天体力学数学理论研讨会
2022.11.24-25，陈省身数学研究所

哈密尔顿系统的辛几何算法

尚在久
中国科学院数学与系统科学研究院

2022年11月25日

Outline of the talk

1. Introduction to geometric numerical integration
2. Hamiltonian systems
3. Symplectic integration
4. Stability analysis

4-1. Numerical resonance

4-2. Nonresonant time-step size

4-3. Numerical KAM theorem

4-4. Backward error analysis

4-5. Homoclinic trajectory splitting analysis

1. Introduction

动力系统研究给定系统的长时间演化行为，对其演化方程的解及其守恒量(或者统计不变量）进行稳定的数值模拟往往具有很大的挑战性。挑战之一是如何对连续系统构造合适的离散化算法，不同的离散化方法会产生截然不同的数值结果。几何算法是根据系统的已知代数或几何结构构造保持系统内在性质的数值方法，我国数学家冯康院士领导开创了这一方向的研究并取得了系统的理论成果,推动了其在科学计算的应用。

动力系统几何算法的一个重要分支 “哈密尔顿系统的辛几何算法” 获1997年度国家自然科学奖一等奖(冯康等)。

1. Introduction

(1) 基本问题：

$$\frac{dx}{dt} = a(x), x \in R^n$$

and initial conditions

例：

Newton’s N-body problem (N is small)
Molecular dynamics (N is very large)
Particle tracking problem in fluid dynamics
Time integration of Schroedinger\Maxwell equations (n=infinity)
More others …

1. Introduction

问题:

Dynamics of the system defined by “$a(x)$” ?

=Long-time behavior of solutions

求解:

Quadrature (very few cases)

Qualitative theory (methods of dynamical systems)

Numerical solution (necessary and practical)

for simulations and understanding to problems

1. Introduction

(2) 数值方法(算例分析)：

Euler (1768): $$\frac{dx}{dt} \approx \frac{x_{n+1} - x_n}{h} = \Delta E_n$$

Euler explicit: $$\Delta E_n = a(x_n)$$

Euler implicit: $$\Delta E_n = a(x_{n+1})$$

Implicit mid-point rule: $$\Delta E_n = a\left(\frac{x_n + x_{n+1}}{2}\right)$$

Runge-Kutta (1895,1901) --- systematicaly developed by J. Butcher,…

1. Introduction

A simple example: Harmonic oscillator

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

- Equations of motion:

$$\frac{dp}{dt}=-q,\ \frac{dq}{dt}=p$$

- Phase orbits:

  - The only equilibrium (p,q)=(0,0) (elliptic);
  - Circles of any radius centered at the origin;

1. Introduction

Simple numerical methods (h is time step**):**

- Explicit Euler: $p_{n+1} = p_n - hq_n, q_{n+1} = q_n + hp_n$

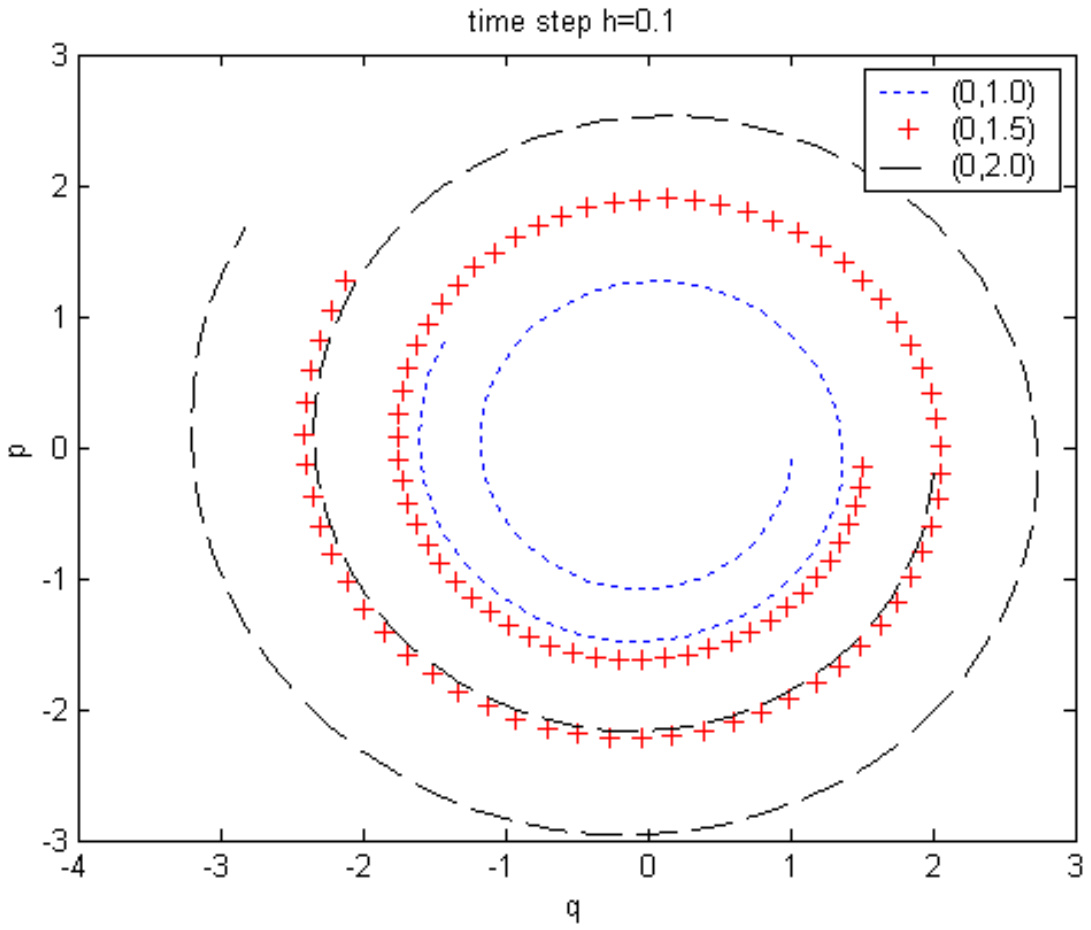
h

- Implicit Euler: $p_{n+1} = p_n - hq_{n+1}, q_{n+1} = q_n + hp_{n+1}$

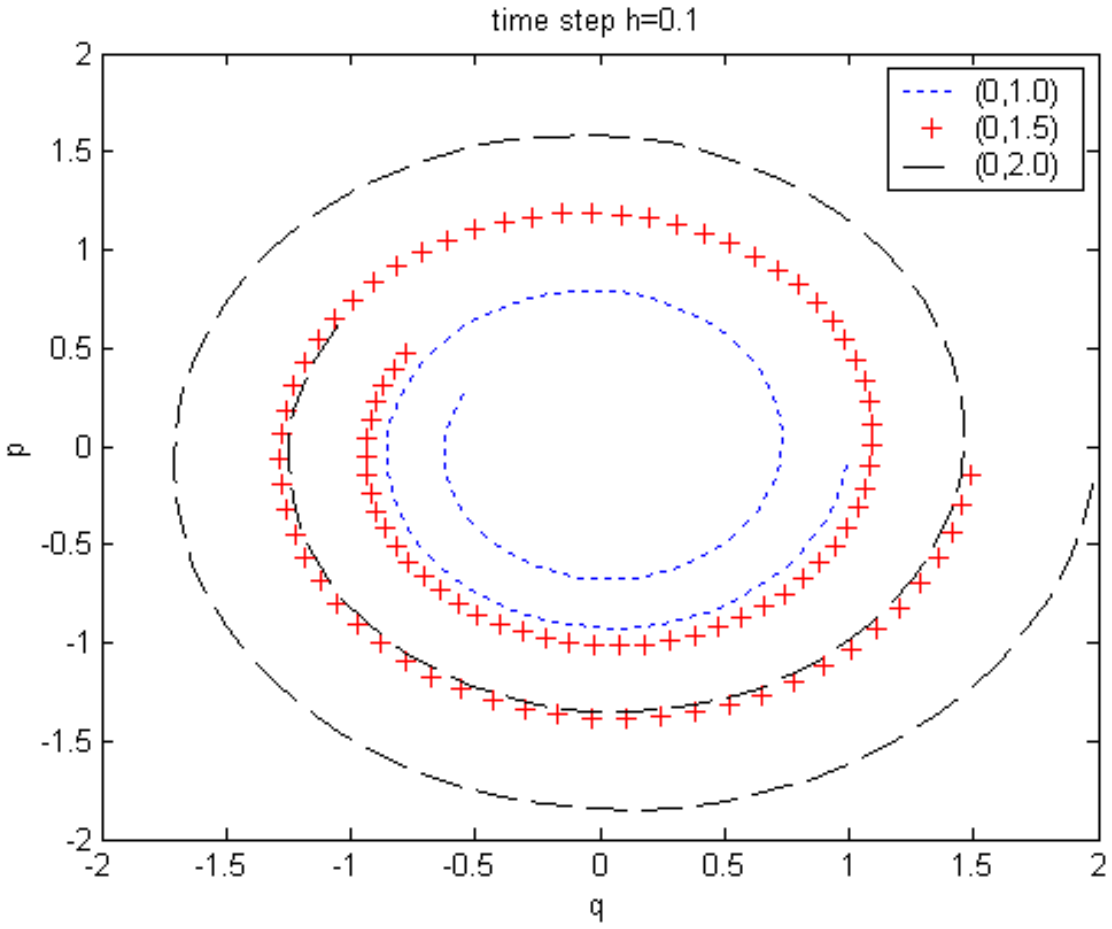
- Midpoint rule:

$$p_{n+1} = p_n - h\left[\left(q_n + q_{n+1}\right)/2\right], q_{n+1} = q_n + h\left[\left(p_n + p_{n+1}\right)/2\right]$$

