Practical methods for geometric integration

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Outline

- Conserving invariants and methods on manifolds
- Symplectic and symmetric methods for Hamiltonian ODE systems
- Symplectic and multisymplectic methods for PDEs

Geometric Integration (GI): Structure Preserving Algorithms

A dynamical system defined by a differential system (DE) typically has some structure. A numerical discretization algorithm for the DE may or may not reproduce this structure exactly.

- **Geometrical structure**: Properties of the phase space.
- **Conservation laws**: Conservation of total quantities such as mass, energy and momentum; casimirs along trajectories; etc.
- **Symmetries**: Galilean symmetries such as translations, reflexions and rotations; time reversal; scaling; Lie group symmetries such as the invariance of a mechanical system to the action of the rotation group SO(3).

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- **Symmetries**: Galilean symmetries such as translations, reflexions and rotations; time reversal; scaling; Lie group symmetries such as the invariance of a mechanical system to the action of the rotation group SO(3).
- **Asymptotic behaviour**: These are the usual dynamical system features.
- **Ordering in the solutions**: For instance, the maximum principle and solution comparisons.

Instances and examples

- Hamiltonian ODEs: symplectic maps
- Constrained mechanical systems
- Hamiltonian PDEs: symplectic and multisymplectic maps
- Conservation laws

Hamiltonian ODEs: symplectic maps

$$q_i' = \frac{\partial H}{\partial p_i}, \qquad\qquad i = 1, \ldots, l.$$
$$p_i' = -\frac{\partial H}{\partial q_i},$$

In vector form

$$\mathbf{q}' = \boldsymbol{\nabla}_{\mathbf{p}} H(\mathbf{q}, \mathbf{p}), \quad \mathbf{p}' = -\boldsymbol{\nabla}_{\mathbf{q}} H(\mathbf{q}, \mathbf{p}) \, .$$

Hamiltonian $H(\mathbf{q}, \mathbf{p})$ (total energy) remains constant:

$$H(\mathbf{q}(t), \mathbf{p}(t)) = H(\mathbf{q}(0), \mathbf{p}(0)) = H(\mathbf{q}_0, \mathbf{p}_0)$$

Famous applications:

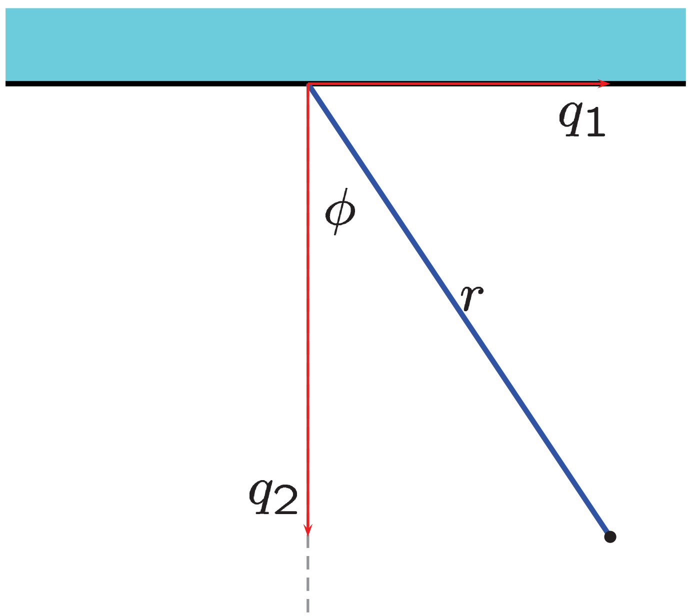
- Celestial mechanics
- Molecular dynamics

Example: Stiff spring pendulum

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2}\mathbf{p}^T\mathbf{p} + (\phi(\mathbf{q}) - \phi_0)^2 + \varepsilon^{-2}(r(\mathbf{q}) - r_0)^2.$$

This Hamiltonian is in separable form.

Stiff spring pendulum



Example: Linear harmonic oscillator

$$H = \frac{\omega}{2}(p^2 + q^2)$$

yields the linear equations of motion

$$q' = \omega p, \quad p' = -\omega q$$

or

$$\begin{pmatrix} q \\ p \end{pmatrix}' = \omega J \begin{pmatrix} q \\ p \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Here $\omega > 0$ is a known parameter. General solution is

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \cos \omega t & \sin \omega t \\ -\sin \omega t & \cos \omega t \end{pmatrix} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix}.$$

General solution is

$$\begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} \cos\omega t & \sin\omega t \\ -\sin\omega t & \cos\omega t \end{pmatrix} \begin{pmatrix} q(0) \\ p(0) \end{pmatrix} .$$

Hence, $S(t)B$ is just a rotation of the set B at a constant rate depending on ω.

In general,

$$\mathbf{y}' = J\boldsymbol{\nabla} H(\mathbf{y}) \quad \text{where } \mathbf{y} = \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}, \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

Jacobian,

$$Y(t;\mathbf{c}) = \frac{\partial \mathbf{y}(t;\mathbf{c})}{\partial \mathbf{c}}$$

$$Y' = J(\nabla^2 H)Y, \quad Y(0) = I.$$

The flow is called *symplectic* if

$$Y^T J^{-1} Y = J^{-1}, \quad \forall t.$$

Constrained mechanical systems

$$
\begin{aligned}
\mathbf{q}' &= \mathbf{v}, \\
M(\mathbf{q})\mathbf{v}' &= \mathbf{f}(\mathbf{q}, \mathbf{v}) - G^T(\mathbf{q})\boldsymbol{\lambda}, \\
\mathbf{0} &= \mathbf{g}(\mathbf{q}).
\end{aligned}
$$

- $\mathbf{q}$ generalized body positions,
- $\mathbf{v}$ generalized velocities,
- $\boldsymbol{\lambda} \in \mathbb{R}^l$ Lagrange multiplier functions,

- $\mathbf{g}(\mathbf{q}) \in \mathbb{R}^l$ holonomic constraints,
- $G = \mathbf{g}_\mathbf{q}$ has full row rank at each t,
- M positive definite generalized mass matrix,
- $\mathbf{f}$ the applied forces.

This is an index-3 differential-algebraic equation (DAE).

Apply two differentiations to the position constraints:

$$\begin{aligned} \mathbf{0} &= G\mathbf{v} \qquad (= \mathbf{g}'), \\ \mathbf{0} &= G\mathbf{v}' + \frac{\partial(G\mathbf{v})}{\partial \mathbf{q}}\mathbf{v} \qquad (= \mathbf{g}'') \, . \end{aligned}$$

Eliminate Lagrange multipliers:

$$\boldsymbol{\lambda}(\mathbf{q},\mathbf{v}) = (GM^{-1}G^T)^{-1}\left(GM^{-1}\mathbf{f} + \frac{\partial(G\mathbf{v})}{\partial \mathbf{q}}\mathbf{v}\right).$$

Obtain ODE

$$\begin{aligned}
\mathbf{q}' &= \mathbf{v}, \\
M\mathbf{v}' &= \mathbf{f} - G^T(GM^{-1}G^T)^{-1}\left(GM^{-1}\mathbf{f} + \frac{\partial(G\mathbf{v})}{\partial \mathbf{q}}\mathbf{v}\right)
\end{aligned}$$

on the manifold defined by constraint and its derivative, $\mathbf{g}(\mathbf{q}) = G(\mathbf{q})\mathbf{v} = \mathbf{0}$.

Hamiltonian PDEs: symplectic and multisymplectic maps

$$
\begin{aligned}
\mathbf{u}_t &= \mathcal{D}\left(\frac{\delta \mathcal{H}}{\delta \mathbf{u}}\right), \\
\mathcal{H}[\mathbf{u}] &= \int H(x, \mathbf{u}, \mathbf{u}_x, \ldots)\,dx \\
\int \frac{\delta \mathcal{H}}{\delta \mathbf{u}} \mathbf{v}\,dx &= \left(\frac{d}{d\varepsilon}\mathcal{H}[\mathbf{u} + \varepsilon \mathbf{v}]\right)_{\varepsilon=0}.
\end{aligned}
$$

$\mathcal{D}$ corresponds to a skew-symmetric matrix.

