

Designing conservative and accurately dissipative numerical integrators in time

Patrick E. Farrell

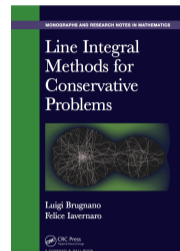
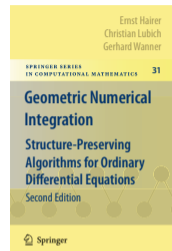
Boris Andrews



University of Oxford

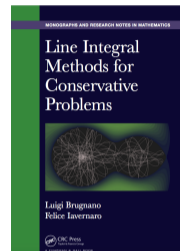
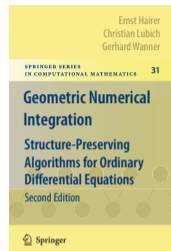
June 13 2024

Structure preservation means different things in different contexts.



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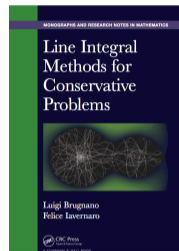
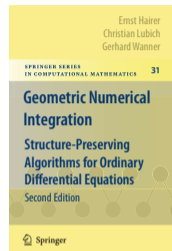
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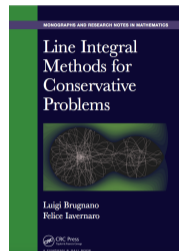
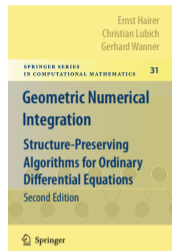
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conservation	dissipation



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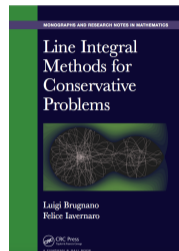
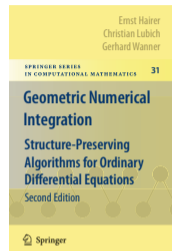
Symplecticity

The differential equation preserves the symplectic 2-form.

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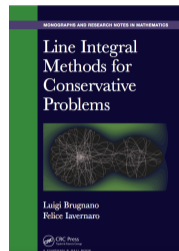
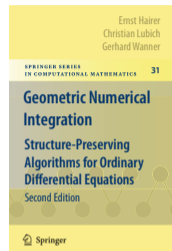
Reversibility

Negating the initial velocity only inverts the direction of motion.

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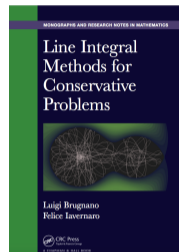
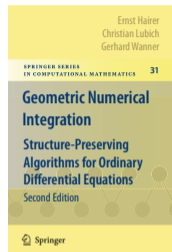
Conservation

The equation preserves invariants, like energy or angular momentum.

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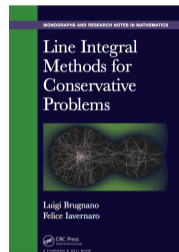
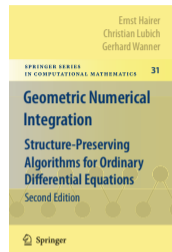
Dissipation

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

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



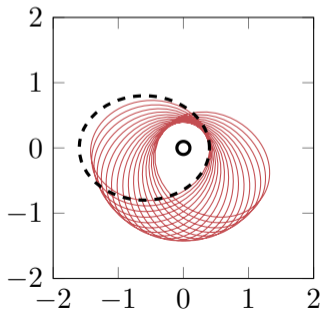
Johannes Kepler

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Implicit midpoint:

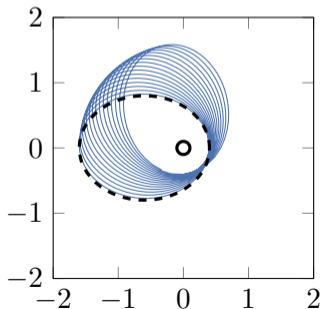
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- ✓ angular momentum
- ✓ energy
- ✗ orientation (LRL)

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LaBudde–Greenspan:

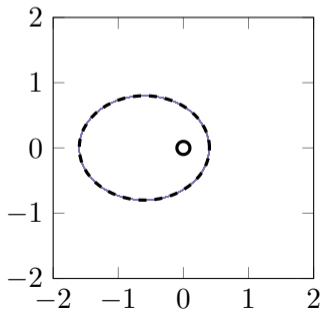
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Johannes Kepler

