SIAM J. SCI. COMPUT.
Vol. 23, No. 4, pp. 1172–1188

PRACTICAL CONSTRUCTION OF MODIFIED HAMILTONIANS*

ROBERT D. SKEEL† AND DAVID J. HARDY†

Abstract. One of the most fruitful ways to analyze the effects of discretization error in the numerical solution of a system of differential equations is to examine the "modified equations," which are equations that are exactly satisfied by the (approximate) discrete solution. These do not actually exist in general but rather are defined by an asymptotic expansion in powers of the discretization parameter. Nonetheless, if the expansion is suitably truncated, the resulting modified equations have a solution which is remarkably close to the discrete solution. In the case of a Hamiltonian system of ordinary differential equations, the modified equations are also Hamiltonian if and only if the integrator is symplectic. Evidence for the existence of a Hamiltonian for a particular calculation is obtained by calculating modified Hamiltonians and monitoring how well they are conserved. Also, energy drifts caused by numerical instability are better revealed by evaluating modified Hamiltonians. Doing this calculation would normally be complicated and highly dependent on the details of the method, even if differences are used to approximate derivatives. A relatively simple procedure is presented here, nearly independent of the internal structure of the integrator, for obtaining highly accurate estimates for modified Hamiltonians. As a bonus of the method of construction, the modified Hamiltonians are exactly conserved by a numerical solution in the case of a quadratic Hamiltonian.

Key words. symplectic, Hamiltonian, modified equation, integrator, backward error, numerical

AMS subject classifications. 65P10, 65L05

PII. S106482750138318X

1. Introduction.

One of the most fruitful ways to analyze the effects of discretization error in the numerical solution of differential equations is to examine the "modified equations," which are equations that are exactly satisfied by the (approximate) discrete solution. These do not actually exist (in general) but rather are defined by an asymptotic expansion in powers of the discretization parameter. Nonetheless, if the expansion is suitably truncated, the resulting modified equations have a solution which is remarkably close to the discrete solution [9] (over relatively short time intervals). In the case of a Hamiltonian system of ordinary differential equations, the modified equations are also Hamiltonian if and only if the integrator is symplectic. The existence of a modified (or "shadow" [4]) Hamiltonian is an indicator of the validity of statistical estimates calculated from long time integration of chaotic Hamiltonian systems [20]. In addition, the modified Hamiltonian is a more sensitive indicator than the original Hamiltonian of drift in the energy (caused by instability). Evidence for the existence of a Hamiltonian for a particular calculation can be obtained by calculating modified Hamiltonians and monitoring how well they are conserved. Doing this calculation would normally be complicated and highly dependent on the details of the method, even if differences are used to approximate higher derivatives. Presented here is a relatively simple procedure, nearly independent of the internal structure of the integrator, for obtaining highly accurate estimates for modified Hamiltonians.

Consider a step by step numerical integrator $x^{n+1} = \Phi_h(x^n)$ which evolves an

*Received by the editors January 4, 2001; accepted for publication (in revised form) June 22, 2001; published electronically November 7, 2001.

http://www.siam.org/journals/sisc/23-4/38318.html

†Department of Computer Science and Beckman Institute, University of Illinois, 1304 West Springfield Avenue, Urbana, Illinois 61801-2987 (skeel@cs.uiuc.edu, dhardy@cs.uiuc.edu). The work of the first author was supported in part by NSF grants DMS-9971830 and DBI-9974555, and NIH grant P41RR05969, and completed while visiting the Mathematics Department, University of California, San Diego.

approximate solution $x^n \approx x(nh)$ for a system of ordinary differential equations $\dot{x} = f(x)$. For such discrete solutions, there exists modified equations $\dot{x}_h = f_h(x_h)$ defined by an asymptotic expansion such that *formally* the numerical solution $x^n = x_h(nh)$. The modified right-hand-side function f_h is defined uniquely by postulating an asymptotic expansion $f_0 + hf_1 + h^2 f_2 + \cdots$ in powers of h, substituting this into the equations for the numerical solution, expanding in powers of h, and equating coefficients [17, 27, 6, 24]. The asymptotic expansion does not generally converge except for (reasonable integrators applied to) linear differential equations.

A Hamiltonian system is of the form

$$\dot{x}(t) = JH_x(x(t)), \qquad J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},$$

for some Hamiltonian $H(x)$, $x = [q^{\mathrm{T}}, p^{\mathrm{T}}]^{\mathrm{T}}$. The modified equation for an integrator Φ_h applied to this system is Hamiltonian; i.e., $f_h = JH_{h,x}(x)$ for some modified Hamiltonian $H_h(x)$ if and only if the integrator is symplectic [25, 22]. The integrator is symplectic if $\Phi_{h,x}(x) J^{\mathrm{T}} \Phi_{h,x}(x) \equiv J$. There is theoretical [18, 2, 8, 20] and empirical evidence that

$$x_n = x_h(nh) + \text{ very small error}$$

for a very long time, where x_h is the solution for a suitably truncated Hamiltonian H_h. In what follows we assume that H_h is such a Hamiltonian and *we neglect the very small error*.

If we plot total energy as a function of time for a numerical integrator such as leapfrog/Störmer/Verlet applied to a molecular dynamics simulation, we get a graph like Figure 3. What we observe are large fluctuations in the original Hamiltonian, as the trajectory moves on a hypersurface of a constant modified Hamiltonian. A small drift or jump in the energy would be obscured by the fluctuations. A plot of a modified Hamiltonian might be more revealing. As an example, the plots of modified Hamiltonians in Figure 4 already show a clear rise in energy in a 400-step simulation. This indicates that plots of suitable modified Hamiltonians can make it easier to test integration algorithms for instability and programming bugs. Details of this and other numerical tests are given in section 2. Before continuing, it is worth emphasizing that the concern of this paper is stability monitoring—not the monitoring and enhancement of accuracy, as in [4] and [16].

The goal is to construct an approximate modified Hamiltonian

$$H_{[2k]}(q,p) = H_h(q,p) + O(h^{2k})$$

that can be conveniently assembled from quantities, such as forces and energies, already available from the numerical integration. These requirements do *not* uniquely determine $H_{[2k]}$. We consider the special separable Hamiltonian $H(q,p) = \frac{1}{2} p^{\mathrm{T}} M^{-1} p + U(q)$ for which the system is of the form

$$\dot{q} = M^{-1} p, \qquad \dot{p} = F(q) \stackrel{\text{def}}{=} -U_q(q).$$

A "brute force" approach would be to determine an asymptotic expansion for H_h and of the quantities available for making an approximation and then to form a suitable linear combination of the latter. By such a matching of asymptotic expansions

one could derive the following modified Hamiltonians for the leapfrog method:

$$H_{[2]}(q^n,p^n) = H(q^n,p^n) - \underbrace{\frac{1}{8}h^2(F^n)^{\mathrm{T}}M^{-1}F^n}_{\text{why?}}, \tag{1.1}$$

$$H_{[4]}(q^n,p^n) = H(q^n,p^n) + \frac{1}{4}\delta^2 U^n + \frac{1}{6}h(p^n)^{\mathrm{T}}M^{-1}\mu\delta F^n + \frac{5}{24}h^2(F^n)^{\mathrm{T}}M^{-1}F^n + \frac{1}{12}h^2(F^n)^{\mathrm{T}}M^{-1}\delta^2 F^n, \tag{1.2}$$

$$H_{[6]}(q^n,p^n) = H(q^n,p^n) + \frac{11}{60}\delta^2 U^n + \frac{1}{10}h(p^n)^{\mathrm{T}}M^{-1}\mu\delta F^n + \frac{17}{120}h^2(F^n)^{\mathrm{T}}M^{-1}F^n + \frac{1}{10}h^2(F^n)^{\mathrm{T}}M^{-1}\delta^2 F^n + \frac{1}{60}h^2(\mu\delta F^n)^{\mathrm{T}}M^{-1}\mu\delta F^n - \frac{1}{240}h^2(\delta^2 F^n)^{\mathrm{T}}M^{-1}\delta^2 F^n. \tag{1.3}$$

Here a superscript n denotes evaluation at q^n, the centered difference operator is defined by $\delta w^n = w^{n+1/2} - w^{n-1/2}$, the averaging operator is defined by $\mu w^n = \frac{1}{2}w^{n+1/2} + \frac{1}{2}w^{n-1/2}$, and values $q^{n\pm1}$, $p^{n\pm1}$ are defined in terms of q^n, p^n by the leapfrog method:

$$p^{n\pm1/2} = p^n \pm \frac{h}{2}F^n, \quad q^{n\pm1} = q^n \pm hM^{-1}p^{n\pm1/2}, \quad p^{n\pm1} = p^{n\pm1/2} \pm \frac{h}{2}F^{n\pm1}.$$

Thus, in principle, analytical expressions for the $H_{[2k]}(q,p)$ could be produced.

