SYMPLECTIC GEOMETRY AND NUMERICAL METHODS IN FLUID DYNAMICS [①]

辛几何与流体动力学中的数值方法

§1 Introduction

It is an honor and a pleasure for me to present the inaugural talk at the Tenth International Conference on Numerical Methods in Fluid Dynamics in Beijing. I want to thank the Organizing Committee, its Secretory, Prof. H. Cabannes, the Conference Chairman, Prof. F.G. Zhuang, and the Co-chairman, Prof. Y.L. Zhu for the kind invitation.

We present a brief survey of considerations and results of a study [1, 2, 3, 4, 6], undertaken by the author and his group, on the links between the *Hamiltonian formalism* and the *numerical methods* for solving dynamical problems expressed in the form of the *canonical system* of differential equations

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

with given *Hamiltonian function* $H(p_1, \ldots, p_n, q_1 \ldots, q_n)$.

The canonical system (1.1) with remarkable elegance and symmetry was introduced by Hamilton as a general mathematical scheme, first for problems of geometrical optics in 1824, then for conservative dynamical problems in 1834. The approach was followed and developed further by Jacobi into a well-established mathematical formalism for analytical dynamics, which is an alternative of, and equivalent to, the Newtonian and Lagrangian formalisms. The geometrization of the Hamiltonian formalism was undertaken by Poincare in 1890's and by Cartan, Birkhoff, Weyl, Siegel, etc., in the 20th century; this gave rise a new discipline, called *symplectic geometry*, which serves as the mathematical foundation of the Hamiltonian formalism.

It is known that, Hamiltonian formalism, apart from its classical links with analytical mechanics, geometrical optics, calculus of variations and non-linear PDE of first order, has inherent connections also with unitary representations of Lie groups, geometric quantization, pseudo-differential 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 fluid dynamics, elasticity, electrodynamics, plasma physics, relativity, etc.. Now it is almost certain that all real physical

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processes with negligible dissipation can be described, in some way or other, by Hamiltonian formalism, so the latter is becoming one of the most useful tools in the mathematical arsenal of physical and engineering sciences. In this way, a systematic study of numerical methods of Hamiltonian systems is motivated and would eventually lead to more general applicability and more direct accessibility of the Hamiltonian formalism. 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. 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.

In the following, vectors are always represented by column matrices, matrix transpose is denoted by prime $'$. Let $z = (z_1, \ldots, z_n, z_{n+1}, \ldots, z_{2n})' = (p_1, \ldots, p_n, q_1, \ldots, q_n)'$,

$$H_z = \left[\frac{\partial H}{\partial p_1}, \cdots, \frac{\partial H}{\partial p_n}, \frac{\partial H}{\partial q_1} \cdots, \frac{\partial H}{\partial q_n}\right]',$$

$$J_{2n} = J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \quad J' = J^{-1} = -J.$$

(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 non-singular anti-symmetric closed differential 2-form

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

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

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 the given Hamiltonian H, of *canonical transformations* of R^{2n} (locally in t and z) such that

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

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 everywhere symplectic, i.e.

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

The canonicity of $G(t)$ implies the preservation of 2-form ω, 4-form $\omega \wedge \omega, \ldots,$ $2n$-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 $\varphi(z)$ is said to be an *invariant integral* of (1.2) if it is invariant under (1.2)

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

which is equivalent to

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

where the *Poisson Bracket* for two functions $\varphi(z), \psi(z)$ are defined as

$$\{\varphi, \psi\} = \varphi_z' J^{-1} \psi_z,$$

H itself is always an invariant integral, see, e.g., [5].

The above digressions on Hamiltonian systems suggest the following *guidelines* for the numerical study of dynamical problems: The problem scold be expressed in some suitable *Hamiltonian formalism*. The numerical schemes should preserve as much as possible the characteristic properties and inner symmetries of the original system. 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 Canonical Difference Schemes for Linear Canonical Systems

Consider the case for which the Hamiltonian is a quadratic form

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

then the canonical system

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

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* if and only if $\alpha = \frac{1}{2}$, i.e. it is the case of *time-centered Euler Scheme* with the transition matrix F_τ,

