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LETTER TO THE EDITOR

Energy drift in reversible time integration

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Abstract
Energy drift is commonly observed in reversible integrations of systems of molecular dynamics. We show that this drift can be modelled as a diffusion and that the typical energy error after time T is $\mathcal{O}(\sqrt{T})$.

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In simulations of conservative systems, the energy H is usually monitored as a check on the calculation. In *symplectic* integration of Hamiltonian systems, it is known that the integrator is very close to the flow of a Hamiltonian system with Hamiltonian close to H, so that one can give conditions under which the energy error is bounded for exponentially long times [14]. However, in *reversible* integration [1–3, 5, 7, 8, 10], one typically sees the energy drift away from its initial value. In this letter we model this drift as a diffusion process, showing that the expected drift after time T is $\mathcal{O}(\sqrt{T})$.

There are several reasons why one might use a reversible integrator on a conservative system. First, if the system is Hamiltonian, a symplectic integrator might be prohibitively expensive. This occurs if one wants to adaptively vary the time step, which can be much cheaper to do reversibly than symplectically, or if the symplectic structure is noncanonical, perhaps as a result of a change of variables. See, e.g., the discussion of the Nosé–Hoover thermostat of molecular dynamics in [2].

Second, if the system is not Hamiltonian but still has a first integral H, then a reversible integrator is the natural choice of geometric method. One can construct integrators which are reversible and preserve energy, but they are expensive, typically fully implicit in the dependent variables and in the (introduced) Lagrange multipliers. It is usually much cheaper to preserve just the reversibility, which is the dominant property characterizing the dynamics, and merely monitor the energy.

We consider systems with phase space M and dynamics $\dot{x} = f(x)$, reversible under the diffeomorphism $R : M \to M$, i.e. $R^* f = -f$ or $f(R(x)) = -T_x R \cdot f(x)\ \forall x \in M$, and

with a symmetric first integral $H : M \to \mathbb{R}$, i.e. $\dot{H} = f(H) = 0$ and $H(R(x)) = H(x)$. (H can be any symmetric integral; we are calling it 'energy' for illustration.) The integrator, a diffeomorphism $\phi_\tau : M \to M$, which approximates the time-τ flow of f, is also assumed to be reversible, i.e. $\phi_\tau(R(x)) = R\big(\phi_\tau^{-1}(x)\big)$. We are interested in the energy drift: for a given initial condition $x_0 \in M$, which we take for convenience to have zero energy, $H(x_0) = 0$, what is the behaviour of the sequence $\big\{H\big(\phi_\tau^n(x_0)\big)\big\}$? Extensive numerical evidence suggests that it is not bounded but wanders erratically: in fact, it looks like a random walk. This is in stark contrast to the behaviour of general purpose, nonreversible integrators, for which the energy error increases linearly in time on a suitable time scale. Note that if the vector field f is Hamiltonian, then the integrator ϕ is close to symplectic. However, this plays no role in our analysis and we believe it is irrelevant.

For any orbit $\{x(t) : t \in \mathbb{R}\}$, we have that $\{R(x(-t))\}$ is also an orbit. If it is the same orbit, it is said to be symmetric. Otherwise, it is said to be nonsymmetric. Any orbit that intersects the fixed set $\{x : R(x) = x\}$ of R is symmetric. Symmetric orbits display typical conservative behaviour, for example, the eigenvalues of symmetric fixed points have the same symmetry as those of Hamiltonian systems, and there is a KAM theorem for symmetric quasiperiodic orbits [9, 15]. Nonsymmetric orbits, on the other hand, cannot 'see' the reversing symmetry and can have any dynamics, including asymptotically stable fixed points and strange attractors (whose image under R must be a strange repellor). This is commonly observed only in low-dimensional systems [9, 15, 6]. For typical high-dimensional systems such as those of molecular dynamics, the phase space consists of an ergodic 'sea' containing tiny islands of regular (e.g. quasiperiodic) orbits. Since there is no known mechanism which could keep a chaotic orbit in the sea bounded away from the fixed set of R, these orbits are believed to be generally symmetric.

(If the system has nonsymmetric first integrals $I : M \to \mathbb{R}^k$, then only orbits starting on the fixed set $\{x : I(x) = I(R(x))\}$ of I can possibly be symmetric. Therefore, we assume that the system either has no nonsymmetric integrals, or the system and integrator are both restricted to the fixed set of I. Momentum and angular momentum are examples of such nonsymmetric integrals.)