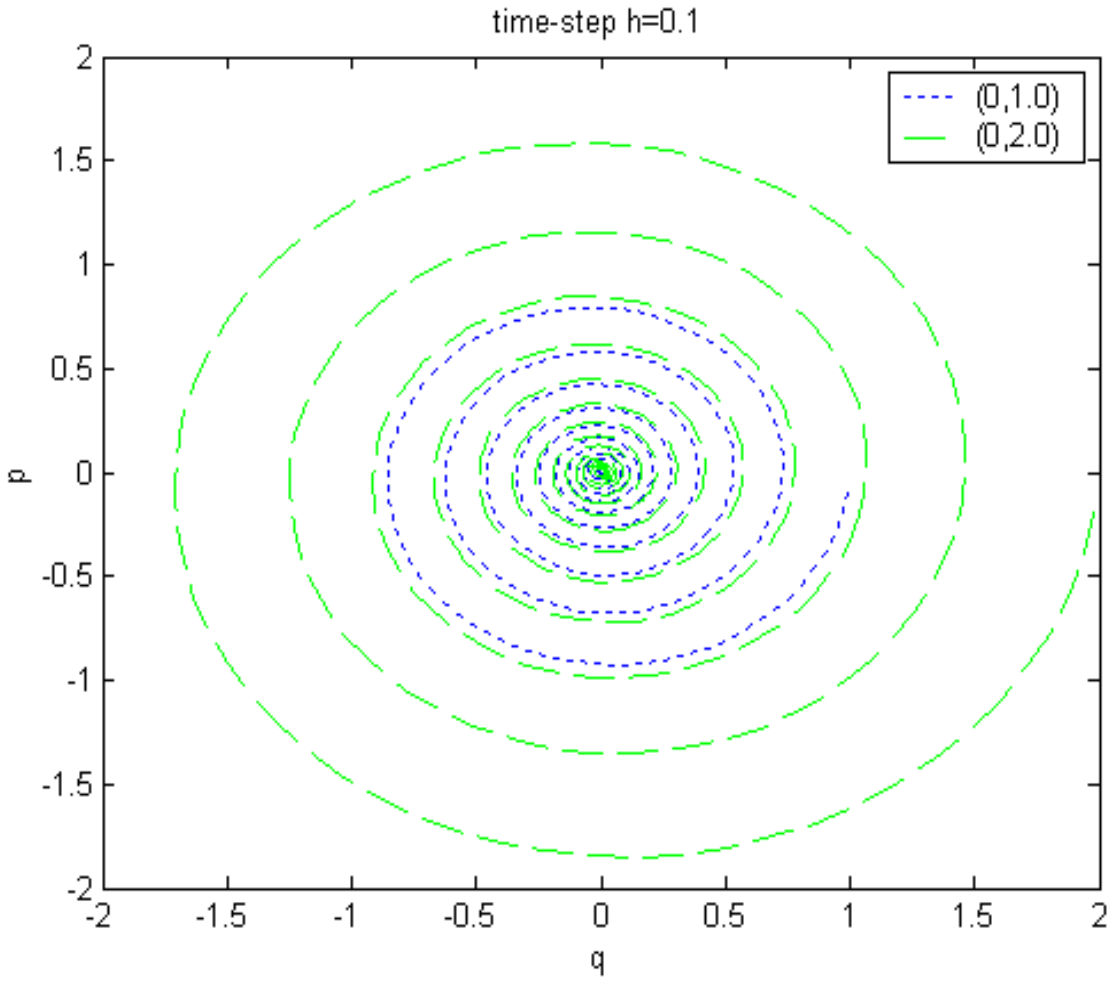
Explicit Euler: orbits expand outward (wrong!)



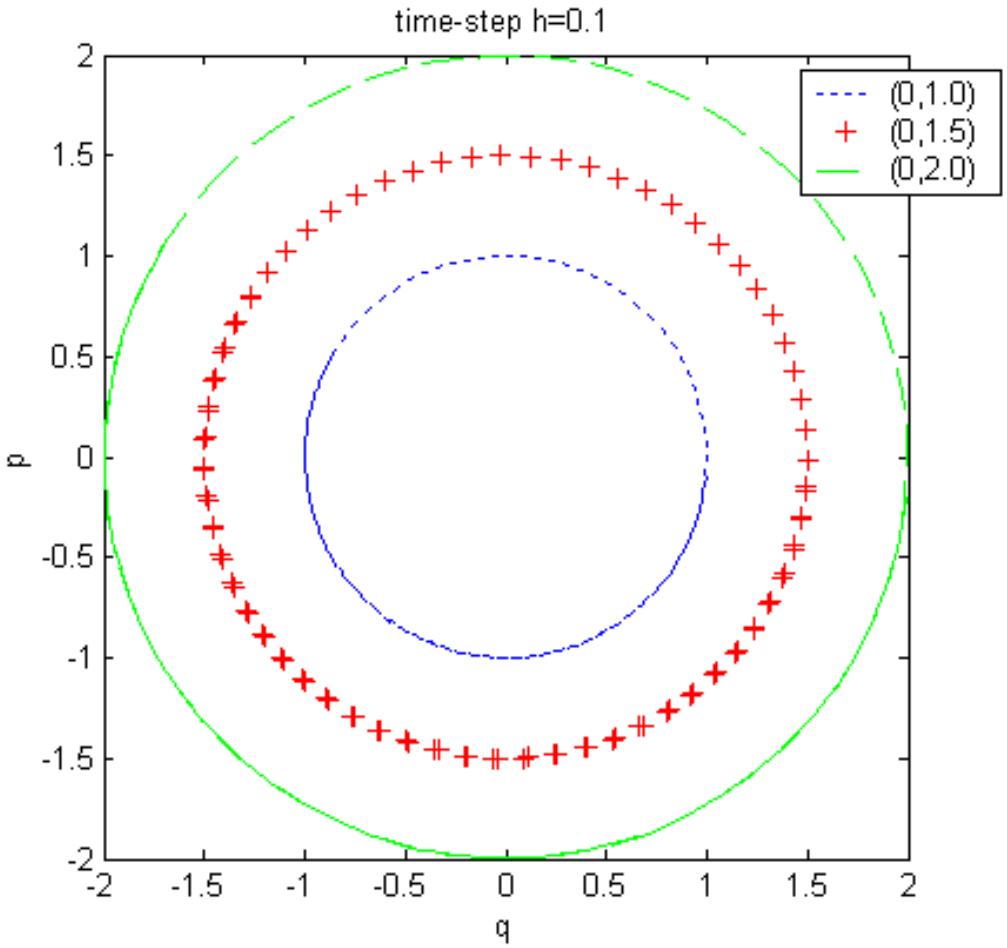
Implicit Euler: orbits contract inward (wrong!)