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

F_τ, as the *Cayley transform* of infinitesimally symplectic τL, is symplectic. The 2nd order canonical Euler scheme (2.3) can be generalized to canonical schemes of arbitrary high order [2, 3]. For example, by taking the matrix transform function $\varphi(\lambda)$ in (2.3) to be the diagonal *Padé approximants* $P_m(\lambda)/P_m(-\lambda)$ to the exponential function $\exp \lambda$, where

$$\begin{aligned}
&P_0(\lambda) = 1, \\
&P_1(\lambda) = 2 + \lambda, \\
&P_2(\lambda) = 12 + 6\lambda + \lambda^2, \\
&\qquad \cdots, \\
&P_m(\lambda) = 2(2m-1) P_{m-1}(\lambda) + \lambda^2 P_{m-2}(\lambda),
\end{aligned}$$

we can prove that the difference schemes

$$z^{k+1} = \frac{P_m(\tau L)}{P_m(-\tau L)} z^k \quad m = 1, 2, \ldots \tag{2.4}$$

for the system (2.2) are symplectic, A-stable, of $2m$-th order of accuracy, and having the same set of quadratic invariant integrals including $H(z)$ as that of system (2.2). The case $m = 1$ is the time-centered Euler scheme (2.3).

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

$$\frac{1}{\tau}(z^{k+1} - z^k) = J^{-1} H_z(\frac{1}{2}(z^{k+1} + z^k)) \tag{2.5}$$

is *canonical*. However, unlike the linear case, the invariant integrals $\varphi(z)$ of system (1.2), including $H(z)$, are conserved only approximately

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

the time-centered Euler schemes (2.3), (2.5) and their canonical generalizations (2.4) are all *implicit*. For the case of *separable* Hamiltonian

$$H(p, q) = U(p) + V(q),$$

one can construct *time-staggered* schemes which are *canonical*, of 2nd order accuracy and *practically explicit* [1, 2], e.g.,

$$\begin{aligned} \frac{1}{\tau}(p^{k+1} - p^k) &= -V_q(q^{k+\frac{1}{2}}), \\ \frac{1}{\tau}(q^{k+1+\frac{1}{2}} - q^{k+\frac{1}{2}}) &= U_p(p^{k+1}). \end{aligned} \tag{2.6}$$

The $p's$ are set at integer times $t = k\tau$, $q's$ at half-integer times $t = (k + \frac{1}{2})\tau$. We need averaging, e.g., using

$$q^k = \frac{1}{2}(q^{k-\frac{1}{2}} + q^{k+\frac{1}{2}})$$

to compute the invariant integrals $\varphi(p, q)$ and get

$$\varphi(p^{k+1}, q^{k+1}) - \varphi(p^k, q^k) = O(\tau^3).$$

For the comparison of stability for the linear system (2.3) and the canonical schemes (2.4), (2.6) and the application of (2.6) to the wave equation, see [1].

§3 Construction of Canonical Difference Schemes via Generating Functions

A major component of the transformation theory in symplectic geometry is the method of *generating functions*, see, e.g., [5], which also play a central role for the construction of canonical difference schemes. In [2, 4] a constructive general theory of generating functions is given, roughly as follows: Let

$$T = \begin{bmatrix} A & B \\ C & D \end{bmatrix}, \quad T^{-1} = \begin{bmatrix} A_1 & B_1 \\ C_1 & D_1 \end{bmatrix},$$

T be a non-singular real matrix of order $4n$ satisfying

$$T' = \begin{bmatrix} 0 & I_{2n} \\ -I_{2n} & 0 \end{bmatrix} T = \mu \begin{bmatrix} -J_{2n} & 0 \\ 0 & J_{2n} \end{bmatrix}, \quad \text{for some } \mu \neq 0. \tag{3.1}$$

T defines a linear transformation in product space $R^{2n} \times R^{2n}$ by

$$\begin{aligned} \hat{w} &= A\hat{z} + Bz \\ w &= C\hat{z} + Dz, \end{aligned} \qquad \begin{bmatrix} \hat{z} \\ z \end{bmatrix}, \begin{bmatrix} \hat{w} \\ w \end{bmatrix} \in R^{2n} \times R^{2n}. \tag{3.2}$$