Our discretisation:

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

The Kovalevskaya top is described by

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

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



Sofya Kovalevskaya

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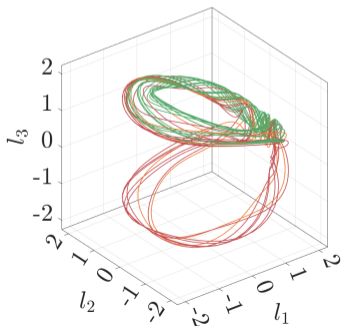
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Implicit midpoint:

- ✓ symplecticity
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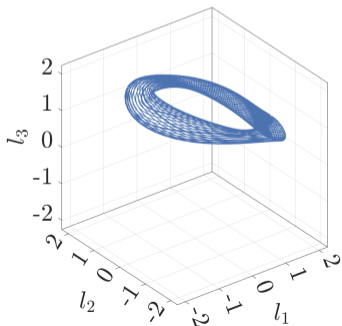
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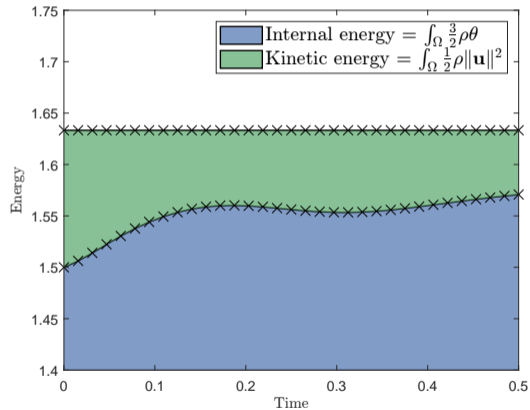
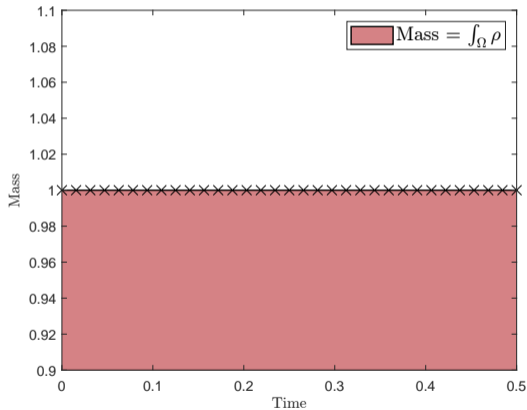
Sofya Kovalevskaya



Our discretisation:

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

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

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

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

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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

$$u(t_n) = u_n,$$

and s other *test conditions*.

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Collocation Runge–Kutta test conditions

Demand that

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

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

We can rewrite the collocation Runge–Kutta test conditions:

Collocation Runge–Kutta test conditions, rephrased (I)

Demand that

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

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

Or we could write them as:

Collocation Runge–Kutta test conditions, rephrased (II)

Demand that

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

for all $v \in \text{span}(\delta_{c_1}, \dots, \delta_{c_s})$.

Collocation Runge–Kutta test conditions, rephrased (II)

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$$\int_{t_n}^{t_{n+1}} i v \, dt = \int_{t_n}^{t_{n+1}} f(u) v \, dt,$$

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The natural FET scheme instead chooses another test set:

Continuous Petrov–Galerkin (cPG) test conditions

Demand that

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

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

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In other words, each conservation law has an

associated test function.

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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.

We call this approach the

auxiliary-variable continuous Petrov–Galerkin (AV-CPG)

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framework.

- 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:

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

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

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v) \, dt = \int_{t_n}^{t_{n+1}} [(u \times (\nabla \times u), v) - \operatorname{Re}^{-1}(\nabla u, \nabla v)] \, dt$$

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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 $s - 1$.