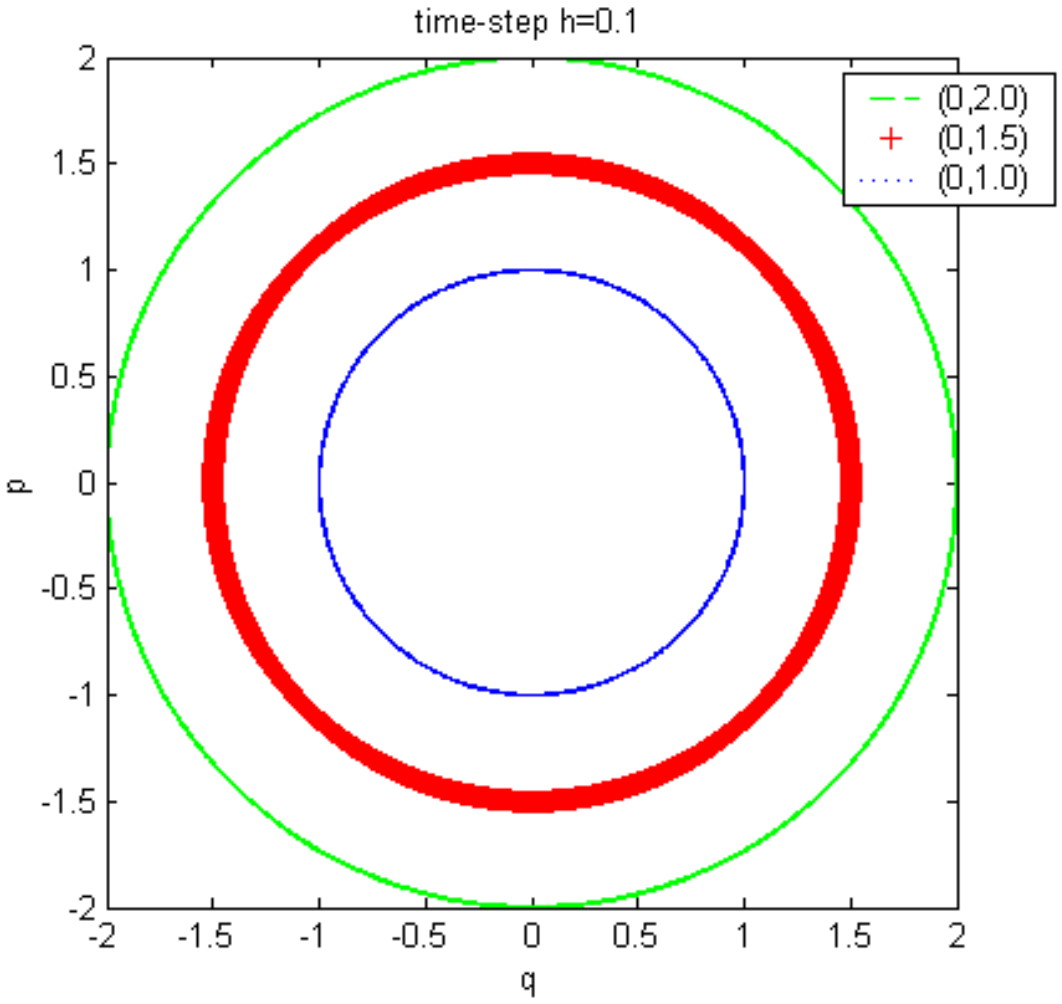
Implicit Euler: “long time” orbits (totally wrong!)



Midpoint rule: almost circles for “long time” (right)



Midpoint rule: almost circles for “very long time” (right)



1. Introduction

A nonlinear system: Pendulum

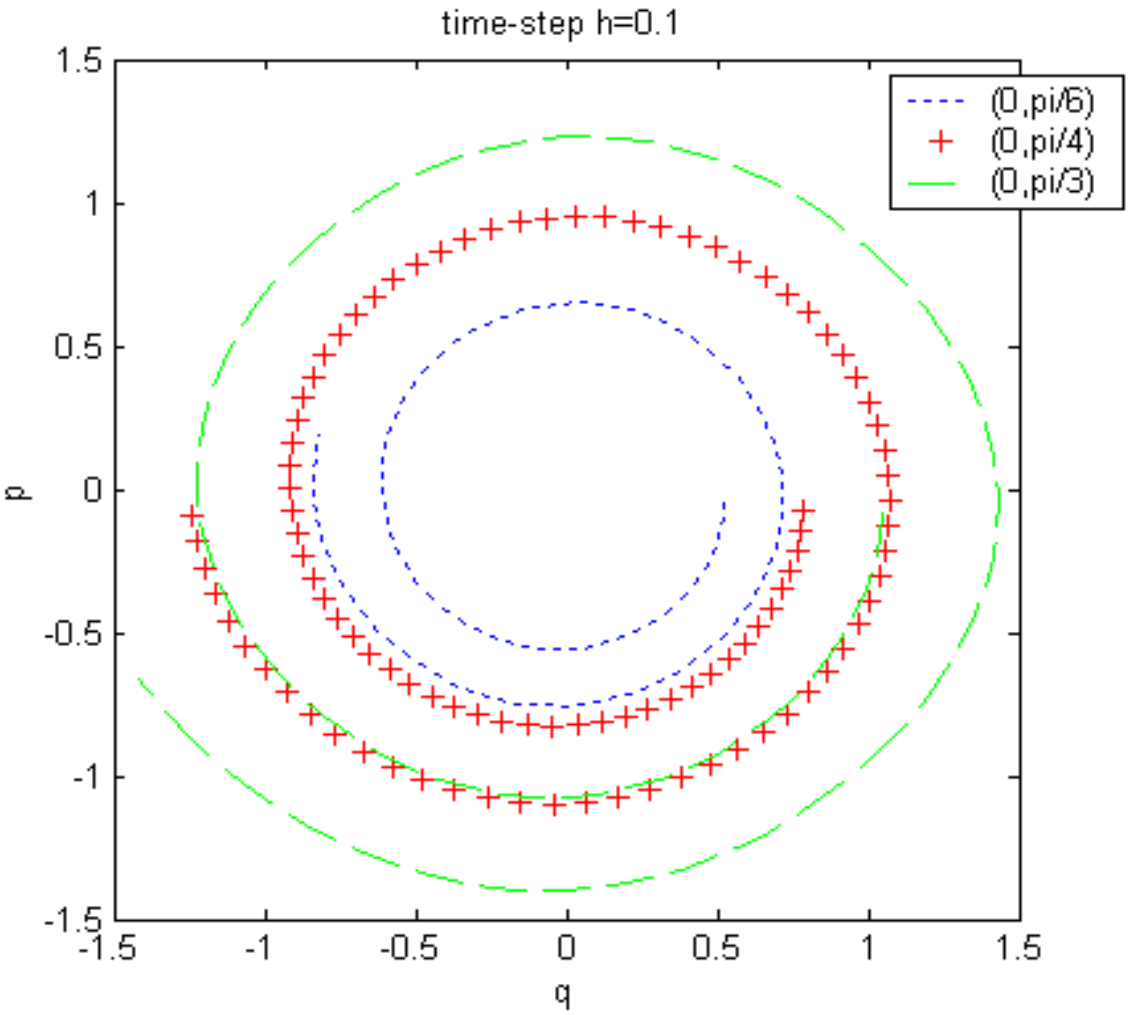
- Hamiltonian function: $H(p,q)=\frac{1}{2}p^2-\cos q$

- Equations of motion:

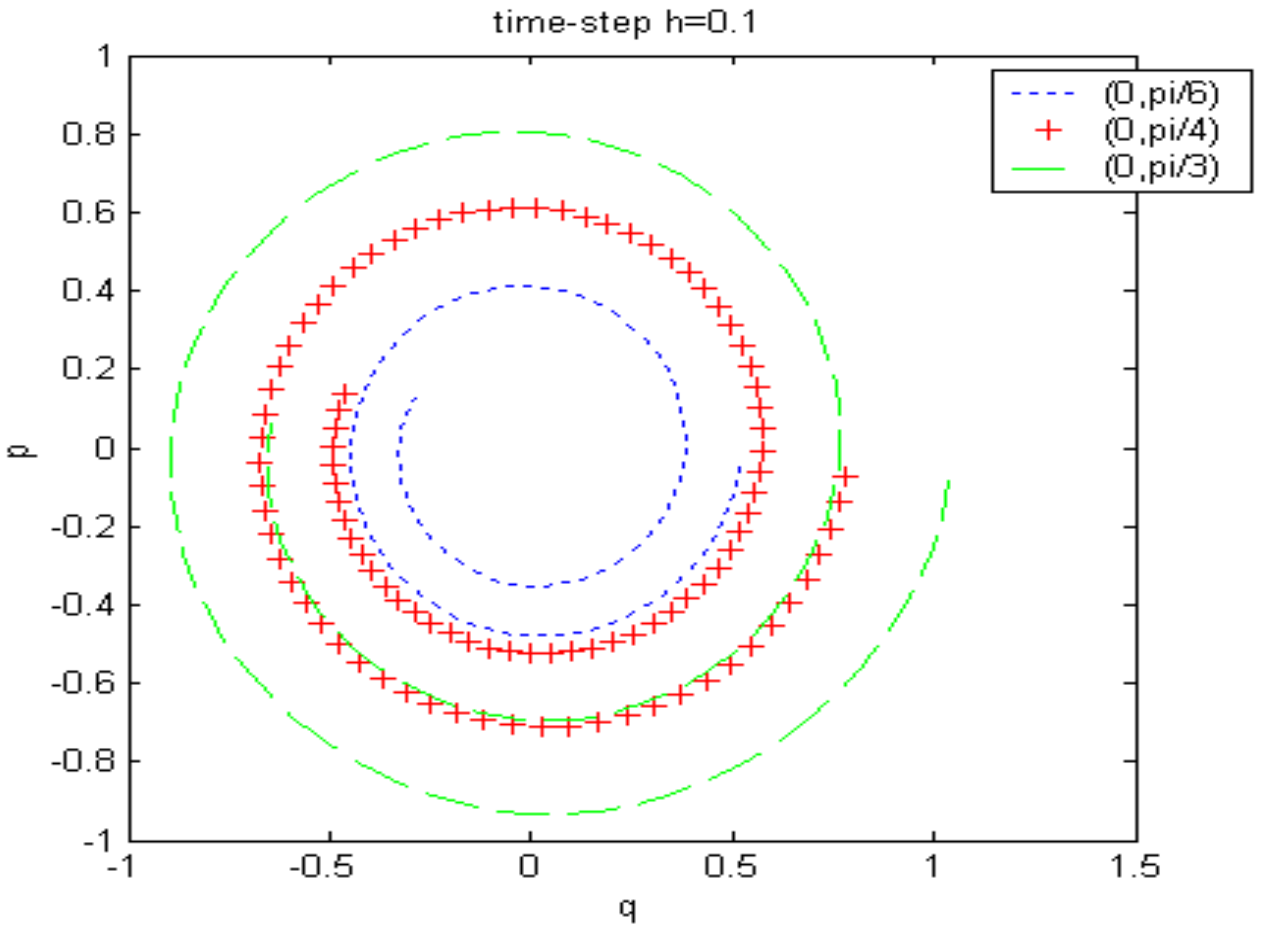
$$\frac{dp}{dt}=-\sin q,\frac{dq}{dt}=p$$