Note. The terms of order h^2 in $H_{[4]}$ and $H_{[6]}$ are different; but if expanded in powers of h, they agree up to $O(h^4)$.

An easier and more elegant construction is presented in sections 3–5. The technique is developed only for splitting methods. It is likely that a similar construction is also possible for symplectic implicit Runge–Kutta methods. The idea is to add a new position variable and a conjugate momentum variable to get an extended Hamiltonian $\bar{H}_h(y)$ which is homogeneous of order 2. For such a Hamiltonian $\bar{H}_h(y_h(t)) \equiv \frac{1}{2}\dot{y}_h(t)^{\mathrm{T}}\bar{J}y_h(t)$. Thus the problem is reduced to that of forming an approximation for $y_h(t)$ using the numerical solution of an extended Hamiltonian system. It is plausible that such a construction might be useful theoretically due to the availability of robust approximation techniques.

Equation (1.1) for $H_{[2]}$ contains an h^2 term which is not needed for achieving second order accuracy. Similarly, the last terms of $H_{[4]}$ and $H_{[6]}$ are not needed for fourth and sixth order, respectively. They are present because the given "truncations" $H_{[2k]}$ are designed to exactly conserve energy for the numerical solution when H is quadratic. (See sections 4.1 and 5.1.) This is a very useful property because typical applications, including molecular dynamics, are dominated by harmonic motion. The existence of a modified Hamiltonian that is exactly conserved for a quadratic Hamiltonian is noted in [19, Eq. (4.7b)], and the search for similar methods having this property was central to the results of this paper. For a quadratic Hamiltonian the modified Hamiltonian H_h actually exists (if h is not too large), but $H_{[2k]} \neq H_h$. (A simple derivation of H_h for the one-dimensional case is given in [24].) It should also be noted that the Hamiltonians $H_{[2k]}$ will not detect numerical instability in the case of quadratic Hamiltonians H.

2. Numerical experiments. The approximate modified Hamiltonians $H_{[2k]}(x)$, $k = 1,2,3,4$, defined by (5.3), (4.4), (5.2), and (4.3) are computed and plotted as

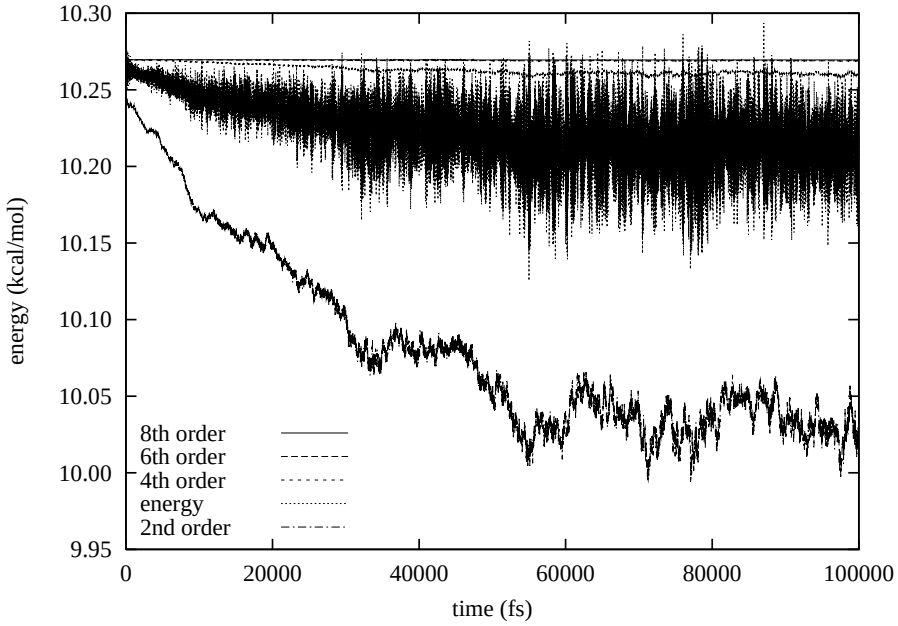

FIG. 1. *Energy and various truncations of the modified Hamiltonian for decalanine.*

functions of time for numerical solutions generated by the leapfrog method. The unmodified Hamiltonians are those of classical molecular dynamics. The testing was done with a molecular dynamics program written by the second author, which is compatible with NAMD [12] but limited in features to facilitate algorithm testing.

The first couple of experiments demonstrate the quality of the modified Hamiltonians. The test problem is a 66-atom peptide, decalanine, in a vacuum [1]. The force field parameters are those of CHARMM 22 for proteins [15, 14] without cutoffs for nonbonded forces.

Figure 1 shows a plot of the Hamiltonian and second, fourth, sixth, and eighth order modified Hamiltonian approximations vs. time for 100,000 fs (femtoseconds) for a step size $h = 1$ fs with the energy sampled every eighth step. The level graph at the top is the eighth order truncation, the one just barely beneath it is sixth order, and the one under that is fourth order. The greatly fluctuating graph is the energy itself, and the undulating one well below it is the second order truncation. Note how well the asymptotic theory holds for the higher order truncations—one could not obtain such flat plots by simply smoothing the original Hamiltonian.

Figure 2 expands the vertical scale to show fluctuations in the eighth, sixth, and fourth order truncations of modified Hamiltonians.

An explanation is in order concerning the initial drop in energy. The initial velocities are zero, so integrating backward in time is the same as integrating forward. Hence the first part of the trajectory is simply the second half of a very unusual fluctuation. In other words, the initial conditions are atypical, i.e., not properly equilibrated (with respect to the original Hamiltonian). This is particularly well revealed by the plot of the second order truncation.

The remaining experiments demonstrate the ability of modified Hamiltonians to detect instability. The test problem is a set of 125 water molecules harmonically