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

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In this example, we care about the dissipation of energy

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

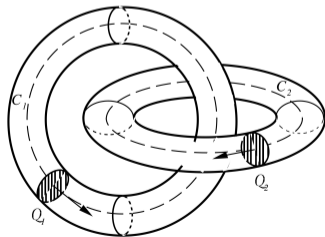
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and the change in *helicity*, a topological measure of the knottedness of the flow,

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



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:

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

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

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

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 \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 \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

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v) \, dt = \int_{t_n}^{t_{n+1}} [(u \times (\nabla \times u), v) - \operatorname{Re}^{-1}(\nabla u, \nabla v)] \, dt,$$

$$\int_{t_n}^{t_{n+1}} (w_1, v_1) \, dt = \int_{t_n}^{t_{n+1}} (u, v_1) \, dt,$$

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

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

$$\int_{t_n}^{t_{n+1}} (\dot{u}, v) \, dt = \int_{t_n}^{t_{n+1}} [(\underline{w_1} \times \underline{w_2}, v) - \operatorname{Re}^{-1}(\nabla \underline{w_1}, \nabla v)] \, dt,$$

$$\int_{t_n}^{t_{n+1}} (w_1, v_1) \, dt = \int_{t_n}^{t_{n+1}} (u, v_1) \, dt,$$

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

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!

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

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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](https://doi.org/10.1137/060651227).



Leo Rebholz

For the compressible Navier–Stokes equations,

$$\dot{\rho} = -\operatorname{div}[\rho u],$$

$$\rho \dot{u} = -\rho u \cdot \nabla u - \nabla[\rho \theta] + \frac{2}{\operatorname{Re}_\mu} \operatorname{div}[\rho \varepsilon[u]] + \frac{1}{\operatorname{Re}_\zeta} \nabla[\rho \operatorname{div} u],$$

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

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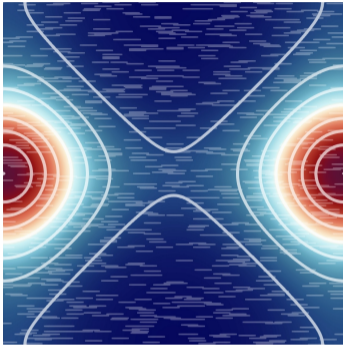
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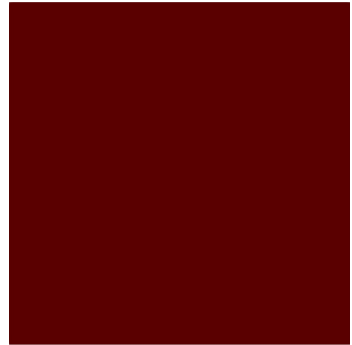
- ▶ mass conservation;
- ▶ momentum conservation;
- ▶ energy conservation;
- ▶ entropy dissipation.



velocity

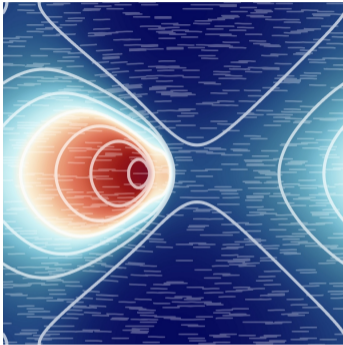


density

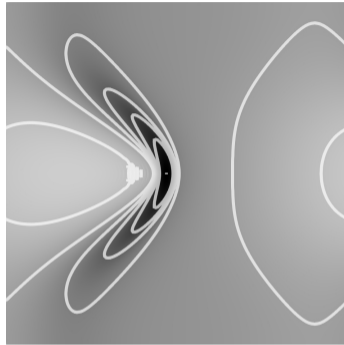


temperature

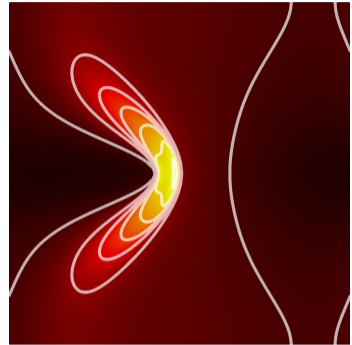
Supersonic compressible Navier–Stokes simulation



