# High-order conservative and accurately dissipative numerical integrators via finite elements in time


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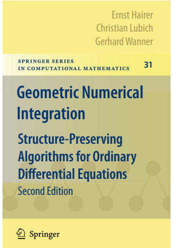
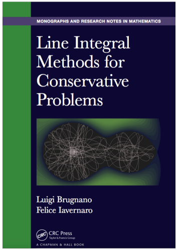
April 4 2024

Structure preservation means different things in different contexts.



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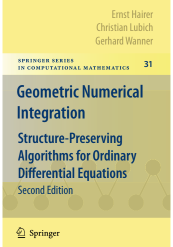


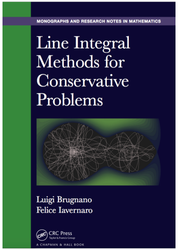

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Here are four properties an initial value problem might have:

| | |
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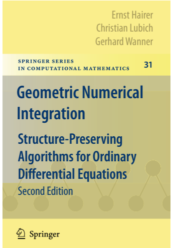
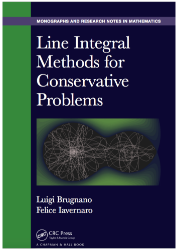
| symplecticity | reversibility |
| conservation | dissipation |



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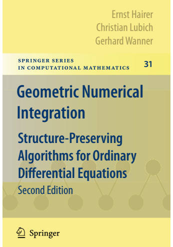


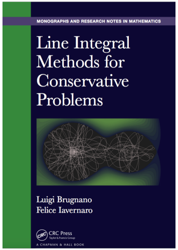


## Symplecticity

The differential equation preserves the symplectic 2-form.

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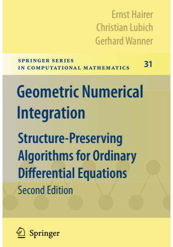


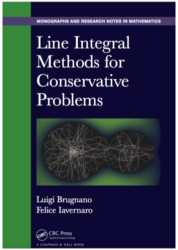


## Reversibility

Negating the initial velocity only inverts the direction of motion.

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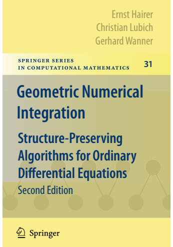


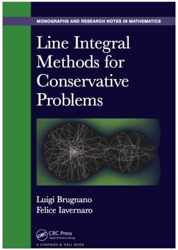


## Conservation

The equation preserves invariants, like energy or angular momentum.

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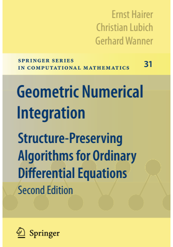


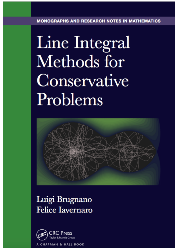


## Dissipation

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

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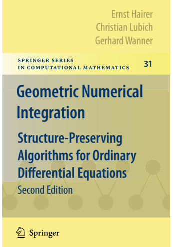
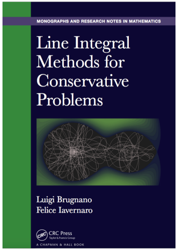



## This talk

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

…without projections onto manifolds or Lagrange multipliers.

Section 1

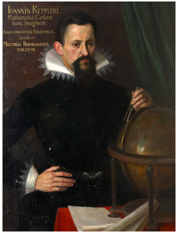
# Examples

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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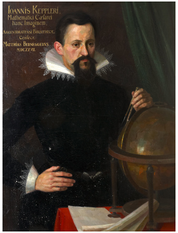


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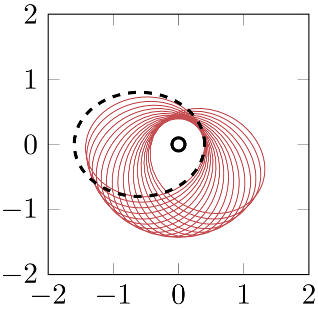


Implicit midpoint:

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

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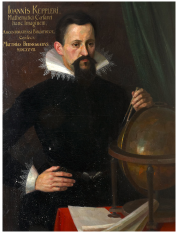

