

Adding an energy-like conservation law to the leapfrog integrator

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Abstract. The leapfrog integrator is widely used because of its excellent stability in molecular dynamics simulation. This is recognized as being due to the existence of a discrete variational structure of the equations. We introduce a modified leapfrog method which includes an additional energy-like conservation law by embedding a molecular dynamics simulation within a larger dynamical system.

1. Introduction

The leapfrog integrator for molecular dynamics is known to display several exceptional features which allow it to have superior long-time stability compared with many higher-order integrators. This exceptional nature is due to the exact conservation of momentum and symplectic structure by the discretization (Hairer et al. 2002). The symplectic nature is particularly important for statistical mechanics applications because it tells us that there is a well defined density in phase space which is conserved – as in the classic Liouville theorem; this density is the basis for the construction of the Gibbsian approach to statistical mechanics (Gibbs 2010). In addition the existence of a backward error analysis (Reich 1999) tells us that we are observing trajectories which are those of a perturbed Hamiltonian which is close to that which we are interested in.

Despite these numerous advantages there is one important quantity which is not exactly conserved; this is the energy. It fluctuates on small time scales and can drift in the very longest simulations. This is normally countered by introducing a coupling to a thermostat (Nosé 1984, Hoover 1985, Frenkel & Smit 2002), but this leads to a change of ensemble from micro-canonical to canonical. The aim of the present paper is the construction of an integrator that is similar in many ways to the leapfrog method, but which is embedded in a larger dynamic system. The dynamics of the larger system are such that the original energy emerges as an additional conservation law.

There are many trivial (and bad) manners to impose energy conservation – for instance one can regularly rescale the particle velocities. However, such arbitrary modifications to the dynamics break the symplectic structure which is a disaster for applications in statistical mechanics. Our approach to build a larger dynamic set of equations via variational methods in such a way that we can construct the discrete Hamiltonian of the system and thus explicitly understand the phase-space structure of the extended dynamical system.

This extended dynamical system is built using several components. We start by considering a discretized Lagrangian, in which the extra conservation is imposed by a Lagrange multiplier. From this dynamic system we build a discretized Hamiltonian. This Hamiltonian has a common defect that occurs in constrained systems (such as electrodynamics) – there is no momentum which corresponds to the multiplier. The solution is to add additional terms to the Hamiltonian which are zero, but which nevertheless generate independent dynamical equations for the multiplier. The logic is very close to the treatment of the potential in electrodynamics which has the formal role of being the Lagrange multiplier in imposing Gauss' law (Dirac 2001).

2. Variational integrators

We firstly resume how to pass from a discretized Lagrangian to the leapfrog integrator before generalizing to our more complicated constrained system: Newton's equations of motion for particles moving under velocity independent forces can be found by considering the variational problem

$$\delta \int \left\{ \frac{m}{2} \left(\frac{dq}{dt} \right)^2 - V(q) \right\} dt = 0 \quad (1)$$

In the following we will take all masses to be identical, and will allow q to denote a $N \times d$ dimensional vector corresponding to N particles moving in d dimensional space. This Lagrangian can be discretized by replacing derivatives by finite differences evaluated every τ so that $t_k = k\tau$ for integer k :

$$L_k = m \frac{(q_{k+1} - q_k)^2}{2\tau^2} - V(q_k) \quad (2)$$

The discretized action principle is then (Guo et al. 2002, Marsden & Ratiu 1999)

$$\delta \sum_k \tau L_k = 0 \quad (3)$$

This variation then gives simple partial derivatives with respect to x_k so that

$$m(q_{k+1} + q_{k-1} - 2q_k) + \tau^2 V'(q_k) = 0 \quad (4)$$

which is indeed a version of the leapfrog algorithm (Frenkel & Smit 2002). In the continuous time limit the energy, U is exactly conserved.

$$U = \frac{m}{2} \left(\frac{dq}{dt} \right)^2 + V(q) \quad (5)$$

However any time stepping procedure such as eq. (4) leads to a breakdown in the conservation of energy. The first step of our modified procedure will be to take the energy eq. (5) and add it as a constraint to the original Lagrangian density eq. (2).

$$L_k = m \frac{(q_{k+1} - q_k)^2}{2\tau^2} - V(q_k) + \lambda_k \left(m \frac{(q_{k+1} - q_k)^2}{2\tau^2} + V(q_k) - U \right) \quad (6)$$

We will call the second line of eq. (6) the *quasi-energy*. In the following the dynamic schemes that we propose will conserve this discretized quasi-energy to machine accuracy. In this expression λ_k is a Lagrange multiplier whose dynamics will be developed in the following sections. In the continuous time limit clearly $\lambda = 0$.