Example: wave equation

$$q_{tt} = c^2 q_{xx} - \frac{dV(q)}{dq},$$

is cast in the Hamiltonian notation using

$$\mathbf{u} = \begin{pmatrix} q \\ p \end{pmatrix}, \quad \mathcal{D} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad H = \frac{cp^2}{2} + \frac{cq_x^2}{2} + c^{-1} V(q).$$

Example: Schrodinger equation

$$\imath\psi_t = -\psi_{xx} - \psi|\psi|^2.$$

It is Hamiltonian with

$$\begin{aligned} \mathcal{D} &= \imath, \\ H(\psi, \bar{\psi}) &= \psi_x\bar{\psi}_x - \frac{1}{2}\psi^2\bar{\psi}^2. \end{aligned}$$

Example: Korteweg - de Vries (KdV)

$$u_t + (\alpha u^2 + \rho u + \nu u_{xx})_x = 0, \qquad -\infty < x < \infty,\ t \geq 0.$$

It is Hamiltonian with

$$\begin{aligned} \mathcal{D} &= \partial_x, \\ H &= -\frac{\alpha}{3}u^3 - \frac{\rho}{2}u^2 + \frac{\nu}{2}u_x^2. \end{aligned}$$

All of these PDE instances also have **multisymplectic structure**. Arises from writing PDE as

$$L\mathbf{z}_t + K\mathbf{z}_x = \boldsymbol{\nabla} S(\mathbf{z})$$

K, L antisymmetric (and constant).

"Multisymplectic = symplectic in both space and time"

Why preserve structure?

Remember: an accurate numerical method typically produces an accurate numerical solution that therefore accurately reproduces structure

- Often, some particular structure is more important to reconstruct or preserve than pointwise accuracy

  e.g., Lorentz chaotic dynamics, population dynamics where initial conditions are unknown, mechanical systems with holonomic constraints, etc.

- Conservation laws and other invariants may be based on more solid physical grounds than the DE system itself

- Often, some particular structure is more important to reconstruct or preserve than pointwise accuracy

- Conservation laws and other invariants may be based on more solid physical grounds that the DE system itself

- Better dynamical features may be recovered by a solution with a given pointwise accuracy

  e.g., better long-time behaviour may occasionally be obtained for Hamiltonian systems.

- Better numerical stability may be had in some instances

Wrong reasons to preserve structure

- "Pete made me do it"

  e.g., physicists often like to reproduce as many conservation laws as possible, regardless of whether this buys anything or not.

- "The more structure is preserved, the better"

  e.g., insisting on reproducing constant energy in a Hamiltonian system may actually destroy structure.

- "GI algorithms should be used regardless of computational cost, because they require, and inspire, a richer, more beautiful mathematics"

Numerical examples

- Drawing a circle: the linear oscillator
- Reconstructing a bagel: modified Kepler
- Unstable numerical integration of a mechanical system with holonomic constraints
- KdV solitons
- When we get it for free: Lorenz butterfly and linear conservation laws

Drawing a circle: the linear oscillator

Discretizing the Hamiltonian ODE

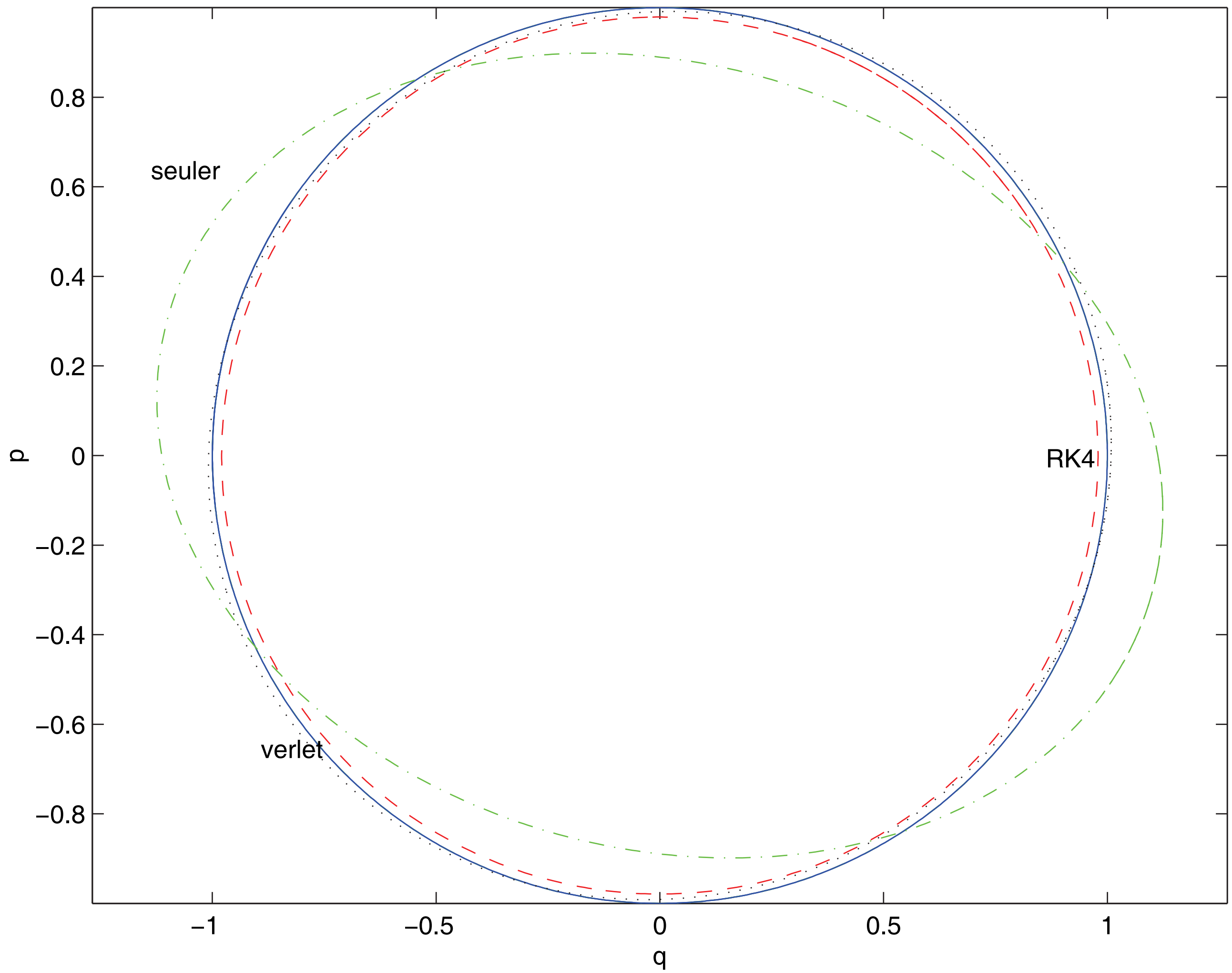
$$q' = p, \;\; p' = -q \;\; q(0) = 1, p(0) = 0$$

to obtain the circle

$$2H = p^2 + q^2 = 1.$$

- Forward Euler: $q_n = q_{n-1} + kp_{n-1}$, $p_n = p_{n-1} - kq_{n-1}$
- Backward Euler: $q_n = q_{n-1} + kp_n$, $p_n = p_{n-1} - kq_n$
- Symplectic Euler: $q_n = q_{n-1} + kp_{n-1}$, $p_n = p_{n-1} - kq_n$
- Verlet: $q_n = q_{n-1} + kp_{n-1/2}$, $p_{n+1/2} = p_{n-1/2} - kq_n$

Evolution of unit circle w RK4, symplectic Euler & Verlet



Reconstructing a bagel: modified Kepler

[Sanz-Serna - Calvo, Hairer-Stoffer]

$r = \sqrt{q_1^2 + q_2^2}$ is a radius;

Hamiltonian

$$H(\mathbf{q}, \mathbf{p}) = \frac{p_1^2 + p_2^2}{2} - \frac{1}{r} - \frac{\delta}{2r^3}$$

Differential system

$$\begin{aligned} \mathbf{q}' &= H_{\mathbf{p}} = \mathbf{p} \\ \mathbf{p}' &= -H_{\mathbf{q}} \end{aligned}$$

Initial conditions and parameters:

$q_1(0) = 1 - e,\; q_2(0) = 0,\; p_1(0) = 0, \; p_2(0) = \sqrt{(1+e)/(1-e)},$

$e = 0.6, \quad \delta = 0.01$

Invariant

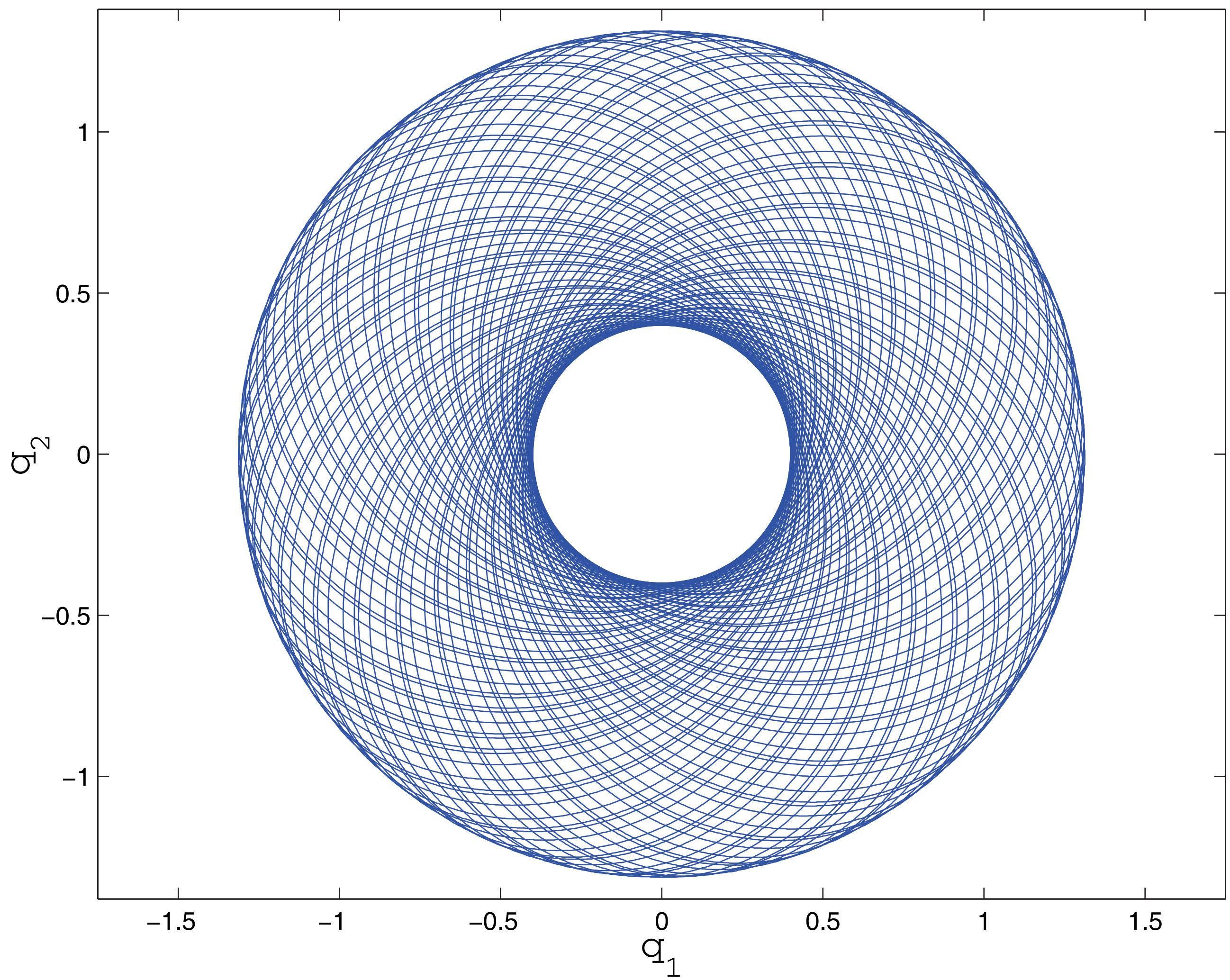
$$h(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}, \mathbf{p}) - H(\mathbf{q}(0), \mathbf{p}(0)) = 0$$

Implicit midpoint scheme (NB method is symplectic)

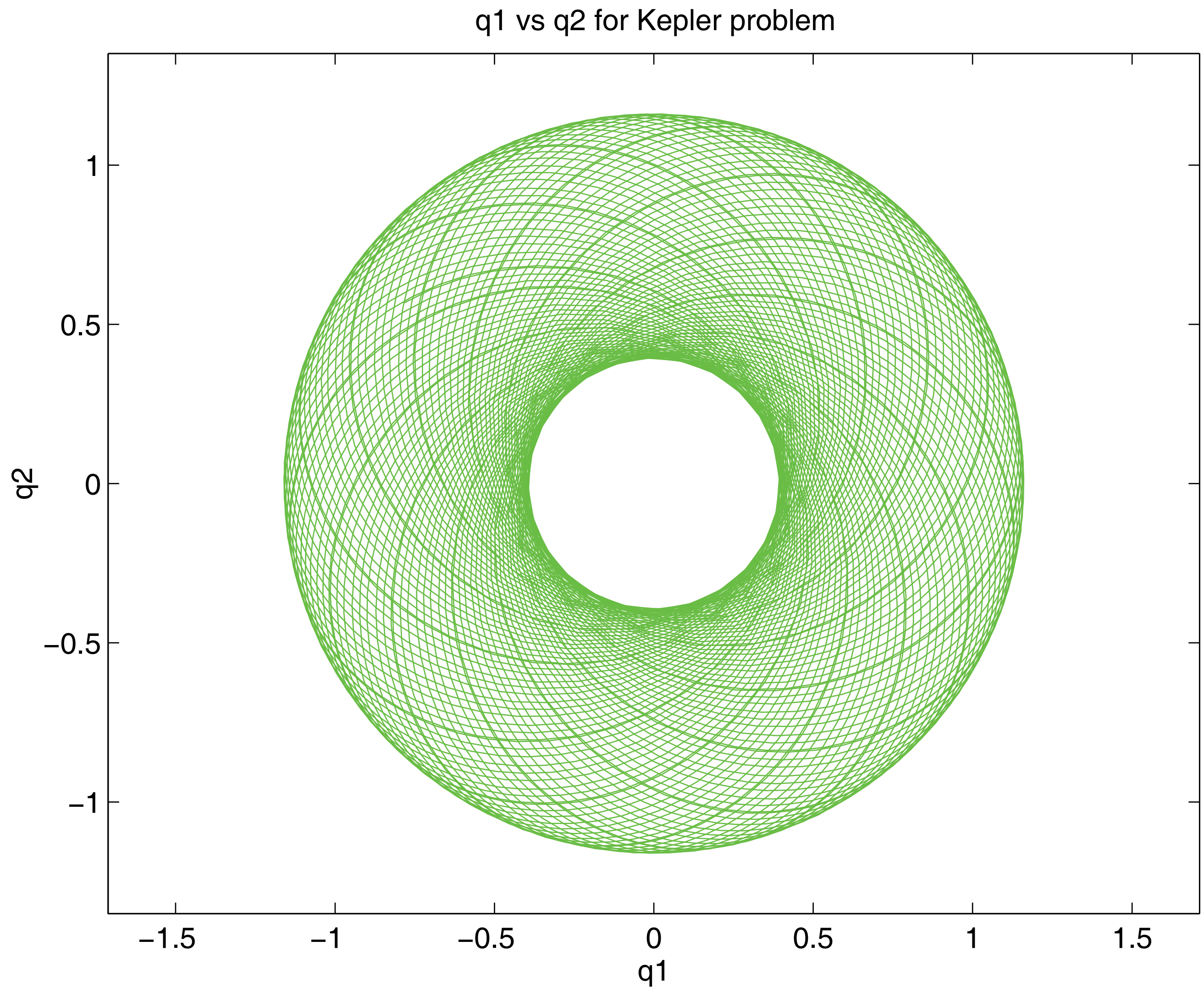
$$\begin{aligned} \mathbf{q}_n - \mathbf{q}_{n-1} &= k\mathbf{p}_{n-1/2} \\ \mathbf{p}_n - \mathbf{p}_{n-1} &= -kH_{\mathbf{q}}(\mathbf{q}_{n-1/2}) \end{aligned}$$

$$\mathbf{q}_{n-1/2} = (\mathbf{q}_n + \mathbf{q}_{n-1})/2, \quad \mathbf{p}_{n-1/2} = (\mathbf{p}_n + \mathbf{p}_{n-1})/2$$