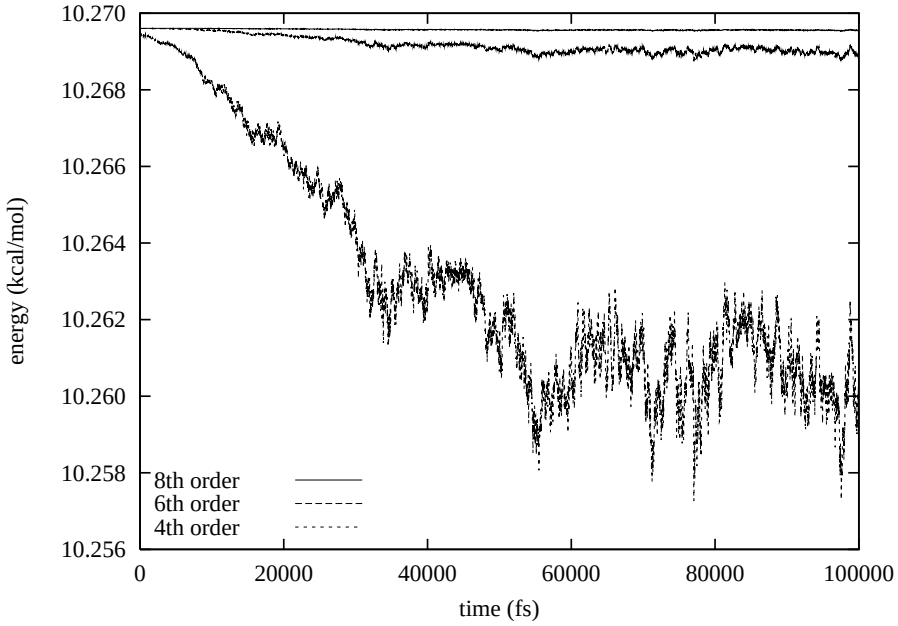

FIG. 2. *A closer look at higher order truncations for decalanine.*

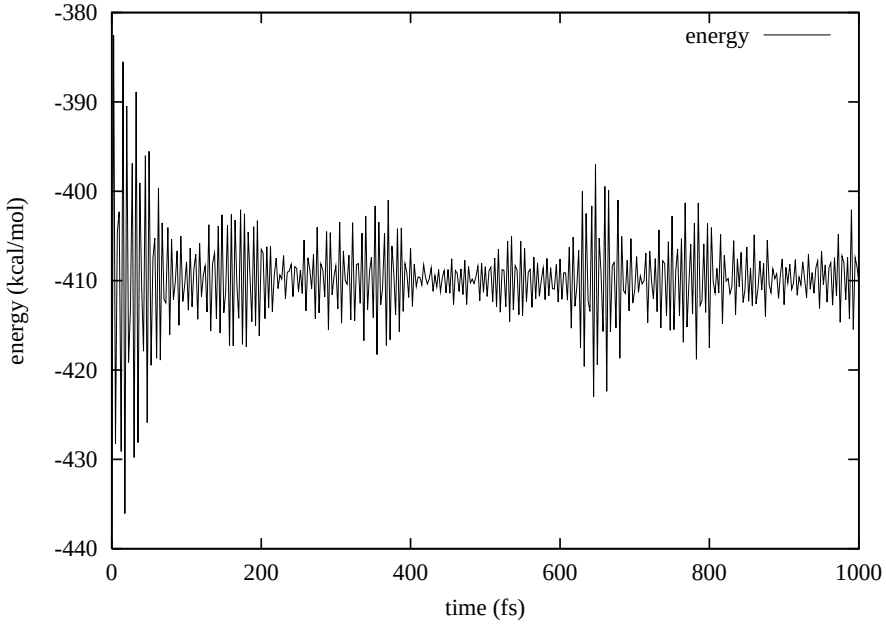

FIG. 3. *Energy for flexible water with step size* 2.5 *fs.*

restrained to a 10 Å-radius sphere. The water is based on the TIP3P model [11] without cutoffs and with flexibility incorporated by adding bond stretching and angle bending harmonic terms (cf. [13]).

Figure 3 shows a plot of the energy vs. time for 1,000 fs for a step size $h = 2.5$ fs with the energy sampled every step. Note that the large fluctuations make it difficult

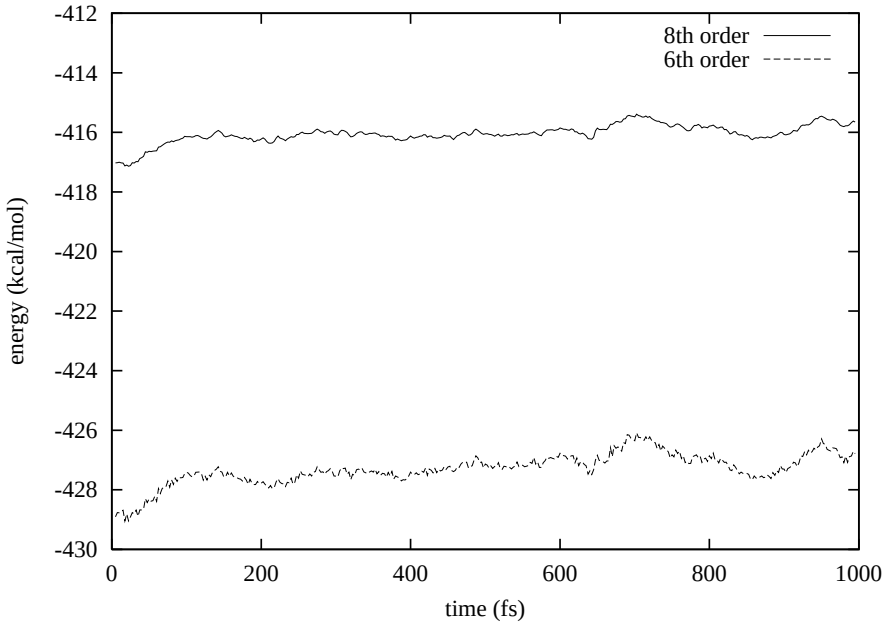

FIG. 4. *Sixth and eighth order truncations with step size* 2.5 *fs.*

to determine whether or not there is energy drift.

Figure 4 shows a plot of the sixth and eighth order modified Hamiltonians for the same step size $h = 2.5$ fs. An upward energy drift is now obvious. The second and fourth order approximations are not shown because neither of them was as flat. Normal mode analysis for this system [10] shows that the 250 fastest frequencies have periods in the range 9.8–10.2 fs and use of the formula in [24, p. 131] shows that a 2.5 fs step size is 30% of the effective period for discrete leapfrog dynamics. It is remarkable that the eighth order approximation is the flattest, even for such a large step size.

Figure 5 shows a plot of the sixth and eighth order modified Hamiltonians for step size $h = 2.15$ fs. There is no apparent upward drift of the energy. Theoretically, instability due to 4:1 resonance [23] should occur for the leapfrog method at $h \cdot$ angular_frequency $= \sqrt{2}$, which is in the range 2.2–2.3 fs for flexible water.

3. Augmenting the integrator. The integrator is augmented to make it homogeneous of order 1. This is motivated by the desire to extend results obtained for homogeneous linear mappings to affine mappings. Affine mappings can be reduced to homogeneous linear mappings through the use of homogeneous coordinates, in which the given set of coordinates is augmented by a scale factor, denoted here by α.

We assume that one step of size h for the given method applied to a system with Hamiltonian H is the composition of exact h-flows for Hamiltonian systems with Hamiltonians H_1, H_2, ..., H_L. Each $H_l(x)$ is assumed to be sufficiently smooth on some domain containing the infinite time trajectory. For example,

1. the leapfrog method for separable Hamiltonian systems $H(q,p) = K(p)+U(q)$ uses $L = 3$, $H_1(x) = \frac{1}{2}U(q)$, $H_2(x) = K(p)$, and $H_3(x) = \frac{1}{2}U(q)$;
2. the Rowlands method [21] for *special* separable Hamiltonian systems uses $H_1(x) = H_3(x) = \frac{1}{2}U(q) - \frac{1}{48}h^2 U_q(q)^{\mathrm{T}} M^{-1} U_q(q)$ and $H_2(x) = \frac{1}{2}p^{\mathrm{T}} M^{-1} p$;

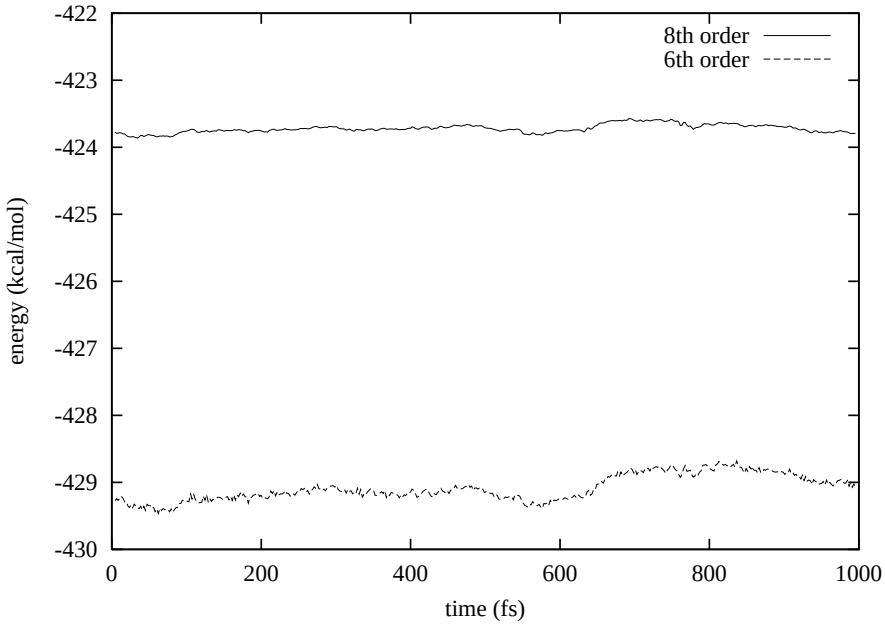

FIG. 5. *Sixth and eighth order truncations with step size* 2.15 *fs.*

3. double time-stepping [7, 26] uses $L = 5$, $H_1(x) = H_5(x) = \frac{1}{2}U^{\text{slow}}(q) + \frac{1}{4}U^{\text{fast}}(q)$, $H_2(x) = H_4(x) = \frac{1}{2}K(p)$, and $H_3(x) = \frac{1}{2}U^{\text{fast}}(q)$,
4. *Molly* [5] does the same as double time-stepping except for the substitution of $U^{\text{slow}}(\mathcal{A}(q))$ for $U^{\text{slow}}(q)$, where $\mathcal{A}(q)$ is a local temporal averaging of q over vibrational motion.

