BERGISCHE UNIVERSITÄT WUPPERTAL

Symplectic and Time-Reversible Projection Methods for Hamiltonian Systems

Dmitry Shcherbakov Matthias Ehrhardt Michael Günther

Bergische Universität Wuppertal

{shcherbakov, ehrhardt, guenther}@math.uni-wuppertal.de

Motivation

BERGISCHE UNIVERSITÄT WUPPERTAL

Structure preservation:

- preserve geometrical properties of the flow of a differential equation
- produce improved qualitative behavior of the numerical solution (even for long-time integration)
- applicable for a wide range of the physical problems

Most geometric properties are not preserves by traditional numerical methods

Example: An integrator for the **Hybrid Monte Carlo algorithm**

- computing samples (p_i, q_i) via ODEs (just one step)
- must be *time-reversible* and *volume-preserving*
- *energy conservation* is an advantage (**no acceptance check needed**)

BERGISCHE UNIVERSITÄT WUPPERTAL

Structure-Preserving Projection Methods for Hamiltonian Systems

Outline

Problem Formulation

BERGISCHE UNIVERSITÄT WUPPERTAL

Equations of Motion

$$\dot{y} = f(x) = J^{-1}\nabla H(y), \qquad y(0) = y_0$$

with $\qquad y = (q,p)^\top, \qquad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

Problems:

- separable linear, e.g. simple harmonic oscillator (SHO)

$$H(q,p) = \frac{1}{2}p^2 + \frac{1}{2}q^2$$

- separable nonlinear, e.g. pendulum equation (PE)

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

- non-separable problem (NS)

$$H(q,p) = (1 + \frac{p^2}{2})^2(1 + q^2)$$

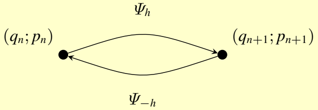
Desired Properties

BERGISCHE UNIVERSITÄT WUPPERTAL

Symmetry

A numerical method Ψ_h is called **symmetric**, if

$$\Psi_h \circ \Psi_{-h} = id \quad \text{or} \quad \Psi_h = \Psi_{-h}^{-1}$$

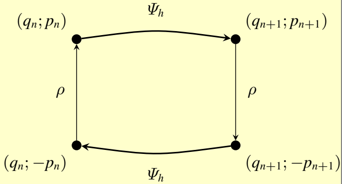


Time-Reversibility

A numerical method Ψ_h is called **time-reversible**, if

$$\rho \circ \Psi_h = \Psi_h^{-1} \circ \rho,$$

where ρ such that $\rho(q, p) = (q, -p)$



Desired Properties

BERGISCHE UNIVERSITÄT WUPPERTAL

Symplecticity

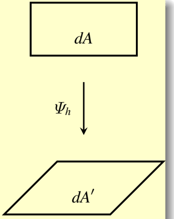
A numerical method Ψ_h is called **symplectic** if

$$\left(\frac{\partial y_{n+1}}{\partial y_n}\right)^\top J \left(\frac{\partial y_{n+1}}{\partial y_n}\right) = J$$

Volume-Preservation

A numerical method Ψ_h is called **volume-preserving** if

$$\left|\det\left(\frac{\partial y_{n+1}}{\partial y_n}\right)\right| = 1$$



$$dA = dA'$$

Outline

Standard Projection Method

BERGISCHE UNIVERSITÄT WUPPERTAL

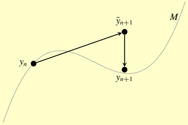
Idea

Assume, $M = \{y; \;\; g(y) = 0\}$ a submanifold on $\mathbb{R}^n$, $g : \mathbb{R}^n \to \mathbb{R}^m$ and $y_n \in M$, then

$$\tilde{y}_{n+1} = \Phi_h(y_n) \qquad \text{compute with arbitrary } \Phi_h$$

$$y_{n+1} = \tilde{y}_{n+1} + G(\tilde{y}_{n+1})^\top \lambda \qquad \text{project on } M$$

$$0 = g(y_{n+1}) \qquad \text{conservation condition}$$



where $G^\top(y) = g'(y)$ and λ is implicitly defined by $g(y_{n+1}) = 0$

Advantages

- preserves the energy of the system
- might improve the long-term behavior of the original method

