Construction of higher order symplectic integrators

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For Hamiltonian systems of the form $H = T(p) + V(q)$ a method is shown to construct explicit and time reversible symplectic integrators of higher order. For any even order there exists at least one symplectic integrator with exact coefficients. The simplest one is the 4th order integrator which agrees with one found by Forest and by Neri. For 6th and 8th orders, symplectic integrators with fewer steps are obtained, for which the coefficients are given by solving a set of simultaneous algebraic equations numerically.

1. Introduction

Symplectic integrators are numerical integration schemes for Hamiltonian systems, which conserve the symplectic two-form $dp \wedge dq$ exactly, so that $(q(0), p(0)) \rightarrow (q(\tau), p(\tau))$ is a canonical transformation [1–6]. For both explicit and implicit integrators, it was shown that the discrete mapping obtained describes the exact time evolution of a slightly perturbed Hamiltonian system and thus possesses the perturbed Hamiltonian as a conserved quantity. This guarantees that there is no secular change in the error of the total energy (which should be conserved exactly in the original flow) caused by the local truncation error. If the integrator is not symplectic, the error of the total energy grows secularly in general. See ref. [7] for more details.

A quite general idea to construct the explicit symplectic integrator for a Hamiltonian

$$H = T(p) + V(q) \tag{1.1}$$

is given by Neri [6]. Although the idea is quite simple, practice is quite another thing. For example, constructing the 6th order integrator just by following the idea of Neri seems to be impossible, or at least, very difficult. In this note, a method is given to construct the symplectic integrator (explicit, time reversible) of any even order (section 4). The simplest non-trivial one, which is the 4th order integrator, agrees with one found by Forest and Ruth [3,4] and by Neri [6]. For 6th and 8th orders, symplectic integrators with fewer steps are also obtained, for which the coefficients are given as a numerical solution of a set of simultaneous algebraic equations (section 5).

2. Problem to be solved

Let A and B be non-commutative operators and τ be a small real number. Then,

Problem. For a given positive integer n which will be called the *order of integrator*, find a set of real numbers $(c_1, c_2, ..., c_k)$ and $(d_1, d_2, ..., d_k)$ such that the difference of the exponential function $\exp[\tau(A + B)]$ and the product of exponential functions

$$\exp(c_1 \tau A) \exp(d_1 \tau B) \exp(c_2 \tau A) \exp(d_2 \tau B) \times ...$$

$$\times \exp(c_k \tau A) \exp(d_k \tau B)$$

is of the order of τ^{n+1}, i.e., the following equality holds,

$$\exp[\tau(A + B)]$$

$$= \prod_{i=1}^{k} \exp(c_i \tau A) \exp(d_i \tau B) + \mathrm{o}(\tau^{n+1}) . \tag{2.1}$$

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For example when $n=1$, a trivial solution is $c_1=d_1=1$ ($k=1$), and we have

$$\exp[\tau(A+B)]=\exp(\tau A)\exp(\tau B)+\mathrm{o}(\tau^2)\ . \quad (2.2)$$

When $n=2$, we find that $c_1=c_2=\frac{1}{2}$, $d_1=1$, $d_2=0$ ($k=2$), thus

$$\exp[\tau(A+B)]$$
$$=\exp(\tfrac{1}{2}\tau A)\exp(\tau B)\exp(\tfrac{1}{2}\tau A)+\mathrm{o}(\tau^3)\ . \quad (2.3)$$

Although the problem above is quite general and may have wide applications, it is directly related to the symplectic integrator of the Hamiltonian system (1.1) as shown by Neri [6].

Introducing the notation $z=(q,p)$, the Hamilton equation is written in the form

$$\dot{z}=\{z,H(z)\}\ , \quad (2.4)$$

where braces stand for the Poisson bracket, $\{F,G\}=F_q G_p-F_p G_q$. If we introduce a differential operator D_G by $D_G F:=\{F,G\}$, (2.4) is written as $\dot{z}=D_H z$, so the formal solution, or the exact time evolution of $z(t)$ from $t=0$ to $t=\tau$ is given by

$$z(\tau)=[\exp(\tau D_H)]z(0)\ . \quad (2.5)$$

For a Hamiltonian of the form (1.1), $D_H=D_T+D_V$ and we have the formal solution

$$z(\tau)=\exp[\tau(A+B)]z(0)\ , \quad (2.6)$$

where $A:=D_T$, and $B:=D_V$.