We define the *homogeneous extension* of a Hamiltonian by

$$\bar{H}(q,\alpha,p,\beta) \stackrel{\text{def}}{=} \alpha^2 H(\alpha^{-1}q, \alpha^{-1}p).$$

Then $\bar{H}$ is homogeneous of order 2:

$$\bar{H}(\sigma y) = \sigma^2 \bar{H}(y), \tag{3.1}$$

where $y \stackrel{\text{def}}{=} [q^{\mathrm{T}}, \alpha, p^{\mathrm{T}}, \beta]^{\mathrm{T}}$. The extended Hamiltonian yields the augmented system

$$\dot{q} = \alpha H_p(\alpha^{-1}q, \alpha^{-1}p), \qquad \dot{p} = -\alpha H_q(\alpha^{-1}q, \alpha^{-1}p),$$

$$\dot{\alpha} = 0, \qquad \dot{\beta} = q^{\mathrm{T}} H_q(\alpha^{-1}q, \alpha^{-1}p) + p^{\mathrm{T}} H_p(\alpha^{-1}q, \alpha^{-1}p) - 2\alpha H(\alpha^{-1}q, \alpha^{-1}p).$$

With initial condition $\alpha(0) = 1$, we have $\alpha \equiv 1$ and the system simplifies to

$$\dot{q} = H_p(q,p), \qquad \dot{p} = -H_q(q,p), \qquad \dot{\beta} = q^{\mathrm{T}} H_q(q,p) + p^{\mathrm{T}} H_p(q,p) - 2H(q,p).$$

For $H(q,p) = \frac{1}{2}p^{\mathrm{T}}M^{-1}p + U(q)$, the extended Hamiltonian is $\bar{H}(q,\alpha,p,\beta) = \frac{1}{2}p^{\mathrm{T}}M^{-1}p + \alpha^2 U(\alpha^{-1}q)$ and the simplified augmented system is

$$\dot{q} = M^{-1}p, \qquad \dot{p} = -U_q(q), \qquad \dot{\beta} = q^{\mathrm{T}} U_q(q) - 2U(q).$$

Remark. The association of α with q rather than with p is of practical importance in that it enables one to get values of $\dot{\beta}$ for free whenever $\dot{p}$ is calculated.

The following proposition shows that the value of the extended Hamiltonian can be calculated knowing only the solution.

PROPOSITION 1. *Let $\bar{H}(y)$ be the homogeneous extension of a given Hamiltonian $H(x)$, and let $y(t)$ be a solution of the extended Hamiltonian system with α initially* 1. *Then*

$$H(x(t)) \equiv \frac{1}{2}\dot{y}(t)^{\mathrm{T}}\bar{J}y(t),$$

where $\bar{J}$ is the matrix $\begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$ of augmented dimension.

Proof. Differentiating (3.1) with respect to σ gives $\bar{H}_y(y)^{\mathrm{T}}y = 2\bar{H}(y)$, so

$$\frac{1}{2}\dot{y}(t)^{\mathrm{T}}\bar{J}y(t) = \frac{1}{2}(\bar{J}\bar{H}_y(y(t)))^{\mathrm{T}}\bar{J}y(t) = \frac{1}{2}\bar{H}_y(y(t))^{\mathrm{T}}y(t) = \bar{H}(y(t)).$$

Because $\bar{H}$ is a homogeneous extension of H, the solution of $\bar{H}$ "includes" that of H and we have $\bar{H}(y(t)) \equiv H(x(t))$. ∎

Of course, the goal is not to calculate the original Hamiltonian for which we know a formula but not the solution; rather, it is to calculate a modified Hamiltonian for which we know the solution (at grid points) but not a formula. Therefore, we must augment the integrator so that its solution at grid points is that of the homogeneous extension of the modified Hamiltonian. For an integrator that is a composition of Hamiltonian flows, this is accomplished by using the homogeneous extension of each of the constituent Hamiltonians. More specifically, we define the augmented method $y^{n+1} = \Psi_h(y^n)$ for $\bar{H}$ to be the composition of exact flows for systems with Hamiltonians $\bar{H}_1, \bar{H}_2, \ldots, \bar{H}_L$, where

$$\bar{H}_l(q, \alpha, p, \beta) \stackrel{\text{def}}{=} \alpha^2 H_l(\alpha^{-1}q, \alpha^{-1}p).$$

LEMMA 1 (commutativity). *The method Ψ_h defined above has a modified Hamiltonian*

$$\bar{H}_h(q, \alpha, p, \beta) = \alpha^2 H_h(\alpha^{-1}q, \alpha^{-1}p),$$

where $H_h(q, p)$ is the modified Hamiltonian of the original method Φ_h, i.e., the following diagram commutes:

$$\begin{array}{ccccc} & & \textit{homogeneous extension} & & \\ & H & \longrightarrow & \bar{H} & \\ \textit{discretization} & \downarrow & & \downarrow & \textit{discretization} \\ & H_h & \longrightarrow & \bar{H}_h & \\ & & \textit{homogeneous extension} & & \end{array}$$

Proof. The modified Hamiltonian $\bar{H}_h$ for method Ψ_h can be expressed as an asymptotic expansion using the Baker–Campbell–Hausdorf formula [22]. This formula combines Hamiltonians using the operations of scalar multiplication, addition, and the Poisson bracket $\{H, N\} = H_x^{\mathrm{T}}\, JN_x$. It is thus sufficient to show that each of these three commute with the operation of forming the homogeneous extension. We show this only for the last of these. The homogeneous extension of the Poisson bracket is

$$\alpha^2 H_x(\alpha^{-1}x)^{\mathrm{T}} J N_x(\alpha^{-1}x).$$

This is exactly the same as the (extended) Poisson bracket of $\alpha^2 H(\alpha^{-1}x)$ and $\alpha^2 N(\alpha^{-1}x)$. ∎

Remark. The aim is to discretize the extended Hamiltonian so that this commutativity property holds. Extension of this technique to implicit Runge–Kutta methods would require an augmentation of the method so that commutativity holds.

The following proposition allows the value of the Hamiltonian to be approximated from known values of $y_h(t)$ at grid points.

PROPOSITION 2. *Let $x_h(t)$ and $y_h(t)$ be the solutions for modified Hamiltonians H_h and $\bar{H}_h$, respectively. Then*

$$H_h(x_h(t)) \equiv \frac{1}{2}\dot{y}_h(t)^{\mathrm{T}} \bar{J} y_h(t). \tag{3.2}$$

Proof. The proof is similar to that of Proposition 1. ∎

4. Using full step values. This section presents the construction of $H_{[2k]}$ for *even values of k*. The idea is to use (3.2) in a judiciously chosen weighted average.

Let $y_h(t)$ be the solution of the modified extended Hamiltonian system with initial condition $y(0) = y$. It has values $y_h(jh) = \Psi_h^j(y)$, $j = 0, \pm 1, \ldots, \pm k/2$. Let $\pi_k(t)$ be the degree k polynomial interpolant of these values. (For large k it may be preferable, instead, to use trigonometric interpolation suitably modified [3].)

