

# A general symplectic integrator for canonical Hamiltonian systems

Yushun Wang

Nanjing Normal University  
Email: wangyushun@njjnu.edu.cn

Joint work with  
Yonghui Bo, Wenjun Cai

# Outline

- 1 Geometric numerical integration
- 2 A novel family of symplectic integrators
- 3 Reconstruction and extension of symplectic schemes
  - Parameterized generating function methods
  - Symmetric composition methods
- 4 Energy and quadratic invariants preserving methods
- 5 Numerical experiments

# Outline

- 1 Geometric numerical integration
- 2 A novel family of symplectic integrators
- 3 Reconstruction and extension of symplectic schemes
  - Parameterized generating function methods
  - Symmetric composition methods
- 4 Energy and quadratic invariants preserving methods
- 5 Numerical experiments

# Geometric numerical integration

The canonical Hamiltonian system has the following form

$$\dot{y} = \mathcal{J}^{-1} \nabla H(y) \xrightarrow{y=(p,q)^T} \dot{p} = -H_q(p, q), \quad \dot{q} = H_p(p, q), \quad (1)$$

where the Hamiltonian  $H$  represents the total energy.

**Geometric numerical integration** deals with numerical schemes that preserve geometric properties of the exact flow of (1). The most characteristic properties are the symplecticity and energy conservation along any flows.

► **Symplecticity conservation:**

$$\frac{d}{dt}(dp(t) \wedge dq(t)) = 0. \quad (2)$$

► **Energy conservation:**

$$\frac{d}{dt}H(p(t), q(t)) = 0. \quad (3)$$

Concerning numerical integration, the numerical one-step method with the time step  $h$  defines the mapping

$$(p_{n+1}, q_{n+1}) = \Phi_h(p_n, q_n). \quad (4)$$

The method (4) is **symplectic**, if

$$\left( \frac{\partial \Phi_h(p_n, q_n)}{\partial (p_n, q_n)} \right)^T \mathcal{J} \left( \frac{\partial \Phi_h(p_n, q_n)}{\partial (p_n, q_n)} \right) = \mathcal{J}, \quad (5)$$

where  $\mathcal{J} = \begin{pmatrix} 0 & \mathcal{I} \\ -\mathcal{I} & 0 \end{pmatrix}$  and  $\mathcal{I}$  is an identity matrix.

The method (4) is **energy-preserving**, if

$$H(p_{n+1}, q_{n+1}) = H(p_n, q_n). \quad (6)$$

Two prominent lines of investigation are currently the study of symplectic methods and energy-preserving methods.

► **Symplectic methods:**

- Generating function methods. Feng Kang, 1984.
- Symplectic Runge-Kutta methods. J.M. Sanz-Serna, 1988.
- Composition methods. Qin Mengzhao, 1992.
- Symplectic partitioned Runge-Kutta methods. Sun Geng, 1993.
- Variational integrators. J.E. Marsden and coauthors, 1998.

.....

► **Energy-preserving methods:**

- Projection methods. Hairer and Wanner, 1996.
- Discrete gradient methods. G.R.W. Quispel and coauthors, 1998.
- Finite element methods. P. Betsch and P. Steinmann, 2000.
- Averaged vector field methods. G.R.W. Quispel and D.I. McLaren, 2008.
- Hamiltonian boundary value methods. L. Brugnano and coauthors, 2010.
- Partitioned averaged vector field methods. Cai Wenjun and coauthors, 2018.
- Energy and quadratic invariants-preserving (EQUIP) methods. L. Brugnano and coauthors, 2012.
- EQUIP multi-symplectic methods. Chen chuchu and Hong Jialin, 2020.

.....

# Outline

- 1 Geometric numerical integration
- 2 A novel family of symplectic integrators**
- 3 Reconstruction and extension of symplectic schemes
  - Parameterized generating function methods
  - Symmetric composition methods
- 4 Energy and quadratic invariants preserving methods
- 5 Numerical experiments

## A novel family of symplectic integrators

There are currently many ways to construct symplectic integrators, but of the methods obtained, only the following methods have the simplest form.