Suppose (c_i,d_i) ($i=1,2,...,k$) is a set of real numbers which satisfy the equality (2.1) for a given integer n. Now consider a mapping from $z=z(0)$ to $z'=z(\tau)$ given by

$$z'=\left(\prod_{i=1}^{k}\exp(c_i\tau A)\exp(d_i\tau B)\right)z\ . \quad (2.7)$$

This mapping is symplectic because it is just a product of elementary symplectic mappings, and approximates the exact solution (2.6) up to the order $\mathrm{o}(\tau^n)$. Furthermore, (2.7) is explicitly computable although (2.6) is only formal. In fact (2.7) gives the succession of the mappings,

$$q_i=q_{i-1}+\tau c_i\frac{\partial T}{\partial p}(p_{i-1})\ ,$$

$$p_i=p_{i-1}-\tau d_i\frac{\partial V}{\partial q}(q_i)\ , \quad (2.8)$$

for $i=1$ to $i=k$, with $(q_0,p_0)=z$ and $(q_k,p_k)=z'$. An nth order symplectic integrator (integration scheme) is thus obtained.

The direct approach to the problem is obviously as follows. We expand the left hand side of (2.1) in powers of τ and equate the coefficients of the equal powers of τ up to the order τ^n. Thus, we obtain a set of non-linear algebraic equations for unknowns c_i and d_i. For example when $n=1$ (1st order integrator), we have two equations from the coefficients of A and B,

$$c_1+c_2+...+c_k=1\ ,\quad d_1+d_2+...+c_k=1\ , \quad (2.9)$$

so that the simplest solution is $k=1$, $c_1=d_1=1$. When $n=2$ (2nd order integrator), in addition to (2.9), we have an equation coming from the coefficient of AB,

$$c_1(d_1+d_2+...d_k)+c_2(d_2+d_3+...+d_k)+...+c_k d_k$$
$$=\tfrac{1}{2}\ , \quad (2.10)$$

and the simplest solution is $k=2$, $c_1=c_2=\frac{1}{2}$, $d_1=1$. In this straightforward way, Neri [6] obtained a 4th order integrator ($k=4$),

$$c_1=c_4=\frac{1}{2(2-2^{1/3})}\ ,\quad c_2=c_3=\frac{1-2^{1/3}}{2(2-2^{1/3})}\ ,$$

$$d_1=d_3=\frac{1}{2-2^{1/3}}\ ,\quad d_2=-\frac{2^{1/3}}{2-2^{1/3}}\ ,\quad d_4=0\ . \quad (2.11)$$

But with this direct method, it is almost hopeless to obtain a much higher integrator.

We now mention that (2.1) is equivalent to

$$S(\tau):=\prod_{i=1}^{k}\exp(c_i\tau A)\exp(d_i\tau B)$$

$$=\exp([\tau(A+B)+\mathrm{o}(\tau^{n+1})])\ , \quad (2.12)$$

and in the following sections we use some indirect method to find the set of coefficients (c_i,d_i) satisfying (2.12).

3. Basic formulas

First we recall the Baker–Campbell–Hausdorff

(BCH) formula [8,4,7]. For any non-commutative operators X and Y, the product of the two exponential functions, $\exp(X)\,\exp(Y)$, can be expressed in the form of a single exponential function as

$$\exp(X)\,\exp(Y) = \exp(Z) ,$$

where

$$Z = X + Y + \tfrac{1}{2}[X, Y]$$
$$+ \tfrac{1}{12}([X, X, Y] + [Y, Y, X]) + \tfrac{1}{24}[X, Y, Y, X]$$
$$- \tfrac{1}{720}([Y, Y, Y, Y, X] + [X, X, X, X, Y])$$
$$+ \tfrac{1}{360}([Y, X, X, X, Y] + [X, Y, Y, Y, X])$$
$$+ \tfrac{1}{120}([X, X, Y, Y, X] + [Y, Y, X, X, Y])$$
$$+ \dots . \tag{3.1}$$

Here we used the notation of the commutator $[X, Y] := XY - YX$, and higher order commutators like $[X, X, Y] := [X, [X, Y]]$. A remarkable feature of this BCH formula is that there appear only commutators of X and Y except for the linear terms in the series (3.1).