Let $z \to \hat{z} = g(z,t)$ be a *time-dependent canonical transformation* defined by

$$g(z,t) = M_0 G(z, -t) \tag{3.3}$$

where $G(w,t)$ is the one-parameter group of canonical transformations for the canonical system (1.2) with given Hamiltonian $H(z)$; M_0 is a constant symplectic *matrix* $\in Sp(2n)$. The Jacobian

$$M(z,t) = \frac{\partial g(z,t)}{\partial z} \in Sp(2n), \quad M(z,0) = M_0.$$

If the transversality condition

$$| CM_0 + D | \neq 0 \tag{3.4}$$

holds, then there exist, for sufficiently small $|t|$ and in (some neighborhood of) R^{2n}, a *time-dependent gradient transformation* $w \to \hat{w} = f(w,t)$ with Jacobian $\frac{\partial f(w,t)}{\partial w} = N(w,t) \in S_m(2n)$, i.e., everywhere *symmetric*, and a *time-dependent generating function* $\phi(w,t)$ with gradient $\phi_{\boldsymbol{w}}(w,t) = f(w,t)$ such that

$$[\hat{w} - f(w,t)]_{\hat{w}=A\hat{z}+Bz,\, w=C\hat{z}+Dz} = 0$$

is an implicit representation of the canonical transformation $\hat{z} = g(z,t)$. The generating function $\phi(w,t)$ satisfies the ***Hamilton-Jacobi equation***

$$\phi_{\boldsymbol{t}}(w,t) = -\mu H(C_1 \phi_{\boldsymbol{w}}(w,t) + D_1 w), \quad w = C\hat{z} + Dz. \tag{3.5}$$

By recursions we can determine explicitly all possible time-dependent generating functions for Hamiltonians $H(z)$ analytic in z :

$$\begin{aligned} \phi(w,t) &= \sum_{k=0}^{\infty} \phi^{(k)}(w) t^k, \qquad (3.6) \\ \phi^{(0)}(w) &= \frac{1}{2} w' N_0 w, \quad N_0 = (AM_0 + B)(CM_0 + D)^{-1}, \\ \phi^{(1)}(w) &= -\mu H(E_0 w), \quad E_0 = (CM_0 + D)^{-1}, \\ k \geq 1: \quad \phi^{(k+1)}(w) &= -\frac{1}{k+1} \sum_{m=1}^{k} \frac{\mu}{m!} \sum_{i_1,\ldots,i_m=1}^{2n} H_{z_{i_1},\ldots,z_{i_m}}(E_0 w) \cdot \\ &\quad \cdot \sum_{\substack{k_1+\cdots+k_m=k \\ k_j \geq 1}} (C_1 \phi_{\boldsymbol{w}}^{(k_1)}(w))_{i_1} \ldots (C_1 \phi_{\boldsymbol{w}}^{(k_m)}(w))_{i_m}. \end{aligned}$$

Choose

$$T = \begin{bmatrix} -I_{\boldsymbol{n}} & 0 & 0 & 0 \\ 0 & 0 & I_{\boldsymbol{n}} & 0 \\ 0 & I_{\boldsymbol{n}} & 0 & 0 \\ 0 & 0 & 0 & I_{\boldsymbol{n}} \end{bmatrix}, \quad \mu = 1, \quad M_0 = J_{2\boldsymbol{n}},$$

we get the generating function of the 1st type for the case $|\frac{\partial \hat{q}}{\partial p}| \neq 0$:

$$\phi = \phi(\hat{q}, q, t), \quad -\hat{p} = \phi_{\hat{q}}, \quad p = \phi_{\boldsymbol{q}}, \quad \phi_{\boldsymbol{t}} + H(\phi_{\boldsymbol{q}}, q) = 0.$$

Choose

$$T=\begin{bmatrix} -I_n & 0 & 0 & 0 \\ 0 & 0 & 0 & -I_n \\ 0 & I_n & 0 & 0 \\ 0 & 0 & I_n & 0 \end{bmatrix}, \quad \mu=1, \quad M_0=I_{2n},$$

we get the generating function of the 2nd type for the case $|\frac{\partial \hat{q}}{\partial q}| \neq 0$:

$$\phi=\phi(\hat{q},p,t), \quad -\hat{p}=\phi_{\hat{q}}, \quad -q=\phi_p, \quad \phi_t+H(p,-\phi_p)=0.$$