► Symplectic Euler methods:

$$\begin{cases} p_{n+1} = p_n - hH_q(p_{n+1}, q_n), \\ q_{n+1} = q_n + hH_p(p_{n+1}, q_n); \end{cases} \quad \text{or} \quad \begin{cases} p_{n+1} = p_n - hH_q(p_n, q_{n+1}), \\ q_{n+1} = q_n + hH_p(p_n, q_{n+1}). \end{cases} \quad (7)$$

► Implicit midpoint rule:

$$\begin{cases} p_{n+1} = p_n - hH_q\left(\frac{p_{n+1} + p_n}{2}, \frac{q_{n+1} + q_n}{2}\right), \\ q_{n+1} = q_n + hH_p\left(\frac{p_{n+1} + p_n}{2}, \frac{q_{n+1} + q_n}{2}\right). \end{cases} \quad (8)$$



► A general symplectic integrator (named Scheme I):

$$\begin{cases} p_{n+1} = p_n - hH_q(\lambda p_{n+1} + (1 - \lambda)p_n, \lambda q_n + (1 - \lambda)q_{n+1}), \\ q_{n+1} = q_n + hH_p(\lambda p_{n+1} + (1 - \lambda)p_n, \lambda q_n + (1 - \lambda)q_{n+1}), \end{cases}$$

where  $\lambda$  is an any real parameter. When  $\lambda = 0, 1, \frac{1}{2}$ , respectively, the symplectic Euler methods and implicit midpoint rule are obtained. When  $\lambda \neq \frac{1}{2}$ , Scheme I is a 1-stage symplectic partitioned RK method of order 1. The Butcher tableau reads

$$\begin{array}{c|c} \lambda & \lambda \\ \hline & 1 \end{array} \quad \begin{array}{c|c} 1 - \lambda & 1 - \lambda \\ \hline & 1 \end{array}.$$

Scheme I represents a mapping

$$\Phi_h^\lambda : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1}). \quad (9)$$

By a straightforward check, the adjoint method of scheme I is

$$(\Phi_h^\lambda)^* = \Phi_h^{1-\lambda}. \quad (10)$$

## Theorem

*Scheme I and its adjoint method are symplectic for any  $\lambda$ .*

By fixing the parameter to specific values, we can obtain more symplectic schemes with simple forms that can be widely applied in practical computations.

$$\lambda = -1 : \begin{cases} p_{n+1} = p_n - hH_q(2p_n - p_{n+1}, 2q_{n+1} - q_n), \\ q_{n+1} = q_n + hH_p(2p_n - p_{n+1}, 2q_{n+1} - q_n); \end{cases}$$

$$\lambda = \frac{1}{3} : \begin{cases} p_{n+1} = p_n - hH_q\left(\frac{2p_n + p_{n+1}}{3}, \frac{2q_{n+1} + q_n}{3}\right), \\ q_{n+1} = q_n + hH_p\left(\frac{2p_n + p_{n+1}}{3}, \frac{2q_{n+1} + q_n}{3}\right); \end{cases}$$

$$\lambda = \frac{3}{2} : \begin{cases} p_{n+1} = p_n - hH_q\left(\frac{3p_{n+1} - p_n}{2}, \frac{3q_n - q_{n+1}}{2}\right), \\ q_{n+1} = q_n + hH_p\left(\frac{3p_{n+1} - p_n}{2}, \frac{3q_n - q_{n+1}}{2}\right); \end{cases}$$

$$\lambda = 2 : \begin{cases} p_{n+1} = p_n - hH_q(2p_{n+1} - p_n, 2q_n - q_{n+1}), \\ q_{n+1} = q_n + hH_p(2p_{n+1} - p_n, 2q_n - q_{n+1}). \end{cases}$$

## Separable Hamiltonian system

For a separable Hamiltonian with the kinetic energy  $T(p) = \frac{1}{2}p^T M^{-1}p$  in some practical situations, where  $M$  is a constant non-degenerate matrix, the dynamics obeys

$$\dot{p} = -\nabla U(q), \quad \dot{q} = M^{-1}p,$$

which are equivalent to the second-order system  $\ddot{q} = -M^{-1}\nabla U(q)$ . We can obtain a one-stage symplectic Nyström method by applying Scheme I to this second-order system as follows

$$\begin{cases} k_1 = -M^{-1}\nabla U(q_n + (1-\lambda)h\dot{q}_n + \lambda(1-\lambda)h^2k_1), \\ q_{n+1} = q_n + h\dot{q}_n + \lambda h^2k_1, \quad \dot{q}_{n+1} = \dot{q}_n + hk_1. \end{cases}$$

This is the version of the Nyström method corresponding to Scheme I.

# Outline

- 1 Geometric numerical integration
- 2 A novel family of symplectic integrators
- 3 Reconstruction and extension of symplectic schemes**
  - Parameterized generating function methods
  - Symmetric composition methods
- 4 Energy and quadratic invariants preserving methods
- 5 Numerical experiments

# Outline

- 1 Geometric numerical integration
- 2 A novel family of symplectic integrators
- 3 Reconstruction and extension of symplectic schemes
  - Parameterized generating function methods
  - Symmetric composition methods
- 4 Energy and quadratic invariants preserving methods
- 5 Numerical experiments

## Generating function with new coordinates

We denote by  $p, q \in \mathbb{R}^d$  the initial values  $p_1, \dots, p_d$  and  $q_1, \dots, q_d$  at  $t_0$ , respectively. Likewise, the solution of the system at  $t_1$  are represented by  $P, Q \in \mathbb{R}^d$ . This implies that the mapping  $(p, q) \mapsto (P, Q)$  is symplectic.

