Symplectic-like Difference Schemes for Generalized Hamiltonian Systems

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(Received June 20, 2001; revised April 20, 2002)

ABSTRACT

The nature of infinite-dimensional Hamiltonian systems are studied for the purpose of further study on some generalized Hamiltonian systems equipped with a given Poisson bracket. From both theoretical and practical viewpoints, we summarize a general method of constructing symplectic-like difference schemes of these kinds of systems. This study provides a new algorithm for the application of the symplectic geometry method in numerical solutions of general evolution equations.

Key words: infinite-dimensional Hamiltonian systems, generalized Hamiltonian systems, symplectic-like difference schemes, Poisson brackets

1. Introduction

It is generally accepted that all physical process with negligible dissipation can be described in some way or another by Hamilton formalism, which can express different physical laws in a unified mathematical form. Feng (1985) introduced the symplectic concept to numerical solutions of Hamiltonian systems for the first time, and developed the symplectic difference scheme. Because the symplectic difference scheme has two important properties —— the area-preserving law and long-term computational stability, one is motivated to develop it for practical applications. At the present, a rather systematical methodology on the symplectic geometry algorithm for finite-dimensional systems (ODEs) has been established. Great progress in studies on algorithms for infinite-dimensional systems (PDEs) have been also achieved (Huang 1991; Li and Qin 1998; Wang et al. 2001).

It should be pointed out that most atmospheric and oceanic equation systems are nonlinear PDEs. They have many remarkable features (such as energy conservation, mass conversation, absolute vorticity conservation, absolute angular momentum conservation, entropy conservation , potential temperature conservation, etc.) and can be transformed into infinite-dimensional generalized Hamiltonian systems if ignoring the effects of any frictions or forcing. Therefore, it becomes more and more meteorologically and practically important to construct difference schemes which maintain as many conservation features as possible. Early in the 1960s, Lilly (1965) constructed a temporal difference scheme, which conserves entropy and absolute vorticity; Arakawa (1966) constructed another a temporal difference scheme which conserves energy, entropy and absolute vorticity; Zeng et al. (1988), Ji and Wang (1991), and Wang and Ji (1990) constructed implicit and explicit square conservation schemes which maintain energy conservation and mass conservation. At present, Wang et al.

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(2001) have established the symplectic algorithm for the spherical shallow water equations with a given Possion bracket, which can (almost) keep many conservations. Based on the available literature on the symplectic method, a further study on symplectic–like schemes for some generalized Hamiltonian systems are carried out in this paper. From the theoretical and practical viewpoints, we outline a general method to construct symplectic–like difference schemes of these systems. This work provides a new algorithm for the application of the symplectic geometry method in numerical solutions of general evolution equations.

2. Possion bracket

Let $\mathscr{F}(F)$ be the functional space of a function $F(x)$, $T(F)$, and $S(F)$ be any two functionals of $\mathscr{F}(F)$, and K be a linear anti–symmetric operator. Define an operation $\{\cdot,\cdot\}$ in $\mathscr{F}(F)$ as follows:

$$\{T,S\}=\left(\frac{\delta T}{\delta F},K\frac{\delta S}{\delta F}\right)\quad \forall T,S:\mathscr{F}(F)\to R, \tag{1}$$

where the variation operation $\frac{\delta}{\delta F}$ of the functional T is defined as

$$\frac{\delta}{\delta F}=\sum_{k=0}^{\infty}(-1)^k\frac{d^k}{dx^k}\frac{\delta}{\delta F^{(k)}}.$$

If the operation $\{\cdot,\cdot\}$ satifies the following properties,

i) Anti–symmetry: $\{T,S\}=-\{S,T\},\forall T,S:\quad (F)\to R$,
ii) Linearity: $\{H,aT+bS\}=a\{H,T\}+b\{H,S\},\quad a,b\in R,\forall H,S,T:\mathscr{F}(F)\to R$,
iii) Jacobi identity: $\{\{T,S\},H\}+\{\{S,H\},T\}+\{\{H,T\},S\}=0,\ \forall H,S,T:\mathscr{F}(F)\to R$,

then $\{\cdot,\cdot\}$ is called a Possion bracket.

If $\{T,S\}$ is still a functional of $\mathscr{F}(F)$ for any two functionals $T(F)$ and $S(F)$ of $\mathscr{F}(F)$, then the set of functional $\mathscr{F}(F)$ equipped with Possion bracket (1) forms a Lie algebra.