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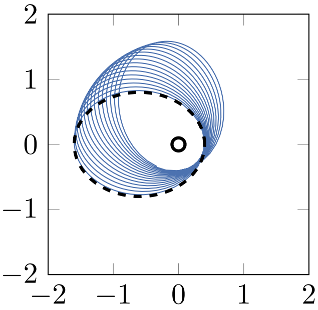


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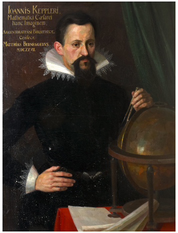


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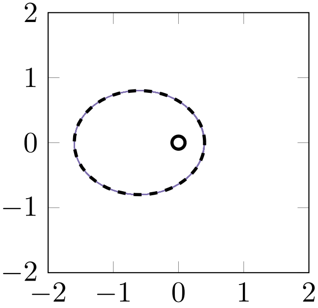


Our discretisation:

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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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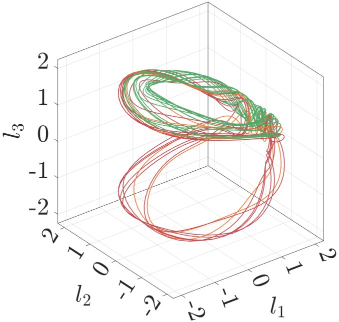


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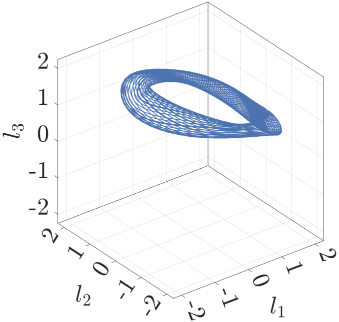


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This approach extends to more complicated problems. The compressible Navier–Stokes equations conserve both mass and energy:

$$M = \int_\Omega \rho \, \mathrm{d}x, \quad E = \int_\Omega \frac{1}{2}\rho\|\mathbf{u}\|^2 + \frac{3}{2}\rho\theta \, \mathrm{d}x.$$

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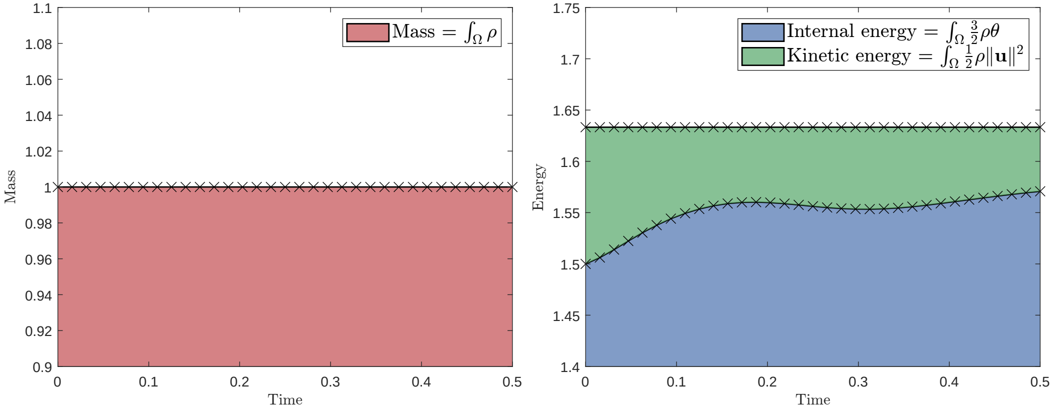

Section 2

# 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 $t = t_n + c_1 \Delta t, t_n + c_2 \Delta t, \ldots, t_n + c_s \Delta t$.

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 $i = 1, \ldots, s$.

Or we could write them as:

## Collocation Runge–Kutta test conditions, rephrased (II)

Demand that

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

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The natural FET scheme instead chooses another test set:

## Continuous Petrov–Galerkin (cPG) test conditions

Demand that

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

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

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## Conservation laws

Conservation laws naturally arise from variational statements:

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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

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framework.