The main questions that will arise are the following: In the presence of the extended dynamical system eq. (6) how do we interpret Liouville's theorem? What are the corresponding momentum variables for the discretized evolution equations that comes from eq. (6). In order to answer these questions we pass from the Lagrangian description to a Hamiltonian form for the dynamics.

3. Discrete Hamiltonians

We will need to introduce a slightly more formal notation in order to pass from the above Lagrangian formulation to a discrete Hamiltonian form. However this notation is such that we find expressions which are very close to those in standard treatments of Hamiltonian dynamics. We firstly introduce the finite time difference operator

$$\Delta q_k = (q_{k+1} - q_k)/\tau \quad (7)$$

We also need its adjoint Δ^* which is defined so that

$$\sum a_k \Delta q_k = - \sum q_k (a_k - a_{k-1})/\tau = \sum a_k \Delta^* q_k \quad (8)$$

for arbitrary vectors a_k . Thus we see that

$$\Delta^* q_k = -\Delta q_{k-1} \quad (9)$$

There is a natural shift of unity in indices when performing the discrete version of integrating by parts.

The Lagrangian equations of motion are then

$$\Delta^* \frac{\partial L}{\partial \Delta q_k} + \frac{\partial L}{\partial q_k} = 0 \quad (10)$$

which is very close to their form in the continuum limit. We now define the momentum variables:

$$p_{k+\frac{1}{2}} = \frac{\partial L}{\partial \Delta q_k} = m(q_{k+1} - q_k)(1 + \lambda_k)/\tau \quad (11)$$

The use of half-integer labels for the momentum variable is motivated by the fact that the momentum $p_{k+\frac{1}{2}}$ couples to both q_k and q_{k+1} . We construct the Hamiltonian as usual as a Legendre transform of the Lagrangian.

$$\begin{aligned} H(q_k, p_{k+\frac{1}{2}}) &= p_{k+\frac{1}{2}} \Delta q_k - L_k \\ &= \frac{p_{k+\frac{1}{2}}^2}{2(1 + \lambda_k)m} + V_k(1 - \lambda_k) + \lambda_k U \end{aligned} \quad (12)$$

Let us consider the equations of motion which come from applying Hamilton's principle to eq. (12). We calculate

$$\delta \sum_k \left[p_{k+\frac{1}{2}} \Delta q_k - H(p_{k+\frac{1}{2}}, q_k) \right] = 0 \quad (13)$$

and find

$$\frac{\partial H}{\partial q_k} = -\Delta p_{k-\frac{1}{2}} \quad (14)$$

$$\frac{\partial H}{\partial p_{k+\frac{1}{2}}} = \Delta q_k \quad (15)$$

which is the discretized form of the Hamiltonian equations of motion, with $\Delta p_{k-\frac{1}{2}} = (p_{k+\frac{1}{2}} - p_{k-\frac{1}{2}})/\tau$. More explicitly we have

$$\tau \Delta p_{k-\frac{1}{2}} = p_{k+\frac{1}{2}} - p_{k-\frac{1}{2}} = -\tau(1 - \lambda_k)V'_k \quad (16)$$

$$\tau \Delta q_k = q_{k+1} - q_k = \tau \frac{p_{k+\frac{1}{2}}}{m(1 + \lambda_k)} \quad (17)$$

When $\lambda_k = 0$ this corresponds to the standard alternating update in the leapfrog algorithm.

Now consider the equation which comes from varying the Lagrange multiplier λ_k :

$$\frac{\partial H}{\partial \lambda_k} = U - V(q_k) - \frac{p_{k+\frac{1}{2}}^2}{2m(1 + \lambda_k)^2} = W_k = 0 \quad (18)$$

which is just the equation for the quasi-energy in the Hamiltonian picture. Note this quasi-energy conservation does not imply that the Hamiltonian eq. (12) is itself conserved, however if they are numerically close one might hope that the stability of the algorithm is also improved for H .

