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Cheap enhancement of symplectic integrators

1 Introduction

We show how to increase the accuracy of symplectic integrations of Hamiltonian systems [17] by cheaply processing the results given by the numerical method being used.

The idea of processing is as follows. Let

$$\frac{dy}{dt} = f(y), \quad y(0) = \alpha \quad (1)$$

be the initial-value problem in \mathcal{R}^D we wish to integrate, and consider a consistent, one-step method given by a mapping $\psi_{h,f}$ in \mathcal{R}^D ; for instance, $\psi_{h,f}(y) = y + hf(y)$ corresponds to Euler's rule. At this stage we do not assume that (1) is a Hamiltonian problem. If $\{Y_n\}_{n=0}^N$ is a sequence computed with the numerical method, $Y_{n+1} = \psi_{h,f}(Y_n)$, $n = 0, \dots, N-1$, then it is standard to interpret Y_n as an approximation to $y(nh)$, where $y(t)$ is the solution of (1). When processing is used, the numerical values Y_n , $n = 0, \dots, N$, are transformed with the help of a suitable mapping $\pi_{h,f}$ in \mathcal{R}^D and the transformed $y_n = \pi_{h,f}(Y_n)$ are seen as approximations to $y(nh)$. The mapping $\pi_{h,f}$ is assumed to be close to the identity $\pi_{h,f} = \text{id} + O(h)$ and to have an inverse $\chi_{h,f} = \pi_{h,f}^{-1}$. In later developments $\chi_{h,f}$ plays a more important role than $\pi_{h,f}$ and to avoid a proliferation of symbols we shall write $\chi_{h,f}^{-1}$ instead of $\pi_{h,f}$.

Note that, when processing is used, $y_0 = \chi_{h,f}^{-1}(Y_0)$ is seen as the approximation to $y(0) = \alpha$, so that in order to remove the initial error $y_0 - \alpha$, Y_0 should be determined as $Y_0 = \chi_{h,f}(\alpha)$. To sum up, to solve with processing (1), the following prescription should be followed:

1. *Preprocessing*: Find the starting value for time-stepping $Y_0 = \chi_{h,f}(\alpha)$.
2. *Time-stepping*: Compute $Y_{n+1} = \psi_{h,f}(Y_n)$, $n = 0, \dots, N-1$.
3. *Postprocessing*: If output at time $t = nh$ is desired, then find $y_n = \chi_{h,f}^{-1}(Y_n)$, which provides the numerical approximation to $y(nh)$.

The preprocessor $\chi_{h,f}$ is applied only once, so that its cost may safely be ignored. Since

$$y_{n+1} = \chi_{h,f}^{-1}(Y_{n+1}) = \chi_{h,f}^{-1}(\psi_{h,f}(Y_n)) = \chi_{h,f}^{-1}(\psi_{h,f}(\chi_{h,f}(y_n))),$$

the processed y_n 's turn out to be the (unprocessed) numerical approximations corresponding to the one-step method given by the mapping

$$\tilde{\psi}_{h,f} = \chi_{h,f}^{-1} \circ \psi_{h,f} \circ \chi_{h,f}. \quad (2)$$

Processing is appealing if $\widehat{\psi}_{h,f}$ is a more accurate method than $\psi_{h,f}$ and the cost of postprocessing is negligible, either because output is not frequently required or because $\chi_{h,f}^{-1}$ is cheaply evaluated. Then, processing provides the accuracy of $\widehat{\psi}_{h,f}$ at the cost of the less accurate method $\psi_{h,f}$.

The idea of processing goes back at least to a 1969 Dundee conference paper by Butcher [2] (see also [9, Chapter II.12]). In [2], $\psi_{h,f}$ and $\chi_{h,f}$ (and therefore $\chi_{h,f}^{-1}$ and $\widehat{\psi}_{h,f}$) are Runge-Kutta methods. Butcher shows that $\widehat{\psi}_{h,f}$ may possess a higher order than $\psi_{h,f}$; the order of $\widehat{\psi}_{h,f}$ is called the *effective order* of $\psi_{h,f}$. Butcher's approach, elegant as it is, never became practically significant, no doubt in view of the difficulties of coupling processing with variable step-sizes.

A revival of the idea of processing has recently taken place [16], [19], [21], [13], [18], [11], in a context where constant step-sizes seem appropriate.

In Section 2 we discuss the modified equation approach to error analysis and its relation to processing, both in the case of general and Hamiltonian systems (1). Thereafter we consider only Hamiltonian problems. In Section 3 we assume that the (Hamiltonian) problem being solved is linear and develop a methodology for finding $\chi_{h,f}$ and $\chi_{h,f}^{-1}$. Our interest is in symplectic methods of orders 2 and 4 that are time-reversible (selfadjoint in the terminology of [9], [17]). In Section 4 we show how the pre- and postprocessors found in Section 3 may be approximately computed at virtually no cost. We demonstrate in Section 5 that these processors apply also to nonlinear problems. To illustrate our general methodology, in Section 6 we look at a family of integrators $\psi_{h,H}$ that includes the standard Verlet method used in molecular dynamics [1] and also a method, of effective order 4, introduced by Rowlands [16]. Section 7 presents some numerical experiments for a highly nonlinear molecular dynamics problem. It turns out that, at essentially no cost, processing very significantly enhances the accuracy of the numerical methods studied. This conclusion is at variance with the rather pessimistic view of processing expressed by McLachlan in [13]. There is a final Section 8 discussing how to evaluate the potential gradient and potential Hessian required by Rowlands and related methods when applied to molecular dynamics problems involving two-body interactions.

2 Processing and Modified Equation Analysis

Some of the recent contributions on processing present this technique in terms of changes of variables in a modified equation, a point of view that we study in this section.