From Proposition 2, $\frac{1}{2}\dot{\pi}_k(t) J \pi_k(t) \approx \bar{H}_h(y)$. Let

$$H_{k,j} \stackrel{\text{def}}{=} \frac{1}{jh}\int_{-jh/2}^{jh/2} \frac{1}{2}\dot{\pi}_k(t)^{\mathrm{T}} J \pi_k(t)\mathrm{d}t, \qquad j = 2, 4, \ldots, k.$$

The interpolant $\pi_k(t) = y_h(t) + e(t)$, where the error $e(t) = (t^2 - \frac{1}{4}k^2h^2)\cdots(t^2 - h^2)t y_h^{[k+1]}(t)$ and $y_h^{[k+1]}(t) \stackrel{\text{def}}{=} y_h[-\frac{1}{2}kh, \ldots, \frac{1}{2}kh, t]$ with the brackets denoting a $(k+1)$th divided difference. Noting that $\dot{e}(t)^{\mathrm{T}} \bar{J} e(t) = O(h^{2k+2})$, we get

$$\begin{aligned} H_{k,j} &= \bar{H}_h + \frac{1}{jh}\int_{-jh/2}^{jh/2} \frac{1}{2}\dot{y}_h(t)^{\mathrm{T}} \bar{J} e(t)\mathrm{d}t - \frac{1}{jh}\int_{-jh/2}^{jh/2} \frac{1}{2} y_h(t)^{\mathrm{T}} \bar{J}\dot{e}(t)\mathrm{d}t + O(h^{2k+2}) \\ &= \bar{H}_h + \frac{1}{jh/2}\int_{-jh/2}^{jh/2} \frac{1}{2}\dot{y}_h(t)^{\mathrm{T}} \bar{J} e(t)\mathrm{d}t + O(h^{2k+2}) \\ &= \bar{H}_h + \frac{1}{jh/2}\int_{-jh/2}^{jh/2} \left(t^2 - \frac{1}{4}k^2h^2\right)\cdots(t^2 - h^2)t\gamma(t)\mathrm{d}t + O(h^{2k+2}), \end{aligned}$$

where the second equation is obtained by integration by parts and where $\gamma(t) \stackrel{\text{def}}{=} \frac{1}{2}\dot{y}_h(t)^{\mathrm{T}} \bar{J} y_h^{[k+1]}(t)$. This can be expressed as an expansion

$$H_{k,j} = \bar{H}_h + c_{j1}h^{k+2}\gamma'(0) + c_{j3}h^{k+4}\gamma'''(0) + \cdots + O(h^{2k+2}).$$

By forming a suitable linear combination of the values $H_{k,j}$, $j = 1, 2, \ldots, k/2$, it is expected that one can get $\bar{H}_h$ with the first $k/2 - 1$ leading error terms eliminated:

$$\text{linear combination of the } H_{k,j} = \bar{H}_h + O(h^{2k}).$$

Note. The value $\dot{\pi}_k(0)^{\mathrm{T}} \bar{J} \pi_k(0)$ contains a leading term that is only $O(h^k)$, so it is not useful for eliminating error terms.

The case $k = 2$ is the fourth order accurate formula

$$H_{[4]}(x) \stackrel{\text{def}}{=} H_{2,2} = \bar{H}_h(y) + O(h^4).$$

For the case $k = 4$, we have

$$\begin{aligned} H_{4,2} &= \bar{H}_h + \frac{1}{h}\int_{-h}^{h} (t^2 - 4h^2)(t^2 - h^2) t\gamma(t)\mathrm{d}t + O(h^{10}) \\ &= \bar{H}_h + \frac{20}{21} h^6 \gamma'(0) + O(h^8) \end{aligned}$$

and

$$\begin{aligned} H_{4,4} &= \bar{H}_h + \frac{1}{2h}\int_{-2h}^{2h} (t^2 - 4h^2)(t^2 - h^2) t\gamma(t)\mathrm{d}t + O(h^{10}) \\ &= \bar{H}_h - \frac{64}{21} h^6 \gamma'(0) + O(h^8), \end{aligned}$$

and hence

$$H_{[8]}(x) \stackrel{\text{def}}{=} \frac{16}{21} H_{4,2} + \frac{5}{21} H_{4,4} = \bar{H}_h(y) + O(h^8).$$

Below are given formulas for $H_{[8]}$ and for $H_{[4]}$ in terms of values of $y_h(t)$ at grid points. Let a_j be the jth centered difference of $y_h(t)$ at $t = 0$:

$$a_j = \begin{cases} \delta^j y_h(0), & j = 0, 2, 4, \ldots, \\ \mu\delta^j y_h(0), & j = 1, 3, \ldots, \end{cases}$$

where the centered difference operator is defined by $\delta w(t) = w(t + h/2) - w(t - h/2)$ and the averaging operator is defined by $\mu w(t) = \frac{1}{2} w(t + h/2) + \frac{1}{2} w(t - h/2)$.

The fourth degree interpolant in divided difference form is

$$\pi_4(t) = y_h(0) + t\frac{\mu\delta y_h(0)}{h} + t^2 \frac{\delta^2 y_h(0)}{2h^2} + t(t^2 - h^2)\frac{\mu\delta^3 y_h(0)}{6h^3} + t^2(t^2 - h^2)\frac{\delta^4 y_h(0)}{24h^4}.$$

Hence,

$$\pi_4(sh) = a_0 + a_1 s + \frac{1}{2} a_2 s^2 + \frac{1}{6} a_3 s(s^2 - 1) + \frac{1}{24} a_4 s^2 (s^2 - 1)$$

and

$$h\dot{\pi}_4(sh) = a_1 + a_2 s + \frac{1}{2} a_3 \left(s^2 - \frac{1}{3}\right) + \frac{1}{6} a_4 s \left(s^2 - \frac{1}{2}\right).$$

Define

$$A_{ij} = a_i^{\mathrm{T}} \bar{J} a_j / (2h),$$

and we have

$$\begin{aligned} \frac{1}{2}\dot{\pi}_4(sh)^{\mathrm{T}} \bar{J} \pi_4(sh) = A_{10} &- \frac{1}{2} A_{12} s^2 + \frac{1}{2} A_{30}\left(s^2 - \frac{1}{3}\right) + \frac{1}{12} A_{32} s^2 (s^2 + 1) \\ &- \frac{1}{8} A_{14} s^2 \left(s^2 - \frac{1}{3}\right) \\ &- \frac{1}{144} A_{34} s^2 (s^2 - 1)^2 + \text{ odd powers of } s. \end{aligned}$$

Averaging over $-1 \le s \le 1$ yields

$$H_{4,2} = A_{10} - \frac{1}{6}A_{12} + \frac{2}{45}A_{32} - \frac{1}{90}A_{14} - \frac{1}{1890}A_{34}, \tag{4.1}$$

and averaging over $-2 \le s \le 2$ yields

$$H_{4,4} = A_{10} - \frac{2}{3}A_{12} + \frac{1}{2}A_{30} + \frac{17}{45}A_{32} - \frac{31}{90}A_{14} - \frac{107}{3780}A_{34}.$$

Therefore,

$$H_{[8]}(x) = \frac{16}{21}H_{4,2} + \frac{5}{21}H_{4,4} \tag{4.2}$$

$$= A_{10} - \frac{2}{7}A_{12} + \frac{5}{42}A_{30} + \frac{13}{105}A_{32} - \frac{19}{210}A_{14} - \frac{1}{140}A_{34}. \tag{4.3}$$

For a second degree interpolant, it follows from (4.1) that

$$H_{[4]}(x) = H_{2,2} = A_{10} - \frac{1}{6}A_{12}. \tag{4.4}$$

An implementation of these formulas might calculate $H_{[2k]}(x^n)$ for consecutive values of n in terms of quantities $A_{ij}^n = (a_i^n)^{\mathrm{T}}\bar{J}a_j^n/(2h)$ defined in terms of centered differences of y^n which can be obtained from the x^n. (Only first and higher differences of β^n are needed.)

Example 1. To make this concrete, we calculate $H_{[4]}(x)$ for the leapfrog method, as given by (1.2). The leapfrog method advances one step by

$$\begin{aligned}
p^{n+1/2} &= p^n + \frac{h}{2}F^n,\\
\beta^{n+1/2} &= \beta^n + \frac{h}{2}(-(q^n)^{\mathrm{T}}F^n - 2U^n),\\
q^{n+1} &= q^n + hM^{-1}p^{n+1/2},\\
p^{n+1} &= p^{n+1/2} + \frac{h}{2}F^{n+1},\\
\beta^{n+1} &= \beta^{n+1/2} + \frac{h}{2}(-(q^{n+1})^{\mathrm{T}}F^{n+1} - 2U^{n+1}).
\end{aligned}$$

We have

$$H_{[4]}(q^n, p^n) = \frac{1}{2h}(\mu\delta y^n)^{\mathrm{T}}\bar{J}\left(y^n - \frac{1}{6}\delta^2 y^n\right).$$