By backward error analysis [5, 14], the integrator ϕ_τ is (exponentially close to) the time-τ flow of the modified vector field

$$\dot{x} = \tilde{f}(x) = f(x) + \tau^p f_p(x) + \mathcal{O}(\tau^{p+1})$$

where $\tilde{f}$ and f_p are R-reversible. Here p is the order of the method. Therefore, the energy evolves according to

$$\dot{H} =: h = i_{\tilde{f}}\,\mathrm{d}H = i_f\,\mathrm{d}H + \tau^p i_{f_p}\,\mathrm{d}H + \mathcal{O}(\tau^{p+1}) = \tau^p i_{f_p}\,\mathrm{d}H + \mathcal{O}(\tau^{p+1}).$$

H is symmetric by assumption, so $\dot{H}$ is antisymmetric:

$$\dot{H} \circ R = R^* i_{\tilde{f}}\,\mathrm{d}H = i_{R^*\tilde{f}} R^*\,\mathrm{d}H = i_{-\tilde{f}}\,\mathrm{d}(R^*H) = -i_{\tilde{f}}\,\mathrm{d}H = -\dot{H}. \tag{1}$$

Under these circumstances the evolution of H for a symmetric ergodic orbit can be modelled as a diffusion process as in [11]. The approximation is valid for time scales which are long enough that one can average over the fast motion in x but short enough that the total energy drift is small. On such an intermediate time scale we think of the orbit as consisting of a fast motion on an energy surface (which plays the role of the 'angles' for a diffusion process) and a slow drift in H (which plays the role of the action) transverse to this surface.

We now make the following key assumptions: (i) the flow of $\tilde{f}$ is ergodic on an invariant set $A \subset M$ with respect to an invariant measure μ and (ii) the set A is symmetric. The measure is necessarily symmetric. Then, we have (recalling $\dot{H} = h$)

$$\lim_{T\to\infty} \frac{H(T)}{T} = \lim_{T\to\infty} \frac{1}{T} \int_0^T h(x(t))\,\mathrm{d}t = \int_A h(x)\mu = \int_{R\circ A} (R^*h)(x) R^*\mu = \int_A -h(x)\mu = 0$$

since the integrand is odd and the measure μ is invariant with respect to R. We write $\langle h\rangle := \int_A h\mu$ for the spatial average of a function.

That is, the mean energy error is zero. For each positive contribution to $\dot{H}$ at x say, there is a negative contribution at $R(x)$ which is visited equally often. The behaviour of H therefore looks something like a random walk with mean zero, except that the deterministic nature of $x(t)$ means that (as typical in these situations) the 'walk' is more autocorrelated than a true random walk. The fast motion in x can be averaged over to give the rate of diffusion of H [4]:

$$\begin{aligned}\lim_{T\to\infty} \frac{H(T)^2}{T} &= \lim_{T\to\infty} \frac{1}{T} \left(\int_0^T h(x(t))\,\mathrm{d}t \right)^2 = \lim_{T\to\infty} \frac{1}{T} \int_0^T \int_0^T h(x(t))h(x(u))\,\mathrm{d}u\,\mathrm{d}t \\ &= \lim_{T\to\infty} \frac{1}{T} \int_0^T \int_{-t}^{T-t} h(x(t))h(x(t+s))\,\mathrm{d}s\,\mathrm{d}t = \int_{-\infty}^{\infty} \langle h(x(0))h(x(s))\rangle\,\mathrm{d}s\end{aligned}$$

which is the integral of the correlation function

$$b_h(s) := \langle h(x(0))h(x(s))\rangle.$$

If the flow is mixing, then

$$\lim_{s\to\infty} b_h(s) = \langle h\rangle^2 = 0$$

so that, provided the correlations are integrable, we have $|H(T)| = \mathcal{O}(\sqrt{T})$. In fact, it is believed that one often has (e.g. for many Anosov systems) exponential decay of correlations, namely $b_h(s) \leqslant C\,\mathrm{e}^{-s/k}$ for some $C, k > 0$, although the precise conditions required to ensure this are not known [4, 12].

We can now check the time scale on which the result is valid. For a method of order p, $h = \mathcal{O}(\tau^p)$ so $|H(T)| = \mathcal{O}(\sqrt{T}\tau^p)$ and we have good mixing but small drift for $k \ll T \ll \tau^{-2p}$. (For longer times, the diffusion rate may change as x moves onto different energy surfaces.) On the other hand, if the simulation is required to estimate an observable of variance σ^2 to within an error ϵ, it must be run for time $T \sim k\sigma^2/\epsilon^2$, so that the energy drift typically is indeed relevant.