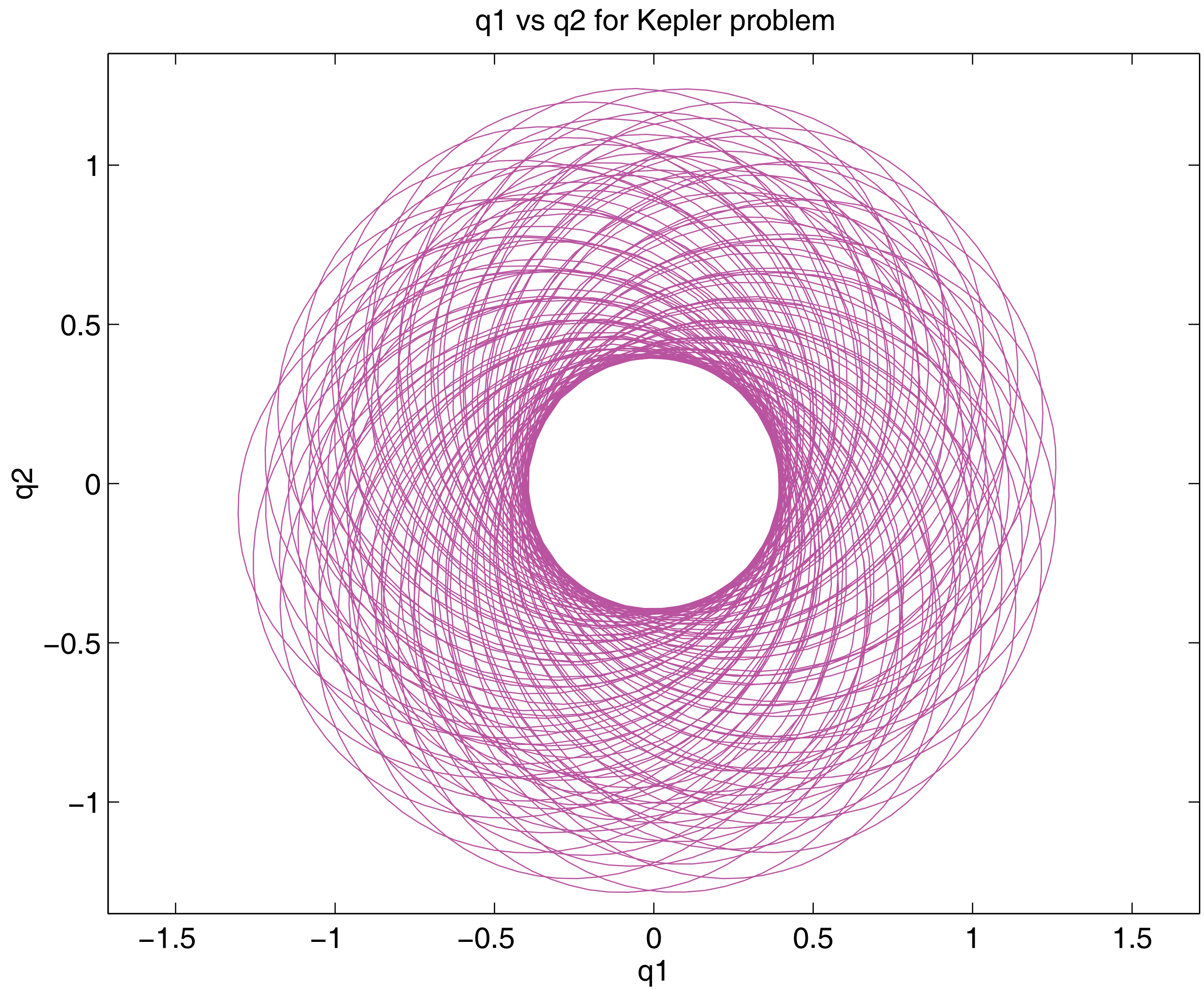
Exact solution for $T = 500$



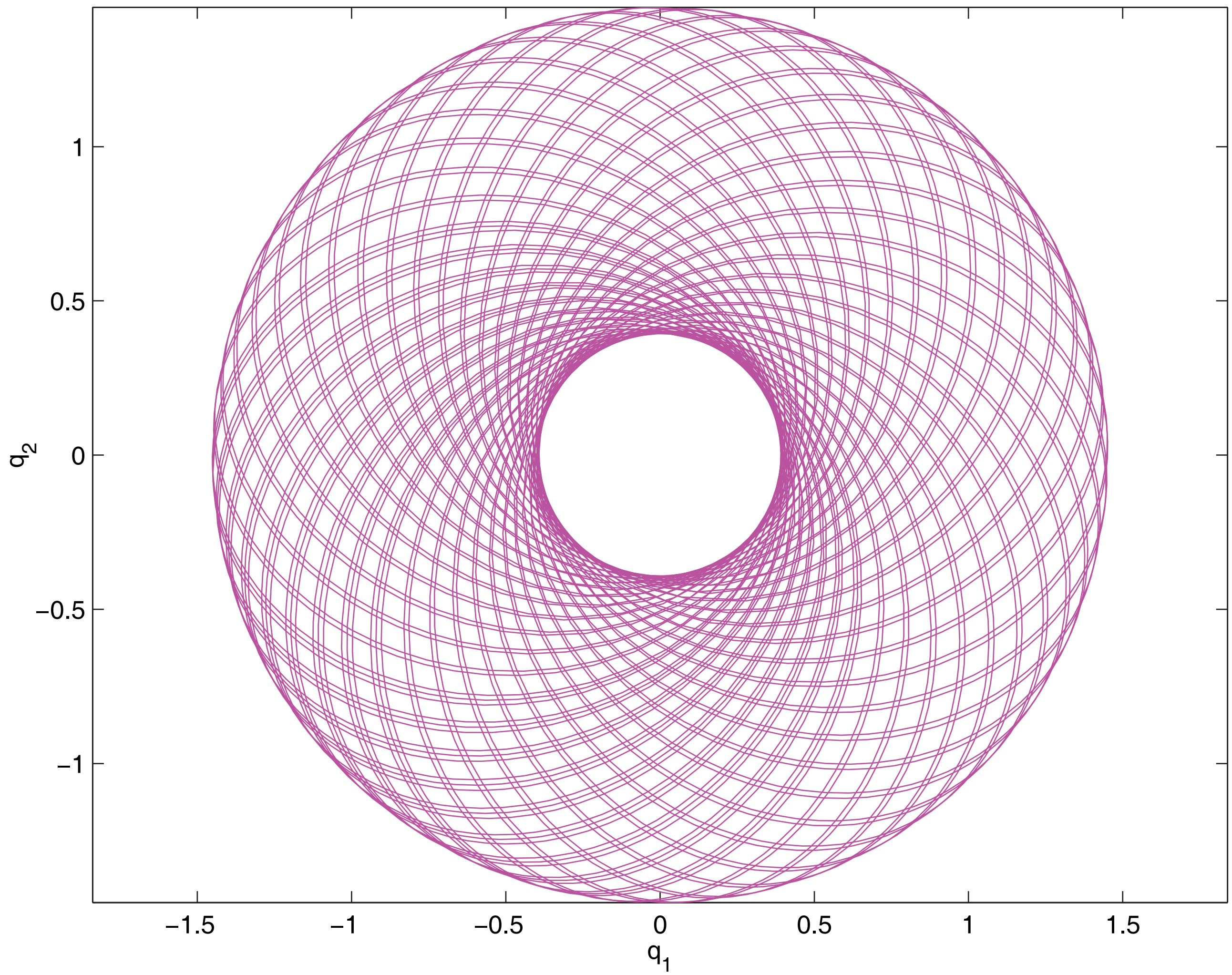
Midpoint, 5000 uniform steps



Explicit RK4, 5000 uniform steps



Verlet, 5000 uniform steps



Unstable numerical integration of a mechanical system with holonomic constraints

Ignoring the fact that the corresponding ODE is on a manifold can cause a numerical integration algorithm to go unstable.

