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Zhu You-lan Guo Ben-yu (Eds.)

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Proceedings, Shanghai 1987

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Preface

This volume of Lecture Notes in Mathematics is the Proceedings of the First Chinese Conference on Numerical Methods for Partial Differential Equations, which was held at the Shanghai University of Science and Technology, Shanghai, China on March 25-29, 1987 and attracted about 100 participants from all parts of China. It includes 16 papers selected from 75 papers presented at the Conference. A complete list of the papers presented at the Conference is also given in this Proceedings. These papers are arranged in alphabetical order of the first author's name and every name is typewritten in "the Chinese way", i.e., the family name is typed first, followed by the given name.

We are indebted to our many colleagues and friends who helped us in preparing the Conference, during the meeting and in editing the Proceedings, but especially, to Yang Zhong-hua who supervised all of the local arrangements. We are also thankful to the Chinese Mathematical Society and the Chinese Society of Computational Mathematics for their support.

Finally, we would like to express our thanks to the series editors and the editorial staff of Springer-Verlag for valuable assistance in preparing the Proceedings.

July, 1987

Zhu You-lan and Guo Ben-yu
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Chang Qian-shun [Institute of Applied Mathematics, Academia Sinica, Beijing, China]: Applications of splitting schemes and multigrid methods to computation of separated flows

Chen Guang-nan [Institute of Applied Physics and Computational Mathematics, P.O. Box 8009, Beijing, China]: A tri-level difference Scheme for one dimensional parabolic systems

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Huang Ming-you [Dept. of Mathematics, Jilin University, Changchun, China]: A Hamiltonian approximation for nonlinear wave equation on n-dimensional spheres S^n

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CONTENTS

THE SYMPLECTIC METHODS FOR THE COMPUTATION OF HAMILTONIAN EQUATIONS*

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Abstract

The present paper gives a brief survey of results from a systematic study, undertaken by the authors and their colleagues, on the symplectic approach to the numerical computation of Hamiltonian dynamical systems in finite and infinite dimensions. Both theoretical and practical aspects of the symplectic methods are considered. Almost all the real conservative physical processes can be cast in suitable Hamiltonian formulation in phase spaces with symplectic structure, which has the advantages to make the intrinsic properties and symmetries of the underlying processes more explicit than in other mathematically equivalent formulations, so we choose the Hamiltonian formalism as the basis, together with the mathematical and physical motivations of our symplectic approach for the purpose of numerical simulation of dynamical evolutions. We give some symplectic difference schemes and related general concepts for linear and nonlinear canonical systems in finite dimensions. The analysis confirms the expectation for them to behave more satisfactorily, especially in the desirable conservation properties, than the conventional schemes. We outline a general and constructive theory of generating functions and a general method of construction of symplectic difference schemes based on all possible generating functions. This is crucial for the developments of the symplectic methods. A generalization of the above theory and method to the canonical Hamiltonian eqs. in infinite dimensions is also given. The multi-level schemes, including the leap-frog one, are studied from the symplectic point of view. We give an application of symplectic schemes, with some indications of their potential usefulness, to the computation of chaos.

CONTENTS

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* Work supported by National Natural Science Foundation of China.

§ 1 Introduction

Recently it is evident that Hamiltonian formalism plays a fundamental role in the diverse areas of physics, mechanics, engineering, pure and applied mathmatics, e. g. geometrical optics, analytical dynamics, nonlinear PDE's of first order, group representations, WKB asymptotics, pseudodifferential and Fourier integral operators, classification of singularities, integrability of non-linear evolution equations, optimal control theory, etc. It is also under extension to infinite dimensions for various field theories, including electrodynamics, plasma physics,elasticity, hydrodynamics etc. It is generally accepted that all real physical processes with negligible dissipation could be expressed, in some way or other, by Hamiltonian formalism, so the latter is becoming one of the most useful tools in the mathematical physics and engineering sciences.

Hamiltonian formalism has the important property of being area-preserving (symplectic) i.e. the sum of the areas of canonical variable pairs, projected on any two-dimensional surface in phase space, is time invariant. In numerically solving these equations one hopes that the approximating equation will hold this property.

In DD-5 Beijing Conference the first author [1] propose an approach for computing Hamiltonian equation from the viewpoint of symplectic geometry. This paper is a brief survey of considerations and developments [1-11,15], obtained by the first author and his group, on the links between the Hamiltonian formalism and the numerical methods.

