# HOW TO COMPUTE PROPERLY NEWTON'S EQUATION OF MOTION ? ①

# 如何正确计算牛顿运动方程？

## §1 Problems and Motivations

The main theme of modern scientific computing is the numerical solution of various differential equations of mathematical physics bearing the names such as Newton, Euler, Lagrange, Laplace, Navier-Stokes, Maxwell, Boltzmann, Einstein, Schrödinger, Yang-Mills, etc. At the top of the list is the most celebrated Newton's equation of motion. The historical, theoretical and practical importance of Newton's equation hardly needs any comment, so is the importance of the numerical solution of such equations. On the other hand, starting from Euler, right down to the present computer age, a great wealth of scientific literature on numerical methods for differential equations has been accumulated, and a great variety of algorithms, software packages and even expert systems had been developed. Under such circumstances we still feel motivated to raise the following two questions:

Question 1: *Are the existing numerical methods adequate for computing Newton's equations of motion?*

Question 2: *What is the proper way to compute Newton's equations of motion?*

Question 1 seems to have never been seriously raised before, so question 2 seems to have never been studied systematically.

We start with the case of Newton's equations of motion in conservative force field in configuration space $\mathbf{R^n}$, which is physically more basic and mathematically more difficult:

$$M\ddot{q} = -V_q(q) \tag{1}$$

where $q = (q_1, \cdots, q_n)$ is the position variable, $M$ is the inertia matrix, $V(q)$ is the potential energy. It is well known that the conservative Newton's equations has two alternative mathematically equivalent formalisms: the Lagrangian formalism as a variational principle and the Hamiltonian formalism in which the Newton's system of differential equations of second order in configuration space is reduced to Hamilton's system of canonical equations of first order in phase space with doubled dimension.

The mathematically equivalent formalisms express the same physical laws, but they look very different in form, so they lead to different technical approaches in problem solving,

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they are not equally effective in practice. So a judicious choice at the start among the alternative mathematically equivalent formalisms is very crucial for the eventual success or failure in problem solving.

We choose the *Hamiltonian* formalism as the basis, i.e. instead of the Newton's system (1) we consider the Hamilton's canonical system

$$\dot{p} = -H_q(p,q), \quad \dot{q} = H_p(p,q)$$

i.e.

$$\dot{z} = JH_z(z), \quad J = J_{2n} = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix} \tag{2}$$

in phase space $\mathbf{R}^{2n}$, defined by the Hamiltonian function $H(z) = H(p,q)$ in $2n$ variables $(z_1, \cdots, z_{2n}) = (p_1, \cdots, p_n, q_1, \cdots, q_n)$ representing the total energy. Our motivations are 1. Hamiltonian formalism is distinctive in its *simplicity*, *symmetry* and *elegance* in form. The laws of motion become more explicit and transparent in Hamiltonian formalism. 2. Hamiltonian formalism is also distinctive in its *ubiquity* and *universality*. It is now beyond doubt that any real physical process with negligible dissipation of classical or relativistic or quantum nature in finite or infinite number of degrees of freedom can always be cast in suitable Hamiltonian form. So, if the algorithms for classical Hamiltonian systems turn to be successful, they are expected to have wide applications. We started with a search in the vast volume of archives on numerical methodology for differential equations; however, we found that the pertinent study specifically for Hamiltonian equations is virtually void, in paradoxical contradiction with the importance and general applicability of Hamiltonian formalism. This situation also motivate us to think hard and to raise the questions as mentioned above.