If λ_k were a true dynamic degree of freedom we would have deduced from eq. (18), in analogy to eq. (14) that

$$-\Delta \pi_{k-\frac{1}{2}} = W_k(q_k, p_{k+\frac{1}{2}}, \lambda_k) \quad (19)$$

where $\pi_{k-\frac{1}{2}}$ the conjugate momentum to λ_k . We discover that in order to have a full Hamiltonian description of the system we must add this extra degree of freedom, but also that $\pi_{k-\frac{1}{2}} = 0$ for all k in order conserve the quasi-energy. We will show this is possible later, but firstly move on to the practical question of implementation of the algorithm.

4. Integration loop

The equations eq. (16), eq. (17) together with the constraint equation $W_k = 0$, eq. (18), tell us how the positions and momenta of the particles evolve within a time step. We now show that the equations have explicit (non-iterative) solutions that require only small modifications of the usual leapfrog step.

We firstly take eq. (18) and substitute eq. (16) for $p_{k+\frac{1}{2}}$.

$$2m(U - V_k) = \frac{(p_{k-\frac{1}{2}} + \tau(1 - \lambda_k)f_k)^2}{(1 + \lambda_k)^2} \quad (20)$$

or

$$S(1 + \lambda_k)^2 = p_{k-\frac{1}{2}}^2 + 2\tau p_{k-\frac{1}{2}} f_k (1 - \lambda_k) + \tau^2 f_k^2 (1 - \lambda_k)^2 \quad (21)$$

with f_k the force. Thus

$$\begin{aligned} & \lambda_k^2 (S - \tau^2 f_k^2) + \lambda_k (2S + 2\tau p_{k-\frac{1}{2}} \cdot f_k + 2\tau^2 f_k^2) + \\ & (S - 2\tau p_{k-\frac{1}{2}} \cdot f_k - \tau^2 f_k^2 - p_{k-\frac{1}{2}}^2) = 0 \end{aligned} \quad (22)$$

with $S = 2m(U - V_k)$. This is a simple quadratic equation for λ_k which involves quantities which are already calculated within a leapfrog integration loop. In practice λ remains small throughout our simulations and its value is close to

$$\lambda \approx -\tau p \cdot f / S \quad (23)$$

We can integrate the equations with the following loop

know $\lambda_{k-1}, q_k, p_{k-\frac{1}{2}}$
 calculate $f_k(q_k)$
 calculate λ_k eq. (22)
 calculate $p_{k+\frac{1}{2}}$ eq. (16)
 eq. (18) satisfied at this moment of cycle
 calculate q_{k+1} eq. (17)
 know $\lambda_k, q_{k+1}, p_{k+\frac{1}{2}}$

This is the practical generalisation of the generalised leapfrog method with the addition of an exact conservation of the quasi-energy. Note that eq. (23) implies that the iteration becomes ill defined if S becomes too small, this is notably the case of a one-dimensional harmonic oscillator where the algorithm becomes unstable. For a system of N particles we expect that S is an extensive variable so that $\lambda \sim \tau/\sqrt{N}$. Already when we simulated with two degrees of freedom we found that the code remains stable; it is unlikely that all particles in a simulation become stationary at the same moment.

The equations of motion as stated above are adequate to implement the algorithm. However they contain a formal weakness. While p and q evolution is the result of a variational principle eq. (13) this is not true of λ . The Lagrange multiplier is simply slaved to impose energy conservation. Such slaved variables are well known in quantum mechanics, indeed the electrostatic potential is an example of such a variable; this explains the initial difficulties in the quantisation in electrodynamics due to the lack of an obvious conjugate momentum. We now show how to render the equation for the evolution of λ autonomous, and thus better understand the phase space of the enlarged dynamic system. We will use methods which are rather similar to those invented in electrodynamics (Dirac 2001, Leimkuhler & Skeel 1994) where the electrostatic potential also has a role which is similar to a Lagrange multiplier. There are clear analogies too with our previous work on local simulation algorithms for charged media (Rottler & Maggs 2004, Maggs 2002, Maggs 2004). The first problem with the equation eq. (12) is that it does not include a momentum variable, π which is conjugate to λ . We correct this deficit with the following ansatz: we add an extra term to the Hamiltonian:

$$\pi_{k+\frac{1}{2}} \mu_k(q_k, p_{k+\frac{1}{2}}, \lambda_k) \quad (24)$$

where μ_k is a function that we will construct later. This leads to the following equations of motion:

$$\Delta \lambda_k = \frac{\partial H}{\partial \pi_{k+\frac{1}{2}}} = \mu_k \quad (25)$$

$$-\Delta \pi_{k-\frac{1}{2}} = \frac{\partial H}{\partial \lambda_k} = W_k + \pi_{k+\frac{1}{2}} \frac{\partial \mu_k}{\partial \lambda_k} \quad (26)$$