Now we will give a review of some facts from Hamiltonian mechanics which are fundamental to what follows. We consider the following canonical system of ordinary first order differential equations on R^{2n}

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad i = 1,2,\cdots n, \tag{1.1}$$

where H(p,q) is some real valued function. We call (1.1) a Hamiltonian system of differential equations (H - system). In the following, vectors are always represented by column matrices, matrix transpose is denoted by prime'. Let $z=(z_1 \cdots z_n, z_{n+1}, \cdots z_{2n})' = (p_1 \ldots p_n, q_1 \ldots q_n)'$, $H_z = [\frac{\partial H}{\partial p_1},\ldots,\frac{\partial H}{\partial p_n}, \frac{\partial H}{\partial q_1},\ldots,\frac{\partial H}{\partial q_n}]'$, $J_{2n} = J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$, $J'=J^{-1} = -J$, where I_n is the $n \times n$ identity matrix. (1.1) can be written as

$$\frac{dz}{dt} = J^{-1} H_z, \tag{1.2}$$

defined in phase space R^{2n} with a standard symplectic structure given by the nonsingular anti-symmetric closed differential 2-form

$$\omega = \Sigma\, dz_i \wedge dz_{n+i} = \Sigma\, dp_i \wedge dq_i .$$

According to Darboux Theorem, the symplectic structure given by any non-singular antisymmetric closed differential 2-form can be brought to the above standard form, at least locally, by suitable change of coordinates.

The right side of equation (1.2) gives a vector field. At each point(p,q) of the phase space, there is a 2n-dimensional vector$(-H_q, H_p)$.

The fundamental theorem on Hamiltonian Formalism says that the solution $z(t)$ of the canonical system (1.2) can be generated by a one-parameter group $G(t)$, depending on given Hamiltonan H, of canonical transformations of R^{2n} (locally in t and z) such that

$$z(t)=G(t)z(0).$$

This group is also called the phase flow

$$G(t): \ (p(o),q(o)) \to \ (p(t), q(t))$$

where $p(t)$, $q(t)$ are the solution of Hamilton's system of equations(1.1).
A transformation $z \to \hat{z}$ of R^{2n} is called canonical, or symplectic, if it is a local diffeomorphism whose Jacobian $\frac{\partial \hat{z}}{\partial z} = M$ is every-where symplectic i.e.

$$M'JM=J, \ \text{ie.} \ M \in Sp(2n).$$

Linear canonical transformation is special symplectic transformation.

The canonicity of $G(t)$ implies the preservation of 2-form ω, 4-form $\omega \wedge \omega$, $\cdots$, 2n-form $\omega \wedge \omega \wedge \cdots \wedge \omega$. They constitute the class of conservation laws of phase area of even dimensions for the Hamiltonian system (1.2).

Moreover, the Hamiltonian system possesses another class of conservation laws related to the energy $H(z)$. A function $\psi(z)$ is said to be an invariant integral of (1.2) if it is invariant under (1.2)

$$\psi(z(t)) \equiv \psi(z(0))$$

which is equivalent to

$$\{\psi, H\} = 0,$$

where the Poisson Brackets for any pair of differentiable functions ϕ and ψ are defined as

$$\{\phi, \psi\} = \phi_z' J^{-1} \psi_z .$$

H itself is always an invariant integral, see, e.g. [12].

For the numerical study , we are less interested in (1.2) as a general system of ODE per se, but rather as a specific system with Hamiltonian structure. It is natural to look for those discretization systems which preserve as much as possible the characteristic properties and inner symmetries of the original continuous systems. To this end the transition $\hat{z} \to z$ from the k-th time step $z^k = \hat{z}$ to the next (k+1)-th time step $z^{k+1} = z$ should be canonical for all k and, moreover, the invariant integrals of the original system should remain invariant under these transitions.

Thus, a difference scheme may be regarded as a transformation from time t^k to time t^{k+1}. We have the following

Definition. A difference scheme may be called symplectic or canonical scheme if its transitional transformation is symplectic. We try to conceive, design, analyse and evaluate difference schemes and algorithms specifically within the framework of symplectic geometry. The approach proves to be quite successful as one might expect, we actually derive in this way numerous "unconventional" difference schemes.

An outline of the paper is as follows. In section 2 we review some symplectic difference schemes (S-scheme) for linear hamiltonian system (LH-system) and nonlinear hamiltonian system (NLH-system) and its related properties are given. In section 3 we systematically outline the general method of construction of S-scheme with any order accuracy via generating function. The constructive theory of generating function and the corresponding construction of S-schemes have been generalized to the case of phase space of infinite dimensions of the form $B^* \times B$, where B is a reflexive Banach space, B^* its dual [3] [8]. Section 4 contains the main idea. The multi-level difference S-schemes of hamiltonian type are described in §5. In §6 we show some computational results and comparison with R-K method. The last section is S-scheme and chaos. It is well known that canonical transformation is an area-preserving mapping. Therefore S-schemes are suitabe tools for studying chaotic behavior in hamiltonian mechanics.