## §2 Hamiltonian Algorithms for Hamiltonian Systems

Our technical approach is *symplectic geometry*, i.e., the geometry of phase space in which an anti-symmetric area metric is basic, in contrast with the Euclidean or Riemannian geometry in which a symmetric distance metric is basic. The fundamental theorem of classical mechanics expressed in symplectic geometry becomes "all dynamical evolutions of Hamiltonian system are *symplectic* (canonical) transformations", i.e. those preserving the anti-symmetric symplectic metric, or more precisely, smooth 1-1 transformation $g : \mathbf{R}^{2n} \to \mathbf{R}^{2n}$ with Jacobian matrix $g_z(z)$ satisfying

$$(g_z(z))^T J_{2n} g_z(z) \equiv J_{2n}.$$

It is natural and mandatory to require that the marching of the discrete algorithm should be also symplectic. Such algorithms are called *symplectic* or *canonical* or *Hamiltonian*. We conceive, design, analyse and assess the algorithms conciously and exclusively within the framework of symplectic geometry. This approach turns out to be successful and fruitful, giving a great variety of symplectic algorithms with remarkable properties and outstanding performance and with sound theoretical foundation [1, 2].

A comparative numerical study for non-symplectic conventional methods and symplectic methods has been carried out on the following set of "benchmarks": 1. Simple harmonic oscillator 2. Nonlinear Duffing oscillator 3. Huygens oscillator 4. Cassini oscillator

5. Stationary flow on plane periodic and quasi-periodic lattices 6. Double harmonic oscillator and Lissajous figures 7. Geodesic flow on ellipsoidal surface 8. Kepler motion. Extensive computer experimentation affirms indisputably the high quality and superiority of symplectic methods; especially in the global, structural and long-term tracking aspects, all conventional non-symplectic methods irretrievably fail without exception while all symplectic methods decently succeed without exception, possessing remarkable very-long-term tracking capability. The contrast is sharp and overwhelming.

Fig 1 shows the linear harmonic oscillator $H = \frac{1}{2}(p^2 + 4q^2)$ computed by different methods. (A): 4th order Runge Kutta method, step size $s = 0.4$, dissipative, a false attractor is formed at the center. (B): 4th order Adams method, $s = 0.2$, anti-dissipative, diverging outwards. (C): Leap-flog method, i.e., explicit 3-level method which is symplectic for linear Hamiltonian systems but non-symplectic for non-linear Hamiltonian systems, $s = 0.1$. Three consecutive 1000 points after the 1st step, after the 5 million-th step and after the 10 million-th step are plotted on the same figure, their coincidence shows the long-term tracking capability of symplectic scheme.

Fig 2: Non-linear Duffing oscillater $H = \frac{1}{2}(p^2 + q^2) - \frac{2}{3}q^4$ (A) and (B): The same Leap-flog method, non-symplectic now, $s = 0.2$, 10000 steps. The first 20 points (not clearly shown in the plot) are on the right track of a near elliptic orbit like that of (C), but long-time tracking goes wrong. (C): Explicit symplectic method of order 2 with $s = 0.1$ up to 100 million steps. Three consecutive 1000 points after the first step, after the 50 million-th step and after the 100 million-th step are plotted on the same figure, their remarkable coincidence shows the very long-term tracking capability of symplectic method for non-linear system. Here some function $=H + O(s^2)$, instead of $H$ itself, is exactly conserved.

Fig 3: Nonlinear Huygens oscillater $H = p^2 - q^2 + q^4$, having two elliptic fixed points. (A) and (B): Runge-Kutta method, 2 artificial attractors at the elliptic fixed points are formed. The same initial point outside the separatrix is attracted randomly either to the left or to the right by minute changes of step sizes from 0.10000005 in (A) to 0.10000004 in (B). (C): Symplectic computation of 4 typical orbits each up to 100000000 steps, showing the striking robustness of the algorithm.

Fig 4–6 show the geodesic flows on ellipsoidal surface and Kepler motion with Hooke potential. Initial data in both cases correspond to rational or irrational frequency ratio, which give closed or dense orbit. (A): Total failure of Runge-Kutta method in long-term tracking. (B): Success of symplectic method in long-term tracking, exhibiting the closedness or denseness of orbits, [7].

Apart from very rare exceptions, almost all conventional methods are non-symplectic, usually they were designed for asymptotically stable systems, providing dissipative mechanisms to guarantee computational stability. Hamiltonian systems can never be asymptotically stable, so the non-symplectic methods inevitably bring in artificial dissipation, false attractors and/or various parasitic effects which are alien to Hamiltonian dynamics, leading eventually to grave distortions. Although practically applicable for short-term simulation of transcient phenomena, they are impotent and possibly misleading in global and structural study and long-term tracking. Since Newton's equations are mathematically equivalent to Hamilton's, so we get at the quite unexpected *negative answer* to Question 1.