- Phase orbits:
- Equilibria $(p,q)=(0,k\pi)$, elliptic (hyperbolic) for even (odd) k;
- Closed curves for $-1<H<1$;
- Separatrix for $H=1$

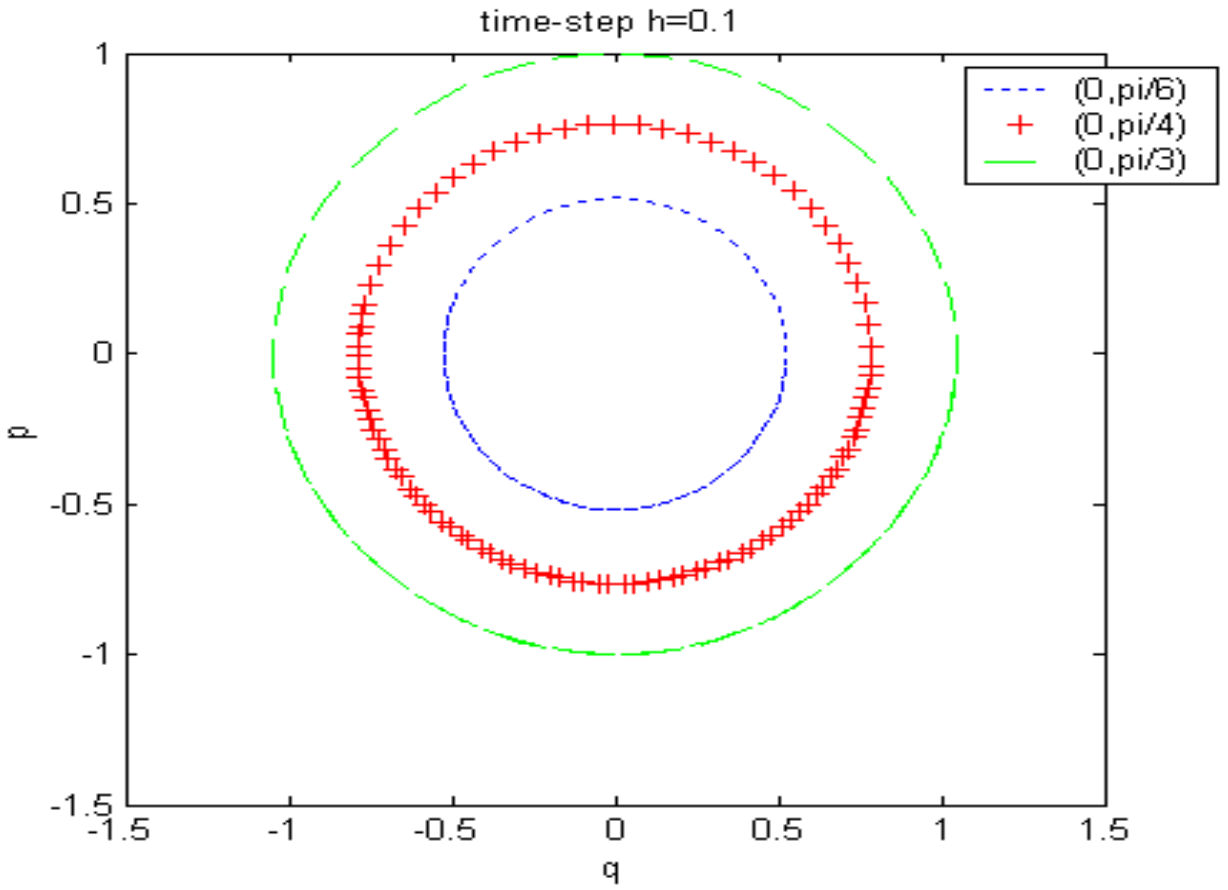
Explicit Euler: orbits expand outward (wrong!)



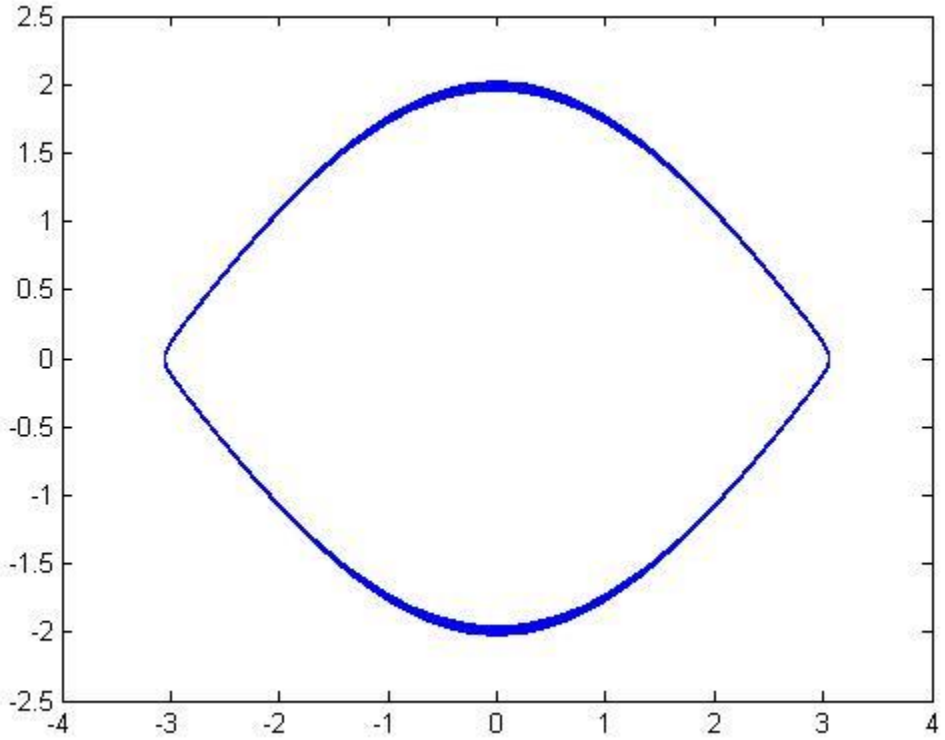
Implicit Euler: orbits contract inward (wrong!)



Midpoint rule: closed curves for “very long time” (right)



Midpoint rule: saddle separatrix for “very long time” (right) (symplectic, area-preserving map)



1. Introduction

Why?

- $H(p_n, q_n)$ increases as *n* increases by Explicit Euler (wrong);
- $H(p_n, q_n)$ decreses as *n* increases by Implicit Euler (wrong);
- $H(p_n, q_n)$ is (nearly) invariant as *n* increases by Midpoint rule (right).

- Area of any domain in *(p,q)* plane (**symplectic structure** of R^2):

➢ expands under Explicit Euler (wrong) ;

➢ contracts under Implicit Euler (wrong);

➢ is preserved by the midpoint rule (right);.

1. Introduction

- 数值方法的目的是尽可能地精确求解或者正确理解系统的动力学（即解的长时间行为), 特别是达到某种宏观平衡态的动力学，如：周期解、拟周期解、几乎周期解、同宿/异宿解…,以及支撑这些解的遍历分支------极小不变集。
- 对这些解的数值模拟是计算数学的巨大挑战。
- 以上的例子初步说明，数值方法是否保持系统的代数/几何结构对实现上述目标至关重要。

- **动力系统几何算法：保持系统代数/几何结构的数值方法。**

1. Introduction

(3) 基本思想（冯康）

- 向量场**李代数**:

$$V_n = \left\{ a : R^n \to R^n, a \in C^\infty \right\}$$

- 李括弧:

$$[a, b] = \frac{\partial a}{\partial x} b - \frac{\partial b}{\partial x} a$$

- 无穷维(局部)**李群**: R^n 上的(局部)微分同胚群 D_n

- **指数影射**: $V_n \xrightarrow{f_a^t} D_n$

1. Introduction

- V_n 的子代数(E.Cartan 的分类, 1904-):
- R^{2n} 上的 哈密尔顿向量场 HV_{2n}

$$a(x) = J\nabla H(x)$$

- R^n 上的无源向量场 SV_n :散度为零
- R^{2n+1} 上的切触向量场 CV_{2n+1}

  ------- R^{2n+2} 上的锥形哈密尔顿向量场

1. Introduction

- 经典数值方法只考虑保持最大的李代数/李群对应关系

$$V_n \xrightarrow{F_a^h} D_n$$

- 冯康的想法:

$$HV_{2n} \xrightarrow{F_a^h} SD_{2n} \quad (辛算法)$$

$$SV_n \xrightarrow{F_a^h} VD_n \quad (保体积算法)$$

$$CV_{2n+1} \xrightarrow{F_a^h} CD_{2n+1} \quad (切触算法)$$

$$LV_n \xrightarrow{F_a^h} LD_n \quad (冯康原理)$$

1. Introduction

- 数值方法的一般原则：

“It is natural to look forward to those discrete systems which preserve as many as possible intrinsic properties of the continuous system.”