Suppressing the n in the superscript,

$$y^{\pm 1} = \begin{bmatrix} q \pm hM^{-1}p + \frac{1}{2}h^2M^{-1}F \\ 1 \\ p \pm \frac{1}{2}hF \pm \frac{1}{2}hF^{\pm 1} \\ \beta \pm \frac{1}{2}h(-2U - q^{\mathrm{T}}F) \pm \frac{1}{2}h(-2U^{\pm 1} - (q^{\pm 1})^{\mathrm{T}}F^{\pm 1}) \end{bmatrix},$$

whence

$$\mu\delta y = \begin{bmatrix} hM^{-1}p \\ 0 \\ hF + \frac{1}{4}h\delta^2 F \\ -2hU - hq^{\mathrm{T}}F - \frac{1}{2}h\delta^2 U - \frac{1}{4}h\delta^2(q^{\mathrm{T}}F) \end{bmatrix}, \quad \delta^2 y = \begin{bmatrix} h^2M^{-1}F \\ 0 \\ h\mu\delta F \\ \text{not needed} \end{bmatrix}. \tag{4.5}$$

From $\delta(ab) = \delta a \cdot \mu b + \mu a \cdot \delta b$ and $\mu^2 = 1 + \frac{1}{4}\delta^2$, we get

$$\delta^2(ab) = \delta^2 a \cdot b + 2\mu\delta a \cdot \mu\delta b + a \cdot \delta^2 b + \frac{1}{2}\delta^2 a \cdot \delta^2 b,$$

so

$$\delta^2(q^{\mathrm{T}}F) = h^2 F^{\mathrm{T}} M^{-1} F + 2hp^{\mathrm{T}} M^{-1}\mu\delta F + q^{\mathrm{T}}\delta^2 F + \frac{1}{2}h^2 F^{\mathrm{T}} M^{-1}\delta^2 F. \tag{4.6}$$

Therefore,

$$\begin{aligned} H_{[4]}(q^n, p^n) = H(q^n, p^n) &+ \frac{1}{4}\delta^2 U^n + \frac{1}{6}h(p^n)^{\mathrm{T}} M^{-1}\mu\delta F^n + \frac{5}{24}h^2 (F^n)^{\mathrm{T}} M^{-1} F^n \\ &+ \frac{1}{12}h^2 (F^n)^{\mathrm{T}} M^{-1}\delta^2 F^n. \end{aligned}$$

4.1. The case of a quadratic Hamiltonian. The following result implies that, in the case where $H(x)$ is quadratic, the numerical solution exactly conserves an approximate modified Hamiltonian which is a linear functional of $\frac{1}{2}\dot{\pi}(t)^{\mathrm{T}}\bar{J}\pi(t)$, where $\pi(t)$ is a linear combination of numerical solution values.

PROPOSITION 3. *Assume that Φ_h is the composition of flows for systems with quadratic Hamiltonians and that Ψ_h is constructed as in Lemma* 1. *Then the quantity*

$$\bar{H}_*(y) \stackrel{\text{def}}{=} \sum_{i,j} a_{i,j}\Psi_h^i(y)^{\mathrm{T}}\bar{J}\Psi_h^j(y),$$

where the sum is taken over a finite set of pairs of integers, is exactly conserved by method Ψ_h.

Proof. The mapping $\Psi_h(y) = Sy$ for some symplectic matrix S because Ψ_h is the composition of flows for systems with homogeneous quadratic Hamiltonians. Then

$$\begin{aligned} \bar{H}_*(\Psi_h(y)) &= \sum_{i,j} a_{i,j}(S^i Sy)^{\mathrm{T}}\bar{J}(S^j Sy) \\ &= \sum_{i,j} a_{i,j}(S^i y)^{\mathrm{T}} S^{\mathrm{T}}\bar{J}S(S^j y) \\ &= \sum_{i,j} a_{i,j}\Psi_h^i(y)^{\mathrm{T}}\bar{J}\Psi_h^j(y). \qquad \square \end{aligned}$$

5. Using intermediate values. This section presents the construction of $H_{[2k]}$ for *odd values of k*.

For most numerical integrators one can define "sensible" midstep values

$$y^{n\pm 1/2}, y^{n\pm 3/2}, \ldots, y^{n\pm k/2},$$

and these can be used instead of full step values to get an estimate accurate up to $O(h^{2k})$. We assume that $\Psi_h = \hat{\Psi}_{-h/2}^{-1} \circ \hat{\Psi}_{h/2}$, where $\hat{\Psi}_{h/2}$ is a composition of exact flows of homogeneously extended Hamiltonians.

Remark. It is not necessary that the midstep values be approximations to $y(t)$ at midpoints nor that Ψ_h be time symmetric ($\Psi_h^{-1} = \Psi_{-h}$). All we need is that $\Psi_h = \Psi_{2,h} \circ \Psi_{1,h}$ where each of $\Psi_{1,h}$, $\Psi_{2,h}$ is a composition of exact flows of homogeneously extended Hamiltonians.

For example, the leapfrog method separates into half steps $\hat{\Psi}_{-h/2}^{-1} \circ \hat{\Psi}_{h/2}$ with $\hat{\Psi}_{h/2}$ as follows:

$$\begin{aligned} p^{n+1/2} &= p^n + \frac{h}{2} F^n, \\ \beta^{n+1/2} &= \beta^n + \frac{h}{2}(-(q^n)^{\mathrm{T}} F^n - 2U^n), \\ q^{n+1/2} &= q^n + \frac{h}{2} M^{-1} p^{n+1/2}. \end{aligned}$$

Remark. For the leapfrog method, the estimate over an interval from $(n - \frac{1}{2}k)h$ to $(n + \frac{1}{2}k)h$, where k is odd, actually uses only values of energy and forces from the shorter interval from $(n - \frac{1}{2}k + \frac{1}{2})h$ to $(n + \frac{1}{2}k - \frac{1}{2})h$.

The midstep values are values at midpoints of some function $z_h(t)$ which can be used to construct the Hamiltonian.

PROPOSITION 4. *Let* $z_h(t) = \Phi_{h/2}(y_h(t - h/2))$. *Then*

$$H_h(x_h(t)) \equiv \frac{1}{2} \dot{z}_h(t)^{\mathrm{T}} \bar{J} z_h(t).$$

Proof. For any real s, we define $\Psi_h^s = sh$-flow for $\dot{y} = \bar{J}\bar{H}_{h,y}(y)$. Then $z_h(t) = \chi_h(y_h(t))$, where $\chi_h = \Phi_{h/2} \circ \Psi_h^{-1/2}$. Because χ_h is symplectic, $z_h(t) = \chi_h(y_h(t))$ satisfies a Hamiltonian system with Hamiltonian $\bar{H}_h \circ \chi_h^{-1}$. Also, $\chi_h(\sigma z) = \sigma \chi_h(z)$ because χ_h is the composition of flows of Hamiltonians that are second order homogeneous, and hence $\bar{H}_h \circ \chi_h^{-1}$ is homogeneous of order 2. Therefore,

$$\frac{1}{2} \dot{z}_h(t)^{\mathrm{T}} \bar{J} z_h(t) \equiv \bar{H}_h \circ \chi_h^{-1}(z_h(t)) = \bar{H}_h(y_h(t)). \qquad \square$$

Let $\pi_k(t)$ be the degree k polynomial interpolant of the values $z_h(jh) = \hat{\Psi}_{h/2} \circ \Psi_h^{j-1/2}(y)$, $j = \pm\frac{1}{2}, \pm\frac{3}{2}, \ldots, \pm k/2$.

As before, let

$$H_{k,j} = \frac{1}{jh} \int_{-jh/2}^{jh/2} \frac{1}{2} \dot{\pi}_k(t)^{\mathrm{T}} \bar{J} \pi_k(t) \mathrm{d}t, \qquad j = 1, 3, \ldots, k.$$

The interpolant $\pi_k(t) = z_h(t) + e(t)$, where the error $e(t) = (t^2 - \frac{1}{4}k^2h^2) \cdots (t^2 - \frac{1}{4}h^2) z_h^{[k+1]}(t)$ and $z_h^{[k+1]}(t) \stackrel{\mathrm{def}}{=} z_h[-\frac{1}{2}kh, \ldots, \frac{1}{2}kh, t]$. Similar to before, we get

$$H_{k,j} = \bar{H}_h + \frac{1}{jh/2} \int_{-jh/2}^{jh/2} \left(t^2 - \frac{1}{4}k^2h^2\right) \cdots \left(t^2 - \frac{1}{4}h^2\right) \gamma(t) \mathrm{d}t + O(h^{2k+2}),$$

where $\gamma(t) \stackrel{\mathrm{def}}{=} \frac{1}{2} \dot{z}_h(t)^{\mathrm{T}} \bar{J} z_h^{[k+1]}(t)$. This can be expressed as an expansion

$$H_{k,j} = \bar{H}_h + c_{j0} h^{k+1} \gamma(0) + c_{j2} h^{k+3} \gamma''(0) + \cdots + O(h^{2k+2}).$$

Again, it is expected that a suitable linear combination of the $(k+1)/2$ different values of $H_{k,j}$ yields $\bar{H}_h$ with the first $(k+1)/2 - 1$ leading error terms eliminated:

$$\text{linear combination of the } H_{k,j} = \bar{H}_h + O(h^{2k}).$$

Note. It does not seem possible to combine values obtained from full steps with those from half steps to further increase the order of accuracy because the error expansions for the two kinds of averages do not have terms in common that can cancel.