### Theorem

*Let  $\lambda$  be a real number and the mapping  $\varphi : (p, q) \mapsto (P, Q)$  be smooth, close to the identity. It is symplectic if and only if there exists locally a function  $S(\lambda P + (1 - \lambda)p, \lambda q + (1 - \lambda)Q)$  such that*

$$(Q - q)^T d(\lambda P + (1 - \lambda)p) - (P - p)^T d(\lambda q + (1 - \lambda)Q) = dS. \quad (11)$$

Let the notations  $u = \lambda P + (1 - \lambda)p$ ,  $v = \lambda q + (1 - \lambda)Q$ , comparing the coefficient functions of  $dS = \partial_u S du + \partial_v S dv$  with the left-hand side of (11), we derive the system

$$\begin{cases} P = p - \partial_v S(\lambda P + (1 - \lambda)p, \lambda q + (1 - \lambda)Q), \\ Q = q + \partial_u S(\lambda P + (1 - \lambda)p, \lambda q + (1 - \lambda)Q). \end{cases} \quad (12)$$

## Remark

*The above theorem gives a more general form of generating functions. When  $\lambda = 0, 1, 1/2$ , respectively, we reproduce the generating functions with the three typical coordinates<sup>a</sup> as follows:*

$$(1) \quad (Q - q)^T dp - (P - p)^T dQ = dS_1(p, Q);$$

$$(2) \quad (Q - q)^T dP - (P - p)^T dq = dS_2(P, q);$$

$$(3) \quad (Q - q)^T d(P + p) - (P - p)^T d(Q + q) = 2dS_3\left(\frac{P+p}{2}, \frac{Q+q}{2}\right).$$

---

<sup>a</sup>E. Hairer, C. Lubich, and G. Wanner. Springer-Verlag, Berlin, 2nd edition, 2006.

- In short, a generating function with new coordinates is introduced, which unifies the traditional three typical generating functions<sup>1</sup> that are widely used to construct symplectic schemes.

- How to determine the generating function  $S(u, v)$ ??

---

<sup>1</sup>K. Feng, H.M. Wu, M.Z. Qin, and D.L. Wang. *J. Comput. Math.*, 7:71–96, 1989.

## The Hamilton-Jacobi equation with new variables

Assuming the point  $(P(t), Q(t))$  to move in the exact flow of the system (1), it is found that a smooth generating function  $S(u, v, t)$  generates via (12) the exact flow of the Hamiltonian system.

### Theorem

*Let  $\lambda$  be a real number. If  $S(u, v, t)$  is a smooth solution of the partial differential equation*

$$\frac{\partial S}{\partial t}(u, v, t) = H(u - (1 - \lambda) \frac{\partial S}{\partial v}(u, v, t), v + \lambda \frac{\partial S}{\partial u}(u, v, t)) \quad (13)$$

*with initial condition  $S(u, v, 0) = 0$ , then the mapping  $(p, q) \mapsto (P, Q)$ , defined by (12), is the exact flow of the Hamiltonian system (1).*

### Remark

*When  $\lambda = 0, 1, 1/2$ , respectively, the Hamilton-Jacobi equations under the three typical variables<sup>a</sup> are obtained.*

<sup>a</sup>E. Hairer, C. Lubich, and G. Wanner. Springer-Verlag, Berlin, 2nd edition, 2006.



## Parameterized generating function methods

An approximate solution of the Hamilton-Jacobi equation (13) can construct symplectic schemes of any order. For this purpose, we consider a convergent power series in  $t$  as follows:

$$S(u, v, t) = \sum_{i=1}^{\infty} K_i(u, v) t^i. \quad (14)$$

Inserting this series into (13) and comparing like powers of  $t$ , this follows

$$K_1(u, v) = H(u, v), \quad (15)$$

$$K_2(u, v) = \left(\lambda - \frac{1}{2}\right) \left( \left( \frac{\partial H}{\partial u} \right)^T \frac{\partial H}{\partial v} \right) (u, v), \quad (16)$$

$$\begin{aligned} K_3(u, v) = & \frac{1}{2} \left( \lambda^2 - \lambda + \frac{1}{3} \right) \left( \left( \frac{\partial H}{\partial u} \right)^T \frac{\partial^2 H}{\partial v^2} \frac{\partial H}{\partial u} + \left( \frac{\partial H}{\partial v} \right)^T \frac{\partial^2 H}{\partial u^2} \frac{\partial H}{\partial v} \right) (u, v) \\ & + \left( \lambda^2 - \lambda + \frac{1}{6} \right) \left( \left( \frac{\partial H}{\partial v} \right)^T \frac{\partial^2 H}{\partial u \partial v} \frac{\partial H}{\partial u} \right) (u, v). \end{aligned} \quad (17)$$

.....