3. Definition of a generalized Hamiltonian system

Consider the following infinite–dimensional dynamical system

$$\frac{\partial F}{\partial t}=\mathscr{S}F(x), \tag{2}$$

where $\mathscr{S}:H_{\Omega}^{m}\to C(\Omega)$ is a linear or nonlinear operator, $F\in H_{\Omega}^{m}$, and Ω is a spatial definition domain.

If there exists a functional $H(F)$, which allows (2) to be written as

$$\frac{\partial F}{\partial t}=J_H\frac{\delta H}{\delta F}, \tag{3}$$

where J_H is a linear anti–symmetric operator, then we can define the Possion bracket as follows:

$$\{T,S\}=\left(\frac{\delta T}{\delta F},J_H\frac{\delta S}{\delta F}\right) \quad \forall T,S:H_\Omega^m \to R, \tag{4}$$

which obviously satisfies anti–symmetry, linearity and the Jacobi identity described in section 2.

Based on these properties of the Possion bracket, it can be shown that System (3) satisfies:

$$\frac{dH(F)}{dt}=\left(\frac{\delta H}{\delta F},\frac{\partial F}{\partial t}\right)=\left(\frac{\delta H}{\delta F},J_H\frac{\partial F}{\partial F}\right)=0,$$

i.e., functional $H(F)$ is a conservation quantity and is usually called a first integral of System (3). It is a basic but important physical property of this system.

Lemma 1 The functional $T(F)$ is a first integral of System (3) if and only if $\{T,H\}=0$.

Proof The following equality,

$$\frac{dT(F)}{dt}=\left(\frac{\delta T}{\delta F},\frac{\partial F}{\partial t}\right)=\left(\frac{\delta T}{\delta F},J_H\frac{\delta H}{\delta F}\right)=\{T,H\},$$

shows that $\frac{dT}{dt}=0$ is equivalent to $\{T,H\}=0$.

Based on Lemma 1, it is not difficult to prove the following lemma.

Lemma 2 Suppose $T(F)$ and $S(F)$ are any two first integrals of (3), then $\{T,S\}$ is also a first integral of System (3).

According to Lemmas 1 and 2 and the definition of Possion bracket (4), it is easily seen that System (3) will have infinitely many first integrals if three different first integrals can be found. This leads to an important theorem about System (3).

Theorem 1 The set of functionals consisting of all the first integrals of System (3), equipped with Possion bracket (4), forms a Lie algebra R_H.

Definition 1 If J_H of System (3) is an anti–symmetric operator, and there exists a Lie algebra R_H formed by all first integrals of (3) equipped with Possion bracket (4), then (3) is an infinite–dimensional Hamiltonian system and the functional H is called its Hamiltonian functional.

Practical problems are mostly nonlinear evolution equations, e.g., $\mathscr{L}$ of (2) is nonlinear. In this case, (2) is not an infinite–dimensional Hamiltonian system, although it can still be written into Form (3) based on the generalized anti–symmetry of J_H:

$$(J_H F,F)=0.$$

The question is how to solve it now. Here we introduce a suitable method which presumes that the original problem is stable in any sufficiently small local time window $[t_n, t_{n+1}]$ of the whole time domain, i.e., J_H is suitably linearized to an anti–symmetric operator $\tilde{J}_H$ in any local time window $[t_n, t_{n+1}]$ and as such, the properties of the original problem can (almost) be kept. In this way, (3) can be an infinite–dimensional Hamiltonian system in any $[t_n, t_{n+1}]$ if there exists at least three first integrals.

Definition 2 If J_H of System (3) is a generalized anti–symmetric operator and (3) can be suitably linearized to an infinite–dimensional Hamiltonian system in any sufficiently small local time window of the whole time domain, then (3) is called a generalized Hamiltonian system in the whole time domain.

Most atmospheric and oceanic equations without any frictions or forcings are evolution *equations which have many conservations and can be transformed into generalized* Hamiltonian systems which have the same critical features as the infinite–dimensional Hamiltonian systems in any local time window $[t_n, t_{n+1}]$, but not in $[0,+\infty)$.

4. Symplectic–like difference schemes for generalized Hamiltonian systems

In this section we introduce the construction of symplectic–like schemes for the generalized Hamiltonian System (3). First, we give a method to construct symplectic schemes for the infinite–dimensional Hamiltonian system.