------K. Feng (1985)

2. Hamiltonian systems

A Hamiltonian system of ordinary differential equations reads:

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, i = 1,2,\cdots,n$$

where

$$q = (q_1, q_{2,} \cdots, q_n)^T \quad \text{and} \quad p = (p_1, p_2, \cdots, p_n)^T$$

are the position and momentum vectors (conjugate variables), respectively,

$$H = H(q, p) : T^*M \cong M \times R^n \subset R^{2n} \to R$$

is the Hamiltonian (total energy in classical mechanics).

M is the configuration manifold.

2. Hamiltonian systems

This is a system of ordinary differential equations of special form with $2n$ unkown variables, but can formulate almost all the physical processes of time evolution of a system with n degrees of freedom without considering dissipation (from classical mechanics to statistical physics).

- Two distinguished properties:
- Hamiltonian is a conservative quantity during time evolution;
- The phase flow preserves the symplectic structure of the phase space T^*M, i.e., the solution map from the initial phase state to the time t state is symplectic.

$$\left(\frac{\partial f_H^t}{\partial z}(z)\right)^T J \frac{\partial f_H^t}{\partial z}(z) = J$$

Where $z = (q^T, p^T)^T$

2. Hamiltonian systems

- Example (Newton's equations): $H(q, p) = T(p) + V(q)$

Question 1:

- Solve the system with given initial states as accurately as possible in as long as possible time intervals (e.g., motions of the planets of the solar system --- N-body problems in which $n = 3N$).

Question 2:

- Give statistical averages of macroscopic physical quantities which are functions of the microscopic phase states of the system of particles whose motions are described by the Hamilton's equations (e.g., molecular dynamics).

2. Hamiltonian systems

- For the both “Questions”, one needs to integrate the Hamilton’s equations in very long time, which is challenging in many interesting problems.
- For “Question 2”, in addition, ergodicity of the sample trajectories should be verified or assumed.

◆ N-body problem: $T(p)=\frac{1}{2}p^T\mathbf{M}^{-1}p, V(q)=\sum_{1\le i<j\le N}\frac{Gm_im_j}{|\mathbf{r_i}-\mathbf{r_j}|}$

$$m_i\frac{d^2\mathbf{r}_i}{d^2t}=\mathbf{F}_i(t,\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N,),i=1,...,N$$

$$\mathbf{F}_i(t,\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N)=\sum_{j\neq i}G\frac{m_im_j}{|\mathbf{r}_i-\mathbf{r}_j|^2}\frac{\mathbf{r}_i-\mathbf{r}_j}{|\mathbf{r}_i-\mathbf{r}_j|}$$

$$q=(\mathbf{r}_1^T,\mathbf{r}_2^T,\cdots,\mathbf{r}_N^T)^T,\ p=\mathbf{M}\dot{q},\mathbf{M}=diag(m_1I_3,m_2I_3,\cdots,m_NI_3)$$

2. Hamiltonian systems

- $N = 2$ (Kepler problem), solutions are conic sections.
- $N \geq 3$ (unsolvable by quadrature!), Analytic solutions are not possible in these more general cases and approximate solutions are necesary.

- Numerical integration methods were developed greatly in the past centuries (Euler, Adams, Runge, Kutta, Stoemer, Dahlquist, Butcher, …);
- Heavily depends on the perturbation theory based on the Lyapunov stability criterion and does not suit very long term solutions of the N-body problem before 1980's.
- Qualitative studies in view of dynamical systems gave rise to a completely new way for numerical solutions of the N-body problem and more general Hamiltonian systems (systematical studies with substantial applications began in 1980's).

2. Hamiltonian systems

- **MR3204187 Reviewed**
  Laskar, Jacques(F-CNRS-ADM)
  Is the solar system stable? (English summary) *Chaos,* 239–270,
  Prog. Math. Phys., 66, *Birkhäuser/Springer, Basel,* 2013.

- Summary: "Since the formulation of the problem by Newton, and during three centuries, astronomers and mathematicians have sought to demonstrate the stability of the Solar System. As mentioned by Poincaré, several demonstrations of the stability of the Solar System have been published. By Laplace and Lagrange in the first place, then by Poisson, and more recently by Arnold. Others came after again. *Were the old demonstrations insufficient, or are the new ones unnecessary?* These rigorous demonstrations are in fact various approximations of idealized systems, but thanks to the numerical experiments of the last two decades, we know now that the motion of the planets in the Solar System is chaotic. This prohibits any accurate prediction of the planetary trajectories beyond a few tens of millions of years. The recent simulations even show that planetary collisions or ejections are possible on a period of less than 5 billion years, before the end of the life of the Sun."
- Here the numerical experiments used the symplectic methods to integrate the Hamilton's equations, which are more stable and reliable than those used before.

3. Symplectic integration

- A symplectic integration method is a discretization method whose step-transition maps from initial states to the computed states are symplectic when it applies to Hamiltonian systems.

- **Pioneering works:**
  - Symplectic Euler （generated already by Jacobi from Hamilton-Jacobi equations, 1st order method proved by **Vogelaere** in 1956 （unpublished report), published in 1990 by Channell and Scovel);
  - Henon-Heiles（1964）： Area-preserving mappings；
  - Mid-pint rule (generated already by Poincaré, 2nd order method hilighted by Kang Feng in 1984);
  - A special method of 3rd order for Newton's euqations (**Ruth**, IEEE on Nuclei 1983, a nontrivial construction);
  - More general types of symplectic maps: generating function approach (**Kang Feng** 1986, first arbitrarily high order method);

3. Symplectic integration

- **Foundational work——Rapid development period (1988-1993)**

- Symplectic Runge-Kutta (Lasagni, Sanz-Serna, Suris 1988);
- Lie-Poisson integrators (Z. Ge's Ph. D thesis in 1988, published with J. Marsden in 1988);
- Symplectic methods do not preserve the Hamiltonian (Z. Ge's Ph. D thesis in 1988, published with J. Marsden in 1988);
- Splitting-composition methods (H. Yoshida 1990);
- Backward error analysis (H. Yoshida 1990, K. Feng 1991);
- Numerical KAM theorem (Z. J. Shang 1991 Ph.D thesis, published in 1999-2000);
- No multistep methods are symplectic (Y. F. Tang 1993);
- Partitioned Runge-Kutta methods (Geng Sun 1993).

2. Symplectic integration

- **Further developments, extensions to other structures and applications (1994-):**

- **Symplectic methods** (more useful integrators for special problems, more extensive and deeper applications, more systematic theories) ;
- **Other structure-preserving methods**:
  - Contact structure (K. Feng 1993);
  - Volume-preserving structure (Z. Shang 1994,1995; R. Quispel 1995);
  - Lie-group structures (Lewis-Simo 1994, Munthe-Kaas 1998, Owren 1999, Iserles-Munthe-Kaas-Norsett-Zanna 2000, …);
  - Variational structure （J. Marsden etc. 2001, …);
  - Multi-symplectic structures for Hamiltonian PDE (Bridge-Reich 2000, …);
- **Applications to various different types of equations**: Schroedinger, High oscillations, Time multiscales, Dirac, Maxwell, Plasma, …

  (C. Lubich's plenary talk at ICM2018)

4. Stability analysis

One may hope that numerical methods are able to simulate stable solutions in a stable way, and moreover, are able to simulate stable dynamics structures in a stable way.

Typical dynamics of systems of differential equations

Skeleton of dynamics

(Steady states in time-invariant sense):

- Equilibrium: elliptic, hyperbolic, mixed…
- Periodic solutions: closed trajectories
- Quasi-periodic solutions: invariant tori,Cantori,…
- Homoclinic/heteroclinic solutions: stable/unstable manifolds
- Irregular solutions: diffusions (no recurrent property),…

Theme of the dynamical system:

- Foliations of the phase space by (minimal) invariant manifolds/sets and the stability under perturbations?