A natural way to approximate  $S$  is take the truncation of (14). More precisely, we replace (14) with the truncated series

$$\bar{S}(u, v) = \sum_{i=1}^r K_i(u, v) h^i. \quad (18)$$

Then we get a symplectic scheme of order  $r$ .

► Scheme I (order 1):

$$\begin{cases} p_{n+1} = p_n - h \partial_{\bar{v}} H(\bar{u}, \bar{v}), \\ q_{n+1} = q_n + h \partial_{\bar{u}} H(\bar{u}, \bar{v}). \end{cases} \quad (19)$$

► Scheme II (order 2):

$$\begin{cases} p_{n+1} = p_n - h \partial_{\bar{v}} H(\bar{u}, \bar{v}) - (\lambda - \frac{1}{2}) h^2 \left( \frac{\partial^2 H}{\partial \bar{v}^2} \frac{\partial H}{\partial \bar{u}} + \frac{\partial^2 H}{\partial \bar{v} \partial \bar{u}} \frac{\partial H}{\partial \bar{v}} \right) (\bar{u}, \bar{v}), \\ q_{n+1} = q_n + h \partial_{\bar{u}} H(\bar{u}, \bar{v}) + (\lambda - \frac{1}{2}) h^2 \left( \frac{\partial^2 H}{\partial \bar{u}^2} \frac{\partial H}{\partial \bar{v}} + \frac{\partial^2 H}{\partial \bar{u} \partial \bar{v}} \frac{\partial H}{\partial \bar{u}} \right) (\bar{u}, \bar{v}). \end{cases} \quad (20)$$

The notations  $\bar{u} = \lambda p_{n+1} + (1 - \lambda) p_n$ ,  $\bar{v} = \lambda q_n + (1 - \lambda) q_{n+1}$  are used.

# Outline

- 1 Geometric numerical integration
- 2 A novel family of symplectic integrators
- 3 Reconstruction and extension of symplectic schemes
  - Parameterized generating function methods
  - Symmetric composition methods
- 4 Energy and quadratic invariants preserving methods
- 5 Numerical experiments

## Symmetric composition methods

We consider the symmetric composition method<sup>2</sup> of Scheme I and get the following symmetric symplectic scheme of order 2.

► Scheme III:

$$\Psi_\tau \triangleq \Phi_{\frac{\tau}{2}}^\lambda \circ (\Phi_{\frac{\tau}{2}}^\lambda)^* = \Phi_{\frac{\tau}{2}}^\lambda \circ \Phi_{\frac{\tau}{2}}^{1-\lambda} : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1}). \quad (21)$$

- The symplecticity of Scheme III follows from the fact that the composition of symplectic schemes is still symplectic.
- Using the idea of composition methods<sup>3</sup>, this procedure can also be repeated all the time to construct the higher order symmetric symplectic scheme without higher derivatives.

---

<sup>2</sup>H. Yoshida. *Phys. Lett. A*, 150:262–268, 1990.

<sup>3</sup>M.Z. Qin and W.J. Zhu. *Computing*, 47:309–321, 1992.

## Concluding remarks

- A general parametric symplectic scheme covers the symplectic Euler methods and the midpoint rule. By fixing the parameter to specific values, we can obtain more symplectic schemes with simple forms that can be widely applied in practical computations.
- A more general form of generating functions and the Hamilton-Jacobi equations is proposed, which generalizes the three typical ones widely used to construct symplectic algorithms.
- Two classes of arbitrary high-order parameterized symplectic schemes enrich the types of available symplectic methods.

# Outline

- 1 Geometric numerical integration
- 2 A novel family of symplectic integrators
- 3 Reconstruction and extension of symplectic schemes
  - Parameterized generating function methods
  - Symmetric composition methods
- 4 Energy and quadratic invariants preserving methods
- 5 Numerical experiments

## Energy and quadratic invariants preserving methods (EQUIP)

Some simple applications are given by the parameter  $\lambda$  serving for clever tuning to obtain energy conservation in the numerical solution.