**A.** Define the base timestepping scheme.
**B.** Identify the test functions for the structures to preserve.
**C.** Introduce corresponding auxiliary variables.
**D.** Modify the right-hand side of the weak formulation.

Section 3

# Navier–Stokes equations

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

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

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

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

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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,

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

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

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

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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} (\dot{u}, \nabla \times u) \ \mathrm{d}t \\
&= \int_{T_n} \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} (\nabla u, \nabla \nabla \times u) \ \mathrm{d}t.
\end{aligned}
$$

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

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

## **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

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

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

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

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!

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

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$$
\begin{aligned}
E(u_{n+1}) - E(u_n) &= \int_{T_n} (\dot{u}, u)\ \mathrm{d}t \\
&= \int_{T_n} (\dot{u}, w_1)\ \mathrm{d}t
\end{aligned}
$$

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&= \int_{T_n} \left[ (w_1 \times w_2, w_1) - \mathrm{Re}^{-1} (\nabla w_1, \nabla w_1) \right] \ \mathrm{d}t,
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&= -\mathrm{Re}^{-1} \int_{T_n} \|\nabla w_1\|^2 \ \mathrm{d}t \leq 0.
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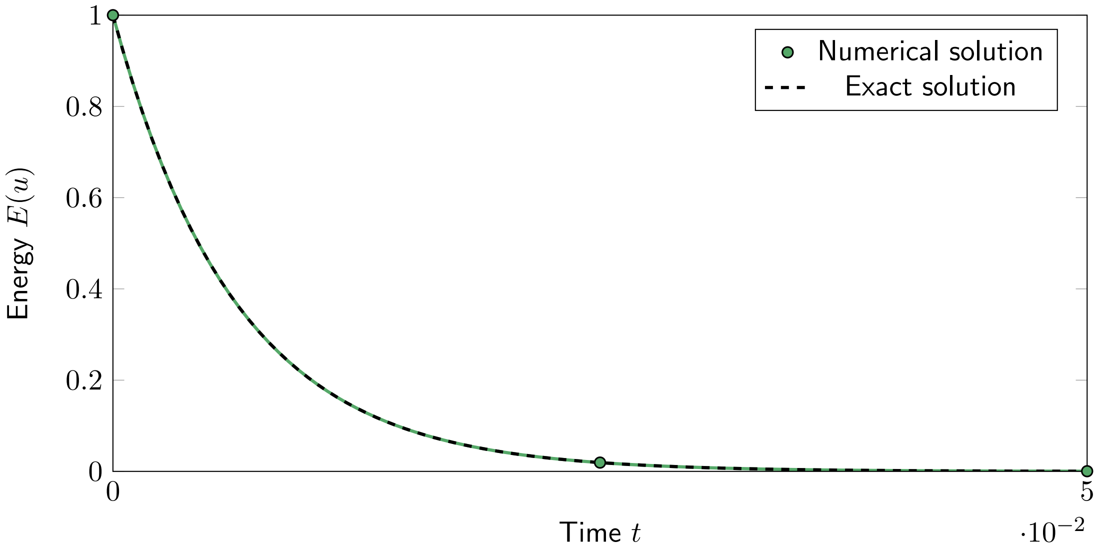
\end{aligned}
$$

We therefore recover a conservation law in the ideal limit.




Energy dissipation for a Taylor–Green vortex.

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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the associated test function for mass conservation is