velocity

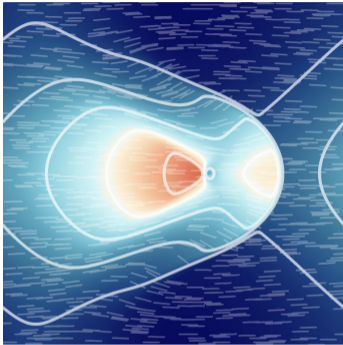


density

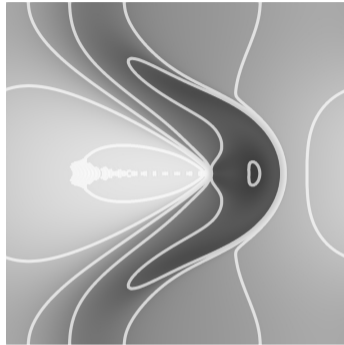


temperature

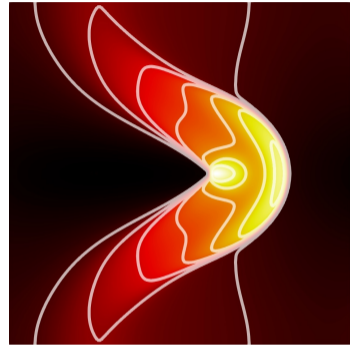
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velocity



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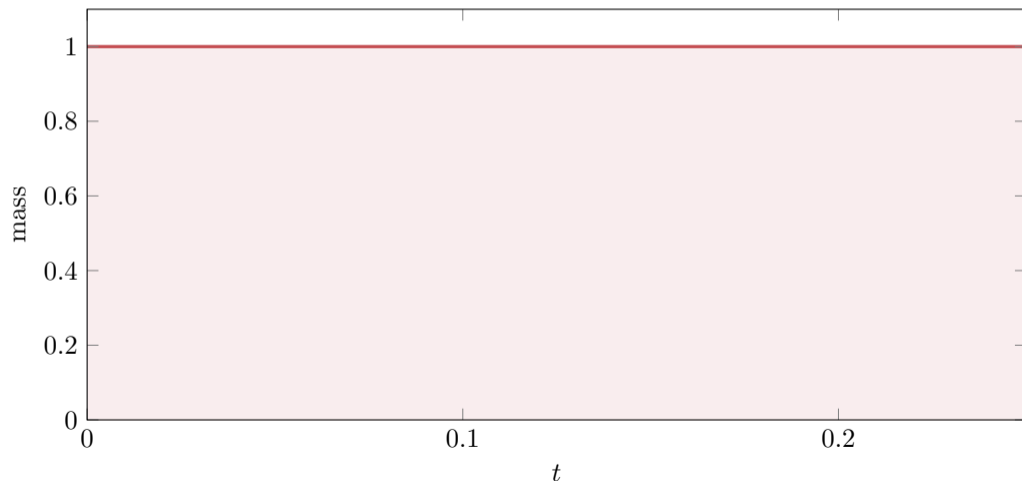
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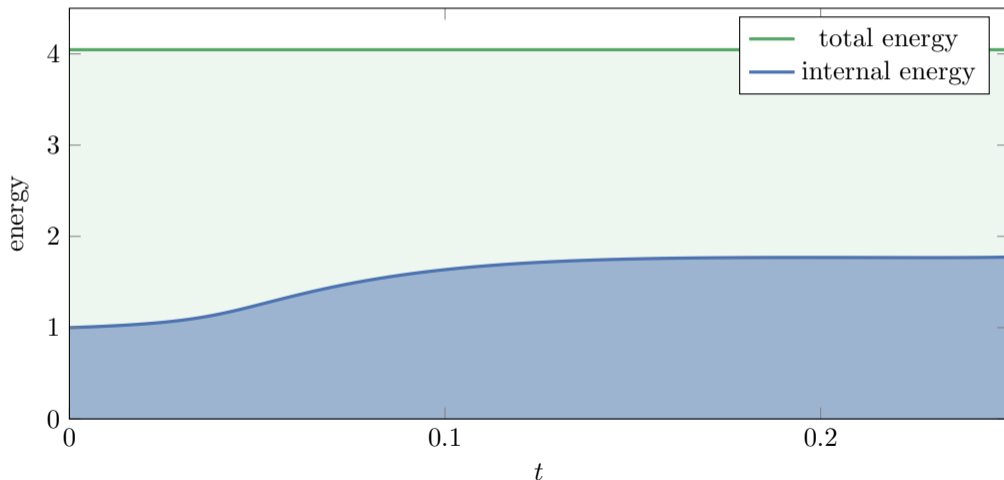