Symplectic methods are inherently free from artificial dissipation and all kinds of non-Hamiltonian pollutions. They are "*clean*" algorithms. The dynamical evolution of Hamiltonian systems are governed by two classes of conservation laws. The first class consists in the conservation of even-dimensional phase area, i.e., the Liouville-Poincaré conservation laws, they are automatically preserved under symplectic algorithms. The second class consists in the conservation of energy and other integrals of motion, i.e., Noether conservation laws. The crucial fact is that any symplectic algorithm possesses its own *formal* integrals of motion depending on the step-size parameter and approximating the original integrals of motion (with the same order of accuracy as that of the method itself) and being invariant under the algorithm [4, 5]. It can also be proved that the majority of invariant tori of integrable systems are preserved under symplectic algorithms; resulting in a new version of the celebrated K.A.M. theorems and the theoretical infinite-time tracking capability of the symplectic algorithms [6], although practically realizable only approximately on computers with finite number of digits.

The high degree of parallelism and proximity between the structure of the time-discrete Hamiltonian system and that of the original system guarantees and explains in a fundamental way the remarkable hi-fi performance of Hamiltonian algorithms. So a *proper* way to compute Newton's equations of motion is *first to Hamiltonize the equations and then to compute them by Hamiltonian algorithm.* This constitutes our answer, by no means trivial, to Question 2.

## §3 Recommendations and Conclusions

We list some very simple and useful Hamiltonian algorithms [1, 2, 8], $s$ = step-size (real number).

1. Centered Eulerian scheme, 2nd order, implicit, preserving all quadratic integrals of motion:

$$z^k \to z^{k+1} =: C^s z^k,$$
$$z^{k+1} = z^k + sJH_z(\frac{1}{2}(z^{k+1} + z^k)).$$

2. Alternating explicit Eulerian schemes for canonically separable Hamiltonian $H(p,q) = \phi(p) + \psi(q)$, preserving all quadratic integrals of motion of angular momentum type $p^T Bq$:

$$z^k \to z^{k+1} =: A_1^s z^k,$$
$$p^{k+1} = p^k - s\psi_q(q^k),$$
$$q^{k+1} = q^k + s\phi_p(p^{k+1}),$$

or

$$z^k \to z^{k+1} =: A_2^s z^k,$$
$$q^{k+1} = q^k + s\phi_p(p^k),$$
$$p^{k+1} = p^k - s\psi_q(q^{k+1}).$$

Both $A_1^s$, $A_2^s$ are of 1st order. Their composite, e.g., $A_2^{s/2} \circ A_1^{s/2} =: A^s$ is 2nd order:

$$z^k \to z^{k+1} =: A_2^{s/2} \circ A_1^{s/2} z^k,$$
$$p^{k+\frac{1}{2}} = p^k - \frac{s}{2}\psi_q(q^k),$$
$$q^{k+1} = q^k + s\phi_p(p^{k+\frac{1}{2}}),$$