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

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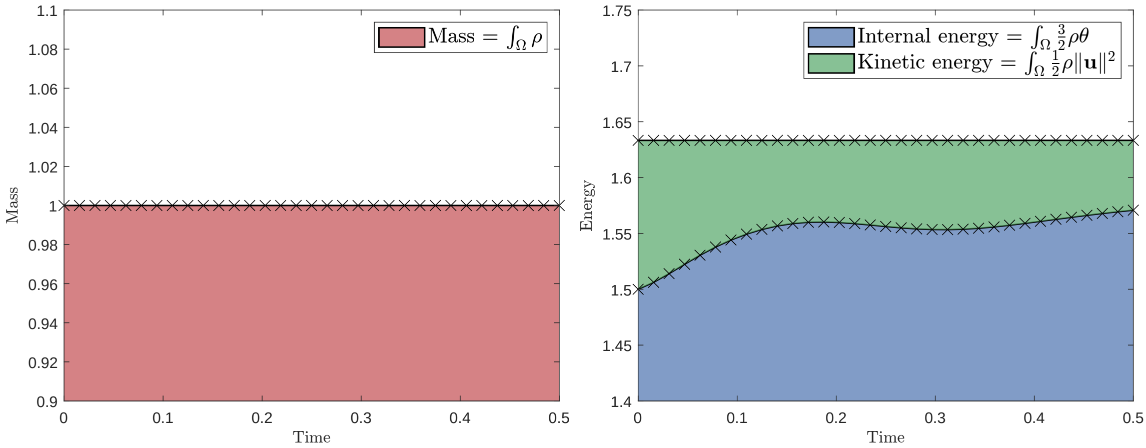
\end{aligned}
$$

the associated test function for mass conservation is

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

and the associated test function for energy conservation is

$$\tilde{\rho} = \|u\|^2, \quad \tilde{u} = u, \quad \tilde{\theta} = 1.$$



Mass = $\int_\Omega \rho$
Mass
Time
1.1
1.08
1.06
1.04
1.02
1
0.98
0.96
0.94
0.92
0.9
0
0.1
0.2
0.3
0.4
0.5
Internal energy = $\int_\Omega \frac{3}{2}\rho\theta$
Kinetic energy = $\int_\Omega \frac{1}{2}\rho\|\mathbf{u}\|^2$
Energy
Time
1.75
1.7
1.65
1.6
1.55
1.5
1.45
1.4
0
0.1
0.2
0.3
0.4
0.5

Section 4

# 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 $\mathbf{x} \in \mathbb{X} := \{\mathbf{y} \in P^s(T_n, \mathbb{R}^4) : \mathbf{y}(t_n) = \mathbf{x}_n\}$ such that

$$\int_{T_n} \mathbf{y}^\top \dot{\mathbf{x}} \, \mathrm{d}t = \int_{T_n} \mathbf{y}^\top B \nabla H(\mathbf{x}) \, \mathrm{d}t$$

for all $\mathbf{y} \in \dot{\mathbb{X}} := P^{s-1}(T_n, \mathbb{R}^4)$.

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**Base cPG discretisation**

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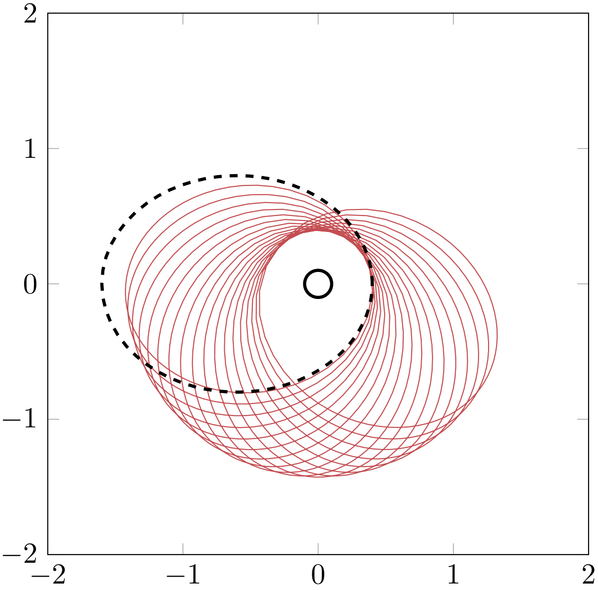
for all $\mathbf{y} \in \dot{\mathbb{X}} := P^{s-1}(T_n, \mathbb{R}^4)$.

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.