Disadvantages

- not symmetric
- not symplectic

Symmetric Projection Method

Idea [Hairer, 2000]

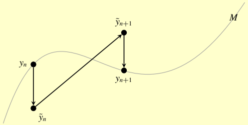
$M = \{y;\ \ g(y) = 0\}$ a submanifold on $\mathbb{R}^n$, $g : \mathbb{R}^n \to \mathbb{R}^m$ and $y_n \in M$

$$\tilde{y}_n = y_n + G(y_n)^\top \mu \qquad \text{perturb } y_n$$

$$\tilde{y}_{n+1} = \Phi_h(\tilde{y}_n) \qquad \text{symmetric method}$$

$$y_{n+1} = \tilde{y}_{n+1} + G(y_{n+1})^\top \mu \qquad \text{project on } M$$

$$0 = g(y_{n+1}) \qquad \text{conservation condition}$$



where $G^\top(y) = g'(y)$ and μ is implicitly defined by $g(y_{n+1}) = 0$

Advantages

- preserves the energy of the system
- symmetric

Disadvantages

- not symplectic (in general)

Outline

Structure-Preserving Method -1

BERGISCHE UNIVERSITÄT WUPPERTAL

Approach

For our problem we have

$$P: \quad \tilde{y}_n = y_n + J^{-1}\nabla H\left(\frac{\tilde{y}_n + y_n}{2}\right)^{\top}\mu \qquad \text{perturbation step}$$

$$\Phi_h: \quad \tilde{y}_{n+1} = \Phi_h(\tilde{y}_n) \qquad \text{intermediate step}$$

$$BP: \quad y_{n+1} = \tilde{y}_{n+1} + J^{-1}\nabla H\left(\frac{y_{n+1} + \tilde{y}_{n+1}}{2}\right)^{\top}\mu \qquad \text{projection step}$$

$$0 = H(y_{n+1}) - H(y_n) \qquad \text{energy conservation}$$

- $\Phi_h(\tilde{y}_n)$ - symplectic, symmetric and time-reversible method
- μ such as $H(y) = const$

Properties

preserving **symmetry**, **time-reversiblity**, **symplecticity** of the method Φ_h and **conserves the energy of the system**

Properties

The method can be represented as

$$\Psi_h := BP \circ \Phi_h \circ P$$

Here we have

- P and BP are **implicit mid-point rules**
- Φ_h is **symmetric**, **time-reversible**, **symplectic** method e.g the **leap-frog method**
- P, BP and Φ_h are **symmetric**, **time-reversible** and **symplectic**

Thus the method is

- **symmetric** $\Rightarrow$ composition of symmetric methods
- **time-reversible** $\Rightarrow$ composition of time-reversible methods
- **symplectic** $\Rightarrow$ composition of symplectic methods
- **energy-conserving** $\Rightarrow$ by the construction of the method

Structure-Preserving Methods -2

Approach

For our problem we have

$$
\begin{aligned}
P: &\quad \tilde{y}_n = y_n + J^{-1}\nabla H\left(\tilde{p}_n, q_n\right)^\top \mu && \text{perturbation step}\\
\Phi_h: &\quad \tilde{y}_{n+1} = \Phi_h(\tilde{y}_n) && \text{intermediate step}\\
BP: &\quad y_{n+1} = \tilde{y}_{n+1} + J^{-1}\nabla H\left(\tilde{p}_{n+1}, q_{n+1}\right)^\top \mu && \text{projection step}\\
&\quad 0 = H(y_{n+1}) - H(y_n) && \text{energy conservation}
\end{aligned}
$$

- $\Phi_h(\tilde{y}_n)$ - symplectic, symmetric and time-reversible method
- μ such as $H(y) = const$