Choose

$$T=\begin{bmatrix} -J_{2n} & J_{2n} \\ \frac{1}{2}I_{2n} & \frac{1}{2}I_{2n} \end{bmatrix}, \quad \mu=-1, \quad M_0=I_{2n},$$

we get the generating function of a new type — the ***Euler type*** —

$$\phi=\phi(w,t), \quad w=\frac{1}{2}(\hat{z}+z), \quad \hat{w}=J(\hat{z}-z)=\phi_w, \quad \phi_t-H(w-\frac{1}{2}J\phi_w)=0.$$

The *general methodology* for the construction of canonical difference schemes is as follows: Choose some suitable type of generating function with its explicit expression (3.6) truncate or approximate it in some way and take gradient of this approximation, then we get automatically the implicit representation of some canonical transformation for the transition of the difference scheme. In this way one can get an abundance of canonical difference schemes. This methodology is *unconventional* in the ordinary sense, but natural from the point of view of symplectic geometry [4]. As an illustration we choose the ***Euler type*** generating function $\phi(w,t)$, which is odd in t :

Take sufficiently small $\tau>0$ as the time-step, define

$$\psi^{(2m)}(w,\tau)=\sum_{k=1}^{m}\phi^{(2k-1)}(w)\tau^{2k-1}, \quad m=1,2,\cdots. \tag{3.7}$$

Then the gradient transformation

$$w \to \hat{w}=\psi_w^{(2m)}(w,\tau) \tag{3.8}$$

represents implicitly a canonical scheme $\hat{z}=z^k \to z^{k+1}=z$ of $2m$-th order accuracy upon substitution (3.2). The case $m=1$ is the centered Euler scheme (2.5). For linear canonical system (2.2), the generating function is the quadratic form

$$\phi(w,t)=\frac{1}{2}w'(2J\tanh(\frac{\tau}{2}L))w, \quad L=J^{-1}S, \quad S'=S,$$

$$\tanh\lambda=\lambda-\frac{1}{3}\lambda^3+\frac{2}{15}\lambda^5-\frac{17}{312}\lambda^7+\cdots=\sum_{k=1}^{\infty}a_{2k-1}\lambda^{2k-1},$$

(3.8) becomes symplectic difference schemes

$$z^{k+1}-z^k=(\sum_{k=1}^{m}a_{2k-1}(\frac{\tau}{2}L)^{2k-1})(z^{k+1}+z^k).$$

The case $m=1$ is the centered Euler scheme (2.3).

§4 Hamiltonian Formalism in Infinite Dimensions for Fluids

Physical processes in continuous media are dynamical systems of infinite dimensions, the corresponding symplectic geometry has not yet been fully developed theoretically. The constructive theory of generating functions [2, 4] of the 2nd type and of the Euler type and the corresponding construction of canonical difference schemes (involving time discretization only) has been generalized by Qing and Li 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 [6], the Hamiltonian canonical systems are of the form

$$\frac{\partial p}{\partial t} = -\frac{\delta H}{\delta q}, \quad \frac{\partial q}{\partial t} = \frac{\delta H}{\delta p}$$

$H = H(p, q)$ is a functional, the right hand sides are variational derivatives. In case B is self-dual, the generalization is valid also for the generating functions of the 1st kind.

The problem of the Hamiltonian structure for the equations of ideal fluids has a long history, dated back to 1850's. There are several different approaches to its solution. We mention here only the oldest one — the representation of velocity by *Clebsch variables*. Take, e.g., the case of compressible ideal fluid,

$$\vec{v} = \frac{\lambda}{\rho}\mathrm{grad}\,\mu + \mathrm{grad}\,\phi$$

where ρ is the density, λ, μ, ϕ are Clebsch potentials. Then the flow equations can be put in the canonical form

$$\frac{\partial \phi}{\partial t} = -\frac{\delta H}{\delta \rho}, \quad \frac{\partial \mu}{\partial t} = -\frac{\delta H}{\delta \lambda},$$
$$\frac{\partial \rho}{\partial t} = \frac{\delta H}{\delta \phi}, \quad \frac{\partial \lambda}{\partial t} = \frac{\delta H}{\delta \mu},$$
$$H = \int \{\frac{1}{2}\rho \vec{v}^2 + e(\rho)\} dr, \quad e(\rho) = \text{internal energy}.$$

Buneman used this formalism (modified) in computer simulation with a scheme *staggered both in space and time* and pointed out the inherent computational advantages of the canonical formalism [7].

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