$$p^{k+1} = p^{k+\frac{1}{2}} - \frac{s}{2}\psi_q(q^{k+1}).$$

The algorithms $C^s, A^s$ are *revertible* in the sense that

$$g^{-s} = (g^s)^{-1}.$$

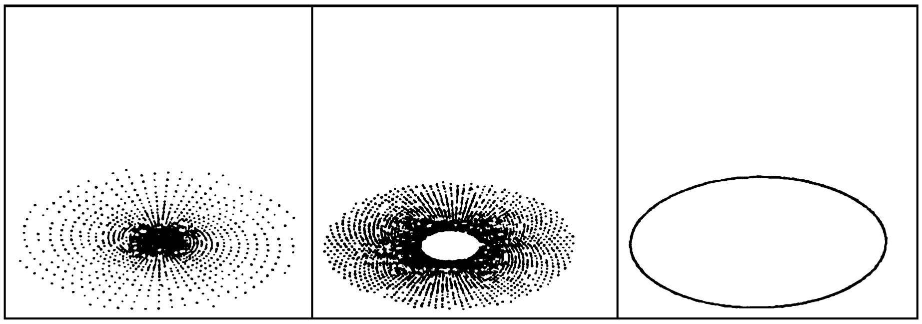
Revertibility is a disirable property of numerical methods, since it is always satisfied by the true solution of the system and it implies that the order of accuracy is necessarilly even. It also provides a practical means for monitoring the inevitable loss of significant digits due to round-off in long-term numerical integration. Moreover, for any revertible Hamiltonian algorithm $g^s$ of order 2, a revertible Hamiltonian algorithm $\tilde{g}^s$ of order 4 can be easily constructed by splitting the time-step of size $s$ into 3 substeps of sizes $\alpha s, \beta s, \alpha s$,

$$\tilde{g}^s = g^{\alpha s} \circ g^{\beta s} \circ g^{\alpha s}$$

with $2\alpha + \beta = 1$, $2\alpha^3 + \beta^3 = 0$, i.e., $\alpha = (2 - \sqrt[3]{2})^{-1} > 0, \beta = 1 - 2\alpha < 0$, [3].

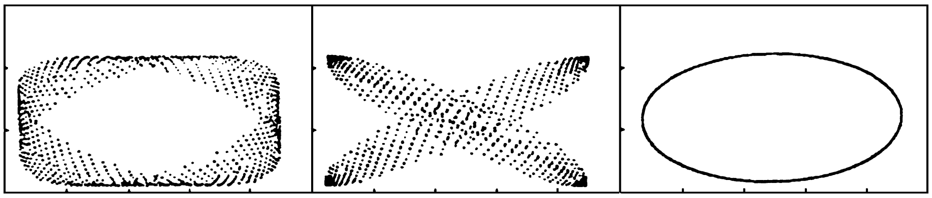
It is important to note that, although Hamiltonian algorithms emerge as the proper methodology for solving Hamiltonian sysems, they are applicable as well to non-Hamilto-nian systems with advantage. Hamiltonian algorithms are *neutral* in the sense that they give the proper amount of dissipation as determined by the systems themselves, without overcharge or discount. The advantage is indiscernible under strong dissipation but becomes ever more prominent with decreasing dissipation. The phenomenal stability property of Hamiltonian algorithms makes them good for solving stiff problems too. So Hamiltonian algorithms are recommented as a safe and high-performance methodology for general usage.

The study of numerical methods for Hamiltonian systems grossly neglected thus far is a new promising and vital field of research at the common frontier of computational physics, computational mechanics and computational mathematics. Owing to the universality of Hamiltonian formalism, Hamiltonian algorithms are promising for wide applications and developments and to have impact on many fields of scientific computing.



| (A) Runge-Kutta non-symplectic 4000 steps | (B) Adams non-symplectic 4000 steps, | (C) Leap-frog symplectic 10000000 steps |
|---|---|---|