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## Energy-conserving discretisation (formal)

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

$$\int_{T_n} \mathbf{y}^\top \dot{\mathbf{x}} \, \mathrm{d}t = \int_{T_n} \mathbf{y}^\top B \widetilde{\nabla H} \, \mathrm{d}t$$

$$\int_{T_n} \mathbf{y}_1^\top \widetilde{\nabla H} \, \mathrm{d}t = \int_{T_n} \mathbf{y}_1^\top \nabla H \, \mathrm{d}t$$

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

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- compute an approximate $\widetilde{\nabla H} \in \dot{\mathbb{X}}$;
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$$\int_{T_n} \mathbf{y}_1^\top \widetilde{\nabla H} \,\mathrm{d}t = \int_{T_n} \mathbf{y}_1^\top \nabla H \,\mathrm{d}t$$

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 $\nabla H$; 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

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

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

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**Energy-conserving discretisation (practical)**

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

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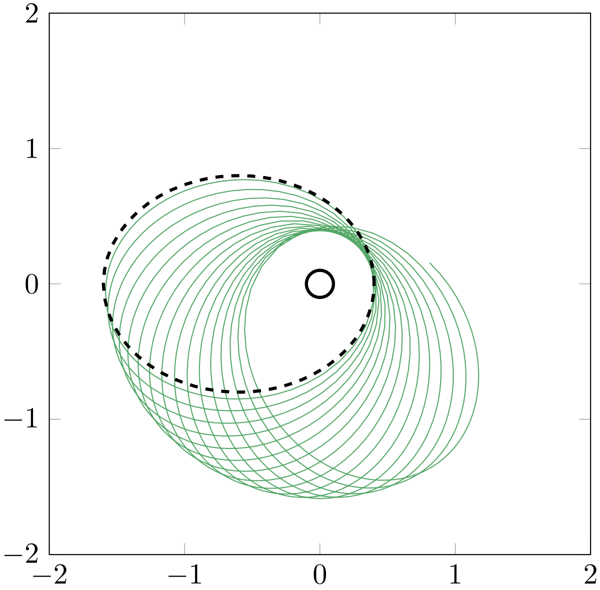
for all $\mathbf{y} \in \dot{\mathbb{X}}$.

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

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We need to modify the right-hand side so that

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

where $\delta B$ is a $\mathcal{O}(\delta t^{s+1})$ skew-symmetric perturbation.

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

where $\delta B$ is a $\mathcal{O}(\delta t^{s+1})$ skew-symmetric perturbation.

We compute $\delta B$ by minimising its Frobenius norm subject to skew-symmetry and the orthogonality above. It requires solving an independent $2 \times 2$ 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

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

$$\int_{T_n} \mathbf{y}_1^\top \widetilde{\nabla H} \, \mathrm{d}t = \int_{T_n} \mathbf{y}_1^\top \nabla H \, \mathrm{d}t$$

$$\int_{T_n} \mathbf{y}_2^\top \widetilde{\nabla A_1} \, \mathrm{d}t = \int_{T_n} \mathbf{y}_2^\top \nabla A_1 \, \mathrm{d}t$$

$$\int_{T_n} \mathbf{y}_3^\top \widetilde{\nabla A_2} \, \mathrm{d}t = \int_{T_n} \mathbf{y}_3^\top \nabla A_2 \, \mathrm{d}t$$

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

## 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

$$\begin{aligned}
\int_{T_n} \mathbf{y}^\top \dot{\mathbf{x}} \, \mathrm{d}t &= \int_{T_n} \mathbf{y}^\top (B + \delta B) \widetilde{\nabla H} \, \mathrm{d}t \\
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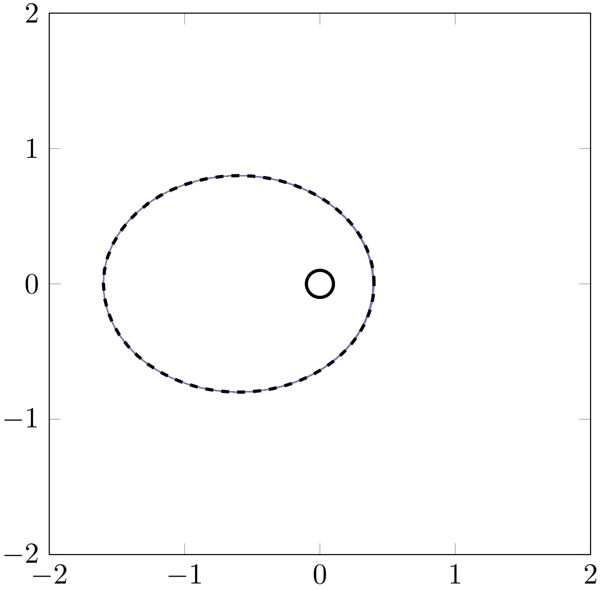
\int_{T_n} \mathbf{y}_2^\top \widetilde{\nabla A_1} \, \mathrm{d}t &= \int_{T_n} \mathbf{y}_2^\top \nabla A_1 \, \mathrm{d}t \\
\int_{T_n} \mathbf{y}_3^\top \widetilde{\nabla A_2} \, \mathrm{d}t &= \int_{T_n} \mathbf{y}_3^\top \nabla A_2 \, \mathrm{d}t
\end{aligned}$$