The associated test function for energy conservation is

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

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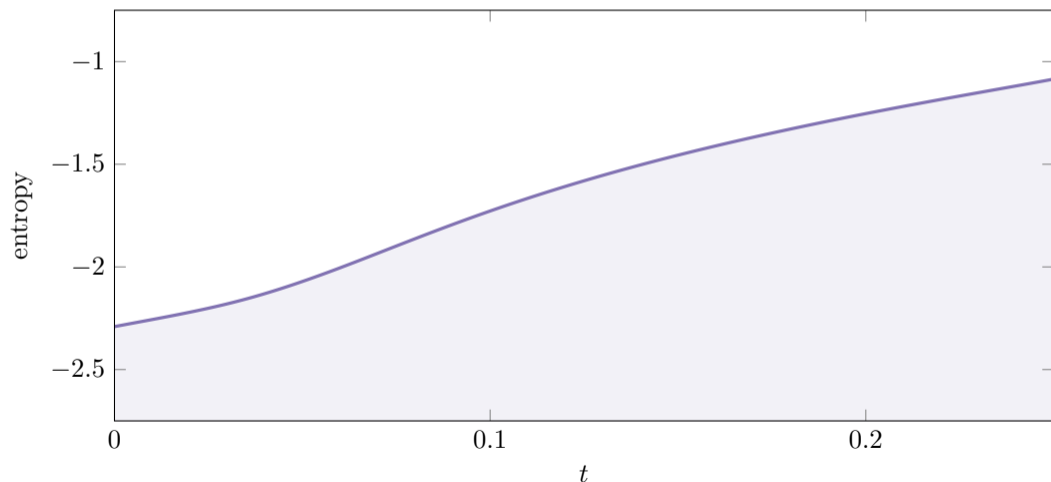


The associated test function for entropy dissipation is

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

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Section 7

The Kepler problem

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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

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

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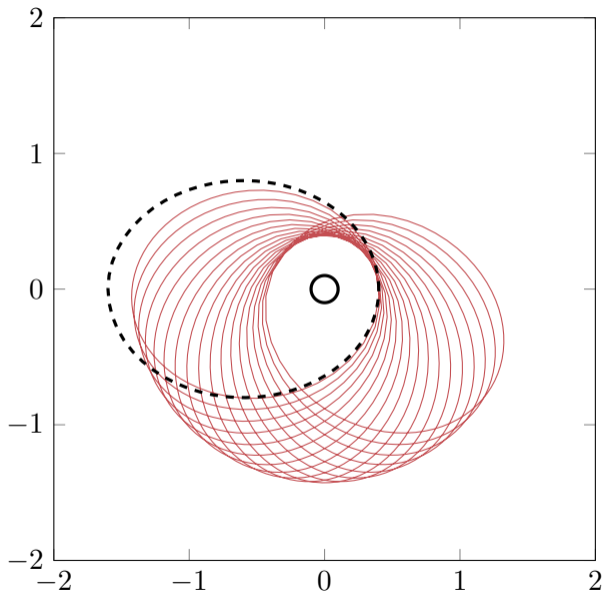
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Setting $s = 1$ and approximating the integrals with a one-point Gauss–Legendre quadrature rule yields the familiar implicit midpoint scheme.



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

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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

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

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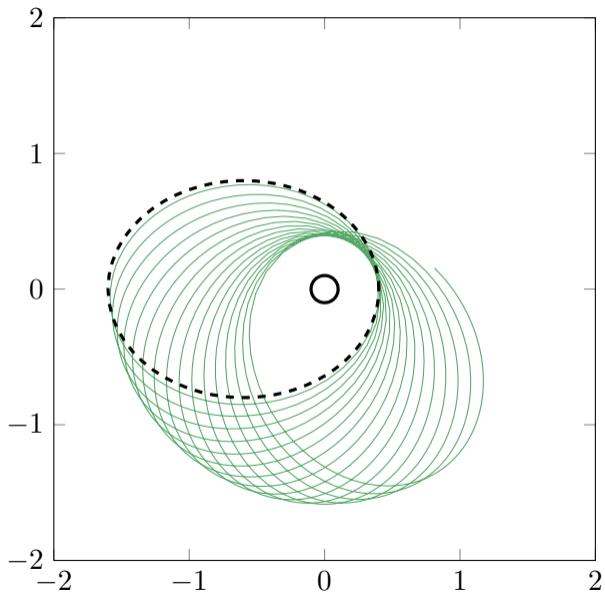
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for all $\mathbf{y} \in \dot{\mathbb{X}}$.