Fig 1. Harmonic oscillator $H = \frac{1}{2}p^2 + 2q^2$

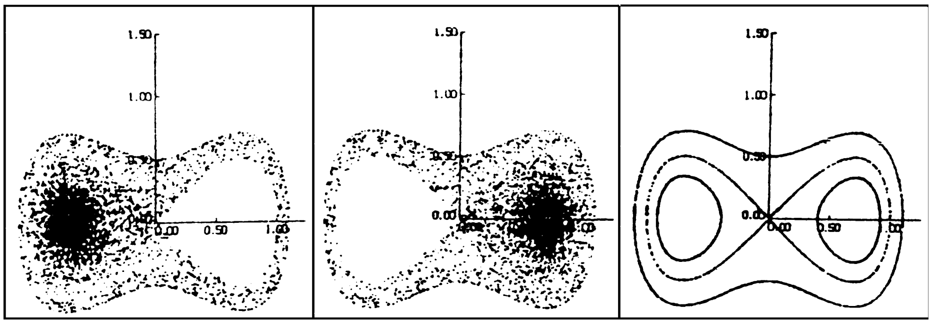


(A) Leap-frog
1-1000 steps

(B) Leap-frog
9000-10000 steps

(C) Symplectic
100000000 steps

Fig 2. Nonlinear Duffing oscillator $H = \frac{1}{2}p^2 + 2q^2 - \frac{2}{3}q^4$

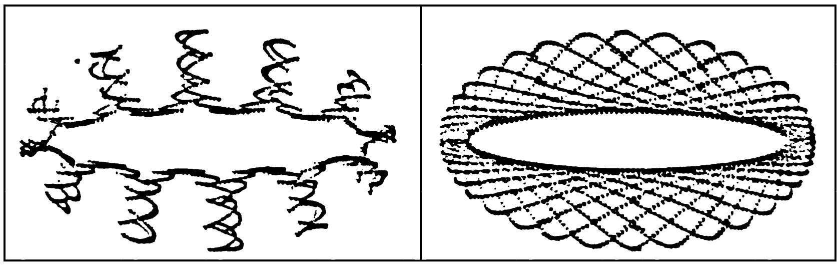



(A) Runge-Kutta, 1 orbit
800000 steps
step size 0.10000005

(B) Runge-Kutta, 1 orbit
800000 steps
step size 0.10000004

(C) Symplectic, 4 orbits
100000000 steps
each

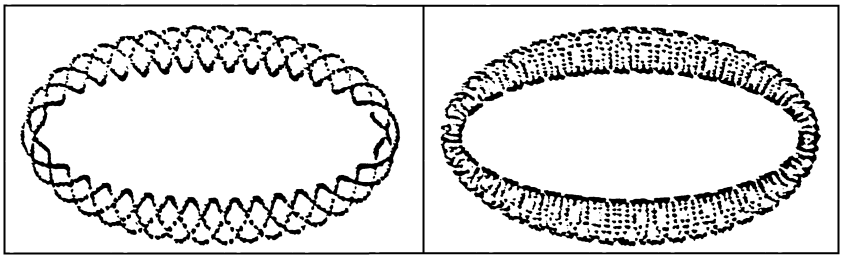
Fig 3. Nonlinear Huygens oscillator $H = p^2 - q^2 + q^4$



(A) Runge-Kutta
100000 steps

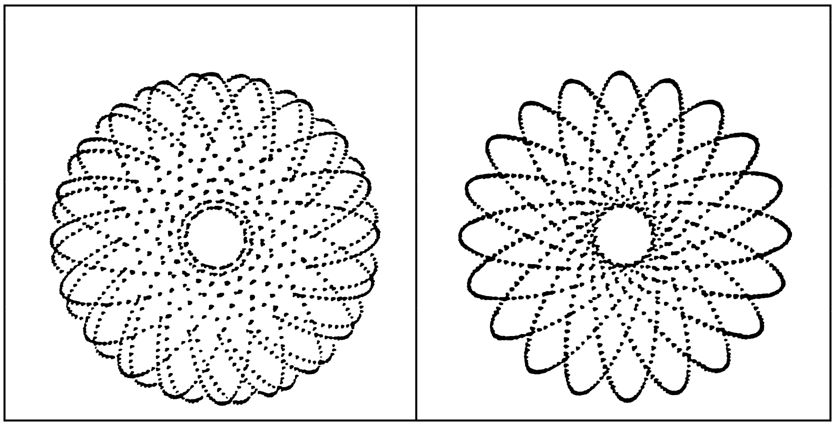
(B) Symplectic
100000 steps

Fig 4. Geodesics on ellipsoid, frequency ratio 11:16, closed orbit.



(A) Runge-Kutta 10000 steps (B) Symplectic 10000 steps

Fig 5. Geodesics on ellipsoid, frequency ratio $\sqrt{5}:4$, dense orbit.



(A) Runge-Kutta 240000 steps (B) Symplectic 240000 steps

Fig 6. Kepler motion, freguency ratio 11:20, closed orbit.

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