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A CANONICAL INTEGRATION TECHNIQUE**

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There are many different ways to integrate differential equations numerically.[1] These various methods are usually characterized by the accuracy of a single step in time. Thus if in a small time step, h, the integration is performed so that it is accurate through order h^n, then the method is referred to as an n^{th} order integration method.

The class of differential equations of interest here is that in which the equations are derivable from a Hamiltonian using Hamilton's equations. The exact solution of such a system of differential equations leads to a symplectic map from the initial conditions to the present state of the system. A characteristic feature of all explicit high order (n>2) integration methods, however, is that they are not exactly symplectic. One manifestation of this is that the Jacobian of the transformation for one time step differs slightly from unity, and so the system will be damped (or excited) artificially. In many applications the salient features of the solutions appear only after long times or large numbers of iterations; in these applications spurious damping or excitation may lead to misleading results.

The purpose of this note is to develop an explicit third order symplectic map (i.e. a third order integration step that preserves exactly the canonical character of the equations of motion) and to indicate the method for higher order maps. For a typical numerical integration, this method can be used to eliminate the noncanonical effects while providing the accuracy corresponding to a third order integration step.

There is in addition another benefit of this approach. If we iterate a map of a given order whether canonical or not, eventually the absolute error in $\vec{x}$ and $\vec{p}$ gets large. In cases where spurious damping occurs, $\vec{x}$ and $\vec{p}$ typically settle into some stable fixed point[2]. If the map is symplectic, this is not the case. A symplectic map generates phase space behaviour which is close to that of the original system with errors in phase which eventually may add up after many interations to yield large absolute errors in $\vec{x}$ and $\vec{p}$.

Therefore, in the symplectic case, it is possible and sometimes attractive to replace the differential equation by a symplectic map. This map then becomes the object of study and so can be iterated as much as we like. This is possible since the map is the solution of some physical Hamiltonian problem which, in some sense, is close to the original problem. For other integration methods this is not the case and iterations must be terminated at some point.

The Problem

Consider a system of differential equations governed by the Hamiltonian,

$$H = \vec{p}^2/2 + V(\vec{x},t). \tag{1}$$

This is just Newton's second law with the potential $V(\vec{x},t)$. The solution of the equations of motion is given by the functions

$$\vec{x}(\vec{x}_0,\vec{p}_0,t) \quad \text{and} \quad \vec{p}(\vec{x}_0,\vec{p}_0,t), \tag{2}$$

where $\vec{x}_0$ and $\vec{p}_0$ are the initial conditions at time t = 0. Due to the canonical character of the equations of motions, Equation (2) constitutes a canonical transformation (or a symplectic map) from the initial conditions to the state at time t which we denote by

$$(x,p) = M(t)(x_0,p_0). \tag{3}$$

Now the question is: if the parameter t is small, can this map be found approximately to some given order in t? If this can be done explicitly, then the process can easily be iterated and the error controlled by adjusting the step size, t. Of course, the typical integration method does just this but sacrifices the canonical character of the map. This we propose to avoid. Let the approximate n^{th} order symplectic map be denoted by

$$(x,p) = M_n(t)(x_0,p_0), \tag{4}$$

where t is the time step (assumed small) and n is the order of the map, i.e.

$$||M(t) - M_n(t)|| = O(t^{n+1}). \tag{5}$$

In the next section we demonstrate a method for finding $M_n(t)$.

The Method

To illustrate the method first start from low order. If we somehow perform the transformation in Equation (3) so that H is expressed in terms of the initial conditions, then the equations of motion are

$$\frac{d\vec{x}_0}{dt} = 0 \qquad \frac{d\vec{p}_0}{dt} = 0, \tag{6}$$

or the new Hamiltonian, H', is identically zero (or at least independent of x_0,p_0). This suggests that we make canonical transformations in such a way as to make H vanish. Thus the program is to make these successive canonical transformations until we arrive at the initial conditions of the problem, or at least to another set of coordinates which approximates (x_0,p_0) through some order in t.