By repeated application of the BCH formula (3.1), we find

$$\exp(X)\,\exp(Y)\,\exp(X) = \exp(W) ,$$

where

$$W = 2X + Y + \tfrac{1}{6}[Y, Y, X] - \tfrac{1}{6}[X, X, Y]$$
$$+ \tfrac{7}{360}[X, X, X, X, Y] - \tfrac{1}{360}[Y, Y, Y, Y, X]$$
$$+ \tfrac{1}{90}[X, Y, Y, Y, X] + \tfrac{1}{45}[Y, X, X, X, Y]$$
$$- \tfrac{1}{60}[X, X, Y, Y, X] + \tfrac{1}{30}[Y, Y, X, X, Y]$$
$$+ \dots . \tag{3.2}$$

Thus the operator for the 2nd order symplectic integrator (2.3) can be written in the form

$$S_{2\text{nd}}(\tau) := \exp(\tfrac{1}{2}\tau A)\,\exp(\tau B)\,\exp(\tfrac{1}{2}\tau A)$$
$$= \exp(\tau\alpha_1 + \tau^3\alpha_3 + \tau^5\alpha_5 + \tau^7\alpha_7 + \dots) , \tag{3.3}$$

where

$$\alpha_1 := A + B , \quad \alpha_3 := \tfrac{1}{12}[B, B, A] - \tfrac{1}{24}[A, A, B] ,$$
$$\alpha_5 := \tfrac{7}{5760}[A, A, A, A, B] + \dots .$$

We now mention that in the expression (3.3) there exist no terms of even powers of τ, i.e.,

$\alpha_2 = \alpha_4 = \alpha_6 = \dots = 0$. This comes from the fact that the operator $S_{2\text{nd}}(\tau)$ is symmetric and has the exact time reversibility

$$S(\tau)S(-\tau) = S(-\tau)S(\tau) = \text{identity} . \tag{3.4}$$

Indeed this is an example of a more general statement as follows.

Lemma. Let $S(\tau)$ be an operator of the form (2.12) which has the time reversibility (3.4). If we expand $S(\tau)$ in the form

$$S(\tau) = \exp(\tau\gamma_1 + \tau^2\gamma_2 + \tau^3\gamma_3 + \tau^4\gamma_4 + \dots) \tag{3.5}$$

then

$$\gamma_2 = \gamma_4 = \gamma_6 = \dots = 0 .$$

To see this, we make the product of $S(\tau)$ and

$$S(-\tau) = \exp(-\tau\gamma_1 + \tau^2\gamma_2 - \tau^3\gamma_3 + \tau^4\gamma_4 - \dots) .$$

By the BCH formula (3.1) we find, for lower orders of τ,

$$S(\tau)S(-\tau) = \exp[2\tau^2\gamma_2 + o(\tau^3)] . \tag{3.6}$$

Since $S(\tau)S(-\tau) = 1$, the argument of the exponential function, $2\tau^2\gamma_2 + o(\tau^3)$, must vanish identically. This requires, at first, that $\gamma_2 = 0$. Now the same product gives

$$S(\tau)S(-\tau) = \exp[2\tau^4\gamma_4 + o(\tau^5)] \tag{3.7}$$

and requires that $\gamma_4 = 0$. By repeating this procedure we get $\gamma_6 = \gamma_8 = \dots = 0$.

Therefore if a symplectic integrator has a symmetric form so that (3.4) holds, it is automatically of an even order. Keeping this fact in mind, we now construct symplectic integrators (4th, 6th, 8th, ...) by a symmetric product of symplectic integrators of a lower order.