KdV solitons

$$
\begin{aligned}
u_t + 3(u^2)_x + u_{xxx} &= 0, \\
u^0(x) = 6\operatorname{sech}^2(x), \\
u(-20,t) = u(20,t).
\end{aligned}
$$

When we get it for free: Lorenz butterfly and linear conservation laws

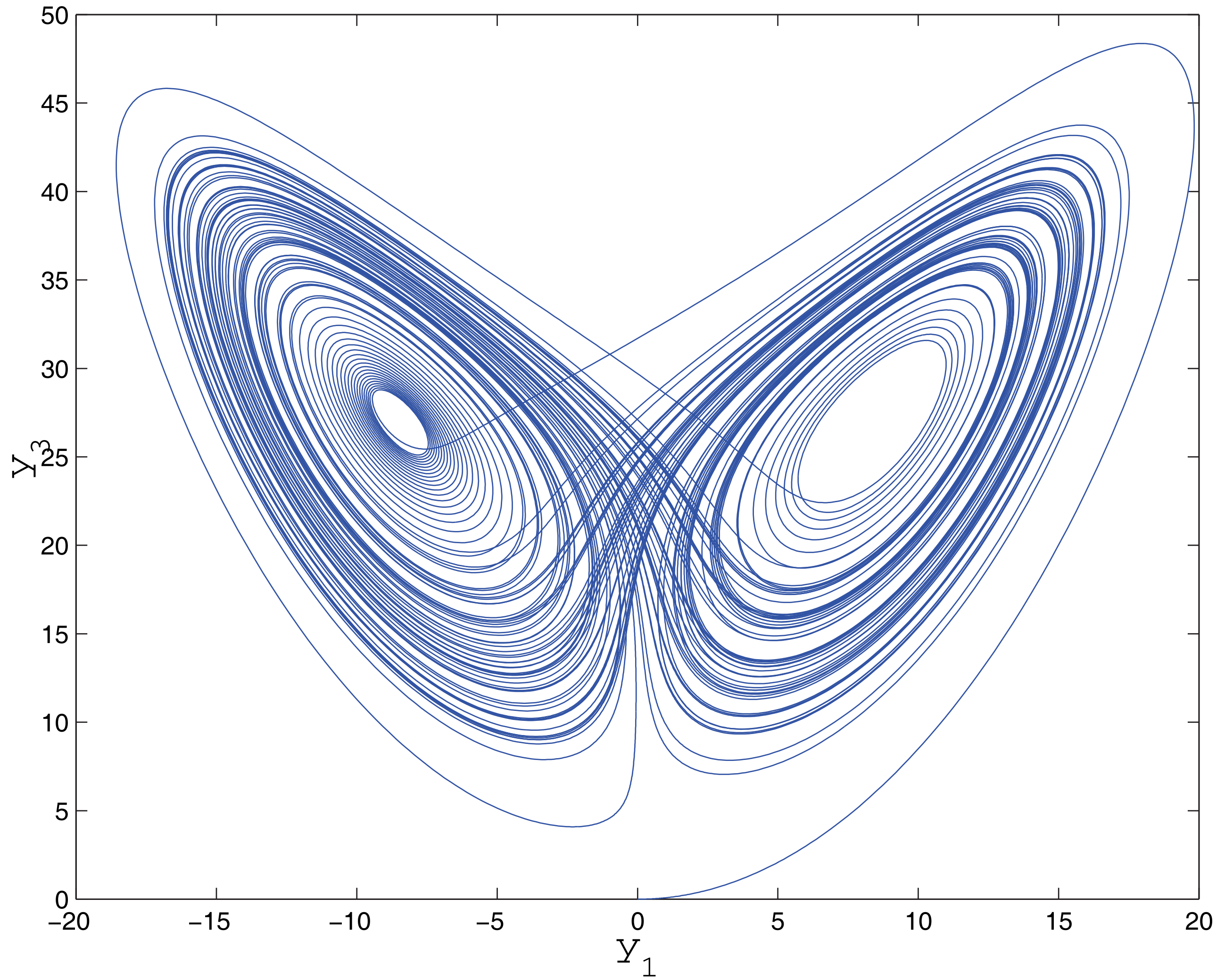
1. Lorenz equations

$$\mathbf{y}' = \mathbf{f}(\mathbf{y}) = \begin{pmatrix} \sigma(y_2 - y_1) \\ ry_1 - y_2 - y_1y_3 \\ y_1y_2 - by_3 \end{pmatrix},$$

$\sigma = 10,\ b = 8/3,\ r = 28.$

Plot y_3 vs. y_1 obtaining the famous “butterfly”

Although system is “chaotic” the attractor is robust. Its accurate numerical construction does not depend strongly on the integration method


50
45
40
35
30
25
20
15
10
5
0
–20
–15
–10
–5
0
5
10
15
20
y_3
y_1

2. Chemical reaction

Robertson: an extremely stiff ODE

$$\begin{aligned} y_1' &= -\alpha y_1 + \beta y_2 y_3, \\ y_2' &= \alpha y_1 - \beta y_2 y_3 - \gamma y_2^2, \\ y_3' &= \gamma y_2^2 \,. \end{aligned}$$

$\alpha = 0.04,\ \beta = 1.\mathrm{e}+4,\ \gamma = 3.\mathrm{e}+7.$

Conservation law:

$$\sum_{i=1}^{3} y_i(t) = constant, \quad \forall t.$$

Any Runge-Kutta method would reproduce this conservation law!

Outline

- Conserving invariants and methods on manifolds
- Symplectic and symmetric methods for Hamiltonian ODE systems
- Symplectic and multisymplectic methods for PDEs

Conserving invariants and methods on manifolds

Consider ODE system

$$\mathbf{y}' = \mathbf{f}(\mathbf{y}), \quad \mathbf{y}(0) = \mathbf{y}_0.$$

Vector function $\mathbf{i}(\mathbf{y})$ is a **first integral** if

$$\mathbf{i}_{\mathbf{y}}\mathbf{f}(\mathbf{y}) = \mathbf{0}, \quad \forall \mathbf{y}.$$

Then $\mathbf{i}(\mathbf{y}(t)) = \mathbf{i}(\mathbf{y}_0), \forall t$.

Also called **invariant** and **conserved quantity**.

Let $\mathbf{h}(\mathbf{y}) = \mathbf{i}(\mathbf{y}) - \mathbf{i}(\mathbf{y}_0)$. Then

$$\begin{aligned} \mathbf{h}_{\mathbf{y}}\mathbf{f}(\mathbf{y}) &= \mathbf{0}, \quad \forall \mathbf{y}, \\ \mathbf{h}(\mathbf{y}(t)) &= \mathbf{0}, \quad \forall t. \end{aligned}$$

Example: In an autonomous Hamiltonian system $H(\mathbf{q}(t), \mathbf{p}(t))$ is invariant.

Example: Mass conservation in a chemical reaction.

Several problem instances can be written as

$$\mathbf{y}' = A(\mathbf{y})\mathbf{y}, \quad A^T = -A, \; \forall \mathbf{y}.$$

Then

$$\mathbf{i}(\mathbf{y}) = \mathbf{y}^T\mathbf{y} = \|\mathbf{y}(t)\|^2$$

is a first integral: solution l_2 norm is conserved.

In fact, $\mathbf{y}$ can be a matrix: conserve orthogonality with $Y(0) = I$,

$$Y^T(t)Y(t) = I, \quad \forall t.$$

Conserving invariants by Runge-Kutta (RK) methods

Here, we want ODE methods which conserve invariants without doing anything special.

- Any RK method conserves linear invariants.
- Only methods based on polynomial **collocation at Gaussian points** (of which **implicit midpoint** is the simplest instance) conserve quadratic invariants.
- No such method conserves a cubic or higher invariant.

Differential equations on a manifold

For our ODE system, consider a submanifold of $\mathbb{R}^m$,

$$\mathcal{M} = \{\mathbf{y}; \mathbf{h}(\mathbf{y}) = \mathbf{0}\}$$

where $\mathbf{h} : \mathbb{R}^m \to \mathbb{R}^l, \ \ l < m$, s.t.

$$\text{if} \ \ \mathbf{y}_0 \in \mathcal{M} \ \ \text{then} \ \ \mathbf{y}(t) \in \mathcal{M} \ \forall t$$

Weaker than requirement of first integral because requires only

$$\mathbf{h}_\mathbf{y}\mathbf{f}(\mathbf{y}) = \mathbf{0}, \quad \forall \mathbf{y} \in \mathcal{M}.$$

Projection methods

For the problem $\mathbf{y}' = \mathbf{f}(\mathbf{y}),\ \mathbf{y}(0) = \mathbf{y}_0$, $\mathbf{h}(\mathbf{y}(t)) = \mathbf{0},\ \forall t$:

1. Apply a one-step method of order p with a step size k for the given ODE

$$\tilde{\mathbf{y}}_n = \phi_k^f(\mathbf{y}_{n-1})$$

2. Project back to the manifold: find $\mathbf{y}_n$ closest to $\tilde{\mathbf{y}}_n$ in l_2-norm that satisfies $\mathbf{h}(\mathbf{y}_n) = \mathbf{0}$.

Can replace projection step by a simpler post-stabilization,

$$\mathbf{y}_n \quad = \quad \tilde{\mathbf{y}}_n - F(\tilde{\mathbf{y}}_n)\mathbf{h}(\tilde{\mathbf{y}}_n)$$

The smaller $\|I - HF\|$ the better; e.g., $F = H^T(HH^T)^{-1}$ (one Newton step of projection) yields $HF = I$.