- Scheme IV (order 1): **Scheme I+energy conservation**

$$\begin{cases} p_{n+1} = p_n - h\partial_q H(\lambda p_{n+1} + (1-\lambda)p_n, \lambda q_n + (1-\lambda)q_{n+1}), \\ q_{n+1} = q_n + h\partial_p H(\lambda p_{n+1} + (1-\lambda)p_n, \lambda q_n + (1-\lambda)q_{n+1}), \\ H(p_{n+1}, q_{n+1}) = H(p_n, q_n). \end{cases}$$

- Scheme V (order 2): **Scheme III+energy conservation**

$$\begin{cases} (p_{n+1}, q_{n+1}) = \Psi_h(p_n, q_n), \\ H(p_{n+1}, q_{n+1}) = H(p_n, q_n). \end{cases}$$

If a real value  $\lambda$  can be found such that the condition  $H(p_{n+1}, q_{n+1}) = H(p_n, q_n)$  is satisfied, we get a one-step scheme

$$\Phi_h^\lambda : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1}). \quad (22)$$

For a fixed  $\lambda$ , the scheme (22) is symplectic so that all quadratic invariants are preserved. If the existence of the parameter  $\lambda$  is verified, there exists a real sequence  $\{\lambda_i\}$  as the following diagram

$$(p_n, q_n) \xrightarrow{\Phi_h^{\lambda_1}} (p_{n+1}, q_{n+1}) \xrightarrow{\Phi_h^{\lambda_2}} (p_{n+2}, q_{n+2}) \xrightarrow{\Phi_h^{\lambda_3}} (p_{n+3}, q_{n+3}) \mapsto \cdots \quad (23)$$

such that the numerical solution  $(p_{n+i}, q_{n+i})$  defined by  $\Phi_h^{\lambda_i}$  satisfies  $H(p_{n+i}, q_{n+i}) = H(p_n, q_n)$ ,  $i = 1, 2, \dots$ . Symplectic schemes with different fixed parameters are used at each step to obtain energy conservation.

### Remark

*Schemes IV and V are energy and quadratic invariants preserving.*



## Solvability

Following the classical formulation of the implicit function theorem, we define the vector equation

$$G(p_{n+1}, q_{n+1}, \lambda, p_n, q_n, h) \triangleq \begin{pmatrix} p_{n+1} - p_n + hH_q(\bar{u}, \bar{v}) \\ q_{n+1} - q_n - hH_p(\bar{u}, \bar{v}) \\ H(p_{n+1}, q_{n+1}) - H(p_n, q_n) \end{pmatrix} = 0 \quad (24)$$

which is equivalent to Scheme IV. The function  $G$  vanishes at point  $(p_n, q_n, \lambda_0, p_n, q_n, 0)$  with any real  $\lambda_0$ . The Jacobi matrix of  $G$  at this point is obtained as

$$\left. \frac{\partial G}{\partial(p_{n+1}, q_{n+1}, \lambda)} \right|_{(p_n, q_n, \lambda_0, p_n, q_n, 0)} = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ H_p(p_n, q_n) & H_q(p_n, q_n) & 0 \end{pmatrix}. \quad (25)$$

This lead to a nonlinear system with a **singular Jacobian** so the usual Newton-type iteration methods are invalid. It is immediately clear that the traditional steps does not help to acquire the solvability of Scheme IV.

The next nonlinear function

$$E(\lambda, h) = H(p_{n+1}(\lambda, h), q_{n+1}(\lambda, h)) - H(p_n, q_n) \quad (26)$$

is introduced as an error function of the numerical Hamiltonian, where  $p_{n+1}(\lambda, h)$  and  $q_{n+1}(\lambda, h)$  are defined by the first two equations of Scheme IV.

It is apparent that the solvability of Scheme IV is equivalent to the existence of a solution in the form  $\lambda = \lambda(h)$  of  $E(\lambda, h) = 0$ , in particular  $E(1/2, 0) = 0$  as the initial condition.

### Theorem

*Assuming that the Hamiltonian is sufficiently smooth, then there exists a function  $\lambda = \lambda(h)$  defined in a neighborhood  $(-h_0, h_0)$  with  $h_0$  small enough, such that*

- (1)  $E(\lambda(h), h) = 0$  for all  $\tau \in (-h_0, h_0)$ ;*
- (2)  $\lambda(h) = 1/2 + \varepsilon(h)h$  with  $\varepsilon(h) = \text{constant} + \mathcal{O}(h)$ .*

## Concluding remarks

- The existence of  $\lambda_*(h) = 1/2 + \varepsilon(h)h$  around  $1/2$  is confirmed to make EQUIP methods solvable, which reveals the superior behavior of the midpoint method in most actual calculations.
- By tuning the free parameter in symplectic schemes, we achieve the energy preservation. Thus, we establish the relation between symplectic schemes and energy-preserving methods.
- A novel methodology is proposed to construct arbitrary high-order energy preserving methods.
- The symplecticity and energy conservation are realized at the same time from a new perspective in a weaker sense.