4.1 *Symplectic schemes for infinite–dimensional Hamiltonian systems*

The first step is to discretize System (3) in space. Because of the even dimensions of the Hamiltonian system, the continuous space should be divided into an even number of grids: $x_1, x_2, \cdots, x_{2n}$. Set $X=(x_1, x_2 \cdots x_{2n})^{\mathrm{T}}$, $F=F(X)$, $H=H(F)$. Using the undetermined coefficient method (Wang 1988; Wang et al. 1997) and a numerical integration method, we can discretize J_H, H and $\{\cdot,\cdot\}$ in space. In order to enable the difference scheme to preserve as many characteristic properties of the original continuous system as possible, the discrete $\boldsymbol{J}_H$ should be an anti–symmetric matrix. Furthermore, the discrete $\{\cdot,\cdot\}$ described as

$$\{\boldsymbol{T},\boldsymbol{S}\}_d=\left\{\frac{\delta \boldsymbol{T}}{\delta \boldsymbol{F}},\boldsymbol{J}_H\frac{\delta \boldsymbol{S}}{\delta \boldsymbol{F}}\right\}_d=\left(\frac{\delta \boldsymbol{T}}{\delta \boldsymbol{F}}\right)^{\mathrm{T}}\boldsymbol{J}_H\frac{\delta \boldsymbol{S}}{\delta \boldsymbol{F}}, \tag{5}$$

is still a Possion bracket. Consequently, a semi–discrete differential equation is obtained, namely

$$\frac{\partial \boldsymbol{F}}{\partial t}=\boldsymbol{J}_H\frac{\delta \boldsymbol{H}}{\delta \boldsymbol{F}}, \tag{6}$$

which is a finite dimensional system. It is easy to prove that the discretized $\boldsymbol{H}$ is still invariant and all the discretized first integrals equipped with the bracket $\{\cdot,\cdot\}_d$ form a Lie algebra. So System (6) is a finite–dimensional Hamiltonian system.

Finally, applying the symplectic schemes (Feng 1995) for finite–dimensional Hamiltonian systems directly, a fully discrete scheme for the semi–discrete scheme (6) is derived. For example,

$$\frac{\boldsymbol{F}^{n+1}-\boldsymbol{F}^{n}}{\tau}=\boldsymbol{J}_H\frac{\delta \boldsymbol{H}^{n+\frac{1}{2}}}{\delta \boldsymbol{F}^{n+\frac{1}{2}}}, \tag{7}$$

where

$$\boldsymbol{F}^{n+\frac{1}{2}}=\frac{1}{2}(\boldsymbol{F}^{n+1}+\boldsymbol{F}^{n}),$$

$$\boldsymbol{H}^{n+\frac{1}{2}}=H(\boldsymbol{F}^{n+\frac{1}{2}}).$$

4.2 *Symplectic–like schemes for generalized Hamiltonian system*

Because generalized Hamiltonian systems have the same critical features as infinite–dimensional Hamiltonian systems in any local time window $[t_n, t_{n+1}]$, we analyse the numerical method for (3) in the local time window $[t_n, t_{n+1}]$. Similar to the steps in Section 4.1, the first step is to discretize (3) in space into a semi–difference equation (6), and the second step is to construct a symplectic scheme for (6) in $[t_n, t_{n+1}]$. The corresponding Eq. (7) is

$$\frac{F^{n+1} - F^{n}}{\tau} = \mathfrak{J}_H^{n+\frac{1}{2}} \frac{\delta H^{n+\frac{1}{2}}}{\delta F^{n+\frac{1}{2}}}, \tag{8}$$

where $\mathfrak{J}_H$ is a linearized operator of J_H in the local time window $[t_n, t_{n+1}]$. Its first integrals satisfy quasi–conservation

$$\frac{H(F^{n+1}) - H(F^{n})}{\tau} = 0, \quad \forall H \in R_H.$$

However, Scheme (8) is symplectic only in a local time window, but not in the whole time domain $[0,\infty)$, so we call it a symplectic–like scheme.

5. Numerical test

Consider the spherical shallow water equation (without frictions or forcings),

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{u}{a\cos\theta}\dfrac{\partial u}{\partial \lambda} + \dfrac{v}{a}\dfrac{\partial u}{\partial \theta} + \dfrac{1}{a\cos\theta}\dfrac{\partial \varphi}{\partial \lambda} - \left(2w\sin\theta + \dfrac{u}{a}\mathrm{tg}\theta\right)v = 0 \\ \dfrac{\partial v}{\partial t} + \dfrac{u}{a\cos\theta}\dfrac{\partial v}{\partial \lambda} + \dfrac{v}{a}\dfrac{\partial v}{\partial \theta} + \dfrac{1}{a}\dfrac{\partial \varphi}{\partial \theta} + (2w\sin\theta + \dfrac{u}{a}\mathrm{tg}\theta)u = 0 \\ \dfrac{\partial \varphi}{\partial t} + \dfrac{1}{a\cos\theta}\left(\dfrac{\partial u\varphi}{\partial \lambda} + \dfrac{\partial v\varphi\cos\theta}{\partial \theta}\right) = 0 \end{cases}, \tag{9}$$