Example: For mechanical systems with holonomic constraints,

$$\mathbf{h}(\mathbf{q}, \mathbf{v}) = \begin{pmatrix} \mathbf{g}(\mathbf{q}) \\ G(\mathbf{q})\mathbf{v} \end{pmatrix}.$$

can choose

$$F = \begin{pmatrix} G^T(GG^T)^{-1} & 0 \\ 0 & G^T(GG^T)^{-1} \end{pmatrix}$$

Then $(I - HF)^2 = 0$, so apply this cheap post-stabilization twice per step.

See textbook [Ascher-Petzold, '98]

Numerical integrators on manifolds

Unfortunately, good long-time behaviour and other dynamical properties may be destroyed by projection.

See [Hairer, Lubich & Wanner, ’02] for:

Differential equations on Lie groups

Specifically, construct **orthogonal matrix functions** and solutions that can be represented as an **exponential matrix function**.

Methods using Magnus series expansion, Crouch et al., Munthe-Kaas et al.

Beautiful mathematical concepts at work, but does any of these lead to something practical?

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- Conserving invariants and methods on manifolds
- **Symplectic and symmetric methods for Hamiltonian ODE systems**
- Symplectic and multisymplectic methods for PDEs

Symplectic and symmetric methods for Hamiltonian ODE systems

- Hamiltonian systems
- Symplectic methods
- Properties of symplectic methods
- Pitfalls in highly oscillatory systems
- Reversible maps and symmetric methods
- Varying step size

Hamiltonian ODEs: symplectic maps

$$q_i' = \frac{\partial H}{\partial p_i}, \qquad i = 1, \ldots, l.$$
$$p_i' = -\frac{\partial H}{\partial q_i},$$

In vector form

$$\mathbf{q}' = \nabla_{\mathbf{p}} H(\mathbf{q}, \mathbf{p}), \quad \mathbf{p}' = -\nabla_{\mathbf{q}} H(\mathbf{q}, \mathbf{p})\,.$$

In general mechanical systems,

$T = T(\mathbf{q}, \mathbf{q}')$: kinetic energy

$V = V(\mathbf{q})$: potential energy

$L = T - V$: Lagrangian

obey Lagrange equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{q}'}\right) = \frac{\partial L}{\partial \mathbf{q}}$$

Introducing momenta and Hamiltonian

$p_i = \frac{\partial L}{\partial q_i'}$: moment

$H = \mathbf{p}^T\mathbf{q}' - L$: Hamiltonian

obtain Hamiltonian system.

Important special case: $T = \frac{1}{2}\mathbf{q}'^T M(\mathbf{q})\mathbf{q}'$, where mass matrix M is symmetric positive definite.

Then $\mathbf{p} = M(\mathbf{q})\mathbf{q}', \Rightarrow \mathbf{p}^T\mathbf{q}' = 2T, \Rightarrow H = T + V$, Hamiltonian is the total energy of mechanical system.

If, further, mass matrix is independent of $\mathbf{q}$, then Hamiltonian is in separable form,

$$H(\mathbf{q}, \mathbf{p}) = T(\mathbf{p}) + V(\mathbf{q})$$

Symplectic methods

- Symplectic Runge-Kutta
- Splitting and composition

Consider a one-step method $(\mathbf{q}_n, \mathbf{p}_n) = \phi_k(\mathbf{q}_{n-1}, \mathbf{p}_{n-1})$. Differentiate

$$Y = \frac{\partial(\mathbf{q}_n, \mathbf{p}_n)}{\partial(\mathbf{q}_{n-1}, \mathbf{p}_{n-1})}$$

and check symplecticity condition $Y^T J^{-1} Y = J^{-1}$.

Symplectic Runge-Kutta

Example: implicit midpoint

$$\mathbf{y}_n = \mathbf{y}_{n-1} + kJ\boldsymbol{\nabla} H((\mathbf{y}_n + \mathbf{y}_{n-1})/2)$$

$$\begin{aligned}
\Rightarrow Y \quad &= \quad I + \frac{k}{2} J\nabla^2 H(Y + I) \\
\Rightarrow Y \quad &= \quad (I - \frac{k}{2} J\nabla^2 H)^{-1}(I - \frac{k}{2} J\nabla^2 H)
\end{aligned}$$

Easy to check that symplecticity condition holds.

More generally: polynomial collocation at Gaussian points is symplectic for same reason that it conserves quadratic invariants.

$$\mathbf{y}'_\Delta(t_{nj}) = J\boldsymbol{\nabla} H(\mathbf{y}_\Delta(t_{nj})), \;\; j = 1, \ldots, s.$$

Therefore, also

$$Y'_\Delta(t_{nj}) = J\nabla^2 H(\mathbf{y}_\Delta(t_{nj}))Y_\Delta(t_{nj}), \;\; j = 1, \ldots, s.$$

We obtain $Y_\Delta^T(t_n)J^{-1}Y_\Delta(t_n) = Y_\Delta^T(t_{n-1})J^{-1}Y_\Delta(t_{n-1})$

Partitioned Runge-Kutta

No other “normal” RK method is symplectic, but there are symplectic partitioned RK methods, where one RK method is applied to $\mathbf{q}' = \boldsymbol{\nabla}_{\mathbf{p}} H$ and another to $\mathbf{p}' = -\boldsymbol{\nabla}_{\mathbf{q}} H$.

Example: symplectic Euler. For separable Hamiltonian it becomes explicit:

$$
\begin{aligned}
\mathbf{q}_n &= \mathbf{q}_{n-1} + k \boldsymbol{\nabla}_{\mathbf{p}} T(\mathbf{p}_{n-1}), \\
\mathbf{p}_n &= \mathbf{p}_{n-1} - k \boldsymbol{\nabla}_{\mathbf{q}} V(\mathbf{q}_n).
\end{aligned}
$$

Splitting and composition

Derive the discrete flow over a time step as a composition of simpler, symplectic flows. **This yields a symplectic map!**

If we can write

$$
\begin{aligned}
H &= H_1 + H_2 + \ldots + H_s \\
(\mathbf{y}^j)' &= J\boldsymbol{\nabla} H_j(\mathbf{y}^j)
\end{aligned}
$$

and for each component can obtain a symplectic flow then compose:

$$
\begin{aligned}
\mathbf{y}^1(t_{n-1}) &= \mathbf{y}_{n-1}, \\
\mathbf{y}^{j+1}(t_{n-1}) &= \mathbf{y}^j(t_n),\ j = 1, \ldots, s-1 \\
\mathbf{y}_n &= \mathbf{y}^s(t_n).
\end{aligned}
$$

Particularly useful for separable Hamiltonians

$$H_1 = T(\mathbf{p}), \;\; H_2 = V(\mathbf{q}).$$

Then

$$(\mathbf{q}^1)' = \boldsymbol{\nabla}_{\mathbf{p}} T(\mathbf{p}^1), \; (\mathbf{p}^1)' = \mathbf{0}, \; \mathbf{y}^1(t_{n-1}) = \begin{pmatrix} \mathbf{q}_{n-1} \\ \mathbf{p}_{n-1} \end{pmatrix}.$$

Exact solution: $\mathbf{p}^1 \equiv \mathbf{p}_{n-1}$ constant, hence $\mathbf{q}_n^1 = \mathbf{q}_{n-1} + k \boldsymbol{\nabla}_{\mathbf{p}} T(\mathbf{p}_{n-1})$.

Now,

$$(\mathbf{q}^2)' = \mathbf{0}, \; (\mathbf{p}^2)' = -\boldsymbol{\nabla}_{\mathbf{q}} V(\mathbf{q}^2), \; \mathbf{y}^1(t_{n-1}) = \begin{pmatrix} \mathbf{q}_n^1 \\ \mathbf{p}_{n-1} \end{pmatrix}.$$

Exact solution: $\mathbf{q}^2 \equiv \mathbf{q}_n = \mathbf{q}_n^1$ constant, hence $\mathbf{p}_n = \mathbf{p}_{n-1} - k \boldsymbol{\nabla}_{\mathbf{q}} V(\mathbf{q}_n)$.

Obtain symplectic Euler yet again

(and prove it is symplectic).