Dynamics match between continuous and discrete systems (Numerical stability analysis for symplectic methods):

■ Continuous system

- Phase space (R^{2n},ω)
- Phase flow g^t_H
- Symplecticity: $(g^t_H)^* \ \omega = \omega$
- Phase orbit
- $\gamma(z) = \{g^t_H(z), t \in R\}$
- Invariant set $S = \overline{\gamma(z)}$
  (minimal in many cases)
- Invariant foliation $\Gamma = \mathrm{U} S$

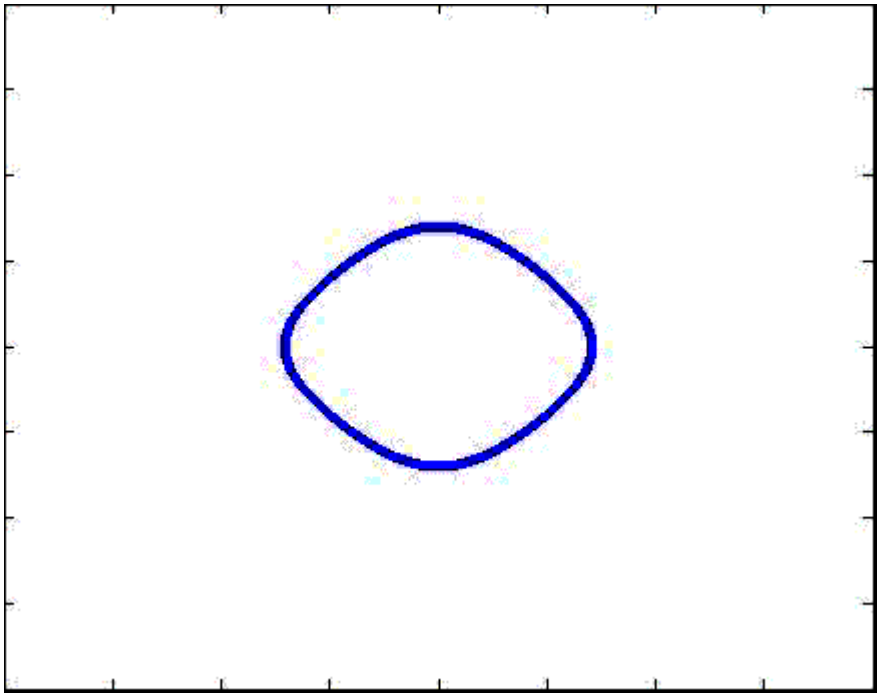
■ Discretized system

- Phase space (R^{2n},ω)
- Discrete flow $G^t_H \backsim g^t_H$
- Symplecticity: $(G^t_H)^* \ \omega = \omega$
- Numerical orbit:

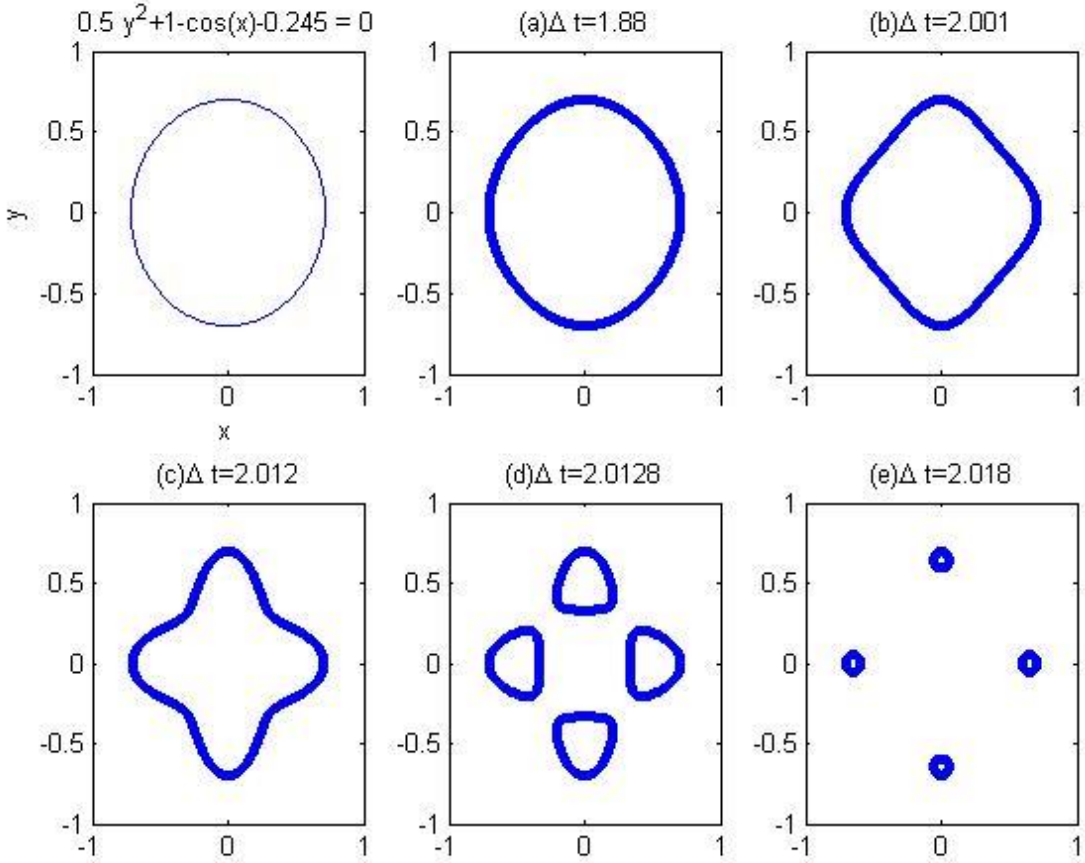
  $\gamma_t(z)=\{z, z_1= G^t_H(z), z_2= G^t_H(z_1), \ldots\}$
- Invariant set $S_t \rightarrow S$ as $t \rightarrow 0$

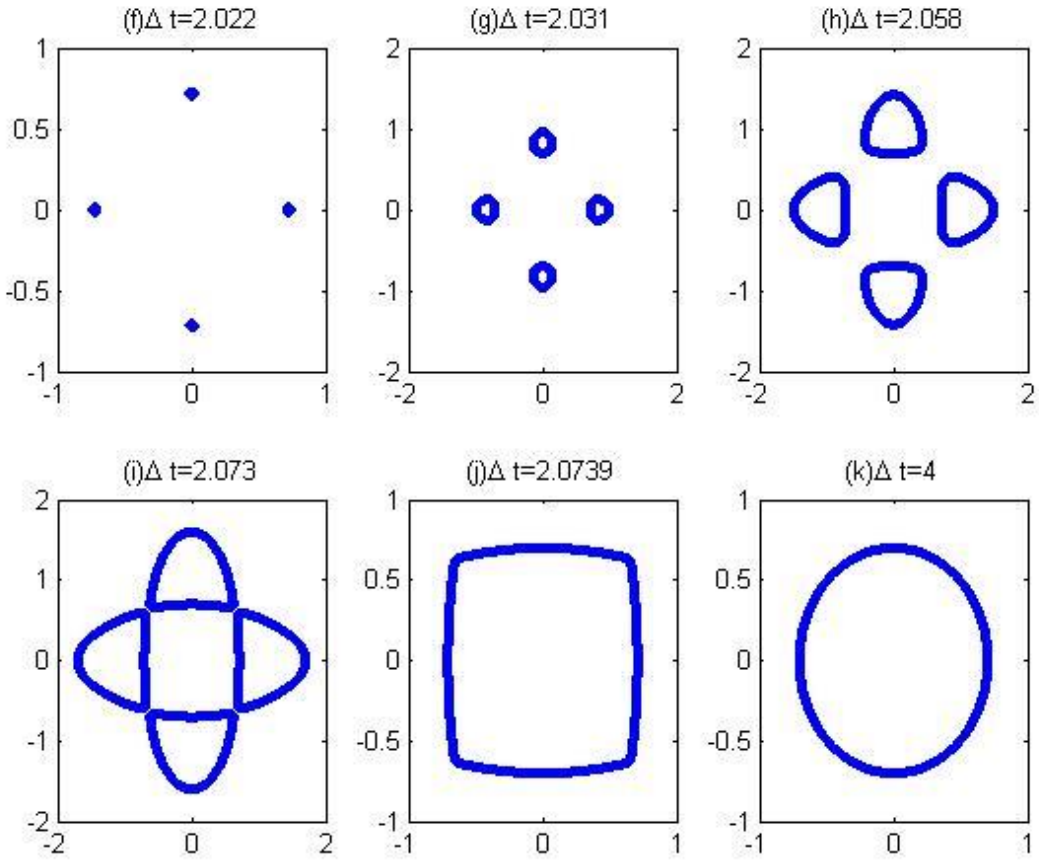
  (has the same topology as S)
- Invariant foliation $\Gamma_t = \mathrm{U} S_t$

Preservation and breakdown of invariant curves by the midpoint rule as time step size changes



Time-stepsize resonance




(f)Δ t=2.022
(g)Δ t=2.031
(h)Δ t=2.058
(i)Δ t=2.073
(j)Δ t=2.0739
(k)Δ t=4

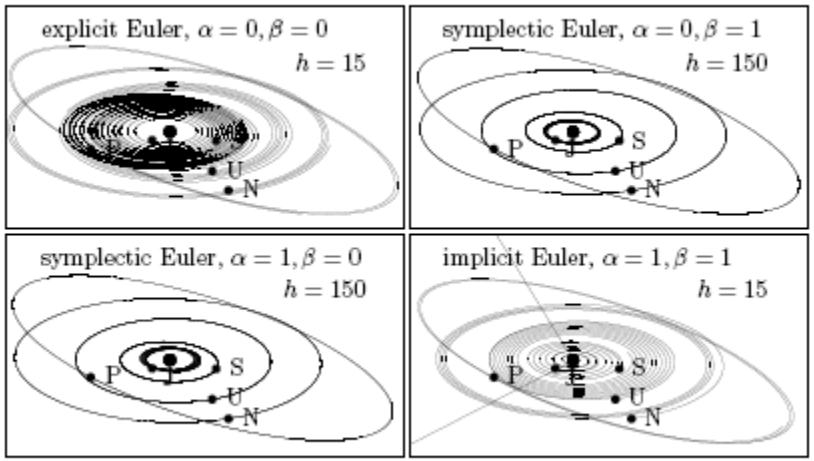


FIGURE 2.1. Numerical simulation of the outer solar system.