# Outline

- 1 Geometric numerical integration
- 2 A novel family of symplectic integrators
- 3 Reconstruction and extension of symplectic schemes
  - Parameterized generating function methods
  - Symmetric composition methods
- 4 Energy and quadratic invariants preserving methods
- 5 Numerical experiments

## The Hénon-Heiles model

The Hénon-Heiles model originates from a problem in celestial mechanics. The dynamics is described by a Hamiltonian of the form

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) + U(q_1, q_2). \quad (27)$$

The following potential  $U$  is chosen as

$$U(q_1, q_2) = \frac{1}{2}(q_1^2 + q_2^2 + 2q_1^2q_2 - \frac{2}{3}q_2^3). \quad (28)$$

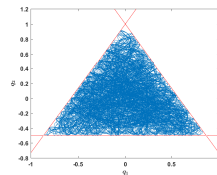
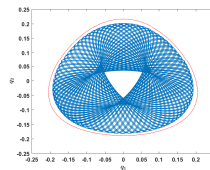
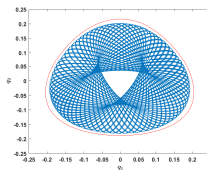
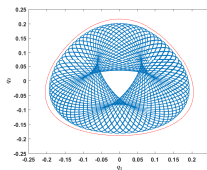
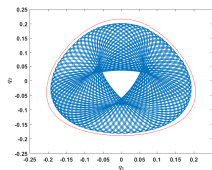
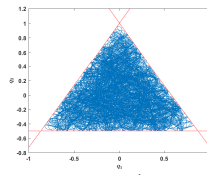
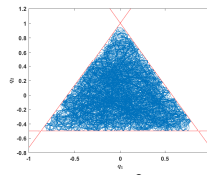
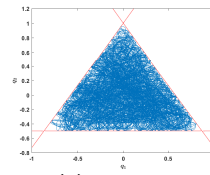
The two classical orbits will be illustrated with the initial value as follows:

(1) box orbit:  $H_0 = 0.02$ ,  $p_2(0) = 0$ ,  $q_1(0) = 0$ ,  $q_2(0) = -0.082$ ;

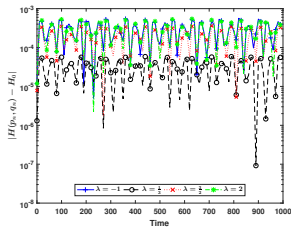
(2) chaotic orbit:  $H_0 = \frac{1}{6}$ ,  $p_2(0) = 0$ ,  $q_1(0) = 0$ ,  $q_2(0) = 0.82$ .

The values of  $p_1(0)$  are found from the Hamiltonian (27).

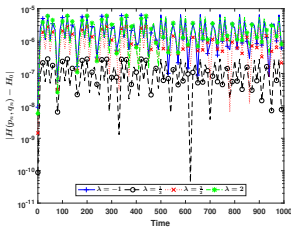
# Box and chaotic orbits of Scheme I

(a)  $\lambda = -1$ (b)  $\lambda = \frac{1}{3}$ (c)  $\lambda = \frac{3}{2}$ (d)  $\lambda = 2$

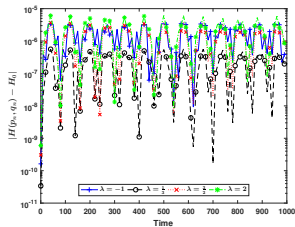
# Energy conservation of box (first row) and chaotic orbits



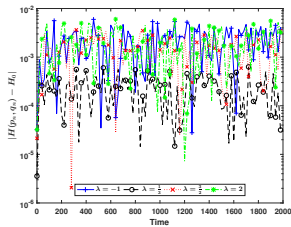
(e) Scheme I (left)



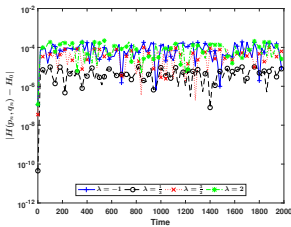
(f) Scheme II (middle)



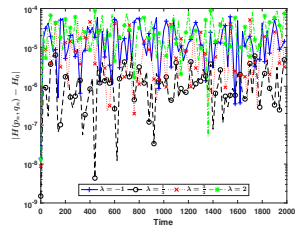
(g) Scheme III (right)



(e) Scheme I (left)



(f) Scheme II (middle)



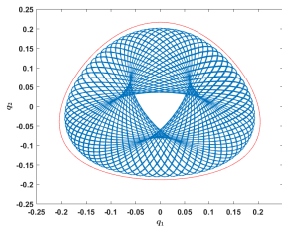
(g) Scheme III (right)