Properties

preserving **symmetry**, **time-reversiblity**, **symplecticity** of the method Φ_h and **conserves the energy of the system**

Properties

Symplecticity(volume-preservation) $\Rightarrow$ composition of symplectic methods

Energy conservation $\Rightarrow$ construction of the method

Symmetry

- exchange $h \leftrightarrow -h$ and $y_n \leftrightarrow y_{n+1}$ we obtain

$$\begin{aligned}
\tilde{y}_n &= y_{n+1} + J^{-1} \nabla H\left(\tilde{p}_n, q_{n+1}\right)^\top \mu \\
\tilde{y}_{n+1} &= \Phi_{-h}(\tilde{y}_n) \\
y_n &= \tilde{y}_{n+1} + J^{-1} \nabla H\left(\tilde{p}_{n+1}, q_n\right)^\top \mu \\
0 &= H(y_n) - H(y_{n+1})
\end{aligned}$$

- replace $\mu, \tilde{y}_n$ and $\tilde{y}_{n+1}$ with $-\mu, \tilde{y}_{n+1}$ and $\tilde{y}_n$ respectively
- obtain the original algorithm $\Rightarrow$ the method is **symmetric**

Properties

Time-reversibility

A symmetric projection method is time-reversible if

- Φ_h satisfies $\rho \circ \Phi_h = \Phi_h^{-1} \circ \rho$
- $\rho G(y_n)^\top = G(\rho y_n)^\top \sigma$, where σ is constant invertible matrix

- Φ_h is chosen to be a time reversible
- then

$$\rho G(y_n)^\top = \rho J^{-1} \nabla H\left(q_n, \tilde{p}_n\right)^\top = \rho \begin{pmatrix} -H_q(q_n, \tilde{p}_n) \\ H_p(q_n, \tilde{p}_n) \end{pmatrix} = \begin{pmatrix} -H_q(q_n, \tilde{p}_n) \\ -H_p(q_n, \tilde{p}_n) \end{pmatrix}$$

$$G(\rho y_n)^\top \sigma = J^{-1} \nabla H\left(q_n, -\tilde{p}_n\right)^\top \sigma = \begin{pmatrix} -H_q(q_n, -\tilde{p}_n) \\ H_p(q_n, -\tilde{p}_n) \end{pmatrix} \sigma$$

$$= \begin{pmatrix} -H_q(q_n, \tilde{p}_n) \\ -H_p(q_n, \tilde{p}_n) \end{pmatrix} \sigma, \quad \text{where} \quad \sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

- thus the method is **time-reversible**

Alternative

Adapted method

For our problem we have

$$\begin{aligned} P: &\quad \tilde{y}_n = y_n + A\, y_n\, \mu && \text{perturbation step} \\ \Phi_h: &\quad \tilde{y}_{n+1} = \Phi_h(\tilde{y}_n) && \text{intermediate step} \\ BP: &\quad y_{n+1} = \tilde{y}_{n+1} + A\, y_{n+1}\, \mu && \text{projection step} \\ &\quad 0 = H(y_{n+1}) - H(y_n) && \text{energy conservation} \end{aligned}$$

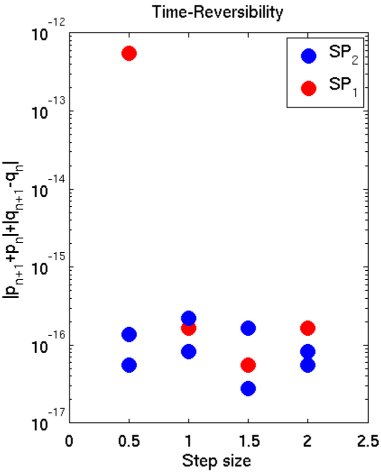
- μ such as $H(y) = const$
- A is a block-diagonal matrix: $A = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}$