We denote by $\phi_{h,f} : \mathcal{R}^D \rightarrow \mathcal{R}^D$ the h -flow of the system in (1), so that, if $\mathbf{y}^* \in \mathcal{R}^D$ and $h \in \mathcal{R}$, then $\phi_{h,f}(\mathbf{y}^*) \in \mathcal{R}^D$ is the value at $t = h$ of the solution of the system in (1) with initial value \mathbf{y}^* at time $t = 0$. The mapping $\psi_{h,f}$ tries to approximate the exact $\phi_{h,f}$; for a method of order r , $\psi_{h,f} = \phi_{h,f} + O(h^{r+1})$. By considering the method of *modified equations* [20], [6], it turns out [17, Section 10.1], that $\psi_{h,f}$ formally coincides

with the exact solution flow ϕ_{h,\tilde{f}_h} of a *modified system*

$$\frac{d\mathbf{y}}{dt} = \tilde{\mathbf{f}}_h(\mathbf{y}), \quad \tilde{\mathbf{f}}_h(\mathbf{y}) = \mathbf{f}(\mathbf{y}) + O(h^r). \quad (1)$$

Thus, when using the numerical integrator $\psi_{h,f}$ instead of the true $\phi_{h,f}$, we obtain solutions of the perturbed (1) rather than solutions of the system in (1) we really wanted to solve. A prescription for finding $\tilde{\mathbf{f}}_h$ for a given $\psi_{h,f}$ was given by Hairer [8] and simplified by Murua [14], [3].

Equipped with the modified system (1), we return to (2), that now becomes

$$\widehat{\psi}_{h,f} = \chi_{h,\tilde{f}_h}^{-1} \circ \phi_{h,\tilde{f}_h} \circ \chi_{h,f}. \quad (2)$$

Let us study the right hand side of this equality. If $\mathbf{y}^* \in \mathcal{R}^D$, then $(\chi_{h,\tilde{f}_h}^{-1} \circ \psi_{h,f} \circ \chi_{h,f})(\mathbf{y}^*)$ is the result of (i) changing variables from \mathbf{y}^* to $\chi_{h,f}(\mathbf{y}^*)$, (ii) evolving in time with (1), (iii) reversing the change of variables. Of course, the end result is the same as evolving from the initial condition \mathbf{y}^* in the system

$$\frac{d}{dt} \chi_{h,f}(\mathbf{y}) = \chi'_{h,f}(\mathbf{y}) \frac{d\mathbf{y}}{dt} = \tilde{\mathbf{f}}_h(\chi_{h,f}(\mathbf{y}))$$

or

$$\frac{d\mathbf{y}}{dt} = \tilde{\tilde{\mathbf{f}}}_h(\mathbf{y}), \quad \tilde{\tilde{\mathbf{f}}}_h(\mathbf{y}) := (\chi'_{h,f}(\mathbf{y}))^{-1} \tilde{\mathbf{f}}_h(\chi_{h,f}(\mathbf{y})) \quad (3)$$

that results when changing variables in (1). The conclusion is that (2) may be rewritten as

$$\widehat{\psi}_{h,f} = \chi_{h,\tilde{f}_h}^{-1} \circ \phi_{h,\tilde{f}_h} \circ \chi_{h,f} = \phi_{h,\tilde{\tilde{\mathbf{f}}}_h},$$

or, in other words, that (3) provides the modified system for the method $\widehat{\psi}_{h,f}$. Discretization of (1) with the method $\psi_{h,f}$ modified \mathbf{f} into $\tilde{\mathbf{f}}_h$. We now look for a change of variables $\chi_{h,f}$ that counteracts that modification by moving from $\tilde{\mathbf{f}}_h$ into an $\tilde{\tilde{\mathbf{f}}}_h$ closer to our target \mathbf{f} . Given $\psi_{h,f}$, one should then aim at finding a transformation $\chi_{h,f}$ for which the function $\tilde{\tilde{\mathbf{f}}}_h$ in (3) is as close to \mathbf{f} as possible.

From now on we deal only with Hamiltonian systems, that is, we suppose that in (1), $D = 2d$, $\mathbf{y} = (\mathbf{q}, \mathbf{p})$, $\mathbf{q}, \mathbf{p} \in \mathcal{R}^d$ and (superscripts number components)

$$f^i(\mathbf{y}) = \frac{\partial H}{\partial p^i}, \quad f^{i+d}(\mathbf{y}) = -\frac{\partial H}{\partial q^i}, \quad i = 1, \dots, d, \quad (4)$$

where $H = H(\mathbf{y}) = H(\mathbf{q}, \mathbf{p})$ is the real-valued Hamiltonian function. Hereafter we write $\psi_{h,H}$, $\phi_{h,H}$, ... instead of $\psi_{h,f}$, $\phi_{h,f}$, ...

We also suppose that the basic method $\psi_{h,H}$ is symplectic (canonical). This is equivalent to saying [17, Section 10.1] that the corresponding modified system (1) is also a Hamiltonian system, i.e., $\tilde{\mathbf{f}}_h$ derives, via the recipe (4), from a suitable Hamiltonian function \tilde{H}_h . Thus a symplectic methods perturbs the Hamiltonian equation

being integrated into another Hamiltonian problem. Nonsymplectic methods replace Hamiltonian problems by nonHamiltonian perturbations. A technique for explicitly finding the modified Hamiltonian \tilde{H}_h when the expansion of $\psi_{h,H}(\mathbf{y})$ in powers of h is known is given in [8] and simplified in [13]. If the method $\psi_{h,H}(\mathbf{y})$ is a composition of simpler methods, then the modified Hamiltonian may be found with the help of the Baker-Campbell-Hausdorff formula as, e.g., in [17, Chapters 12 and 13].