Convergence rates with chaotic orbits at  $t = 1$ 

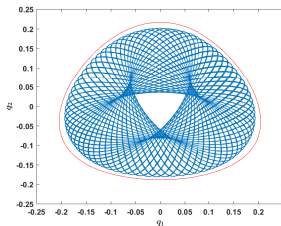
Scheme	$h$	$\lambda = -1$		$\lambda = \frac{1}{3}$		$\lambda = \frac{3}{2}$		$\lambda = 2$	
		error	order	error	order	error	order	error	order
I	0.02/2	4.31E-03	-	4.38E-04	-	2.63E-03	-	3.85E-03	-
	0.02/4	2.09E-03	1.04	2.23E-04	0.98	1.34E-03	0.98	1.98E-03	0.96
	0.02/8	1.03E-03	1.02	1.12E-04	0.99	6.73E-04	0.99	1.00E-03	0.98
	0.02/16	5.13E-04	1.01	5.63E-05	0.99	3.38E-04	0.99	5.06E-04	0.99
II	0.02/2	5.09E-04	-	2.35E-05	-	2.24E-04	-	4.77E-04	-
	0.02/4	1.25E-04	2.02	5.87E-06	2.00	5.67E-05	1.98	1.21E-04	1.98
	0.02/8	3.11E-05	2.01	1.47E-06	2.00	1.42E-05	1.99	3.06E-05	1.99
	0.02/16	7.74E-06	2.01	3.67E-07	2.00	3.57E-06	2.00	7.68E-06	1.99
III	0.02/2	1.12E-04	-	3.54E-06	-	5.04E-05	-	1.18E-04	-
	0.02/4	2.79E-05	2.00	8.84E-07	2.00	1.26E-05	2.00	2.94E-05	2.00
	0.02/8	6.97E-06	2.00	2.21E-07	2.00	3.15E-06	2.00	7.34E-06	2.00
	0.02/16	1.74E-06	2.00	5.52E-08	2.00	7.88E-07	2.00	1.84E-06	2.00



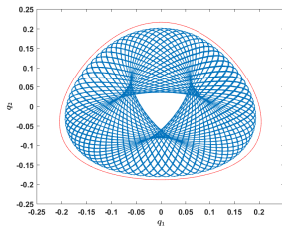
# Box (first row) and chaotic orbits of AVF, Schemes IV and V till $t = 1000$



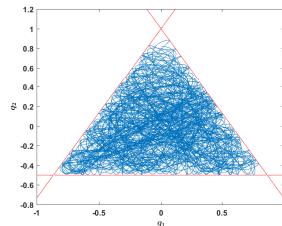
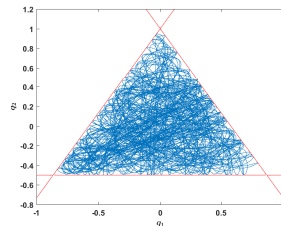
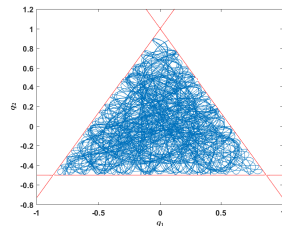
(h) AVF (left)



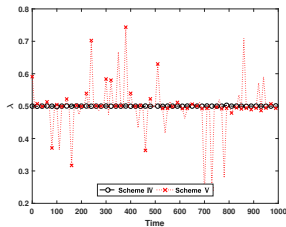
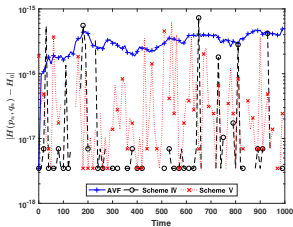
(i) Scheme IV (middle)



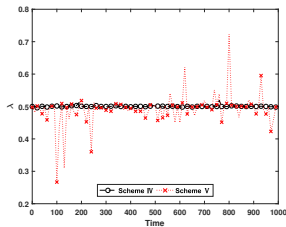
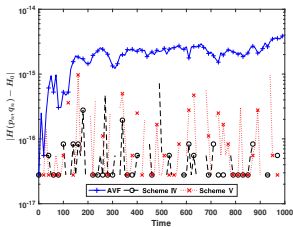
(j) Scheme V (right)



# Energy conservation of AVF, Schemes IV and V



(k) Box orbits



(l) Chaotic orbits

Convergence tests with chaotic orbits at  $t = 1$ 

$h$	AVF		Scheme IV		Scheme V	
	<i>error</i>	<i>order</i>	<i>error</i>	<i>order</i>	<i>error</i>	<i>order</i>
0.02/2	1.78E-05	-	2.50E-03	-	4.23E-06	-
0.02/4	4.46E-06	2.00	1.24E-03	1.01	1.06E-06	2.00
0.02/8	1.11E-06	2.00	6.22E-04	0.99	2.64E-07	2.00
0.02/16	2.78E-07	2.00	3.10E-04	1.00	6.60E-08	2.00

## The perturbed Kepler problem

Our second experiment is the motion of a planet in the Schwarzschild potential for Einstein's general relativity theory. The Hamiltonian of the dynamics reads