The introduction of the modified vector field $\tilde{f}$ is not necessary. Working directly on the integrator, the increment $\Delta H = H(\phi_\tau(x)) - H(x)$ is odd, not under R, but under $R \circ \phi$:

$$\Delta H \circ R \circ \phi_\tau = H \circ \phi_\tau \circ R \circ \phi_\tau - H \circ R \circ \phi_\tau = H - H \circ R \circ \phi_\tau = -\Delta H.$$

If the map ϕ_τ is ergodic on an R-invariant set with respect to an R-invariant measure, then the measure (being ϕ_τ-invariant by assumption) must also be $R \circ \phi_\tau$-invariant. The argument then proceeds as before: the spatial average of ΔH is zero and the mean energy drift is zero.

There is one important case in which the correlation $b_h(s)$ is *not* integrable. If the orbit $x(t)$ is quasiperiodic then $b_h(s)$ is quasiperiodic. In this case, however, the energy error $H(T)$ is the integral of a quasiperiodic function $h(t)$ with mean zero, and hence is bounded for all time. In this case, we expect to observe bounded energy errors for all time. This is also observed in reversible integrations when the orbit is quasiperiodic.

Also, if the integrator in fact preserves a quantity which is close to H on the orbit, such as the modified energy of a symplectic integrator, then of course there will be no energy

drift. The above argument is still valid, but in this case we will have $\lim_{T\to\infty} H(T)^2/T = \int_{-\infty}^{\infty} b_h(s)\,\mathrm{d}s = 0$.

While we have no way of checking whether the orbit is ergodic on a symmetric set, we believe that this argument does describe the mechanism of energy drift. If the orbit were not symmetric, there is no reason for $\langle \dot{H} \rangle$ to be zero. When integrating a (nonsymmetric) strange attractor, we expect that one would observe the linear growth of energy errors.

Example. Nonholonomic mechanical systems form a natural class of systems which are reversible and energy-preserving but not Hamiltonian. We illustrate the typical $\mathcal{O}(\sqrt{T})$ energy drift by a reversible integration of a nonholonomic system. We consider the configuration space $\mathbb{R}^{2n+1}$ with coordinates $q = (x, y_1, \ldots, y_n, z_1, \ldots, z_n)$, conjugate momenta $p = \left(p_x, \ldots, p_{z_n}\right)$, energy

$$H = \frac{1}{2}\left(\|p\|_2^2 + \|q\|_2^2 + z_1^2 z_2^2 + \sum_i y_i^2 z_i^2 \right),$$

and a single nonholonomic constraint

$$f(q)^T p = 0, \qquad f(q) = (1, 0, \ldots, 0, y_1, \ldots, y_n)^T.$$

The equations of motion are

$$\dot{q} = H_p = p, \qquad \dot{p} = -H_q + \lambda f.$$

It can be checked that $\dot{H} = 0$ and that the system is reversible under $(q, p) \mapsto (q, -p)$.

The following integrator is second order, reversible and, because of the simple constraint, explicit [13]. Given initial conditions (q_n, p_n) satisfying the constraint $f(q_n)^T p_n = 0$, we calculate

$$\begin{aligned} \widetilde{q} &= q_n + \tfrac{1}{2}\tau p_n \\ p_{n+1} &= p_n + \tau(-H_q(\widetilde{q}) + \lambda f(\widetilde{q})) \\ q_{n+1} &= \widetilde{q} + \tfrac{1}{2}\tau p_{n+1} \end{aligned} \tag{2}$$

where the Lagrange multiplier λ is chosen so that $f(q_{n+1})^T p_{n+1} = 0$ (it can be determined explicitly in this example). As far as we can tell, this system does not preserve any symplectic structure.

We have taken $n = 3$ (so the phase space is $\mathbb{R}^{14}$) and 10 000 initial conditions roughly equally spaced on the energy surface $H(0) = 3.06$. The results are shown in figure 1 for two different time steps, $\tau = 0.02$ and $\tau = 0.05$. To detect the rate of energy drift, we have calculated the variance $\sigma^2(T)$ of the 10 000 energy errors and scaled out the expected $\mathcal{O}(\tau^4)$ dependence on the step size. We do indeed then see a dominant $\mathcal{O}(T)$ increase in the variance. For this method on this energy surface, we can say that the energy error will be approximately

$$|H(T) - H(0)| \sim \sigma(T) \sim 0.01\tau^2\sqrt{T}.$$

The diffusion rate depends strongly on the energy, because of the quartic nonlinearities in H. In fact, as $H \to 0$, the system becomes integrable and no energy drift is seen; the diffusion rate is found to vary approximately as $\|q\|^4$.