4. Symmetric integrator with exact coefficients

A 4th order integrator is obtained by a symmetric repetition (product) of the 2nd order integrator (3.3) in the form

$$S_{4\text{th}}(\tau) := S_{2\text{nd}}(x_1\tau)S_{2\text{nd}}(x_0\tau)S_{2\text{nd}}(x_1\tau) , \tag{4.1}$$

where x_0 and x_1 are two real unknowns to be deter-

mined. If we apply formula (3.2) to (4.1), with

$$S_{2nd}(x_1\tau) = \exp(\tau x_1\alpha_1 + \tau^3 x_1^3\alpha_3 + \tau^5 x_1^5\alpha_5 + ...) ,$$
$$(4.2)$$

and

$$S_{2nd}(x_0\tau) = \exp(\tau x_0\alpha_1 + \tau^3 x_0^3\alpha_3 + \tau^5 x_0^5\alpha_5 + ...) ,$$
$$(4.3)$$

we have

$$S_{4th}(\tau) = \exp[\tau(x_0 + 2x_1)\alpha_1 + \tau^3(x_0^3 + 2x_1^3)\alpha_3$$
$$+ \tau^5(x_0^5 + 2x_1^5)\alpha_5 + ...] .$$
$$(4.4)$$

In order that (4.4) gives a 4th order integrator, we need two conditions

$$x_0 + 2x_1 = 1 , \quad x_0^3 + 2x_1^3 = 0 ,$$
$$(4.5)$$

so that $S_{4th}(\tau) = \exp[\tau(A+B) + o(\tau^5)]$. The unique real solution is obviously

$$x_0 = -\frac{2^{1/3}}{2 - 2^{1/3}} , \quad x_1 = \frac{1}{2 - 2^{1/3}} .$$
$$(4.6)$$

If we compare the operator (4.1) with (2.12), we find the relations between the two sets of coefficients;

$$d_1 = d_3 = x_1 , \quad d_2 = x_0 ,$$

$$c_1 = c_4 = \tfrac{1}{2}x_1 , \quad c_2 = c_3 = \tfrac{1}{2}(x_0 + x_1) .$$

With the values (4.6), we find that (4.1) is exactly the same as the known 4th order integrator (2.11).

Once a 4th order integrator is found, it is easy to obtain a 6th order integrator using the 4th order one by the same process. By definition a 4th order (symmetric) integrator has an expansion

$$S_{4th}(\tau) = \exp[\tau\alpha_1 + \tau^5\tilde{\alpha}_5 + \tau^7\tilde{\alpha}_7 + o(\tau^9)] .$$
$$(4.7)$$

We try to get a 6th order integrator by the symmetric product

$$S_{6th}(\tau) := S_{4th}(y_1\tau)S_{4th}(y_0\tau)S_{4th}(y_1\tau) .$$
$$(4.8)$$

As before, by formula (3.2), (4.8) has the expansion

$$S_{6th}(\tau) = \exp[\tau(y_0 + 2y_1)\alpha_1 + \tau^5(y_0^5 + 2y_1^5)\tilde{\alpha}_5$$
$$+ o(\tau^7)] .$$
$$(4.9)$$

In order to be a 6th order integrator we must have

$$y_0 + 2y_1 = 1 , \quad y_0^5 + 2y_1^5 = 0 ,$$
$$(4.10)$$

or

$$y_0 = -\frac{2^{1/5}}{2 - 2^{1/5}} , \quad y_1 = \frac{1}{2 - 2^{1/5}} .$$
$$(4.11)$$