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)

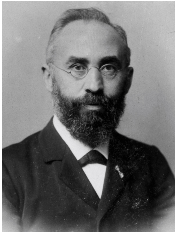
Section 5

# Current work: charged particles in electromagnetic fields

The motion of a charged particle in an electromagnetic field is described by

$$\dot{\mathbf{x}} = \mathbf{v},$$
$$\dot{\mathbf{v}} = \mathbf{E} + \Omega \mathbf{v} \times \mathbf{B},$$

where $\Omega$ is the (nondimensional, large) gyrofrequency.



Hendrik Lorentz

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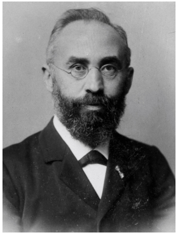

Hendrik Lorentz

This is a Hamiltonian system with

$$H(\mathbf{x}, \mathbf{v}) = \phi(\mathbf{x}) + \frac{1}{2}\|\mathbf{v}\|^2,$$

where $\mathbf{E} = -\nabla\phi$, inducing the differential equations

$$\begin{pmatrix} \dot{\mathbf{x}} \\ \dot{\mathbf{v}} \end{pmatrix} = \begin{pmatrix} & I \\ -I & -\Omega \mathbf{B}\times \end{pmatrix} \begin{pmatrix} \nabla_{\mathbf{x}} H \\ \nabla_{\mathbf{v}} H \end{pmatrix}.$$

Two quantities of major concern are the *magnetic moment*,

$$\mu = \frac{\|\mathbf{v}_\perp\|^2}{2\Omega\|\mathbf{B}\|},$$

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These vary with timescale $\Omega \gg 1$, whereas $\mathbf{v}$ varies with $\Omega^{-1} \ll 1$.

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$$\xi = \mathbf{x} + \frac{1}{\Omega\|\mathbf{B}\|^2}\mathbf{v} \times \mathbf{B}.$$

These vary with timescale $\Omega \gg 1$, whereas $\mathbf{v}$ varies with $\Omega^{-1} \ll 1$.

The standard algorithm for this problem, the Boris algorithm, gives excellent performance . . .

Jay Paul Boris

Two quantities of major concern are the *magnetic moment*,

$$\mu = \frac{\|\mathbf{v}_\perp\|^2}{2\Omega\|\mathbf{B}\|},$$

and the *gyrocentre*,

$$\xi = \mathbf{x} + \frac{1}{\Omega\|\mathbf{B}\|^2}\mathbf{v} \times \mathbf{B}.$$

These vary with timescale $\Omega \gg 1$, whereas $\mathbf{v}$ varies with $\Omega^{-1} \ll 1$.

The standard algorithm for this problem, the Boris algorithm, gives excellent performance . . .

. . . but requires very small timesteps, of about

$$\Delta t \approx (2\Omega)^{-1}$$

to accurately capture gyrocentre drifts and conserve the magnetic moment with varying $\mathbf{B}$.

Jay Paul Boris

## Current research

Can we devise a provably

- energy-conserving,
- asymptotic-preserving (for $\mu$ and $\xi$),
- arbitrary-order,

timestepping scheme that works with timesteps of size $\mathcal{O}(1)$?

## 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 . . . .