Finally, if the preprocessor $\chi_{h,H}$ is also a canonical mapping, then $\tilde{\psi}_{h,H}$, being a composition (2) of canonical mappings, will also be symplectic and its modified system (3) will also be a Hamiltonian system. What is the corresponding Hamiltonian function \tilde{H}_h ? Recall that (3) comes from changing variables in (1). A well-known result of the Hamiltonian formalism [17, Section 11.2] states that to canonically change variables in a Hamiltonian system is equivalent to forming the Hamiltonian system obtained by changing variables in the Hamiltonian function:

$$\tilde{H}_h(\mathbf{y}) = \tilde{H}_h(\chi_{h,H}(\mathbf{y})). \quad (5)$$

Given $\psi_{h,H}$, one should then aim at finding a symplectic $\chi_{h,H}$ for which the right hand side of (5) is as close to H as possible.

3 Determining the Processors

In this section and the next we assume that the Hamiltonian function is quadratic

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2} \mathbf{p}^T M^{-1} \mathbf{p} + \frac{1}{2} \mathbf{q}^T S \mathbf{q}, \quad (1)$$

with M and S constant, symmetric matrices, M regular. The corresponding Hamiltonian system (1), (4) is then linear. The \mathbf{p} quadratic form in (1) is the kinetic energy and the \mathbf{q} term is the potential energy.

If the method is time-reversible, then the expansion of \tilde{H}_h in powers of h includes only even powers. This expansion will be of the form [17, Section 11.5.3], [8], [14]

$$\begin{aligned} \tilde{H}_h(\mathbf{q}, \mathbf{p}) = & H(\mathbf{q}, \mathbf{p}) \\ & + h^2 \frac{A}{2} [\mathbf{p}^T M^{-1} S M^{-1} \mathbf{p}] \\ & + h^2 \frac{B}{2} [\mathbf{q}^T S M^{-1} S \mathbf{q}] \\ & + h^4 \frac{C}{2} [\mathbf{p}^T M^{-1} S M^{-1} S M^{-1} \mathbf{p}] \\ & + h^4 \frac{D}{2} [\mathbf{q}^T S M^{-1} S M^{-1} S \mathbf{q}] + O(h^6). \end{aligned} \quad (2)$$

Here A, B, C, D are method-dependent constants ($A = B = 0$ for order 4) and the scalar expressions in brackets are *elementary Hamiltonians*. The right hand side of (2)

provides an example of an *H-series* [14]. Note that here the elementary Hamiltonians involving \mathbf{p} (resp. \mathbf{q}) represent perturbations to the true kinetic (resp. potential) energy.

Since the transformation $(\mathbf{Q}, \mathbf{P}) = \chi_{h,H}(\mathbf{q}, \mathbf{p})$ is required to be symplectic and close to the identity, it will be the h -flow ϕ_{h,H_χ} of some Hamiltonian system with Hamiltonian function H_χ (see, e.g., [5, Theorem 2]). The H-series for H_χ is sought in the form

$$H_\chi = h\lambda[\mathbf{p}^T M^{-1} S \mathbf{q}] + h^3 \mu[\mathbf{p}^T M^{-1} S M^{-1} S \mathbf{q}] + O(h^5)$$

for undetermined parameters λ and μ ; no $O(1)$ nor $O(h^2)$ contribution is included because (2) possesses no $O(h)$ nor $O(h^3)$ term. Application of the Taylor series method to the Hamiltonian system with Hamiltonian H_χ reveals that $\chi_{h,H} = \phi_{h,H_\chi}$ is

$$\begin{aligned} \mathbf{Q} &= \mathbf{q} + h^2 \lambda [M^{-1} S \mathbf{q}] + h^4 \left(\frac{\lambda^2}{2} + \mu \right) [M^{-1} S M^{-1} S \mathbf{q}] + O(h^6), \\ \mathbf{P} &= \mathbf{p} - h^2 \lambda [S M^{-1} \mathbf{p}] + h^4 \left(\frac{\lambda^2}{2} - \mu \right) [S M^{-1} S M^{-1} \mathbf{p}] + O(h^6). \end{aligned} \quad (3)$$

Here the d -vectors in square brackets are *elementary differentials*; series like (3) are called P-series [7], see also [9, Chapter II.15]. It is perhaps useful to mention that systematic rules for computing the flow corresponding to a given Hamiltonian can be found in [14]. Substitution of \mathbf{Q} and \mathbf{P} given by (3) for \mathbf{q} and \mathbf{p} in (2) leads, according to (5), to the modified Hamiltonian of the processed method. The result is

$$\begin{aligned} \tilde{H}_h(\mathbf{q}, \mathbf{p}) = & H(\mathbf{q}, \mathbf{p}) \\ & + h^2 \left(\frac{A}{2} - \lambda \right) [\mathbf{p}^T M^{-1} S M^{-1} \mathbf{p}] \\ & + h^2 \left(\frac{B}{2} + \lambda \right) [\mathbf{q}^T S M^{-1} S \mathbf{q}] \\ & + h^4 \left(\frac{C}{2} + \lambda^2 - A\lambda - \mu \right) [\mathbf{p}^T M^{-1} S M^{-1} S M^{-1} \mathbf{p}] \\ & + h^4 \left(\frac{D}{2} + \lambda^2 + B\lambda + \mu \right) [\mathbf{q}^T S M^{-1} S M^{-1} S \mathbf{q}] + O(h^6). \end{aligned} \quad (4)$$

Once more, Murua [14] has derived rules for systematically finding the H-series resulting from substituting P-series like (3) into H-series like (2).

We now determine the processing parameters λ and μ so as to bring (4) as close to H as possible. Our strategy is as follows:

1. We first choose λ so as to minimize the quantity $(A/2 - \lambda)^2 + (B/2 + \lambda)^2$ that measures the size of the $O(h^2)$ terms in (4). Clearly this leads to the choice

$$\lambda = \frac{A - B}{4} \quad (5)$$

and implies

$$\frac{A}{2} - \lambda = \frac{B}{2} + \lambda, \quad (6)$$

so that, according to (4), the processed method perturbs the true potential and kinetic energies by equal $O(h^2)$ amounts. In the special case where the basic method $\psi_{h,H}$ has

$$A = -B \quad (7)$$

both sides of (6) are 0 and the $O(h^2)$ terms in (4) vanish: the effective order of $\psi_{h,H}$ is 4 (by (2) the conventional order is 2, unless $A = -B = 0$).

