

Volume or Energy: You Cannot Have Both

— What a Symplectic Integrator Preserves Is Volume, Not Accuracy: Liouville Discretised and the Ge–Marsden Theorem (the Yamagishi Census of Numerics) — [Paper 135]

Yuuki YAMAGISHI (山岸 勇輝)

Yamagishi Complexity Torus Lab, Japan

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— *From thinking to syncing.* —

ABSTRACT

Paper 77 recorded Liouville's theorem, that a Hamiltonian flow **preserves phase-space volume**. This paper calls the roll on its discrete counterpart and separates what a numerical method preserves from what it does not. **NO NEW MATHEMATICAL THEOREM AND NO NEW PHYSICAL LAW IS CLAIMED**. First, the preservation of volume is **exact**. Computing symbolically the Jacobian determinant of one step, leapfrog gives **exactly 1** and semi-implicit Euler gives **exactly 1**, whereas **explicit Euler gives $1 + h^2k$** and **inflates the volume** and **classical fourth-order Runge–Kutta gives $1 - h^6k^3/72 + h^8k^4/576$** and **contracts it** (Section 2). Second, one of the two cores. Being symplectic is not **conserving the energy**. Running a harmonic oscillator for 10^7 steps at $h = 0.1$, the leapfrog energy **keeps oscillating inside the band $[0.99750, 1]$** and **the band itself does not move**, while fourth-order Runge–Kutta **falls to 0.87048**. What a symplectic method preserves exactly is not the true Hamiltonian but a nearby “shadow” Hamiltonian (Section 3). Third, being symplectic is not being accurate either. After 20 periods at $h = 0.05$ the position error is 9.4×10^{-5} for leapfrog and 3.6×10^{-7} for fourth-order Runge–Kutta. **Over short times the fourth-order method is more than two orders better**. Symplecticity buys long-time qualitative behaviour, not accuracy (Section 4). Fourth, secular drift has a clear signature in the Kepler problem. At eccentricity 0.5 and $h = 0.01$ the relative energy error of fourth-order Runge–Kutta is 3.032×10^{-8} after 10 orbits, 3.032×10^{-7} after 100 and 3.032×10^{-6} after 1000: **exactly proportional to the number of orbits, which is the signature of secular drift**. Leapfrog's is **four to six orders smaller and does not follow that law** (Section 5). Fifth, the other core. **You cannot have both**. The Ge–Marsden theorem (1988) states that an integrator that is **both symplectic and exactly energy-conserving** can only be **the exact flow itself, up to a reparametrisation of time**. **Volume or energy. Not both, unless one already has the answer** (Section 6).

Scope of this paper: NO NEW MATHEMATICAL THEOREM AND NO NEW PHYSICAL LAW IS CLAIMED.

Liouville's theorem, symplectic integrators, backward error analysis (the shadow Hamiltonian) and the Ge–Marsden theorem are **all standard**. What this paper adds is only **separating three virtues – volume, energy and accuracy – and showing the separation numerically, writing the signature of secular drift as a proportionality, and placing the impossibility of having both as a theorem. It is not said that being symplectic makes a method good.**

1. Notation and position

The flow of a Hamiltonian $H(q, p)$ is **symplectic**, and in consequence **preserves phase-space volume** (Liouville's theorem, Paper 77). A numerical method with the same property is called **symplectic**.

Position: existing results are laid side by side and what does not follow from what is written down. No new theorem is claimed. Paper 17 said that **calling things distinct-rooted is half the work; only writing the addresses makes the claim checkable. This paper does that for the phrase “a good numerical method”.**

2. The preservation of volume is exact

Verification 2.1 (the Jacobian of one step): For the harmonic oscillator $H = p^2/2 + kq^2/2$, the Jacobian determinant of one step of each method was computed symbolically.

method	$\det J$	the volume
leapfrog (velocity Verlet)	1	exactly preserved
semi-implicit Euler	1	exactly preserved
explicit Euler	$1 + h^2 k$	inflates
classical fourth-order Runge–Kutta	$1 - \frac{h^6 k^3}{72} + \frac{h^8 k^4}{576}$	contracts

At $h = 0.1$ and $k = 1$ the Runge–Kutta determinant is **0.9999999861...** (QED)

Observation 2.2 (this is Liouville discretised)

$\det J = 1$ means the phase-space volume is preserved exactly at every step (Paper 77). It is not an approximation. However coarse the step, 1 is 1.

Observation 2.3 (the standing of that 1)

Paper 16 counted six roots of the equals sign. The $\det J = 1$ here is an identity, independent of the step and of the force. The ≈ 1 of the energy, seen below, is not. One word “preserved” is naming two standings.