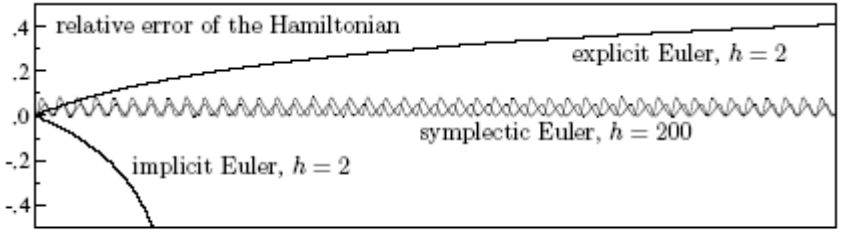


FIGURE 2.2. Relative error of the Hamiltonian on the interval $0 \le t \le 200000$.

From L. Gauckler, E. Hairer, C. Lubich, Dynamics, Numerical analysis, and some geometry, preprint for the plenary talk at ICM 2018 by C. Lubich.

Mercury, Venus, Earth, Mars**, J**upiter**, S**aturn, **U**ranus, **N**eptune, **P**luto

Preservation of equilibia

------Linear Stability analysis

(Thinking in Dahlquist's way)

Test equation: Harmonic oscillator

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

- **Analytic methods (RK, Multi-step, Composition, B-series)**: Dahlquist analysis works for scalar test equation in the complex plane!
- **Nonanalytic methods (PRK, Splitting, LobattoIIIA-IIIB)**: Harmonic oscillator systems in the real plane

Test Hamiltonian

$$H(p,q)=\frac{1}{2}\omega\left(p^2+q^2\right),\omega\in R$$

- Step transition map of numerical method applied to the test system

$$\begin{pmatrix}p_{n+1}\\q_{n+1}\end{pmatrix}=L(z)\begin{pmatrix}p_n\\q_n\end{pmatrix},z=h\omega$$

- Stability matrix

$$L(z)\approx\exp(zJ)=\begin{pmatrix}\cos z & -\sin z\\ \sin z & \cos z\end{pmatrix},J=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}$$

- **Stability set:**

$$\Lambda = \left\{ z \in R \middle| \lambda_{1,2} \right| = 1, \lambda_{1,2} = \sigma(L(z)) \Big\}$$

- **Eigenvalues satisfy the equation:**

$$\lambda^2 - tr(L(z))\lambda + 1 = 0$$

- The trace of the matrix $L(z)$ is a rational function of z.
  It is a hard job to estimate the eigenvalues!

- **Symplectic Euler:**

$$p_{n+1} = p_n - \frac{\partial S_k}{\partial q}(p_{n+1}, q_n), q_{n+1} = q_n + \frac{\partial S_k}{\partial p}(p_{n+1}, q_n)$$

where s_k is the *k–th* truncation of the formal solution of the Hamilton-Jacobi equation of type *(P,q)* and (p_0, q_0) is the initial value.

$$\Lambda_1 = [-2,2], \Lambda_{k+1} \overset{?}{\subset} \Lambda_k, \Lambda_\infty = \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$$

- **Lobatto III A-IIIB pairs:**

---------Non-analytic symmetric methods

$$\Lambda_2 = [-2,2]$$

$$\Lambda_4 = \left[-\sqrt{24},-\sqrt{12}\right] \cup \left[-\sqrt{8},\sqrt{8}\right] \cup \left[\sqrt{12},\sqrt{24}\right]$$

- **Conjecture** (-Shang, Oberwolfach 2006, FoCM 2008):

$$\Lambda_{2k} \overset{?}{\subset} \Lambda_{2k+2}$$

$\Lambda_\infty = R$ (proved by **McLachlan, Sun and Tse** SIAM Numer Anal. 2011)

Linear stability analysis
---- equilibrium analysis

- **Analytic symplectic methods** (SRK) : $\Lambda = \mathbb{R}$

  if the stability function is meroholomorphic.

  (JCM 2020 in Chinese, S-Song)

- **Splitting symplectic methods** with as big as possible stability set to apply in some problems (N-body problem)

  (Blanes, Casas, Murua, McLachlan, Laskar,…)

Preservation of equilibria

- **All the existing methods** preserve equilibrium points of the systems;

- **Symplectic methods** preserve the type of elliptic equilibrium points and, therefore, preserve the linear stability of Hamiltonian systems at elliptic equilibrium points when the step size is in **the stability set**;
- **Symplectic methods** preserve the type of hyperbolic equilibrium points and hence preserve chaotic structure of Hamiltonian systems near the hyperbolic equilibrium points except for some exceptional step sizes.

Preservation of invariant tori: Numerical KAM

------An approach of nonlinear stability analysis

- **KAM theorem** (Kolmogorov-Arnold-Moser, 1954-1963):

  Completely integrable Hamiltonian systems have only periodic or quasi-periodic solutions which densely fill on the invariant tori foliating the phase space. Most of invariant tori survive under small Hamiltonian perturbations.

  Dynamics is ergodic on every surviving invariant torus.

- **Numerical KAM theorem** (Shang 1999, 2000):

✓ Preserve most of foliations by invariant tori of phase space of general completely integrable systems in measure sense;

✓ Perpetual stability of any numerical solution of completely integrable systems of one degree of freedom by symplectic methods (e.g., simple pendulum);

✓ Perpetual stability of most of numerical solutions of completely integrable systems of many degrees of freedom by symplectic methods in measure sense;

✓ **Time-step-size resonance** occurs even when the degree of freedom equal to 1.

- **Time-step size resonance set:** for $\omega \in R^n$,

$$D(\omega) = \{h \in R : \exists k \in Z^n, l \in Z, |\langle k, h\omega \rangle + 2\pi l| = 0\}$$

- **Lemma 1:** $D(\omega)$ *is dense in R for any* $\omega \in R^n$ *!*

- This lemma shows that it seems not possible to compute invariant tori with any given frequency (even diophantine)

  ---------- contradict the numerical observations!

- "KAM tori are very stiff" and can be simulated numerically stably.

Ergodicity-preservation

- With an rationally independent frequency vector, the solutions of the continuous system are ergodic on the whole invariant torus!

- But with resonant time steps, the numerical orbits can only be ergodic on a lower dimensional torus (an invariant measure concentrates on it)!

- It is important to preserve the ergodicity of dynamics of the system on the invariant tori!

Diophantine step-sizes:

- For any given Diophantine frequency $\omega = (\omega_1, \omega_2, ..., \omega_n)$,

$$\left|\langle k, \omega \rangle\right| \geq \frac{\gamma}{|k|^{\nu}}, \forall k = (k_1, ..., k_n) \in Z^n, k \neq 0$$

- **Diophantine step size set:**

$$I(\omega) = \left\{ h \in R : \left| h - \frac{2\pi l}{\langle k, \omega \rangle} \right| \geq \frac{\lambda}{\left(l^{\mu} |k|^{\nu} \right)}, 0 \neq k \in Z^n, 0 < l \in Z \right\}$$

- **Large measure of the diophantine step size set:**

$$\lim_{\delta \to 0} \frac{meas(I(\omega)\Pi(-\delta,\delta))}{meas(-\delta,\delta)} = 1$$

if suitably choose the indecies μ and ν

e.g., $\lambda > 0, \mu \geq -1, \nu > n, \mu + \nu > n + 1.$

具有Diophantine时间步长的数值不变环面的存在性

(from a survey article by R. McLachlan-Quispel in Acta Numerica 2002 **):**

Theorem 2. (Shang 2000) Let there be an analytic, nondegenerate and integrable Hamiltonian system of n degrees of freedom, together with a frequency ω, in the domain of frequencies of the system, which satisfies a Diophantine condition of the form

$$|\langle k, \omega \rangle| \geq \frac{\gamma}{|k|^{\nu}} \quad 0 \neq k = (k_1, \ldots, k_n) \in \mathbb{Z}^n,$$

for some $\gamma > 0$ and $\nu > 0$. Then there exists a Cantor set $I(\omega)$ of $\mathbb{R}$, for any symplectic algorithm applied to the system, and a positive number δ_0, such that, if the step size τ of the algorithm falls into the set $(-\delta_0, \delta_0) \cap I(\omega)$, then the algorithm, if applied to the integrable system, has an invariant torus of frequency $\tau\omega$. The invariant torus of the algorithm approximates the invariant torus of the system in the sense of Hausdorff, with the order equal to the order of accuracy of the algorithm. The Cantor set $I(\omega)$ has

- It is easy to prove that **“good”** time step sizes are

$$h = \frac{1}{N}, N = 1,2,3,\ldots$$

for most of dionphantine frequency vectors, which was already checked numerically by E. Faou etc.