2. Having determined λ , we choose μ to minimize $(C/2 + \lambda^2 - A\lambda - \mu)^2 + (D/2 + \lambda^2 + B\lambda + \mu)^2$. This results in

$$\mu = \frac{C-D}{4} + \frac{B^2 - A^2}{8} \quad (8)$$

and implies

$$\frac{C}{2} + \lambda^2 - A\lambda - \mu = \frac{D}{2} + \lambda^2 + B\lambda + \mu, \quad (9)$$

so that, at the $O(h^4)$ level, the processed method perturbs the kinetic and potential energies by equal amounts. In the special case where (7) holds and furthermore $C + D = A^2$, one has that both sides of (9) vanish and the effective order (for the linear Hamiltonian problems being considered) is 6.

There is an alternative argument leading to (5) and (8). Let us compute the variation of the true energy H along solutions of the Hamiltonian problem with Hamiltonian function (4). It turns out that

$$\begin{aligned} \frac{1}{2} \frac{dH}{dt} &= h^2 \left(\left(\frac{A}{2} - \lambda \right) - \left(\frac{B}{2} + \lambda \right) \right) [\mathbf{p}^T M^{-1} S M^{-1} S \mathbf{q}] \\ &+ h^4 \left(\left(\frac{C}{2} + \lambda^2 - A\lambda - \mu \right) - \left(\frac{D}{2} + \lambda^2 + B\lambda + \mu \right) \right) \\ &\times [\mathbf{p}^T M^{-1} S M^{-1} S M^{-1} S \mathbf{q}] + O(h^6). \end{aligned}$$

By (6) and (9) our choice of parameters clearly ensures that for linear systems, along solutions of the processed method, $dH/dt = O(h^6)$ (recall that $dH/dt = 0$ along true solutions of the system being solved).

Let us finally look at the inverse transformation $\chi_{h,H}^{-1}$. To generate this we simply reverse the sign of the Hamiltonian H_χ that was used to find the expansion of $\chi_{h,H}$. This reverses the signs of λ and μ in (3) so that $(\mathbf{q}, \mathbf{p}) = \chi_{h,H}^{-1}(\mathbf{Q}, \mathbf{P})$ is given by

$$\begin{aligned} \mathbf{q} &= \mathbf{Q} - h^2 \lambda [M^{-1} S \mathbf{Q}] + h^4 \left(\frac{\lambda^2}{2} - \mu \right) [M^{-1} S M^{-1} S \mathbf{Q}] + O(h^6), \\ \mathbf{p} &= \mathbf{P} + h^2 \lambda [S M^{-1} \mathbf{P}] + h^4 \left(\frac{\lambda^2}{2} + \mu \right) [S M^{-1} S M^{-1} \mathbf{P}] + O(h^6). \end{aligned} \quad (10)$$

4 Cheap Processing

Now that the preprocessor (3) has been determined, we consider the task of finding the processed \mathbf{Q}_0 and \mathbf{P}_0 corresponding to \mathbf{q}_0 and \mathbf{p}_0 . To this end we take two forward steps with the basic method, $(\mathbf{q}_1, \mathbf{p}_1) = \psi_{h,H}(\mathbf{q}_0, \mathbf{p}_0)$, $(\mathbf{q}_2, \mathbf{p}_2) = \psi_{h,H}(\mathbf{q}_1, \mathbf{p}_1)$, and two backward steps, $(\mathbf{q}_{-1}, \mathbf{p}_{-1}) = \psi_{-h,H}(\mathbf{q}_0, \mathbf{p}_0)$, $(\mathbf{q}_{-2}, \mathbf{p}_{-2}) = \psi_{-h,H}(\mathbf{q}_{-1}, \mathbf{p}_{-1})$, and form the standard second and fourth order central differences $\delta^2 \mathbf{q}_0$, $\delta^2 \mathbf{p}_0$, $\delta^4 \mathbf{q}_0$, $\delta^4 \mathbf{p}_0$. Since $\psi_{h,H} = \phi_{h,H,h}$, we may find the expansion in powers of h of \mathbf{q}_i , \mathbf{p}_i , $i = \pm 1, \pm 2$ by applying the Taylor series method to the Hamiltonian system with Hamiltonian (2). From those expansions one gets

$$\begin{aligned} \delta^2 \mathbf{q}_0 &= -h^2 [M^{-1} S \mathbf{q}_0] + h^4 \left(\frac{1}{12} - (A+B) \right) [M^{-1} S M^{-1} S \mathbf{q}_0] + O(h^6), \\ \delta^2 \mathbf{p}_0 &= -h^2 [S M^{-1} \mathbf{p}_0] + h^4 \left(\frac{1}{12} - (A+B) \right) [S M^{-1} S M^{-1} \mathbf{p}_0] + O(h^6), \end{aligned}$$

and

$$\begin{aligned} \delta^4 \mathbf{q}_0 &= h^4 [M^{-1} S M^{-1} S \mathbf{q}_0] + O(h^6), \\ \delta^4 \mathbf{p}_0 &= h^4 [S M^{-1} S M^{-1} \mathbf{p}_0] + O(h^6). \end{aligned}$$

Hence

$$\begin{aligned} h^2 [M^{-1} S \mathbf{q}_0] &= -\delta^2 \mathbf{q}_0 + \left(\frac{1}{12} - (A+B) \right) \delta^4 \mathbf{q}_0 + O(h^6), \\ h^2 [S M^{-1} \mathbf{p}_0] &= -\delta^2 \mathbf{p}_0 + \left(\frac{1}{12} - (A+B) \right) \delta^4 \mathbf{p}_0 + O(h^6). \end{aligned}$$