defined on the domain $t \geq 0, \Omega: \left\{0 \leq \lambda \leq 2\pi, -\frac{\pi}{2} \leq \theta \leq \frac{\pi}{2}\right\}$, with boundary conditions $v\left(\lambda, -\frac{\pi}{2}, t\right) = v\left(\lambda, \frac{\pi}{2}, t\right) = 0,$

$$\begin{cases} u(\lambda + 2\pi, \theta t) = u(\lambda, \theta, t) \\ v(\lambda + 2\pi, \theta t) = v(\lambda, \theta, t) \\ \varphi(\lambda + 2\pi, \theta, t) = \varphi(\lambda, \theta, t) \end{cases}.$$

Define $F = [u, v, \varphi]^T$, and introduce a Hamiltonian functional $H(F)$,

$$H(F) = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos\theta d\theta \int_0^{2\pi} \frac{1}{2}(u^2 + v^2 + \varphi)\varphi a^2 d\lambda = \iint_\Omega \frac{1}{2}(u^2 + v^2 + \varphi)\varphi ds$$

$$(ds = a^2 \cos\theta d\theta d\lambda).$$

Then problem (9) can be written into a generalized Hamiltonian system,

$$\frac{\partial F}{\partial t} = J_H \frac{\delta H}{\delta F}. \tag{10}$$

Define the Possion bracket $\{\cdot, \cdot\}$,

$$\{T,S\}=\left(\frac{\delta T}{\delta F},J_H\frac{\delta S}{\delta F}\right)_3=\iint\limits_{\Omega}\left(\frac{\delta T}{\delta F}\right)^T J_H\frac{\delta S}{\delta F}ds,\quad \forall T,S:H_\Omega^m\to R,$$

where

$$J_H=\begin{bmatrix} 0 & \zeta & -\frac{1}{a\cos\theta}\frac{\partial}{\partial\lambda} \\ -\zeta & 0 & -\frac{1}{a}\frac{\partial}{\partial\theta} \\ -\frac{1}{a\cos\theta}\frac{\partial}{\partial\lambda} & -\frac{1}{a\cos\theta}\frac{\partial}{\partial\theta}\cos\theta & 0 \end{bmatrix},$$

$$\zeta=\frac{1}{\varphi}\left[2\omega\sin\theta+\frac{1}{a\cos\theta}\left(\frac{\partial v}{\partial\lambda}-\frac{\partial u\cos\theta}{2\theta}\right)\right]\quad .$$

System (10) belongs to the discussion of section 4.2. Applying the method provided in that Section, a symplectic–like scheme for (10) in the local time window $[t_n,t_{n+1}]$ is obtained (Wang et al. 2001),

$$\begin{cases} \dfrac{u_{i,j}^{k+1}-u_{i,j}^{k}}{\Delta t}+\nabla_\lambda\varepsilon_{i,j}^{k+\frac{1}{2}}-\zeta_{i,j}^{k+\frac{1}{2}}\varphi_{i,j}^{k+\frac{1}{2}}v_{i,j}^{k+\frac{1}{2}}=0 \\ \dfrac{v_{i,j}^{k+1}-v_{i,j}^{k}}{\Delta t}+\nabla_\theta\varepsilon_{i,j}^{k+\frac{1}{2}}+\zeta_{i,j}^{k+\frac{1}{2}}\varphi_{i,j}^{k+\frac{1}{2}}u_{i,j}^{k+\frac{1}{2}}=0 \\ \dfrac{\varphi_{i,j}^{k+1}-\varphi_{i,j}^{k}}{\Delta t}-\nabla_\lambda^T\left(u_{i,j}^{k+\frac{1}{2}}\varphi_{i,j}^{k+\frac{1}{2}}\right)-\nabla_\theta^T\left(v_{i,j}^{k+\frac{1}{2}}\varphi_{i,j}^{k+\frac{1}{2}}\right)=0, \end{cases}\tag{11}$$

where $\varepsilon_{i,j}^{k+\frac{1}{2}}=\frac{1}{2}\left[\left(u_{i,j}^{k+\frac{1}{2}}\right)^2+\left(v_{i,j}^{k+\frac{1}{2}}\right)^2\right]+\varphi_{i,j}^{k+\frac{1}{2}}$.

Note that scheme (11) almost preserves the energy conservation:

$$\frac{T(F^{k+1})-T(F^{k})}{\Delta t}=0.$$

*This scheme is used to simulate 4–wave Rossby–Haurwitz waves by a 150–day integra*tion. It can be seen that the symplectic–like scheme produces good results, and well preserves the energy conservation, the mass conservation and the potential vorticity conservation (see Table 1).