3. Symplectic is not energy-conserving

Verification 3.1 (energy over long times): Harmonic oscillator, $h = 0.1$, initial energy normalised to 1.

steps	method	final	minimum	maximum
10^3	leapfrog	0.99945	0.99750	1.00000
10^3	RK4	0.99999	0.99999	1.00000
10^5	leapfrog	0.99763	0.99750	1.00000
10^5	RK4	0.99861	0.99861	1.00000
10^7	leapfrog	0.99811	0.99750	1.00000
10^7	RK4	0.87048	0.87048	1.00000

Leapfrog's minimum stays at 0.99750 at 10^5 steps and at 10^7 steps alike: the band has not moved. Runge–Kutta's band descends as a whole. (QED)

Observation 3.2 (what is exactly preserved)

What a symplectic method preserves exactly is **not the true Hamiltonian**. By backward error analysis it preserves **a different Hamiltonian close to the true one — the shadow Hamiltonian** — exactly, or more precisely over exponentially long times. **That the energy error stays bounded is a consequence of this.**

Observation 3.3 (correcting the phrase)

“A symplectic method conserves energy” is not right. The correct statement is that the energy error stays bounded and does not grow secularly. What is conserved is a different quantity.

4. Symplectic is not accurate either

Verification 4.1 (short-time error): Position error for the harmonic oscillator at $h = 0.05$.

periods	leapfrog	RK4	better
1	2.14×10^{-5}	2.43×10^{-8}	RK4
5	4.68×10^{-5}	9.41×10^{-8}	RK4
20	9.37×10^{-5}	3.62×10^{-7}	RK4

(QED)

Observation 4.2 (three virtues, three things)

virtue	what guarantees it	how it is bought
preservation of volume	symplecticity	exactly, and it is available
bounded energy error	a consequence of symplecticity	bounded, not zero
accuracy	the order (a power of h)	bought separately

Leapfrog is second order and classical Runge–Kutta is fourth. Order and symplecticity are independent attributes and must not be conflated.

5. Secular drift has a signature

Verification 5.1 (the Kepler problem): Eccentricity 0.5, $h = 0.01$, relative energy error.

orbits	leapfrog	RK4
10	7.60×10^{-13}	-3.032×10^{-8}
100	7.40×10^{-12}	-3.032×10^{-7}
1000	4.48×10^{-10}	-3.032×10^{-6}

Multiplying the number of orbits by ten multiplies the Runge–Kutta error by exactly ten, to four significant figures. That is the signature of secular drift. Leapfrog's error is four to six orders smaller and does not obey that law. (QED)

Observation 5.2 (why the signature is useful)

Whether an error in a numerical experiment is a drift or a mere oscillation cannot be told from its size. It can be told from how it scales with time. As Paper 117 said of scale invariance, the right test is to look at the exponent.

6. You cannot have both

Established Fact 6.1 (Ge–Marsden 1988): An integrator that is symplectic and also conserves the energy exactly can only be the exact flow itself, up to a reparametrisation of time.

Observation 6.2 (this closes the question)

Preserving volume and preserving energy are two demands that cannot both be met — except by already having the answer. Designing a numerical method therefore is choosing which of them to make exact.

what is made exact	what is given up	where it belongs
volume (symplectic)	the energy oscillates, boundedly	long-time orbits
energy (projection, etc.)	the volume is not preserved	when the invariant is the point
neither	both drift secularly	short times, high accuracy

Observation 6.3 (an isomorph in the corpus)

Paper 126 said that an existence theorem delivers existence and nothing more; Papers 127 and 133 said that uniqueness lives only inside a fence. What this paper adds is the case in which two virtues exclude each other. Deciding to make something exact is deciding to give something else up.

Observation 6.4 (on adaptive stepping)

A method that varies its step according to the solution generally loses symplecticity. Adding two good things does not always make a better one. A fence cannot be crossed by addition.

7. Conclusion

1. **The preservation of volume is exact** (Ver. 2.1). Leapfrog and semi-implicit Euler give $\det J = 1$; explicit Euler inflates by $1 + h^2 k$ and Runge–Kutta contracts by $1 - h^6 k^3/72 + \dots$. This is Liouville's theorem discretised (Paper 77).
2. **Symplectic is not energy-conserving** (Ver. 3.1). At 10^7 steps leapfrog never leaves the band $[0.99750, 1]$ while Runge–Kutta falls to 0.87048. What is preserved is the shadow Hamiltonian.
3. **Symplectic is not accurate either** (Ver. 4.1). After 20 periods the errors are 9.4×10^{-5} and 3.6×10^{-7} . Order and symplecticity are independent.
4. **Secular drift has a signature** (Ver. 5.1). Runge–Kutta's error is proportional to the number of orbits to four significant figures. Look at the scaling, not the size (Paper 117).
5. **You cannot have both** (Fact 6.1). By Ge–Marsden, an integrator both symplectic and exactly energy-conserving is the exact flow.
6. **Adaptive stepping generally destroys symplecticity** (Obs. 6.4). A fence cannot be crossed by addition.

Closing: One phrase, “a good numerical method”, names three different virtues — volume, energy and accuracy. They are bought separately, and the first two exclude each other. A design that has not decided what to make exact has decided nothing.

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Yuuki YAMAGISHI (山岸 勇輝)

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