Now that the elementary differentials have been expressed in terms of differences, from the expansion (3) of the preprocessor we may write

$$\begin{aligned} \mathbf{Q}_0 &= \mathbf{q}_0 - \lambda \delta^2 \mathbf{q}_0 + \left(\frac{\lambda^2}{2} + \mu + \frac{\lambda}{12} - \lambda(A+B) \right) \delta^4 \mathbf{q}_0 + O(h^6), \\ \mathbf{P}_0 &= \mathbf{p}_0 + \lambda \delta^2 \mathbf{p}_0 + \left(\frac{\lambda^2}{2} - \mu - \frac{\lambda}{12} + \lambda(A+B) \right) \delta^4 \mathbf{p}_0 + O(h^6). \end{aligned}$$

In practice we disregard the remainder and preprocess according to the following formulae

$$\begin{aligned} \mathbf{Q}_0 &= \mathbf{q}_0 - \lambda \delta^2 \mathbf{q}_0 + \left(\frac{\lambda^2}{2} + \mu + \frac{\lambda}{12} - \lambda(A+B) \right) \delta^4 \mathbf{q}_0, \\ \mathbf{P}_0 &= \mathbf{p}_0 + \lambda \delta^2 \mathbf{p}_0 + \left(\frac{\lambda^2}{2} - \mu - \frac{\lambda}{12} + \lambda(A+B) \right) \delta^4 \mathbf{p}_0. \end{aligned} \quad (1)$$

Note that the omission of the remainder will turn the computed $\chi_{h,H}$ into a non-symplectic transformation. This should not be bad for the overall algorithm; it just

introduces a nonsymplectic $O(h^6)$ error at the beginning of the integration, while the actual time stepping is still being done with the symplectic $\psi_{h,H}$.

Similar considerations apply to the postprocessor $\chi_{h,H}^{-1}$. We approximate it by

$$\begin{aligned} \mathbf{q}_n &= \mathbf{Q}_n + \lambda \delta^2 \mathbf{Q}_n + \left(\frac{\lambda^2}{2} - \mu - \frac{\lambda}{12} + \lambda(A+B) \right) \delta^4 \mathbf{Q}_n, \\ \mathbf{p}_n &= \mathbf{P}_n - \lambda \delta^2 \mathbf{P}_n + \left(\frac{\lambda^2}{2} + \mu + \frac{\lambda}{12} - \lambda(A+B) \right) \delta^4 \mathbf{P}_n, \end{aligned} \quad (2)$$

where the vectors required to form the divided differences come again from the basic method $\psi_{h,H}$. Finding these vectors is completely free of cost: they are the numerical approximations at the two preceding and two next grid points. Again (2) will not in general be symplectic but this has no effect in the long term properties of the processed method because the postprocessor is only used for output purposes.

5 Nonlinear Problems

The processors (1)–(2), with parameter values (5), (8) have been derived under the assumption of a quadratic Hamiltonian (1). We now look at the more general case

$$H(\mathbf{q}, \mathbf{p}) = \frac{1}{2} \mathbf{p}^T M^{-1} \mathbf{p} + V(\mathbf{q}), \quad (1)$$

where the potential energy V is not necessarily quadratic. The discussion that follows is not too detailed; full details will be given in a forthcoming paper.

For (1), the expansion of the modified Hamiltonian will be of the form (cf. (2))

$$\begin{aligned} \tilde{H}_h(\mathbf{q}, \mathbf{p}) &= H(\mathbf{q}, \mathbf{p}) \\ &+ h^2 \frac{A}{2} [\mathbf{p}^T M^{-1} V_{\mathbf{q}\mathbf{q}} M^{-1} \mathbf{p}] \\ &+ h^2 \frac{B}{2} [V_{\mathbf{q}}^T M^{-1} V_{\mathbf{q}}] + O(h^4). \end{aligned} \quad (2)$$

Here $V_{\mathbf{q}}$ and $V_{\mathbf{q}\mathbf{q}}$ are respectively the gradient vector and the Hessian matrix of V . For simplicity, the $O(h^4)$ elementary Hamiltonians have been hidden in the remainder of (2). There are four such elementary Hamiltonians; only two appeared in (2) because the other two vanish identically for quadratic potentials.

In a similar way, the transformation $\chi_{h,H}$ is now (cf. (3))

$$\begin{aligned} \mathbf{Q} &= \mathbf{q} + h^2 \lambda [M^{-1} V_{\mathbf{q}}] + O(h^4), \\ \mathbf{P} &= \mathbf{p} - h^2 \lambda [V_{\mathbf{q}\mathbf{q}} M^{-1} \mathbf{p}] + O(h^4), \end{aligned} \quad (3)$$

and by substitution in (2) we find (cf. (4))

$$\tilde{\tilde{H}}_h(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}, \mathbf{p})$$

$$\begin{aligned} &+ h^2 \left(\frac{A}{2} - \lambda \right) [\mathbf{p}^T M^{-1} V_{\mathbf{q}\mathbf{q}} M^{-1} \mathbf{p}] \\ &+ h^2 \left(\frac{B}{2} + \lambda \right) [V_{\mathbf{q}}^T M^{-1} V_{\mathbf{q}}] + O(h^4). \end{aligned} \quad (4)$$

We still use our (1)–(2), with parameter values (5), (8). The preprocessor (1) provides an $O(h^4)$ approximation to the exact $\chi_{h,H}$ in (3) and the processed numerical solutions differ in $O(h^4)$ terms from the solutions of (4). Due to the choice (5), we are minimizing the sum of squares of the $O(h^2)$ coefficients in (4). Furthermore, we see from (5), (6) and (4) that the condition (7), that was shown in Section 3 to imply effective order 4 for linear problems, leads to $\tilde{\tilde{H}}_h = H + O(h^4)$. Therefore, when (7) holds, the processed method is also fourth-order accurate for nonlinear Hamiltonians. (It should be noted that order $r > 2$ for linear Hamiltonian problems does not imply order r for general Hamiltonian problems. As pointed out above, for $r > 2$ there are relevant elementary Hamiltonians that vanish in the linear case; annihilating the coefficients of the linear elementary Hamiltonians is then not sufficient to keep order r for general Hamiltonian systems.)