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 need to modify the right-hand side so that

$$\widetilde{\nabla A}_j(B + \delta B)\widetilde{\nabla H} = 0, \quad j = 1, 2,$$

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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

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

$$\int_{t_n}^{t_{n+1}} \mathbf{y}_1^\top \widetilde{\nabla H} \, dt = \int_{t_n}^{t_{n+1}} \mathbf{y}_1^\top \nabla H \, dt$$

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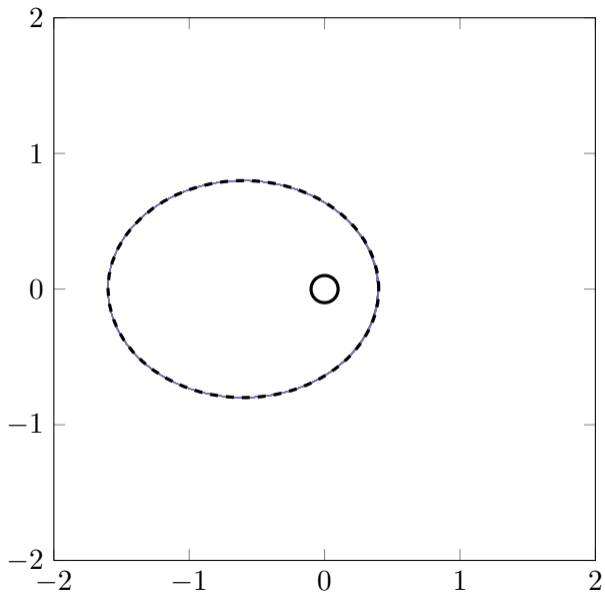
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Again, this can be rewritten purely as a problem in \mathbf{x} .



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:

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

with Hamiltonian

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



T. Brooke Benjamin



Jerry Bona



John Joseph Mahony

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The equation has exactly two other invariants:

$$I_1(u) = \int_{\Omega} u \, dx,$$

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



T. Brooke Benjamin



Jerry Bona

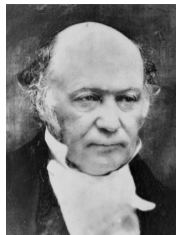


John Joseph Mahony

Our general formulation is

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

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



William Rowan Hamilton

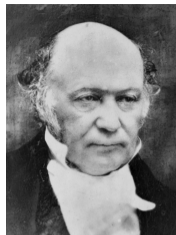
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$$H(u(t_{n+1})) - H(u(t_n)) = \int_{t_n}^{t_{n+1}} \dot{H} dt$$



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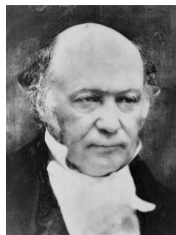
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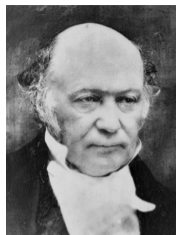
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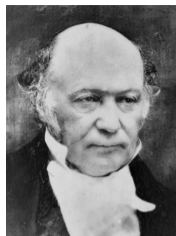
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William Rowan Hamilton

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

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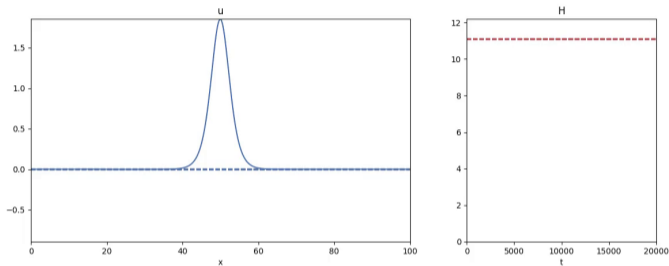
Energy-conserving discretisation

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

$$\begin{aligned} \int_{t_n}^{t_{n+1}} v M[\dot{u}] \, dt &= \int_{t_n}^{t_{n+1}} v B M^*[w_1] \, dt \\ \int_{t_n}^{t_{n+1}} w_1 M[v_1] \, dt &= \int_{t_n}^{t_{n+1}} H'[u] v_1 \, dt \end{aligned}$$

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 $t = 0$.