We repeated this calculation using the fourth-order reversible integrator $\phi_{\alpha\tau}^2 \phi_{(1-4\alpha)\tau} \phi_{\alpha\tau}^2$ where $\alpha = 1/(4 - 4^{1/3})$ and ϕ_τ is the second-order method used above. Again, $\mathcal{O}(\sqrt{T})$ energy drift was seen; numerically, for this fourth-order method on $H(0) = 3.06$,

$$|H(T) - H(0)| \sim 0.003\tau^4\sqrt{T}.$$

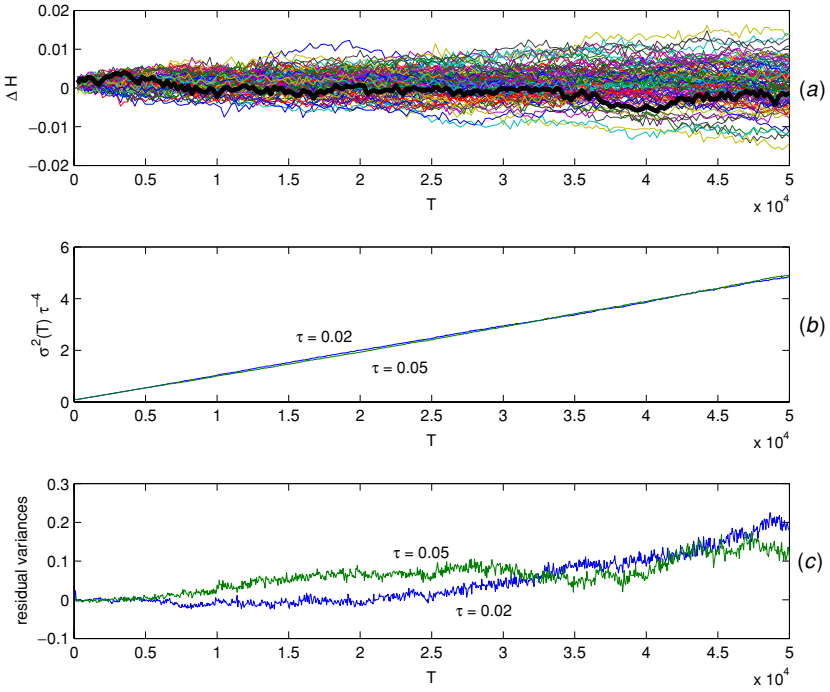

Figure 1. Energy drift on $H(0) = 3.06$ for the reversible integrator (2). (*a*) The observed energy error for 100 different initial conditions with time step $\tau = 0.05$ integrated up to time $T = 50\,000$. One typical simulation is singled out in bold. (*b*) The variance $\sigma^2(T)$ of the energy errors for 10 000 different initial conditions integrated up to time $T = 50\,000$ for two different time steps, scaled by their expected τ^4 dependence on the time step. The growth is roughly linear in time and the two results are almost indistinguishable. (*c*) The residual variance from (*b*) with the expected linear trend subtracted. Only a relatively small nonlinear behaviour remains.

(This figure is in colour only in the electronic version)

As another example we considered the family of systems

$$\dot{q} = p, \qquad \dot{p} = -\nabla V(q) + \epsilon f(q)g(p), \qquad (q, p) \in \mathbb{R}^{2n}$$

where $V = \|q\|^2/2 + \sum_{i=1}^{n}(q_i - q_{i+1})^4/4$ (setting $q_{n+1} = q_1$) and $g(p) = p_1(p_2, -p_1, 0, \ldots, 0)$. Because $p^T g(p) = 0$, the system preserves energy $\frac{1}{2}\|p\|^2 + V(q)$ for all f; and because $g(p) = g(-p)$, it is reversible for all f. When the system is integrated by a second-order splitting method (with the subsystem $\dot{q} = 0$, $\dot{p} = \epsilon f(q)g(p)$ integrated exactly), energy diffusion is observed with a diffusion constant proportional to $\epsilon\tau^2$, which is a measure of the amount by which the integrator fails to be symplectic. The diffusion constant increases markedly with the dimension n.

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