Splitting: Stormer-Verlet for separable Hamiltonian

Error in splitting method is due to splitting: for simple splitting it depends on

$$e^{k(L+M)} - e^{kL}e^{kM}.$$

Generally, for local error

$$e^{kL}e^{kM} - e^{k(L+M)} = \frac{1}{2}k^2(ML - LM) + O(k^3),$$

so overall $O(k)$ may result if L and M do not commute.

Instead restore second order accuracy using Strang splitting:

$$e^{k(L+M)} \approx e^{\frac{k}{2}L}e^{kM}e^{\frac{k}{2}L}.$$

For spearable Hamiltonian obtain Stormer-Verlet

$$
\begin{aligned}
\mathbf{q}_n &= \mathbf{q}_{n-1} + k\boldsymbol{\nabla}_{\mathbf{p}} T(\mathbf{p}_{n-1/2}), \\
\mathbf{p}_{n+1/2} &= \mathbf{p}_{n-1/2} - k\boldsymbol{\nabla}_{\mathbf{q}} V(\mathbf{q}_n).
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{p}_{1/2} &= \mathbf{p}_0 - \frac{k}{2}\boldsymbol{\nabla}_{\mathbf{q}} V(\mathbf{q}_0), \\
\mathbf{p}_n &= \mathbf{p}_{n-1/2} - \frac{k}{2}\boldsymbol{\nabla}_{\mathbf{q}} V(\mathbf{q}_n).
\end{aligned}
$$

Variational integrators

Another approach to symplectic integrators: Use discretized versions of Hamilton's principle determining (discrete) equations of motion from variational principle

Just like splitting-type methods are adaptations of general splitting methods to symplectic context, here there is also a general principle for PDE-optimization: discretize first, then derive necessary conditions.

Properties of symplectic methods

Why is it important to use a symplectic method? Are there disadvantages?

- Favorable error accummulation properties for long times (many, small, constant time steps) observed and proved [Sanz-Serna & Calvo]. The Hamiltonian conservation is particularly well-approximated (without enforcing it)

- However, for symplectic map the step size must be constant or varied carefully - a serious practical limitation!

- An implicit (symplectic) method necessitates solving a large system of possibly nonlinear algebraic equations at each step.

- An implicit (symplectic) method necessitates solving a large system of possibly nonlinear algebraic equations at each step. If iterative methods are used then the symplectic property may be lost unless the iteration is carried out to a very high accuracy. This may also contribute to yield an expensive method.

- Roundoff errors exist, and they are not expected to be structured. Linear accummulation of roundoff errors cannot be avoided, and when billions of time steps are considered this may become a factor.

- A symplectic method discretizing a Hamiltonian system yields (in infinite precision) a solution which is arbitrarily close to the exact flow of a perturbed Hamiltonian system.

  Result obtained independently by E. Hairer and S. Reich in the mid 1990's using backward error analysis.

Pitfalls in highly oscillatory systems

The excellent results obtained by symplectic methods are for **small** (many) time steps. Remember, Hamiltonian systems are only marginally stable, and so are symplectic methods: unfortunate perturbations may cause havoc if the time steps are not relatively small

Highly oscillatory Hamiltonian:

$$H(\mathbf{q},\mathbf{p}) = \frac{1}{2}\mathbf{p}^T\mathbf{p} + V(\mathbf{q}) + \frac{1}{2\varepsilon^2}\mathbf{g}(\mathbf{q})^T\mathbf{g}(\mathbf{q})$$

Differential system

$$\begin{aligned} \mathbf{q}' &= H_{\mathbf{p}} = \mathbf{p} \\ \mathbf{p}' &= -H_{\mathbf{q}} = -\boldsymbol{\nabla} V(\mathbf{q}) - \varepsilon^{-2}G(\mathbf{q})^T\mathbf{g}(\mathbf{q}) \end{aligned}$$

Quest: a numerical discretization that for any step size k and any ε

- conserves the Hamiltonian;
- is stable and efficient;
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Well, maybe not. But the question is of interest and relevance when both fast and slow solution features are present and the numerical scheme ought to approximate slow solution features well.

Highly oscillatory Hamiltonian systems and ghost DEs

[Ascher-Reich]

Consider implicit midpoint scheme.

- Linear oscillator with slowly varying frequency
- Stiff spring pendulum
- “Reversed” stiff spring pendulum

Linear oscillator with slowly varying frequency

$$\begin{aligned} q' &= \omega^2(t)p \\ p' &= -\varepsilon^{-2}q \end{aligned}$$

e.g. $\omega(t) = 1 + t$

Hamiltonian is not constant in t, But **adiabatic invariant**

$$J(q,p,t) = H(q,p,t)/\omega(t) \; = \; \omega(t)p^2/2 + \varepsilon^{-2}\omega^{-1}(t)q^2/2$$

satisfies for $T = c_1\, e^{c_2/\varepsilon}$,

$$\left[J(t) - J(0)\right]/J(0) = O(\varepsilon).$$

Ghost DE

Apply midpoint:

$$\begin{aligned}(q_n - q_{n-1})/k &= \omega(t_{n-1/2})^2\,(p_n + p_{n-1})/2\\ (p_n - p_{n-1})/k &= -\varepsilon^{-2}\,(q_n + q_{n-1})/2\end{aligned}$$

What DE does this really approach when $\varepsilon \ll k \to 0$?

Let

$$u_n = (-1)^n \varepsilon^{-1} q_n, \;\; v_n = (-1)^{n+1} p_n, \;\; \alpha = \frac{k^2}{4\varepsilon}$$

Obtain

$$\begin{aligned}(u_n + u_{n-1})/2 &= -\omega(t_{n-1/2})^2\, \alpha\, (v_n - v_{n-1})/k \\ (v_n + v_{n-1})/2 &= \alpha\, (u_n - u_{n-1})/k\end{aligned}$$

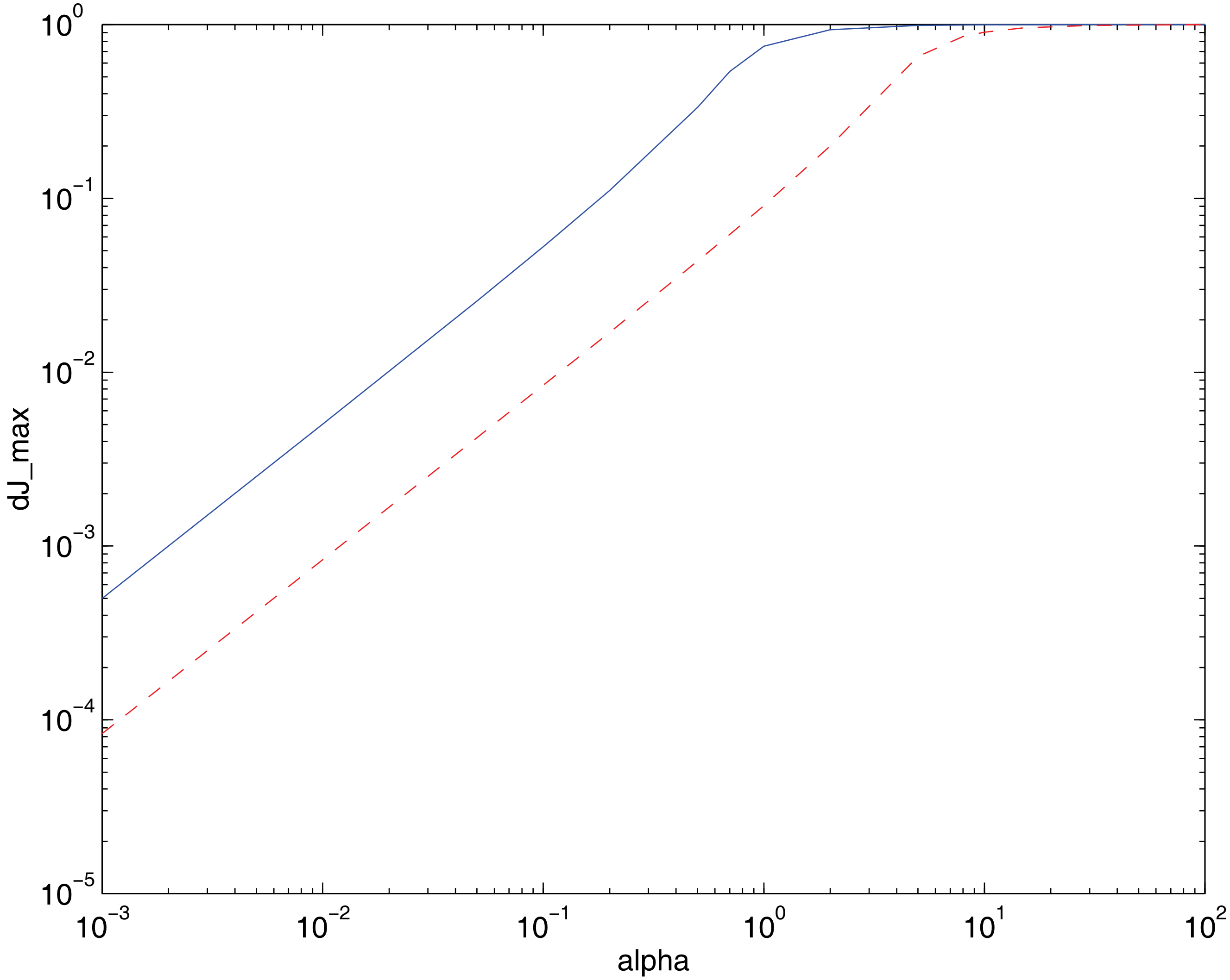
Observe as $k \to 0$ for a fixed α:

$$-\omega^2(t)\alpha v' = u, \quad \alpha u' = v$$

So, the ghost DE is an oscillator with α essentially replacing ε. Hence,

$$\left[\hat{J}(t) - \hat{J}(0)\right]/\hat{J}(0) = O(\alpha)$$
$$\hat{J}(u_n, v_n, t_n) = \hat{J}(\epsilon^{-1}q_n, p_n, t_n) = J(q_n, p_n, t_n)\,.$$

Error in adiabatic invariant vs. $\alpha = \frac{k^2}{4\epsilon}$



Comments and observations

- Whereas no instability is encountered, these results are misleading.

- More generally, may obtain misleading results for highly oscillatory problems, where smooth manifold of Hamiltonian system

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2}\mathbf{p}^T\mathbf{p} + V(\mathbf{q}) + \frac{1}{2\varepsilon^2}[\mathbf{g}(\mathbf{q})]^2$$

$$\begin{aligned}\mathbf{q}' &= \mathbf{p} \\ \mathbf{p}' &= -\boldsymbol{\nabla}_{\mathbf{q}} V(\mathbf{q}) - \varepsilon^{-2} G^T \mathbf{g}(\mathbf{q})\end{aligned}$$

is **not** solution of DAE

$$\begin{aligned}\mathbf{q}' &= \mathbf{p} \\ \mathbf{p}' &= -\boldsymbol{\nabla}_{\mathbf{q}} V(\mathbf{q}) - G^T \boldsymbol{\lambda} \\ 0 &= \mathbf{g}(\mathbf{q})\end{aligned}$$

Stiff spring pendulum

$$\begin{aligned} \mathbf{q}' &= \mathbf{p} \\ \mathbf{p}' &= -(\phi(\mathbf{q}) - \phi_0)\boldsymbol{\nabla}\phi(\mathbf{q}) - \varepsilon^{-2}(r(\mathbf{q}) - r_0)\boldsymbol{\nabla} r(\mathbf{q})) \end{aligned}$$

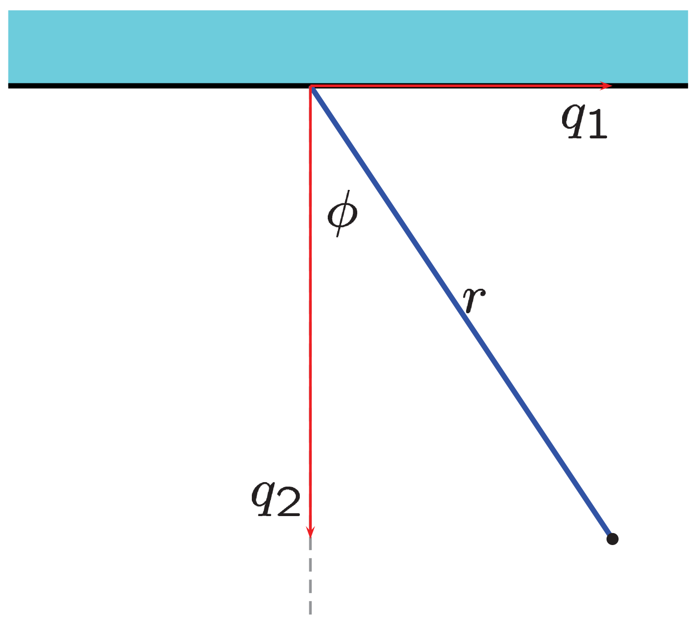
where

$$\begin{aligned} r &= |\mathbf{q}| = \sqrt{q_1^2 + q_2^2} \\ \cos\phi &= q_1/|\mathbf{q}|. \end{aligned}$$

Obtain poor results when discretizing this system by the midpoint scheme when $\alpha = \frac{k^2}{4\epsilon}$ is large, as $k \to 0, \quad \alpha$ fixed.

This is because fast and slow solution modes are strongly coupled! Here r is fast and ϕ is slow: transforming first to DE system in r, ϕ, a subsequent midpoint discretization works very well.

Stiff spring pendulum



“Reversed” stiff spring pendulum

Now r is slow, ϕ is fast (relevant in molecular dynamics).

$$\begin{aligned}\mathbf{q}' &= \mathbf{p}\\ \mathbf{p}' &= -\varepsilon^{-2}(\phi(\mathbf{q})-\phi_0)\boldsymbol{\nabla}\phi(\mathbf{q})-(r(\mathbf{q})-r_0)\boldsymbol{\nabla}r(\mathbf{q}))\end{aligned}$$

This combines the previous two sources of trouble: both coupling of slow and fast modes and poor reconstruction of adiabatic invariant.

Now, even in coordinates r, ϕ must have $\alpha = \frac{k^2}{4\epsilon}$ small: otherwise a wrong limit ghost DAE is discretized in effect.

Comments and observations

- Easy to construct examples, not just *resonance*, where midpoint method blows up (unstable) when $\varepsilon \ll k$.

- Distinguish between two aspects:

  1. Reproducing slow solution features
  2. Coupling of slow solution modes and fast solution modes.

- Of crucial importance is the question to what extent the numerical method is able to **decouple** between fast and slow modes.

  [Simo-Gonzales, Ascher-Reich]

Reversible maps and symmetric methods

Let ρ be an invertible linear transformation in phase space of $\mathbf{y}' = \mathbf{f}(\mathbf{y})$. The DE and vector field are called ρ-reversible if

$$\rho\mathbf{f}(\mathbf{y}) = -\mathbf{f}(\rho\mathbf{y}), \quad \forall\mathbf{y}.$$

Cannical Example: the partitioned system

$$\mathbf{q}' = \mathbf{f}(\mathbf{q},\mathbf{v}), \;\; \mathbf{v}' = \mathbf{g}(\mathbf{q},\mathbf{v})$$

where $\mathbf{f}(\mathbf{q},-\mathbf{v}) = -\mathbf{f}(\mathbf{q},\mathbf{v}), \;\; \mathbf{g}(\mathbf{q},-\mathbf{v}) = \mathbf{g}(\mathbf{q},\mathbf{v})$

Then $\rho(\mathbf{q},\mathbf{v}) = (\mathbf{q},-\mathbf{v})$.

This occurs for conservative mechanical systems.

A numerical map Φ_k is symmetric or time-reversible if

$$\Phi_k \circ \Phi_{-k} = I$$

i.e., if we integrate backwards (replace k by $-k$ and exchange $\mathbf{y}_n$ and $\mathbf{y}_{n-1}$) then the same discretization results.

If a numerical method applied to a ρ-reversible DE satisfies

$$\rho \circ \Phi_k = \Phi_{-k} \circ \rho$$

then numerical flow is ρ-reversible iff method is symmetric.

- All symplectic methods we have seen are symmetric. But also nonsymplectic methods can be symmetric, e.g., trapezoidal.
- Symplectic does not imply symmetric.
- Collocation is symmetric iff the collocation points are symmetric.
- Can use symmetric composition to construct high order symmetric methods.
- Can construct symmetric projection for ODE on manifold
- Symmetric Lie group methods
- Energy-momentum conservation methods

Varying step size

Until now everything has been using a fixed step size. But modern "normal" codes all use automatic local error control by adapting step size!

- Reversible adaptive step size selection
- Time transformation
  - Symplectic integration
  - Reversible integration

None of these techniques come close to the efficiency of normal step-size control, but they do offer significant performance improvements for a given local pointwise error tolerance while yielding qualitatively correct structure preservation.