More generally, if a symmetric integrator of order $2n$, $S_{2n}(\tau)$, is already known, a $(2n+2)$th order integrator is obtained by the product

$$S_{2n+2}(\tau) := S_{2n}(z_1\tau)S_{2n}(z_0\tau)S_{2n}(z_1\tau) ,$$
$$(4.12)$$

where z_0 and z_1 must satisfy

$$z_0 + 2z_1 = 1 , \quad z_0^{2n+1} + 2z_1^{2n+1} = 0 ,$$
$$(4.13)$$

or

$$z_0 = -\frac{2^{1/(2n+1)}}{2 - 2^{1/2(2n+1)}} ,$$

$$z_1 = \frac{1}{2 - 2^{1/(2n+1)}} .$$
$$(4.14)$$

The combination of (4.1) and (4.8) gives

$$S_{6th}(\tau) := S_{2nd}(x_1 y_1\tau)S_{2nd}(x_0 y_1\tau)S_{2nd}(x_1 y_1\tau)$$

$$\times S_{2nd}(x_1 y_0\tau)S_{2nd}(x_0 y_0\tau)S_{2nd}(x_1 y_0\tau)$$

$$\times S_{2nd}(s_1 y_1\tau)S_{2nd}(x_0 y_1\tau)S_{2nd}(x_1 y_1\tau) ,$$
$$(4.15)$$

which implies the exact coefficients in (2.12) as

$$d_1 = d_3 = d_7 = d_9 = x_1 y_1 , \quad d_2 = d_8 = x_0 y_1 ,$$

$$d_4 = d_6 = x_1 y_0 , \quad d_5 = x_0 y_0 ,$$

and

$$c_1 = \tfrac{1}{2}d_1 , \quad c_{10} = \tfrac{1}{2}d_9 ,$$

$$c_i = \tfrac{1}{2}(d_{i-1} + d_i) , \quad i = 2, 3, ..., 9 .$$

In this way we can construct symplectic integrators of an arbitrary even order with exact coefficients. However, with this construction, the $(2n)$th order integrator requires the operator S_{2nd}, 3^{n-1} times. This means that the number of steps k is $k = 3^{n-1} + 1$, which grows rapidly as n increases. In the next section, an alternative method is shown to obtain more economically integrators, though the coefficients cannot be given analytically.

5. 6th and 8th order integrators with fewer steps

Let us define a symmetric operator $S^{(m)}(\tau)$ by

$$S^{(m)}(\tau) := S_{2nd}(w_m \tau) \times ... \times S_{2nd}(w_1 \tau) S_{2nd}(w_0 \tau)$$

$$\times S_{2nd}(w_1 \tau) \times ... \times S_{2nd}(w_m \tau) , \qquad (5.1)$$

with unknowns w_0, w_1, ..., w_m. If we apply formula (3.2) to express (5.1) in the form of a single exponential function, like (4.4), we find that in addition to the operators α_1, α_3, α_5, α_7, ..., there appear

$$\beta_5 := [\alpha_1, \alpha_1, \alpha_3]$$

at the order τ^5, and

$$\beta_7 := [\alpha_1, \alpha_1, \alpha_5] , \quad \gamma_7 := [\alpha_3, \alpha_3, \alpha_1] ,$$

$$\delta_7 := [\alpha_1, \alpha_1, \alpha_1, \alpha_1, \alpha_3]$$

at the order τ^7. Thus we write down (5.1) as

$$S^{(m)}(\tau) = \exp[\tau A_{1,m}\alpha_1 + \tau^3 A_{3,m}\alpha_3$$

$$+ \tau^5 (A_{5,m}\alpha_5 + B_{5,m}\beta_5)$$

$$+ \tau^7 (A_{7,m}\alpha_7 + B_{7,m}\beta_7 + C_{7,m}\gamma_7 + D_{7,m}\delta_7)$$

$$+ o(\tau^9)] . \qquad (5.2)$$

Comparing the both sides of

$$S^{(m+1)}(\tau) = S_{2nd}(w_{m+1}\tau) S^{(m)}(\tau) S_{2nd}(w_{m+1}\tau) \qquad (5.3)$$

with use of (3.2), we find recursion relations for the coefficients. Those for $A_{j,m}$ are simply