6 An Illustration

The preceding material will now be applied to a simple one-parameter family of methods of interest in molecular dynamics. We describe these methods as applied to the Hamiltonian (1) A step $0 \rightarrow 1$ of the method with parameter value α is given by the formula

$$\begin{aligned} \mathbf{p}^{1/2} &= \mathbf{p}^0 + \frac{h}{2} [-V_{\mathbf{q}} + \alpha h^2 V_{\mathbf{q}\mathbf{q}} M^{-1} V_{\mathbf{q}}]^0, \\ \mathbf{q}^1 &= \mathbf{q}^0 + h M^{-1} \mathbf{p}^{1/2}, \\ \mathbf{p}^1 &= \mathbf{p}^{1/2} + \frac{h}{2} [-V_{\mathbf{q}} + \alpha h^2 V_{\mathbf{q}\mathbf{q}} M^{-1} V_{\mathbf{q}}]^1. \end{aligned} \quad (1)$$

Here the superscripts 0 and 1 in the square brackets mean evaluation at \mathbf{q}^0 or \mathbf{q}^1 . When $\alpha = 0$ we retrieve the well-known Verlet method, which does not require the Hessian $V_{\mathbf{q}\mathbf{q}}$.

Our first task is to find the values of the values of A, B, C, D in the expansion (2) of the modified Hamiltonian \tilde{H}_h . This can be done by finding the expansions of (2) and of $(\mathbf{p}^1, \mathbf{q}^1)$ and matching the coefficients of the different elementary Hamiltonians. Alternatively, one may use the Baker-Campbell-Hausdorff formula, as mentioned in Section 2. The result turns out to be

$$A = \frac{1}{6}, \quad B = -\frac{1}{12} - \alpha, \quad C = \frac{1}{30} - \frac{\alpha}{6}, \quad D = -\frac{1}{120} + \frac{\alpha}{6};$$

from these values we compute λ and μ via (5) and (8).

Since $A \neq 0$, we see in (2) that $\tilde{H}_h = H + O(h^2)$ and the order of (1) is 2 regardless of the value of α . The condition (7) for effective order 4 leads to $\alpha = 1/12$. With this value of α , (1) was first suggested by [16] and rediscovered by Wisdom *et al.* [21]. However these authors do not use our simple processors.

7 Numerical Results

We have applied the methods above to the simulation of the motion of $N = 256$ atoms of liquid argon, a typical test in molecular dynamics, see, e.g., [15], [10], [12]. The motion of the atoms is governed by a Hamiltonian of the form (1) with $d = 3N$. The variables q^i are given by $q^{3i-2} = x_i$, $q^{3i-1} = y_i$, $q^{3i} = z_i$, with $\mathbf{r}_i = (x_i, y_i, z_i)$ the position vector of the i -th atom. Similarly, \mathbf{p} collects the momenta of the atoms: $p^{3i-2} = m\dot{x}_i$, $p^{3i-1} = m\dot{y}_i$, $p^{3i} = m\dot{z}_i$, where m is the mass of an atom and $(\dot{x}_i, \dot{y}_i, \dot{z}_i)$ are the components of the velocity of the i -th atom. Then the mass matrix is the diagonal matrix $M = mI$. The potential energy V is given by a sum

$$V(\mathbf{q}) = \sum_{i < j} \Phi(\|\mathbf{r}_i - \mathbf{r}_j\|^2) \quad (1)$$

of the potential energies $\Phi(\|\mathbf{r}_i - \mathbf{r}_j\|^2)$ associated with each pair (i, j) of atoms. For argon, a Lennard-Jones potential

$$\Phi(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right]$$

with $\epsilon = 1.65324 \times 10^{-21}$ joules and $\sigma = 3.405 \times 10^{-10}$ metres is suitable [1]. Note that the corresponding Hamiltonian problem is highly nonlinear.

Periodic boundary conditions were imposed in the manner explained in [12]. We also used the initial condition in [12] and worked with the nondimensional form of the equations of motion described in that paper. It is perhaps useful to mention that the (nondimensional) step $h = 0.064$ corresponds to 0.02 picoseconds of physical time and may be considered as a typical step to be used with the (unprocessed) Verlet algorithm [10].

The integration has been carried out for $0 \leq t \leq 65.536$ and output has been produced at intervals of length $\Delta t = 1.024$ (this yields 64 output points $t = i\Delta t$, $i = 1, \dots, 64$). At each output point, we have measured the error ΔH_i in total energy H and then found the root mean square $\langle \Delta H \rangle = (\sum_i \Delta H_i^2 / 64)^{1/2}$. We also measured in the same way the error in temperature. Measuring global quantities like energies and temperatures is typical of molecular dynamics, where there is little interest in computing accurate solutions of the equations of motion, i.e., in following in detail the motion of the individual atoms. The energy error is relevant for symplectic integrators: it measures the difference between the exact and modified Hamiltonians.

Verlet's method or any other Runge-Kutta-Nyström method [17] for the system with Hamiltonian function (1) requires the evaluation of the vector $-V_{\mathbf{q}}$ that collects

the N forces on the N atoms. Since here each atom is attracted by all others this evaluation has an $O(N^2)$ cost and, in fact, the force evaluation accounts for most of the (rather large) work required in molecular dynamics simulations when Runge-Kutta-Nyström methods are used. For $\alpha \neq 0$, the method (1) also requires the computation of $V_{\mathbf{q}\mathbf{q}}M^{-1}V_{\mathbf{q}}$. It can be shown (see the next section) that, for the liquid argon problem and other molecular dynamics problems involving only two-body interactions the cost of evaluating $V_{\mathbf{q}}$ and $V_{\mathbf{q}\mathbf{q}}M^{-1}V_{\mathbf{q}}$ at a given \mathbf{q} is approximately twice as large as the cost of evaluating only $V_{\mathbf{q}}$. Thus, for the problem at hand, the cost per step of (1) with $\alpha \neq 0$ is twice the cost per step of the Verlet ($\alpha = 0$) algorithm. [p]

We here report results for $\alpha = 0$ (Verlet) and $\alpha = 1/12$ (Rowlands): Verlet has the advantage of its lower cost per step, Rowlands possesses a higher effective order.