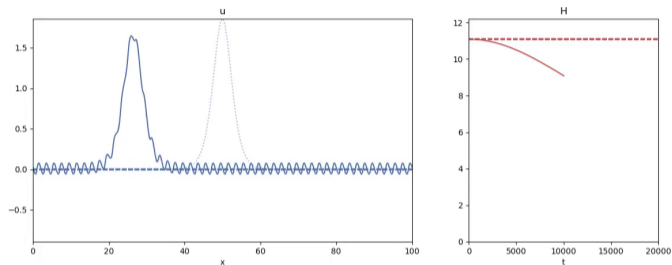


Carl Friedrich Gauss

Gauss method:

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

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Simulation near $t = 10000$.

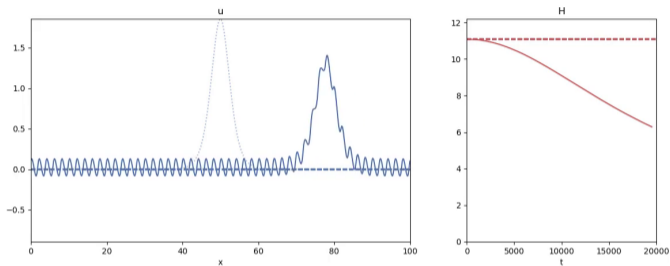


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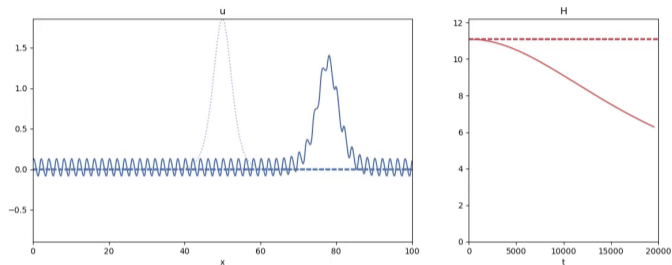


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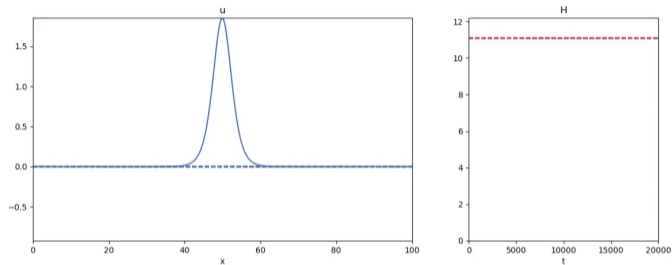
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Spurious oscillations

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

The same soliton, again:



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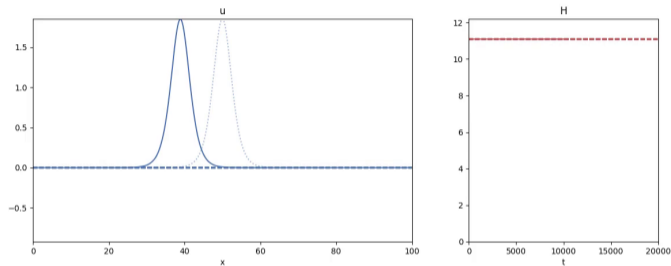


Boris Andrews

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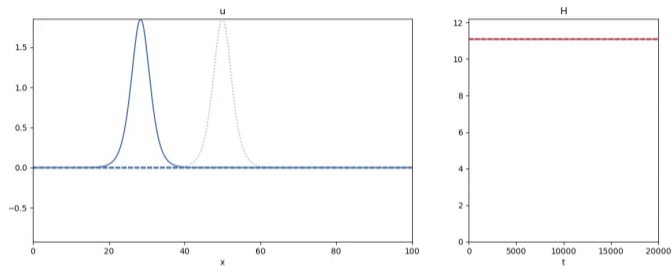


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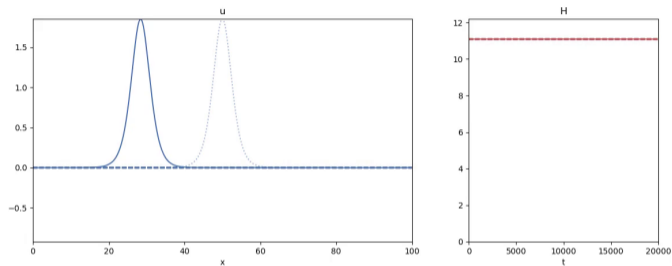


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Good news

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