$$A_{1,m+1} = A_{1,m} + 2w_{m+1} , \qquad (5.4)$$

$$A_{3,m+1} = A_{3,m} + 2w_{m+1}^3 , \qquad (5.5)$$

$$A_{5,m+1} = A_{5,m} + 2w_{m+1}^5 , \qquad (5.6)$$

$$A_{7,m+1} = A_{7,m} + 2w_{m+1}^7 , \quad ... , \qquad (5.7)$$

with initial conditions

$$A_{1,0} = w_0 , \quad A_{3,0} = w_0^3 , \quad A_{5,0} = w_0^5 ,$$

$$A_{7,0} = w_0^7 , \quad ... .$$

For the other coefficients we find

$$B_{5,m+1} = B_{5,m} + \tfrac{1}{6}(A_{1,m}^2 w_{m+1}^3 - A_{1,m} A_{3,m} w_{m+1})$$

$$- \tfrac{1}{6}(A_{3,m} w_{m+1}^2 - A_{1,m} w_{m+1}^4) , \qquad (5.8)$$

$$B_{7,m+1} = B_{7,m} + \tfrac{1}{6}(A_{1,m}^2 w_{m+1}^5 - A_{1,m} A_{5,m} w_{m+1})$$

$$- \tfrac{1}{6}(A_{5,m} w_{m+1}^2 - A_{1,m} w_{m+1}^6) , \qquad (5.9)$$

$$C_{7,m+1} = C_{7,m} + \tfrac{1}{6}(A_{3,m}^2 w_{m+1} - A_{1,m} A_{3,m} w_{m+1}^3)$$

$$- \tfrac{1}{6}(A_{1,m} w_{m+1}^6 - A_{3,m} w_{m+1}^4) , \qquad (5.10)$$

$$D_{7,m+1} = D_{7,m} + \tfrac{7}{360}(A_{3,m} w_{m+1}^4 - A_{1,m} w_{m+1}^6)$$

$$+ \tfrac{7}{180}(A_{1,m} A_{3,m} w_{m+1}^3 - A_{1,m}^2 w_{m+1}^5)$$

$$- \tfrac{1}{45}(A_{1,m}^3 w_{m+1}^4 - A_{1,m}^2 A_{3,m} w_{m+1}^2)$$

$$- \tfrac{1}{360}(A_{1,m}^4 w_{m+1}^3 - A_{1,m}^3 A_{3,m} w_{m+1})$$

$$- \tfrac{1}{6}(B_{5,m} w_{m+1}^2 + A_{1,m} B_{5,m} w_{m+1}) , \qquad (5.11)$$

with initial conditions

$$B_{5,0} = B_{7,0} = C_{7,0} = D_{7,0} = 0 .$$

For $A_{j,m}$ we have obviously

$$A_{1,m} = w_0 + 2(w_1 + w_2 + ... + w_m) , \qquad (5.12)$$

$$A_{3,m} = w_0^3 + 2(w_1^3 + w_2^3 + ... + w_m^3) , \qquad (5.13)$$

$$A_{5,m} = w_0^5 + 2(w_1^5 + w_2^5 + ... + w_m^5) , \qquad (5.14)$$

$$A_{7,m} = w_0^7 + 2(w_1^7 + w_2^7 + ... + w_m^7) . \qquad (5.15)$$

But for other coefficients, the result is not concise. The obvious fact is that for a given m, we have $B_{5,m} = B_{5,m}(w_0, w_1, ..., w_m)$ which is a homogeneous polynomial of degree 5 in w, and $B_{7,m}$, $C_{7,m}$, $D_{7,m}$ which are homogeneous polynomials of degree 7 in w.

Now in order that (5.1) gives a 6th order integrator, we have the four conditions

$$A_{1,m} = 1 , \quad A_{3,m} = 0 , \quad A_{5,m} = 0 , \quad B_{5,m} = 0 , \qquad (5.16)$$

so that $m = 3$ is necessary and sufficient. Thus (5.16) is considered as a set of simultaneous algebraic equations for unknowns (w_0, w_1, w_2, w_3). In order to obtain an 8th order integrator, we need further four conditions

$$A_{7,m} = 0 , \quad B_{7,m} = 0 , \quad C_{7,m} = 0 , \quad D_{7,m} = 0 , \qquad (5.17)$$

in addition to (5.16). Therefore $m = 7$, and we have a set of simultaneous algebraic equations (5.16) and (5.17) for unknowns $(w_0, w_1, ..., w_7)$. We can always reduce one order of the simultaneous algebraic equations by eliminating w_0 using $A_{1,m} = 1$, i.e.,

$$w_0 = 1 - 2(w_1 + w_2 + ... + w_m) . \qquad (5.18)$$

Table 1
6th order symplectic integrators.