We present our results through log-log efficiency charts where the vertical axis measures the relative energy error $\langle \Delta H \rangle / H$ and the horizontal axis corresponds to cost. For the Verlet algorithm cost is measured by the number of evaluations of the force $V_{\mathbf{q}}$. For Rowlands method an evaluation of $V_{\mathbf{q}\mathbf{q}}M^{-1}V_{\mathbf{q}}$ and an evaluation of $V_{\mathbf{q}}$ are counted as two evaluations of $V_{\mathbf{q}}$. In all figures the vertical axis corresponds to the range 10^{-2} to 10^{-6} and the horizontal axis goes from 10^2 to 10^4 . Efficiency plots were also obtained for the temperature errors; they are not shown here because they are similar to and lead to the same conclusions as the energy efficiency plots.

Fig. 1 corresponds to the Verlet method. The circles joined by a solid line are the results of the unprocessed method with $h = 0.128, 0.064, \dots, 0.008$ ($h = 0.256$ leads to instability). The stars joined by the dotted line are the results with processing, $h = 0.128, 0.064, \dots, 0.016$. We see that processing reduces errors by a factor of more than 4, or, in other words, that the processed method with steplength h gives more accuracy than the unprocessed method with steplength $h/2$. Therefore processing cuts by a factor larger than 2 the work required to achieve a target error. We also tried a simplified version of the pre- and postprocessors obtained by leaving out the terms involving δ^4 in (1) and (2). The results for the simplified processing are displayed by plus signs. For h small, the inclusion of the δ^4 terms does not improve the accuracy. This was to be expected: those terms represent an $O(h^4)$ correction and the error itself is $O(h^2)$.

For Rowlands's method the results are given in Fig. 2. The circles joined by a solid line are the results of the unprocessed method with $h = 0.128, \dots, 0.016$ ($h = 0.256$ is unstable). From the slope of the solid line we see that the order of the unprocessed method is 2. The stars joined by the dotted line correspond to the processed results with $h = 0.128, 0.064$ and clearly show a 4-th order behaviour. The plus signs with dash-dot line are the results of the simplified processing: the order is still 4 (because the simplified processor still cancels the leading term of the error), but clearly the full processors should be preferred. The error reduction accomplished by processing in Fig. 2 is truly remarkable.

In Fig. 3 we have again displayed the results of the processed Verlet and Rowlands methods. Verlet is more efficient than Rowlands for low accuracies, but the picture is

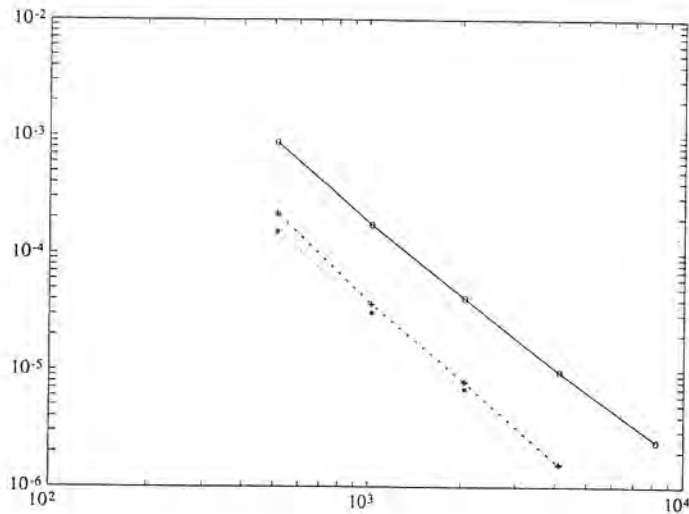


Figure 1: Relative energy error against number of function evaluations. Verlet method: unprocessed (solid line), processed (dotted line) and with simplified processing (dash-dot line)

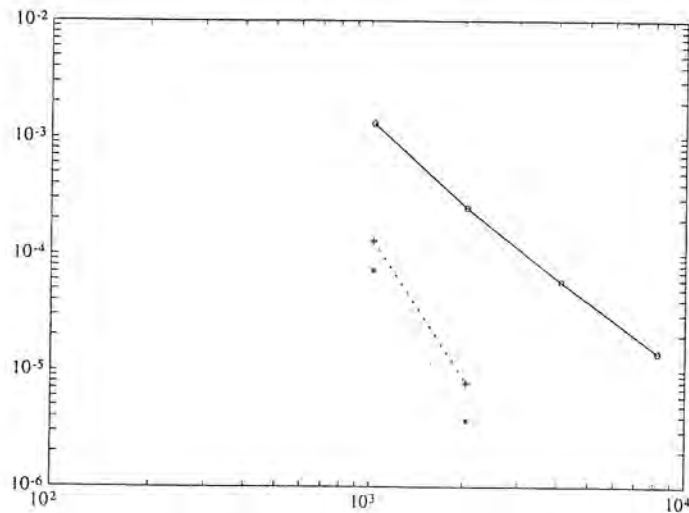


Figure 2: Relative energy error against number of function evaluations. Rowlands method: unprocessed (solid line), processed (dotted line) and with simplified processing (dash-dot line)