§2. S-schemes for Linear and Nonlinear Hamiltonian Systems

Consider the case for which the Hamiltonian is a quadratic form

$$H(z) = \frac{1}{2} z'Sz, \qquad S' = S, \quad H_z = Sz \tag{2.1}$$

Then the canonical system

$$\frac{dz}{dt} = Lz, \qquad L = J^{-1}S \tag{2.2}$$

is linear, where L is infinitesimally symplectic, i.e. L satisfies $L'J + JL = 0$.

The solution of (2.2) is

$$z(t) = G(t)z(0)$$

where $G(t) = \exp tL$, as the exponential transform of infinitesimally symplectic tL, is symplectic.

It is easily seen that the weighted Euler scheme

$$\frac{1}{\tau}(z^{k+1} - z^k) = L(\alpha z^{k+1} + (1-\alpha)z^k)$$

for the linear system (2.2) is symplectic iff $\alpha = \frac{1}{2}$, i.e. it is the case of time-centered Euler scheme with the transition matrix F_τ,

$$z^{k+1} = F_\tau z^k, \quad F_\tau = \psi(\tau L), \qquad \psi(\lambda) = \frac{1+\frac{\lambda}{2}}{1-\frac{\lambda}{2}}, \tag{2.3}$$

F_τ, as the Cayley transform of infinitesimally symplectic τL, is symplectic.

In order to generalize the time-centered Euler scheme, we need, apart from the exponential or Cayley transforms, other matrix transforms carrying infinitesimally symplectic matrices into symplectic ones.

Theorem 1. Let $\psi(\lambda)$ be a function of complex variable λ satisfying

(I) $\psi(\lambda)$ is analytic with real coefficients in a neighborhood D of $\lambda = 0$,

(II) $\psi(\lambda)\psi(-\lambda) \equiv 1$ in D,

(III) $\psi'(0) \neq 0$.

A is a matrix of order 2n, then $(\psi(\tau L))' A \psi(\tau L) = A$ for all τ with sufficiently small $|\tau|$, iff

$$L'A + AL = 0$$

If, more, $\exp \lambda - \psi(\lambda) = 0(|\lambda|^{m+1})$, then

$$z^{k+1} = \psi(\tau L) z^k \tag{2.4}$$

considered as an approximative scheme for the canonical system (2.2) is symplectic, of m-th order of accuracy and has the property that $z'Aw$ is invariant under $\psi(\tau L)$ iff it is invariant under G_t of (2.2).

Remark 1. The last property is remarkable in the sense that, all the bilinear invariants of the system(2.2), no more and no less, are kept invariant under the scheme(2.4), in spite of the fact that the latter is only approximate.

Remark 2. The approximative scheme in theorem 1 becomes difference schemes only when $\psi(\lambda)$ is a rational function. As a concrete application to the construction of symplectic difference schemes, we take the diagonal Padé approximants to the exponential function

$$\exp \lambda - \frac{P_m(\lambda)}{P_m(-\lambda)} = 0(|\lambda|^{2m+1})$$

where $P_0(\lambda) = 1$, $P_1(\lambda) = 2 + \lambda$, $P_2(\lambda) = 12 + 16\lambda + \lambda^2$, $\cdots$ $P_m(\lambda) = 2(2m-1)P_{m-1}(\lambda) + \lambda^2 P_{m-2}(\lambda)$.

Theorem 1'. Difference schemes

$$z^{k+1} = \frac{P_m(\tau L)}{P_m(-\tau L)} z^k, \quad m = 1, 2, \cdots \tag{2.5}$$

for the eq. (2.2) are symplectic, A-stable, of 2m-th order of accuracy, and having the same set of bilinear invariants as that of eq. (2.2), and the case m=1 is the centered Euler scheme [5].

For the general non-linear canonical system (1.2), the time-centered Euler scheme is

$$\frac{1}{\tau}(z^{k+1} - z^k) = J^{-1} H_z\left(\frac{1}{2}(z^{k+1} + z^k)\right). \tag{2.6}$$

The transition $z^{k+1} \to z^k$ is canonical with Jacobian

$$F_\tau = \left[I - \frac{\tau}{2} J^{-1} H_{zz}\left(\frac{1}{2}(z^{k+1} + z^k)\right)\right]^{-1} \left[1 + \frac{\tau}{2} J^{-1} H_{zz}\left(\frac{1}{2}(z^{k+1} + z^k)\right)\right]$$

symplectic everywhere. However, unlike the linear case, the invariant integrals ψ, not quadratic in z, including H(z), are conserved only approximately:

$$\psi(z^{k+1}) - \psi(z^k) = 0(\tau^3).$$