We now use the idea of weak constraints: For arbitrary functions μ_k we have a Hamiltonian system. We will show that the correct choice of the function $\mu_k(p_{k+\frac{1}{2}}, q_k, \lambda_k)$ allows us to impose both the conservation of eq. (18) but is also compatible with $\Delta \pi_{k-\frac{1}{2}} = 0$. We then start the dynamic system in the state $\pi = 0$ and this remains true for all further times in the dynamics.

We now show that the function μ_k is indeed only a function of the objects $(q_k, p_{k+\frac{1}{2}}, \lambda_k)$. We proceed by considering W_k at two successive time steps, imposing

conservation of the quasi-energy

$$W_k(q_k, p_{k+\frac{1}{2}}, \lambda_k) = W_{k+1}(q_{k+1}, p_{k+\frac{3}{2}}, \lambda_{k+1}) \quad (27)$$

We now eliminate the variables q_{k+1} and $p_{k+\frac{3}{2}}$ from the right hand side using eq. (17) and eq. (16). If we do so the right hand side of eq. (27) is a function of $q_k, p_{k+\frac{1}{2}}, \lambda_{k+1}$. We can thus, in principle solve for λ_{k+1} and write the evolution in the form

$$\lambda_{k+1} = \lambda_k + \mu_k(q_k, p_{k+\frac{1}{2}}, \lambda_k) \quad (28)$$

as needed for the dynamics of $\pi_{k-\frac{1}{2}}$, eq. (24), eq. (25)

5. Phase space and Liouville

We have succeeded in embedding our original system of particle dynamics in a larger system such that the quasi-energy is exactly conserved. To do so we were obliged to introduce two new variables λ_k which started as a simple Lagrange multiplier and $\pi_{k-\frac{1}{2}}$ which is the conjugate momentum. For a system of N particles in d -dimensional space this gives us a phase-space of dimensions $2dN + 2$.

We now study the Jacobian of the discrete evolution equations to show that the constrained dynamical systems are compatible with the assumed measure. The maps eq. (16) and eq. (17) are easily seen to have unit Jacobians on the phase space defined by the variables (q, p, λ, π) . The evolution equations for λ require slightly more study. The Jacobian for $\lambda_{k+1} = \lambda_k + \mu_k(q_k, p_{k+\frac{1}{2}}, \lambda_k)$ is given by $J = 1 + \partial\mu_k/\partial\lambda_k$. while we see we can re-arrange eq. (26) to give $\pi_{k+\frac{1}{2}} = \pi_{k-\frac{1}{2}}/(1 + \partial\mu_k/\partial\lambda_k)$. It is thus the product of these two factors which ensures that the Jacobian of a full time-step is indeed unity. We thus see that introduction of the ‘‘dummy’’ momentum π has absorbed the fluctuations in phase space volumes that would otherwise result from the use of the Lagrange multiplier.

Thus we have a complete set of Hamiltonian dynamics on the extended phase space with the extra pair of variables λ, π which are now fully autonomous. We however *choose special initial conditions* $\pi = 0$ that lead to the exact imposition of quasi-energy conservation. We conclude that we have a phase space measure of the form $dq dp d\lambda d\pi$, with conservation laws imposing constant quasi-energy, particle momentum, and π (Khinchin 1949).

6. Time reversal

While we have added a conservation law to the leapfrog integrator we have also lost a symmetry which is present in the standard leapfrog algorithm – it is time reversible: The more complicated quasi-energy conserving version does not re-trace its trajectory when momenta are reversed. This extra symmetry can be imposed in our algorithm by alternating the direct step (described above in section 4) with a version in which each step is implemented in reverse order, with $\tau \rightarrow -\tau$. The main technical difficulty is that the equation of λ_{k-1} given q_k and $p_{k-\frac{1}{2}}$ becomes implicit and must be solved by iteration. In practice we find that a simple iteration procedure converges to machine precision in two steps if we use eq. (23) as a starting guess for λ . The algorithm in which direct and reversed steps are alternated then displays time reversal symmetry.