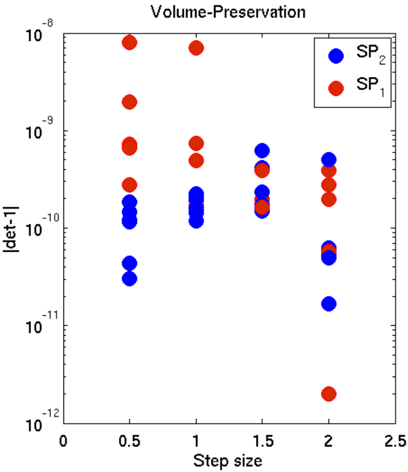
Properties

The method is **symmetric**, **time-reversible**, **symplectic** and **conserves the energy of the system**

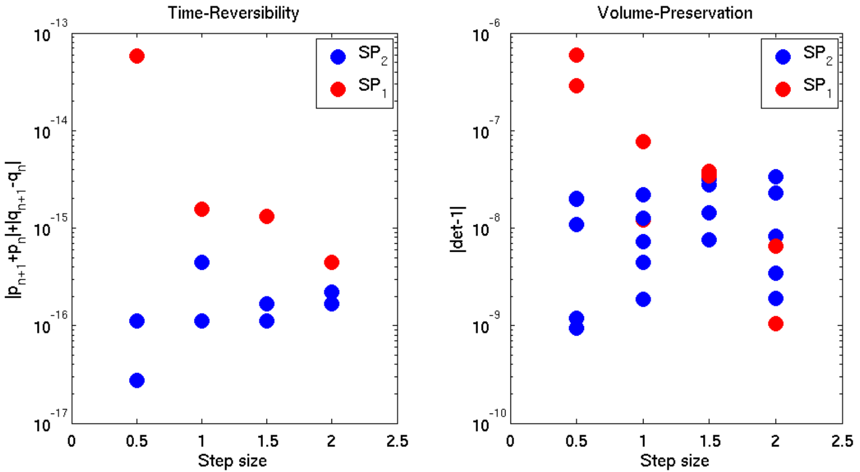
Outline

Numerical Results - SHO

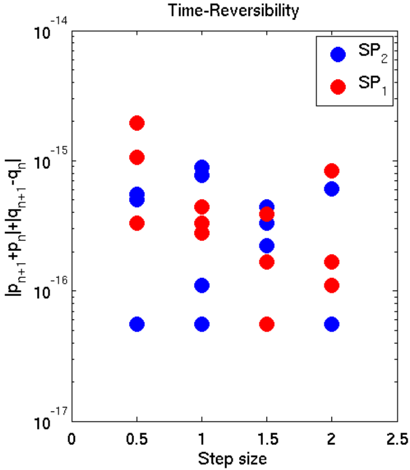


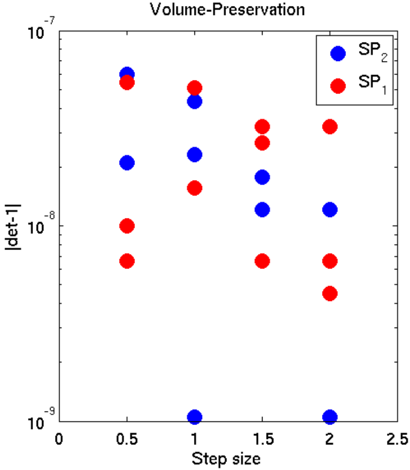


Numerical Results - PE



Numerical Results - NS





Outline

Conclusion & Outlook

Conclusions

- Combining structure preserving numerical methods with projection: **symmetric, time-reversible, volume-preserving, energy-preserving**
- Analytical and numerical proofs of the desired properties
- Applicable for separable and non-separable problems

Outlook

- Application in Quantum Chromodynamics (QCD)
- Applicable for more general non-Abelian structures?

THANK YOU!

ITN STRONGNET

Dmitry Shcherbakov
shcherbakov@math.uni-wuppertal.de

Matthias Ehrhardt
ehrhardt@math.uni-wuppertal.de

Michael Günther
guenther@math.uni-wuppertal.de