	Solution A	Solution B	Solution C
w_1	−0.117767998417887E1	−0.213228522200144E1	0.152886228424922E−2
w_2	0.235573213359357E0	0.426068187079180E−2	−0.214403531630539E1
w_3	0.784513610477560E0	0.143984816797678E1	0.144778256239930E1

Table 2
8th order symplectic integrators.

	Solution A	Solution B	Solution C
w_1	−0.161582374150097E1	−0.169248587770116E−2	0.311790812418427E0
w_2	−0.244699182370524E1	0.289195744315849E1	−0.155946803821447E1
w_3	−0.716989419708120E−2	0.378039588360192E−2	−0.167896928259640E1
w_4	0.244002732616735E1	−0.289688250328827E1	0.166335809963315E1
w_5	0.157739928123617E0	0.289105148970595E1	−0.106458714789183E1
w_6	0.182020630970714E1	−0.233864815101035E1	0.136934946416871E1
w_7	0.104242620869991E1	0.148819229202922E1	0.629030650210433E0

	Solution D	Solution E
w_1	0.102799849391985E0	0.227738840094906E−1
w_2	−0.196061023297549E1	0.252778927322839E1
w_3	0.193813913762276E1	−0.719180053552772E−1
w_4	−0.158240635368243E0	0.536018921307285E−2
w_5	−0.144485223686048E1	−0.204809795887393E1
w_6	0.253693336566229E0	0.107990467703699E0
w_7	0.914844246229740E0	0.130300165760014E1

A set of algebraic equations is thus obtained, which has the general form

$$f_1(w_1, w_2, ..., w_m) = 0 ,$$

$$f_2(w_1, w_2, ..., w_m) = 0 ,$$

...

$$f_m(w_1, w_2, ..., w_m) = 0 ,$$

and must be solved numerically. The Newton–Raphson method is familiar to solve this kind of equations. However it is difficult to derive the expression for the Jacobian matrix $\partial f_i / \partial w_j$, which is necessary for the Newton–Raphson method. Here we have used the Brent method [9] which does not need the Jacobian matrix and is suitable for our problem.

Using the Brent method, three solutions (w_1, w_2, w_3) for the 6th order integrator have been obtained. It seems that there is no other solution. For the 8th

order integrator at least five solutions (w_1, w_2, ..., w_7) have been obtained. These numerical values are listed in tables 1 and 2. Once the values of the w_i are obtained, we get the original coefficients in (2.12) as ($k = 2m + 2$)

$$d_1 = d_{2m+1} = w_m , \quad d_2 = d_{2m} = w_{m-1} , \quad ... ,$$

$$d_m = d_{m+2} = w_1 , \quad d_{m+1} = w_0 ,$$

and

$$c_1 = c_{2m+2} = \tfrac{1}{2} w_m , \quad c_2 = c_{2m+1} = \tfrac{1}{2}(w_m + w_{m-1}) ,$$

$$... , \quad c_{m+1} = c_{m+2} = \tfrac{1}{2}(w_1 + w_0) .$$

For the 6th order integrator ($n = 3$) the number of steps is $k = 8$, and for the 8th order integrator, $k = 16$. On the other hand in the case of the previous section, $k = 10$ for the 6th order integrator and $k = 28$ for the 8th order one. Therefore the integrators in this section are really time-saving.

Application of these integrators to the gravitational N-body problem is now is progress [5] and will be published elsewhere. In order to obtain 10th order integrators in this way, the next order of the BCH formulae (3.1) and (3.2) becomes necessary, and the order of the simultaneous algebraic equations becomes much higher.

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