7. Numerical studies

In this section we give concrete examples of the stability of the integration procedure applied to an interacting particle system. We take $N = 10$ particles interacting in two dimensions with a non-truncated Lennard-Jones potential. The system is simulated at low temperatures to form a stable droplet. Our thermostat seems in many ways similar to velocity scaling methods such as iso-kinetic dynamics so we compare our method to two thermostating methods. In the first “isoT” we scale the velocities after each integration step so that the total kinetic energy is constant, this is an interesting, historic method of controlling temperatures in simulations. In a very similar manner we also introduce an “isoE” ensemble in which the kinetic energy is also scaled to render the total energy constant. As a measure of the stability of the method we then measure the drift of a physical quantity which is known to be conserved in the continuum limit, and which is not controlled explicitly in the algorithm. For this we chose the z-component of the angular momentum defined by

$$L_z = \sum_i (x^i p_y^i - y^i p_x^i)$$

where the sum is over all particles. In both simulation we launch the simulation in a state where the centre of mass positions and momenta are zero. These conditions are conserved by the thermostating.

During a simulation of the droplet (using a time step of 10^{-3} in Lennard-Jones time units) over a period of 10^6 time steps in both methods there is a systematic drift of the angular momentum of the system. We then simulated using our method based on conserved quasi-energy. Using the quasi-energy methods at no time in the simulation did the absolute value of L_z become larger than 10^{-12} . We see that the integration errors coming from simple velocity scaling are far larger than the round-off errors in the quasi-energy method, errors or already $O(1)$ after this short simulation. During this simulation the quasi-energy remains stable to within 10^{-15} , see Fig. 1.

8. Conclusion

We have constructed a variational integrator which includes an additional conserved quasi-energy. Due to the variational Hamiltonian form we are able to study the phase space measure and understand the discrete Liouville theorem that is implied by the dynamics. Implementation of the algorithm requires a small overhead in computational effort compared with the standard leapfrog integrator. We have implemented a version of the code for the molecular dynamics study of a truncated Lennard-Jones potential and verified the stability of the quasi-energy during simulation.

Comparison with algorithms that look similar – such as velocity scaling algorithms to preserve energy or kinetic energy show that the quasi-energy method better conserves other properties that can be important for long time dynamical studies. The example that we gave was the angular momentum.

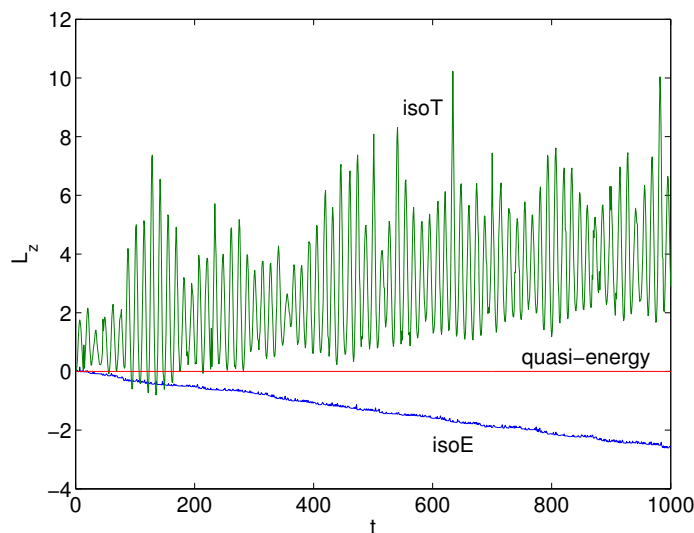


Figure 1. Evolution in the z -component of the angular momentum for three simulations. Topmost curve: the velocities are scaled to conserve kinetic energy. Bottom curve: the scaling conserves the total energy. The quasi-energy method gives a stable angular momentum with fluctuations which are invisible on the scale of the other curves. The amplitude of the quasi-energy fluctuations is a factor 10^{12} smaller than the two other methods.

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