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DIFFERENCE SCHEMES FOR HAMILTONIAN FORMALISM AND SYMPLECTIC GEOMETRY[*1)]

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§ 1. Introduction

The present program [1] that the author and his group have started is a systematic study of the numerical methods for the solution of differential equations of mathematical physics expressed in Hamiltonian formalism. As is well known, Hamiltonian canonical systems serve as the basic mathematical formalism, for diverse areas of physics, mechanics, engineering, as well as pure and applied mathematics, e.g., geometrical optics, analytical dynamics, non-linear PDE's of first order, group representations, WKB asymptotics, pseudo-differential and Fourier integral operators, electrodynamics, plasma physics, elasticity, hydrodynamics, relativity, control theory, etc. It is generally accepted that all real physical processes with negligible dissipation could be expressed, in some way or other, in suitable Hamiltonian forms. So the general methods developed for the numerical solution of Hamiltonian equations, if good, would have wide applications.

Since symplectic geometry is the mathematical foundation of Hamiltonian formalism, a wealth of theoretical results is already accumulated which should be and could be explored for numerical purposes. So the proper mode of research in this area should be geometrical. 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, and we actually derive in this way numerous "unconventional" difference schemes.

Due to historical reasons, classical symplectic geometry, however, lacks the "computational" component in the modern sense. Our present study might be considered as an attempt to fill the blank. We got a number of results (e.g. Th. 1, § 2) which are crucial for the construction of symplectic difference schemes on the one hand and which have independent theoretical interest in themselves on the other hand.

In this paper, we consider the canonical system in finite dimensions

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

with Hamiltonian $H(p_1, \cdots, p_n, q_1, \cdots, q_n)$.

In the following, vectors are always represented by column matrices, and matrix transpose is denoted by prime. Let $z=(z_1, \cdots, z_n, z_{n+1}, \cdots, z_{2n})' = (p_1, \cdots, p_n,$

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$q_1, \cdots, q_n)'$, $H_z = (H_{z_1}, \cdots, H_{z_{2n}})'$. (1.1) can be written as

$$\frac{dz}{dt} = J^{-1}H_z, \quad J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \tag{1.2}$$

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

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

The Fundamental Theorem on Hamiltonian Formalism says that the solution of the canonical system (1.2) can be generated by a one-parameter group G_t of canonical transformations of R^{2n} (locally in t and z) such that

$$G_{t_1}G_{t_2} = G_{t_1+t_2},$$

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

A transformation $z \to \hat{z}$ of R^{2n} is called canonical if it is a local diffeomorphism whose Jacobian $\frac{\partial \hat{z}}{\partial z} = M$ is everywhere symplectic, i.e.

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

Linear canonical transformations are simply symplectic transformations.

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 $\phi(z)$ is said to be an invariant integral of (1.2) if it is invariant under (1.2)

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

which is equivalent to

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

where the Poisson bracket for two functions $\phi(z)$, $\psi(z)$ are defined as

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

H itself is always an invariant integral, see, e.g., [2].

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 many as possible the characteristic properties and inner symmetries of the original continuous systems. We hope that this might lead to more satisfactory theoretical foundation and practical performance.

The above digressions on Hamiltonian systems suggest the following guideline for difference schemes to be constructed. The transition from the k-th time step z^k to the next $(k+1)$-th time step z^{k+1} should be canonical for all k and, moreover, the invariant integrals of the original system should remain invariant under these transitions.

§2. Some Difference Schemes for Hamiltonian Systems

2.1. *The Centered Euler Scheme and Its Generalizations*

Consider first the case for which the Hamiltonian is a quadratic form