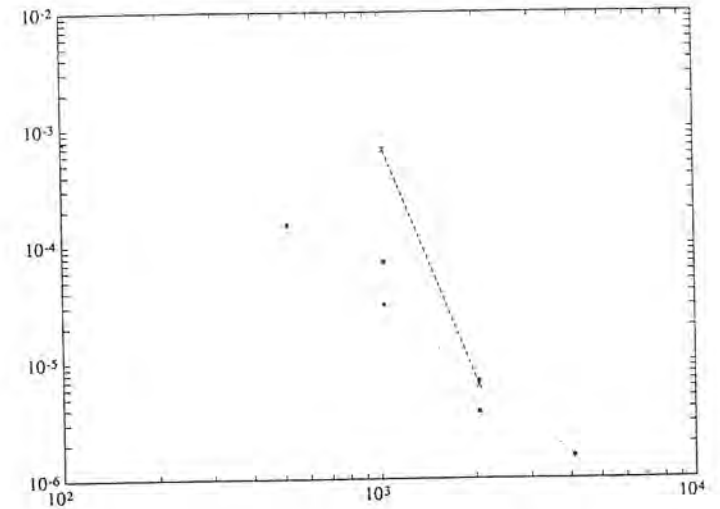


Figure 3: Relative energy error against number of function evaluations. Calvo's method (dashed line) compared to the processed Verlet and Rowlands methods of the preceding figures

reversed when high accuracy is required. In the figure we have also included (dashed line) the results corresponding to an explicit, order 4, optimized, symplectic method introduced by Calvo in her thesis, see, e.g., [4]. This method uses four evaluations of V_q per step and has been run with $h = 0.256$ and $h = 0.128$ ($h = 0.512$ turned out to be unstable). Calvo's method is amongst the best available symplectic integrators [17, Chapters 9 and 13]. It is then encouraging to see in Fig. 3 that, for the problem at hand, the simple processed methods considered in this paper improve on Calvo's scheme. (The slope of the dashed line in Fig. 3 shows an order higher than 4; this is due to the fact that for the values of h considered there is cancellation between the $O(h^4)$ and $O(h^5)$ terms of the expansion of the global error.)

8 Computing the Hessian of the Potential

For a two-body potential of the form (1),

$$V_q = \sum_{i < j} 2\Phi'_{ij} \begin{bmatrix} \vdots \\ 0 \\ -\mathbf{r}_{ij} \\ 0 \\ \vdots \\ 0 \\ \mathbf{r}_{ij} \\ 0 \\ \vdots \end{bmatrix}, \quad (1)$$

where $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$, $\Phi'_{ij} = \Phi'(\mathbf{r}_{ij}^2)$ and the nonzero entries in the $3N$ -dimensional column vector are associated with the i -th and j -th atom, respectively.

Similarly,

$$V_{qq} = \sum_{i < j} \begin{bmatrix} \vdots \\ 0 \\ -I \\ 0 \\ \vdots \\ 0 \\ I \\ 0 \\ \vdots \end{bmatrix} (2\Phi'_{ij}I + 4\Phi''_{ij}\mathbf{r}_{ij}\mathbf{r}_{ij}^T) \begin{bmatrix} \cdots & 0 & -I & 0 & \cdots & 0 & I & 0 & \cdots \end{bmatrix}, \quad (2)$$

where I and O are the unit and zero 3×3 matrices.

Consider now $3N$ -dimensional column vector of accelerations $\mathbf{a} = M^{-1}V_q$, denote by \mathbf{a}_i each of its N 3-dimensional blocks and set $\mathbf{a}_{ij} = \mathbf{a}_j - \mathbf{a}_i$. Then, from (2),

$$V_{qq}M^{-1}V_q = \sum_{i < j} \begin{bmatrix} \vdots \\ O_3 \\ -I_3 \\ O_3 \\ \vdots \\ O_3 \\ I_3 \\ O_3 \\ \vdots \end{bmatrix} (2\Phi'_{ij}\mathbf{a}_{ij} + 4\Phi''_{ij}(\mathbf{r}_{ij}^T\mathbf{a}_{ij})\mathbf{r}_{ij}). \quad (3)$$

To evaluate V_q and $V_{qq}M^{-1}V_q$ at a given q we go twice over all pairs (i, j) of atoms. In the first sweep, for each pair (i, j) we compute and save \mathbf{r}_{ij} , Φ'_{ij} and Φ''_{ij} . We also add to the sum in (1) the contribution of the pair (i, j) . In the second sweep we compute the sum in (3). If $V_{qq}M^{-1}V_q$ is not required, only one sweep is involved and only Φ' (rather than Φ' and Φ'') has to be evaluated. Therefore the evaluation of V_q and $V_{qq}M^{-1}V_q$ should be twice as costly as the evaluation of V_q . Numerical experiments confirm this expectation.

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K W MORTON

Finite volume methods

Abstract To a numerical analyst, finite volume methods are low order, nonconforming Petrov-Galerkin methods of no particular significance. But to the aeronautical engineer they are key design tools, well suited to the efficient modelling of nonlinear conservation laws in complicated three-dimensional geometries. In view of their dominance in this area of computational fluid dynamics, and because of the need to resolve a number of important issues and make improvements in key areas, these methods merit and require more attention from numerical analysts.

In this lecture, I will briefly review the range of methods on structured and unstructured meshes that are in use, and their links to more familiar finite difference and finite element methods. This will be followed by a selection from the numerical analysis results that have been established, particularly in regard to their robustness for singular perturbation problems. Finally, I will outline some of the outstanding issues and situations for which more analysis is needed. In each case the cell vertex scheme will be used as a key exemplar of the methods.

1 Introduction

As young men, ignorant of finite element methods, Ron Mitchell and I shared an enthusiasm for finite difference methods; and I well remember participating in my first Dundee conference (held at St. Andrews!) when their analysis was by far the dominant topic. In middle age we were both fierce advocates of the distinctive advantages of finite element methods, which were nearly as dominant a theme by the time we come to the Dundee conference of 1973. And now, over the last dozen years, I have found myself fascinated by finite volume methods which share properties with each of these more established methods.

Few things have given me as much pleasure as being invited to open this conference with the A.R. Mitchell lecture, and hence to have the opportunity to tell you something of these practically important and theoretically challenging methods. Dundee conferences over the last thirty years have transformed the numerical-analysis scene in the UK, providing the perfect forum for us all to share our ideas with colleagues from around the world.