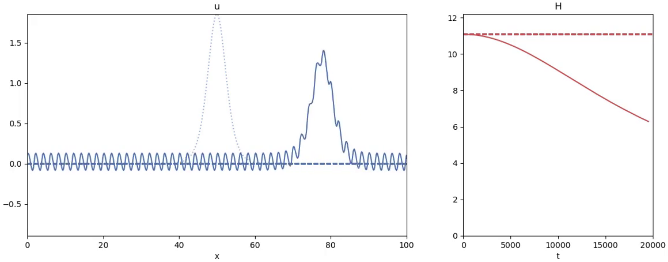

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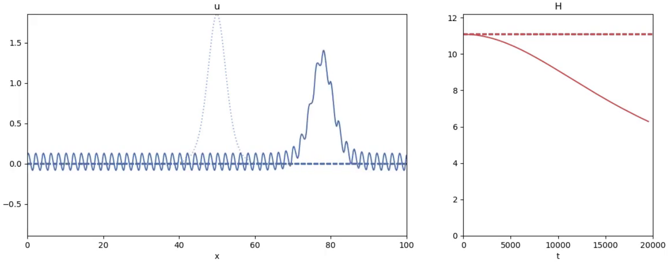

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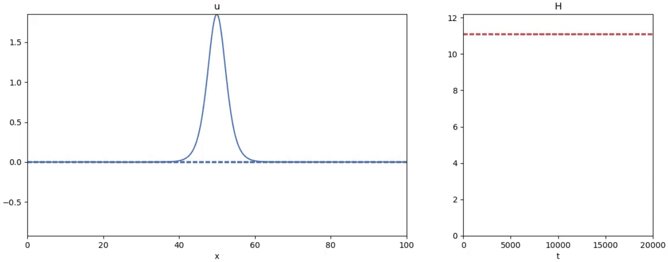
Spurious oscillations

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

The same soliton, again:



Simulation near $t = 0$.

Boris Andrews

AV–CPG method:

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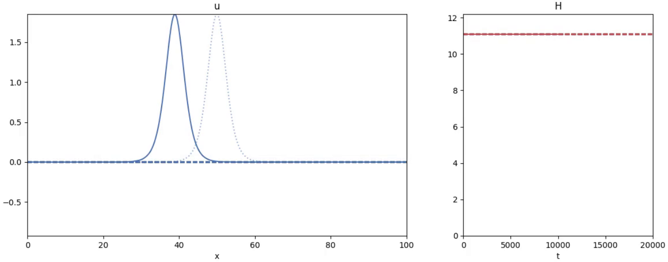
- ✓ H^1-norm
- ✓ energy

The same soliton, again:



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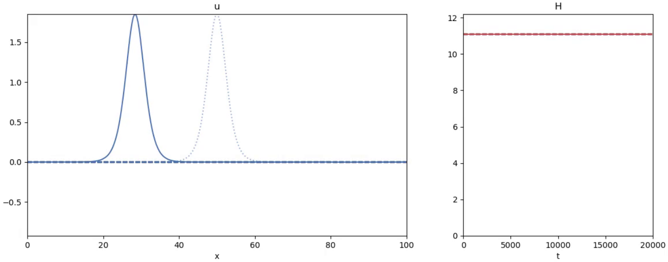

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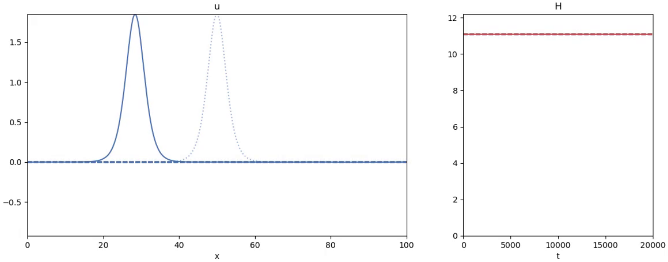

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Good news

Soliton character is preserved even over very long timescales.

Section 9

Conclusions

Good news

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

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Potential applications

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