(Oberwolfach workshop “Geometric numerical integration” , March 19-25, 2006, Numer. Math. 2008 and their other papers)

Numer. Math. (2007) 108:223–262
DOI 10.1007/s00211-007-0119-5

Numerische Mathematik

Normal form and long time analysis of splitting schemes for the linear Schrödinger equation with small potential

Guillaume Dujardin · Erwan Faou

2.3 Numerical experiments

We consider the case where the potential function and the initial wave function are given by

$$V(x) = \frac{3}{5 - 4\cos(x)} \quad \text{and} \quad \varphi^0(x) = \frac{2}{2 - \cos(x)}.$$

We use two different time steps:

$$h = 0.2 \quad \text{and} \quad h = \frac{2\pi}{6^2 - 2^2} = 0.196\ldots. \tag{2.17}$$

The first time step satisfies the non-resonance condition[3] (1.7) while the second one is obviously resonant. We use fast Fourier transformations to compute the solution of (1.3). In Fig. 1, we take $2^7 + 1 = 129$ Fourier modes. We make 10^6 iterations, and we set $\lambda = 0.1$. We plot the first 5 energies $|\varphi^n|_k$, $k = 0, \ldots, 4$ in logarithmic scale. We see that if the non-resonance condition is not satisfied, the conservation properties are lost.

[3] We thank Z. Shang who showed us this fact.

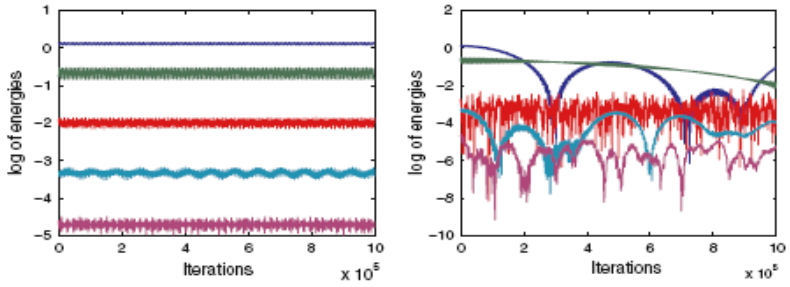


Fig. 1 Energies of the 5 first modes in logarithmic scale, $\lambda = 0.1$. Non-resonant stepsize (*left*) and resonant stepsize (*right*)

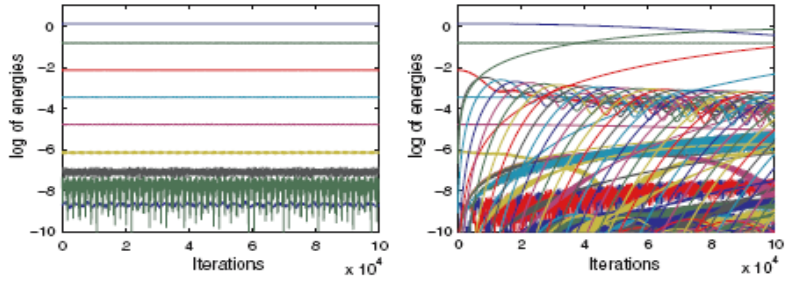


Fig. 2 Energies in logarithmic scale, $\lambda = 0.01$. Non-resonant stepsize (*left*) and resonant stepsize (*right*)

In Fig. 2, we use $2^9 + 1 = 513$ Fourier modes and plot all the energies for 10^5 iterations with $\lambda = 0.01$. We see the growth of high order modes (recall that the L^2-norm is conserved).

- **Quantitative estimates:**

$$d_H(T_\omega, T_h) \leq o(h^p)$$

- **Numerical first integrals** $F_{1,h} = \overline{H}, F_{2,h}, \ldots, F_{n,h}$ exist and

well defined on the union of the numerical invariant tori, in the Whitney's sense, with large Lebesgue measure in the phase space. The numerical tori are the level sets of these first integrals.

$\overline{H}$ is the backward Hamiltonian of the symplectic integrator.

- **A numerical KAM theorem for nearly integrable systems** (Yang Xu's thesis, 2022)
- The results can be extended to systems with Ruessman's nondegeneracy condition, which is the most weak nondegeneracy condition guaranteeing invariant tori.

Periodic points and lower-dimensional tori

- Some studies of preservation and destruction of lower dimensional invariant tori (P. Moan 2004, D R J O' Neale and R. McLachlan 2010).

More numerical KAM results

- **Exponential (Effective) stability** (Hairer & Lubich (1997)

  ------ in the exponentially close sense, numerical invariant tori exist and approximate the invariant tori of the discretized nearly integrable systems

- **Nekhoroshev stability** (Moan (2004, ? incorrect statement and proof)

  ------Any numerical solution is still "very stable" even after "very long" time steps.

  -------Proved by Zhaodong Ding and –S.

- **Problem:** the step size is required to be "very small" and stability conditions are checked "very difficultly"!

  (dissipative invariant tori: Stoffer (1998), Hairer & Lubich (1999))

Nonlinear stability analysis in the KAM setting is numerically not useful!

Nonlinear analysis based on the backward analysis

- Backward Hamiltonian (formal power series in the time step)

$$\bar{H}_h(q,\,p) \;=\; H(q,\,p) + \sum_{k=p+1}^{\infty} h^k H_k(q,\,p) \;:\; f^t_{\bar{H}_h}\Big|_{t=h} \;=\; F^h_H$$

- If the formal Hamiltonian were convergent, then the symplectic integrator would preserve this Hamiltonian function.

- **In general, however, the formal Hamiltonian is not convergent!**
- **Numerical KAM $\Longrightarrow$ convergent in a large set of the phase space!**

A conjecture about the formal Hamiltonian

- Numerical results showed that the modified Hamiltonian function is still bounded in many typical cases;
- The formal Hamiltonian function should still be a "good function" in some generalized sense (KAM theorem gives an indirect proof)!

Conjecture: Take truncations

$$\bar{H}_{h,N} = H + \sum_{k=p+1}^{N+p} h^k H_k$$

We have

$$\left| \bar{H}_{h,N}(q, p) - H(q, p) \right| \leq Ch^p$$

- **Nonlinear stability** by R. I. McLachlan, M. Perlmutter, and G. R. W. Quispel (BIT, 2004):

The level set of $\overline{H}$ (in stead, some finite truncation) is compact if original energy surface is compact.

(Example: nonlinear oscillation)

--- it is still difficult to give out an effective bound of time step size guaranteeing the numerical stability!

Nonlinear stability analysis --- backward+homoclinic analysis

- **Backward/homoclinic criterion** (-L. Song's thesis, 2009**):**

  --- Model example $H(p,q)=\frac{1}{2}(p^2+q^2)-\frac{1}{3}q^3$

- **Theorem.** As the time step size increases from zero, the energy of the modified system at the augmented saddle point increases from minus infinity. When the energy equals to the energy at the preserved saddle point, then the homoclinic trajectory is totally destroyed. This gives a time step size bound which is not too small and when the time step size is below this bound, then there will be full of invariant curves inside the homoclinic trajectory for the modified system.

- **Symplectic Euler (first order truncation of the modified Hamiltonian)**:

$$h^*=\frac{2\sqrt{3}}{3}<2$$

- **Remark:** as the truncation order of the modified system increases, the stability bound decreases. The convergent limit is the nonlinear stability bound of the symplectic integrator.
- This bound can be easier verified for concrete symplectic integrators, and even can be applied to more general systems with stable motions.

Homoclinic/heteroclinic splitting under symplectic integrators

Theorem (L. Song's thesis, 2009). Assume that a Hamiltonian system of one degrees of freedom has a homoclinic trajectory. When a symplectic integrator applies to this system, then the homoclinic trajectory of the system will be split into stable and unstable trajectories of the integrator which intersect transversally in general and span a chaotic web with exponentially small maximal width with respect to the p-th power of time-step size of the integrator, where p is the accuracy order of the integrator.

Conclusions

- Symplectic integrators can simulate foliation structure of dynamics of integrable and nearly integrable Hamiltonian systems in a relatively correct way;
- In general, a homoclinic/heteroclinic trajectory (separatrix) of a Hamiltonian system splits under a symplectic integrator and forms a chaotic web of some width near the separatrix. It is fortunate, however, symplectic methods can give a smaller width of the chaotic web than other generally-purposed methods do.
- Combining the KAM theorem and the homoclinic splitting results, we know that symplectic discretization generates numerical chaos, in general, but the chaotic part is very small in the phase space in significantly long time if the step-size is sufficiently small.

Thank you for your attention!