For $k = 1$, we have the second order formula

$$H_{[2]}(x) \stackrel{\text{def}}{=} H_{1,1} = \bar{H}_h(y) + O(h^2).$$

For $k = 3$, we have

$$\begin{aligned} H_{3,1} &= \bar{H}_h + \frac{1}{h/2}\int_{-h/2}^{h/2}\left(t^2 - \frac{9}{4}h^2\right)\left(t^2 - \frac{1}{4}h^2\right)\gamma(t)\mathrm{d}t + O(h^8) \\ &= \bar{H}_h + \frac{11}{15}h^4\gamma(0) + O(h^6) \end{aligned}$$

and

$$\begin{aligned} H_{3,3} &= \bar{H}_h + \frac{1}{3h/2}\int_{-3h/2}^{3h/2}\left(t^2 - \frac{9}{4}h^2\right)\left(t^2 - \frac{1}{4}h^2\right)\gamma(t)\mathrm{d}t + O(h^8) \\ &= \bar{H}_h - \frac{3}{5}h^4\gamma(0) + O(h^6), \end{aligned}$$

whence

$$H_{[6]}(x) \stackrel{\text{def}}{=} \frac{9}{20}H_{3,1} + \frac{11}{20}H_{3,3} = \bar{H}_h(y) + O(h^6).$$

Let b_j be the jth centered difference of $z_h(t)$ at $t = 0$ using midstep values

$$b_j = \begin{cases} \mu\delta^j z_h(0), & j = 0, 2, 4, \ldots, \\ \delta^j z_h(0), & j = 1, 3, \ldots. \end{cases}$$

The third degree interpolant is

$$\pi_3(t) = \mu z_h(0) + t\frac{\delta z_h(0)}{h} + \left(t^2 - \frac{1}{4}h^2\right)\frac{\mu\delta^2 z_h(0)}{2h^2} + \left(t^2 - \frac{1}{4}h^2\right)t\frac{\delta^3 z_h(0)}{6h^3}.$$

Hence,

$$\pi_3(sh) = b_0 + b_1 s + \frac{1}{2}b_2\left(s^2 - \frac{1}{4}\right) + \frac{1}{6}b_3 s\left(s^2 - \frac{1}{4}\right)$$

and

$$h\dot{\pi}_3(sh) = b_1 + b_2 s + \frac{1}{2}b_3\left(s^2 - \frac{1}{12}\right).$$

Define

$$B_{ij} = b_i^{\mathrm{T}}\bar{J}b_j/(2h),$$

and we have

$$\begin{aligned} \frac{1}{2}\dot{\pi}_3(sh)^{\mathrm{T}}\bar{J}\pi_3(sh) = B_{10} &- \frac{1}{2}B_{12}\left(s^2 + \frac{1}{4}\right) + \frac{1}{2}B_{30}\left(s^2 - \frac{1}{12}\right) \\ &+ \frac{1}{12}B_{32}\left(s^2 - \frac{1}{4}\right)^2 + \text{ odd powers of } s. \end{aligned}$$

Averaging over $-\frac{1}{2} \le s \le \frac{1}{2}$ yields

$$H_{3,1} = B_{10} - \frac{1}{6}B_{12} + \frac{1}{360}B_{32}, \tag{5.1}$$

and averaging over $-\frac{3}{2} \le s \le \frac{3}{2}$ yields

$$H_{3,3} = B_{10} - \frac{1}{2}B_{12} + \frac{1}{3}B_{30} + \frac{7}{120}B_{32}.$$

Therefore,

$$H_{[6]}(x) = B_{10} - \frac{7}{20}B_{12} + \frac{11}{60}B_{30} + \frac{1}{30}B_{32}. \tag{5.2}$$

For a first degree interpolant, it follows from (5.1) that

$$H_{[2]}(x) = B_{10}. \tag{5.3}$$

Example 2. We calculate $H_{[2]}(x)$ for the leapfrog method, as given by (1.1). We have

$$H_{[2]}(q^n, p^n) = \frac{1}{2h}(\delta y^n)^{\mathrm{T}} \bar{J}(\mu y^n).$$

Suppressing the n in the superscript,

$$y^{\pm 1/2} = \begin{bmatrix} q \pm \frac{1}{2}hM^{-1}p + \frac{1}{4}h^2M^{-1}F \\ 1 \\ p \pm \frac{1}{2}hF \\ \pm\frac{1}{2}h(-2U - q^{\mathrm{T}}F) \end{bmatrix},$$

whence

$$\delta y = \begin{bmatrix} hM^{-1}p \\ 0 \\ hF \\ -2hU - hq^{\mathrm{T}}F \end{bmatrix}, \qquad \mu y = \begin{bmatrix} q + \frac{1}{4}h^2M^{-1}F \\ 1 \\ p \\ 0 \end{bmatrix}. \tag{5.4}$$

Therefore,

$$H_{[2]}(q^n, p^n) = H(q^n, p^n) - \frac{1}{8}h^2(F^n)^{\mathrm{T}}M^{-1}F^n.$$

Example 3. We calculate $H_{[6]}(x)$ for the leapfrog method, as given by (1.3). From (5.4) we have

$$\delta^3 y = \begin{bmatrix} hM^{-1}\delta^2 p \\ 0 \\ h\delta^2 F \\ -2h\delta^2 U - h\delta^2(q^{\mathrm{T}}F) \end{bmatrix}, \qquad \mu\delta^2 y = \begin{bmatrix} \delta^2 q + \frac{1}{4}h^2M^{-1}\delta^2 F \\ 0 \\ \delta^2 p \\ 0 \end{bmatrix}.$$

We have $\delta^2 q = h^2M^{-1}F$ and $\delta^2 p = h\mu\delta F$ from the second part of (4.5), and $\delta^2(q^{\mathrm{T}}F)$ is given by (4.6). Then

$$b_1^{\mathrm{T}}\bar{J}b_0 = 2hU + hp^{\mathrm{T}}M^{-1}p - \frac{1}{4}h^3F^{\mathrm{T}}M^{-1}F,$$
$$b_1^{\mathrm{T}}\bar{J}b_2 = h^2p^{\mathrm{T}}M^{-1}\mu\delta F - h^3F^{\mathrm{T}}M^{-1}F - \frac{1}{4}h^3F^{\mathrm{T}}M^{-1}\delta^2F,$$
$$b_3^{\mathrm{T}}\bar{J}b_0 = 2h\delta^2U + 3h^2p^{\mathrm{T}}M^{-1}\mu\delta F + h^3F^{\mathrm{T}}M^{-1}F + \frac{1}{4}h^3F^{\mathrm{T}}M^{-1}\delta^2F,$$
$$b_3^{\mathrm{T}}\bar{J}b_2 = -h^3F^{\mathrm{T}}M^{-1}\delta^2F + h^3(\mu\delta F)^{\mathrm{T}}M^{-1}\mu\delta F - \frac{1}{4}h^3(\delta^2F)^{\mathrm{T}}M^{-1}\delta^2F,$$

and, therefore,

$$\begin{aligned}H_{[6]}(q^n,p^n) = H(q^n,p^n) &+ \frac{11}{60}\delta^2U^n + \frac{1}{10}h(p^n)^{\mathrm{T}}M^{-1}\mu\delta F^n + \frac{17}{120}h^2(F^n)^{\mathrm{T}}M^{-1}F^n\\ &+ \frac{1}{10}h^2(F^n)^{\mathrm{T}}M^{-1}\delta^2F^n + \frac{1}{60}h^2(\mu\delta F^n)^{\mathrm{T}}M^{-1}\mu\delta F^n\\ &- \frac{1}{240}h^2(\delta^2F^n)^{\mathrm{T}}M^{-1}\delta^2F^n.\end{aligned}$$

5.1. The case of a quadratic Hamiltonian.

PROPOSITION 5. *Assume that Φ_h is the composition of flows for systems with quadratic Hamiltonians, that Ψ_h is constructed as in Lemma* 1*, and that $\hat{\Psi}_{h/2}$ is as assumed at the beginning of this section. Then the quantity*

$$\bar{H}_*(y) \stackrel{\text{def}}{=} \sum_{i,j} a_{i,j}\hat{\Psi}_{h/2}\circ\Psi_h^i(y)^{\mathrm{T}}\bar{J}\hat{\Psi}_{h/2}\circ\Psi_h^j(y),$$

where the sum is taken over a finite set of pairs of integers, is exactly conserved by method Ψ_h.