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}} - \frac{\mu}{3\sqrt{(q_1^2 + q_2^2)^3}}, \quad (29)$$

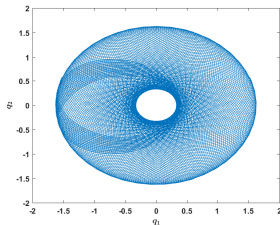
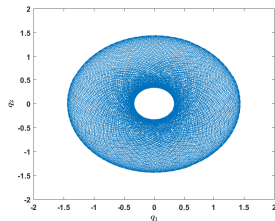
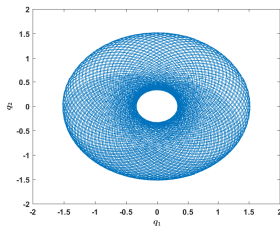
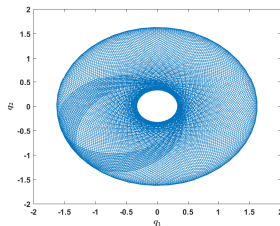
where  $\mu$  is a positive or negative small number. Moreover, the angular momentum of this system

$$L(p_1, p_2, q_1, q_2) = q_1 p_2 - q_2 p_1 \quad (30)$$

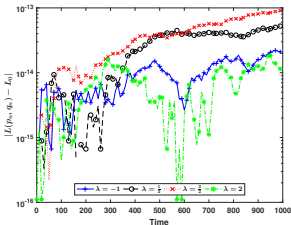
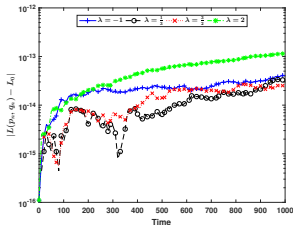
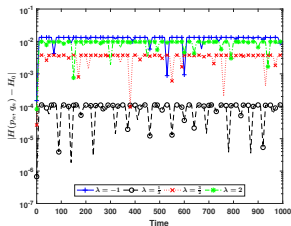
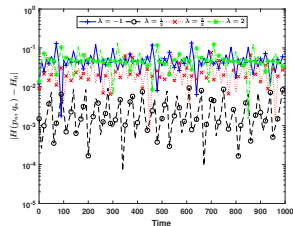
is a quadratic first integral. We choose the initial points as

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

which confers an eccentricity  $e$  on the orbit. We set  $e = 0.6$  and  $\mu = 0.0075$  in this experiment. Then  $H(p, q) = H_0 \approx -0.5391$ ,  $L(p, q) = L_0 = 0.8$ . The system (29) represents approximately an ellipse orbit with eccentricity  $e$  for  $H_0 < 0$ .

Orbits of Scheme I till  $t = 1000$ (m)  $\lambda = -1$ (n)  $\lambda = \frac{1}{3}$ (o)  $\lambda = \frac{3}{2}$ (p)  $\lambda = 2$

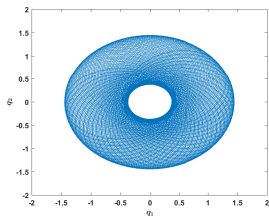
# Energy (first row) and angular momentum conservation of Schemes I and III



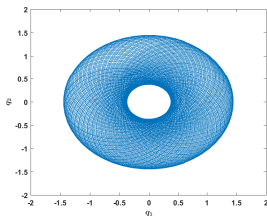
(q) Scheme I (left)

(r) Scheme III (right)

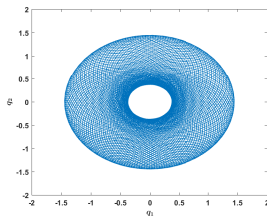
# Numerical results of AVF, Schemes IV and V



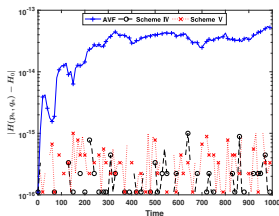
(s) AVF



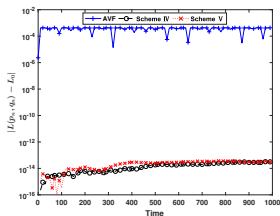
(t) Scheme IV



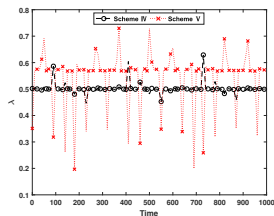
(u) Scheme V



(v) Energy conservation



(w) Momentum conservation

(x) Value distribution of  $\lambda$

# Outline

- 1 Geometric numerical integration
- 2 A novel family of symplectic integrators
- 3 Reconstruction and extension of symplectic schemes
  - Parameterized generating function methods
  - Symmetric composition methods
- 4 Energy and quadratic invariants preserving methods
- 5 Numerical experiments



Thanks for your attention!