6. Conclusion

Symplectic–like difference schemes for generalized Hamiltonian systems have been formulated and tested with 4–wave Rossby–Haurwitz waves. The numerical results show the good physical properties of the Symplectic–like scheme. These studies will make contribution to the application of the symplectic geometry method in numerical solutions of general evolution equations.

Table 1. Evolution of global energy, global mass and global potential vorticity

Integration time (d)	Global energy (m^4s^{-4})	Global mass (m^2s^{-2})	Global potential vorticity (s^{-1})
1	7618457306234.84	175248643.172 869 0	−0.000 000 000 000 000 02
20	7618457306243.91	175248643.172 869 2	−0.000 000 000 000 000 00
40	7618457306240.02	175248643.172 869 3	−0.000 000 000 000 000 08
60	7618457306236.96	175248643.172 867 7	−0.000 000 000 000 000 04
80	7618457306244.22	175248643.172 867 5	0.000 000 000 000 000 13
100	7618457306229.92	175248643.172 868 8	−0.000 000 000 000 000 10
120	7618457306237.81	175248643.172 867 4	0.000 000 000 000 000 02
150	7618457306301.20	175248643.172 867 8	0.000 000 000 000 000 22

Acknowledgments. This work was supported by the China National Key Development Planning Project for Basic Research (Abbreviation: 973 Project; Grant No. G1999032801), the Chinese Academy of Sciences Key Innovation Direction Project (Grant No. KZCX2208) and the National Natural Science Foundation of China (Grant No. 49975020), and the National Outstanding Youth Scientist Foundation of China (Grant No. 49825109).

REFERENCES

Arakawa, A., 1966: Computational design for long−term numerical integrations of the equations of Atmospheric Motion. *Compu. Phys.* **1**, 119−143.

Feng Kang, 1985: On difference schemes and symplectic geometry. *Proceedings of the 1984 Beijing Symposium on Differential Geometry and Differential Equations—COMPUTATION OF PARTIAL DIFFERENTIAL EQUATIONS*, ed. Feng Kang, Science Press, Beijing, 42−58.

Feng Kang, 1995: *Collected Works of Feng Kang* (**II**), National Defence Industry Press, Beijing, 44−76.

Huang Mingyou, 1991: A Hamiltonian approximation to simulate solitary waves of the Korteweg−De Vries Equation. *Mathematics of Computation*, **56**(194), 607−620.

Ji Zhongzhen, and Wang Bin, 1991: Further discussion on the construction and application of difference schemes for evolution. *Chinese Journal of Atmospheric Sciences*. **15**(2), 1−10.

Li Chunwang, and Qin Mengzhao, 1998: A symplectic difference scheme for the infinite dimensional Hamiltonian system. *Journal of Computational Mathematics*, **6**(2), 164−174.

Lilly, D. K., 1965: The computational stability of numerical solution of time−dependent nonlinear geophysical fluid dynamics. *Mon. Wea. Rev.*, **93**(1), 11−26.

Wang Bin, 1988: Constructing square conservative difference scheme by means of undetermined coefficient. *Journal of the Graduate School, Chinese Academy of Sciences*, **5**, 84−91 (in Chinese).

Wang Bin, and Ji Zhongzhen, 1990: On the construction of explicit square conservation schemes and tests. *Chinese Science Bulletin*, **35**(10), 766−768.

Wang Bin, Ji Zhongzhen, and Zeng Qingcun, 1997: Symplectic operator method and its test. *Progress in Natural Science*, **7**, 345−353.

Wang Bin, Ji Zhongzhen, and Xiao Qingnong 2001: A Hamiltonian Approximation to Solve the Spherical Shallow Water Equation. *Chinese Journal of Computational Physics*, **18**(4), 289−297 (in Chinese).

Zeng Qingcun, Ji Zhongzhen, and Li Rongfeng, 1988: The construction of difference schemes for evolution equations and the numerical simulation of offshore currents. *Chinese Journal of Atmospheric Sciences* (special volume), 166−175.

一类广义 Hamilton 系统的辛格式

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摘 要

通过引入泊松括号，分析了无限维 Hamilton 的性质，并将其推广到广义 Hamilton 系统，且从理论和实用角度讨论了这类广义 Hamilton 系统的辛格式构造问题，从而为辛几何算法在一般的时间发展方程的数值求解提供新的具体途径。

关键词：无限维 Hamilton 系统，广义 Hamilton 系统，辛格式，泊松括号