Proof. Because $\hat{\Psi}_{h/2}$, Ψ_h are the compositions of flows for systems with homogeneous quadratic Hamiltonians, the mappings $\hat{\Psi}_{h/2}(y) = S_1y$ and $\Psi_h(y) = S_2S_1y$ for some symplectic matrices S_1, S_2. Then

$$\begin{aligned}\bar{H}_*(\Psi_h(y)) &= \sum_{i,j} a_{i,j}(S_1S^iSy)^{\mathrm{T}}\bar{J}(S_1S^jSy)\\ &= \sum_{i,j} a_{i,j}(S_1S^iy)^{\mathrm{T}}(S_1S_2)^{\mathrm{T}}\bar{J}S_1S_2(S_1S^jy)\\ &= \sum_{i,j} a_{i,j}\hat{\Psi}_{h/2}\circ\Psi_h^i(y)^{\mathrm{T}}\bar{J}\hat{\Psi}_{h/2}\circ\Psi_h^j(y). \qquad \square\end{aligned}$$

Acknowledgment. The authors are grateful for the assistance of Justin Wozniak, who did preliminary tests of the second order truncation for the Hénon–Heiles Hamiltonian and for decalanine.

REFERENCES

[1] http://www.ks.uiuc.edu/Research/namd/utilities.

[2] G. BENETTIN AND A. GIORGILLI, *On the Hamiltonian interpolation of near to the identity symplectic mappings with application to symplectic integration algorithms*, J. Statist. Phys., 74 (1994), pp. 1117–1143.

[3] J. GANS, J. I. CHAN, AND D. SHALLOWAY, *Residual Acceleration as a Measure of the Accuracy of Molecular Dynamics Simulations*, manuscript.

[4] J. GANS AND D. SHALLOWAY, *Shadow mass and the relationship between velocity and momentum in symplectic numerical integration*, Phys. Rev. E (3), 61 (2000), pp. 4587–4592.

[5] B. García-Archilla, J. M. Sanz-Serna, and R. D. Skeel, *Long-time-step methods for oscillatory differential equations*, SIAM J. Sci. Comput., 20 (1998), pp. 930–963.
[6] D. F. Griffiths and J. M. Sanz-Serna, *On the scope of the method of modified equations*, SIAM J. Sci. Statist. Comput., 7 (1986), pp. 994–1008.
[7] H. Grubmüller, H. Heller, A. Windemuth, and K. Schulten, *Generalized Verlet algorithm for efficient molecular dynamics simulations with long-range interactions*, Molecular Simulation, 6 (1991), pp. 121–142.
[8] E. Hairer and C. Lubich, *The life-span of backward error analysis for numerical integrators*, Numer. Math., 76 (1997), pp. 441–462.
[9] E. Hairer and C. Lubich, *Asymptotic expansions and backward analysis for numerical integrators*, in Dynamics of Algorithms, R. de la Llave, L. Petzold, and J. Lorenz, eds., IMA Vol. Math. Appl. 118, Springer-Verlag, New York, 2000, pp. 91–106.
[10] J. Izaguirre, S. Reich, and R. D. Skeel, *Longer time steps for molecular dynamics*, J. Chem. Phys., 110 (1999), pp. 9853–9864.
[11] W. L. Jorgensen, J. Chandrasekhar, J. D. Madura, R. W. Impey, and M. L. Klein, *Comparison of simple potential functions for simulating liquid water*, J. Chem. Phys., 79 (1983), pp. 926–935.
[12] L. Kalé, R. Skeel, R. Brunner, M. Bhandarkar, A. Gursoy, N. Krawetz, J. Phillips, A. Shinozaki, K. Varadarajan, and K. Schulten, *NAMD2: Greater scalability for parallel molecular dynamics*, J. Comput. Phys, 151 (1999), pp. 283–312.
[13] A. R. Leach, *Molecular Modelling: Principles and Applications*, Addison-Wesley, Reading, MA, 1996.
[14] A. D. MacKerell Jr., D. Bashford, M. Bellott, R. L. Dunbrack Jr., J. D. Evanseck, M. J. Field, S. Fischer, J. Gao, H. Guo, S. Ha, D. Joseph-McCarthy, L. Kuchnir, K. Kuczera, F. T. K. Lau, C. Mattos, S. Michnick, T. Ngo, D. T. Nguyen, B. Prodhom, W. E. Reiher, III, B. Roux, M. Schlenkrich, J. C. Smith, R. Stote, J. Straub, M. Watanabe, J. Wiorkiewicz-Kuczera, D. Yin, and M. Karplus, *All-atom empirical potential for molecular modeling and dynamics studies of proteins*, J. Phys. Chem. B, 102 (1998), pp. 3586–3616.
[15] A. D. MacKerell Jr., D. Bashford, M. Bellott, R. L. Dunbrack Jr., M. J. Field, S. Fischer, J. Gao, H. Guo, S. Ha, D. Joseph, L. Kuchnir, K. Kuczera, F. T. K. Lau, C. Mattos, S. Michnick, T. Ngo, D. T. Nguyen, B. Prodhom, B. Roux, M. Schlenkrich, J. C. Smith, R. Stote, J. Straub, J. Wiorkiewicz-Kuczera, and M. Karplus, *Self-consistent parameterization of biomolecules for molecular modeling and condensed phase simulations*, FASEB J., 6 (1992), p. A143.
[16] A. K. Mazur, *Common molecular dynamics algorithms revisited: Accuracy and optimal time steps of Störmer–leapfrog*, J. Comput. Phys., 136 (1997), pp. 354–365.
[17] J. K. Moser, *Lectures in Hamiltonian systems*, Mem. Amer. Math. Soc., 81 (1968), pp. 1–60.
[18] A. I. Neishtadt, *The separation of motions in systems with rapidly rotating phase*, J. Appl. Math. Mech., 48 (1984), pp. 133–139.
[19] R. W. Pastor, B. R. Brooks, and A. Szabo, *An analysis of the accuracy of Langevin and molecular dynamics algorithm*, Molecular Phys., 65 (1988), pp. 1409–1419.
[20] S. Reich, *Backward error analysis for numerical integrators*, SIAM J. Numer. Anal., 36 (1999), pp. 1549–1570.
[21] G. Rowlands, *A numerical algorithm for Hamiltonian systems*, J. Comput. Phys., 97 (1991), pp. 235–239.
[22] J. Sanz-Serna and M. Calvo, *Numerical Hamiltonian Problems*, Chapman and Hall, London, 1994.
[23] T. Schlick, M. Mandziuk, R. D. Skeel, and K. Srinivas, *Nonlinear resonance artifacts in molecular dynamics simulations*, J. Comput. Phys., 139 (1998), pp. 1–29.
[24] R. D. Skeel, *Integration schemes for molecular dynamics and related applications*, in The Graduate Student's Guide to Numerical Analysis, M. Ainsworth, J. Levesley, and M. Marletta, eds., Springer Ser. Comput. Math. 26, Springer-Verlag, Berlin, 1999, pp. 119–176.
[25] D. M. Stoffer, *Some Geometric and Numerical Methods for Perturbed Integrable Systems*, Ph.D. thesis, Swiss Federal Institute of Technology, Zürich, Switzerland, 1988.
[26] M. Tuckerman, B. J. Berne, and G. J. Martyna, *Reversible multiple time scale molecular dynamics*, J. Chem. Phys., 97 (1992), pp. 1990–2001.
[27] R. F. Warming and B. J. Hyett, *The modified equation approach to the stability and accuracy analysis of finite difference methods*, J. Comput. Phys., 14 (1974), pp. 159–179.