Let (x_1,p_1) be the new coordinates. Then the convenient form for the generating function of the canonical transformation is that involving the new coordinates and old momenta:[3]

$$(x,p)\rightarrow(x_1,p_1)$$

$$\text{Gen. Function:} \quad F_3(x_1,p,t) = -x_1p + G(x_1,p,t) \tag{7}$$

$$x = \frac{-\partial F_3}{\partial p} = x_1 - G_p, \qquad p_1 = \frac{-\partial F_3}{\partial x_1} = p - G_{x_1}$$
$$H_1 = H + \frac{\partial F_3}{\partial t} = H + G_t, \tag{8}$$

where subscripts have been used to denote partial derivatives. Equations (8) suggest that we select

$$G = -\{p^2/2 + V(x_1,0)\}t \tag{9}$$

so that

$$p_1 = p - f(x_1,0)t \qquad x = x_1 + pt, \tag{10}$$

where the force, f, has been introduced,

$$f(x,0) = -\partial V(x,0)/\partial x. \tag{11}$$

Subsituting into the Hamiltonian yields

$$H_1 = V(x_1 + t(p_1 + f(x_1,0)t),t) - V(x_1,0) \tag{12}$$

and expanding on the small parameter t, we have

$$H_1 = tV_t(x_1,0) - tp_1f(x_1,0) + O(t^2). \tag{13}$$

Since H_1 is O(t), the right hand sides of the differential equations from Hamilton's Equations are also O(t). Therefore, the solution is

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$$x_1 = \text{const} + O(t^2) \qquad p_1 = \text{const} + O(t^2). \tag{14}$$

So if x_1 and p_1 are used as initial conditions, the error introduced is $O(t^2)$. Thus this approach has yielded a first order symplectic map, $M_1(t)$.

Since this is such a low order method, it could have been derived by inspection; however, it illustrates the method which will be used in the next and subsequent sections. Notice that if (x_1, p_1) are viewed as initial conditions in Equation (10), then the momentum p must be calculated first and then used to evaluate x. This is a characteristic feature of the method. In addition note that the transformation leads back to the initial conditions; thus, the momentum equation must be inverted (trivial in this case).

The Second Order Map

It is possible to continue from the results of the previous section to obtain a second order map; however, there is a well known method (the leap frog method) which is exactly canonical, is second order and which requires only one evaluation of the force. In order to understand that method and to lay the groundwork for a third order map, it is useful to modify the approach in the previous section. The modification consists of performing two canonical transformations rather than one. These are given by:

$$(x,p)\to(x_1,p_1): \qquad x = x_1 + apt, \quad p_1 = p - tf(x_1,bt)$$
$$F = -x_1 p - a\frac{p^2 t}{2} - tV(x_1,bt), \tag{15}$$
$$(x_1,p_1)\to(x_2,p_2): \qquad x_1 = x_2 + (1-a)p_1 t, \quad p_2 = p_1$$
$$F = -x_2 p_1 - \frac{(1-a)}{2}p_1^2 t.$$

Thus, there is an intermediate step at which the force is evaluated. At this time the parameters a and b are undetermined; however, these can be used to generate a second order map. Substituting the two transformations into the Hamiltonian and expanding in the small parameter, t, yields

$$H_2 = t(1-2a)p_2 f(x_2,0) + t(1-2b)V_t(x_2,0) + O(t^2). \tag{16}$$

The purpose of the expansion in t is to identify the coefficients of various powers in H_2. The transformation equations in Equation (15), however, must be kept exactly in order to preserve the canonical character.

Now recall from the previous section that if H is of $O(t^n)$, and if (p_2,x_2) are used as initial conditions, the resulting map is n^{th} order. Therefore, if we choose

$$a = b = 1/2, \tag{17}$$

then H_2 is $O(t^2)$, and the total map is second order.

To summarize the preceding results shift the notation $(x_2\to x_0, p_2\to p_0)$, rewrite the transformations in the reverse order and perform the obvious generalisation to many dimensions. Then the second order map is given by the scheme following:

Second Order

$H = \vec{p}^2/2 + V(\vec{x},t)$, $\qquad \vec{f} = -\partial V/\partial \vec{x}$

time step = h, initial conditions = $(\vec{x}_0,\vec{p}_0,t_0)$

Map : $(\vec{x},\vec{p}) = M_2(h)(\vec{x}_0,\vec{p}_0)$
given by two step process: (18)

1) $\vec{p}_1 = \vec{p}_0$, $\qquad \vec{x}_1 = \vec{x}_0 + \vec{p}_1 h/2$

2) $\vec{p} = \vec{p}_1 + t\vec{f}(\vec{x}_1, t_0+h/2)$, $\quad \vec{x} = \vec{x}_1 + \vec{p}h/2$

This method is well known (the leap frog method) and used frequently in circumstances where anomolous damping or excitation is undesirable. Note that it is written somewhat differently than usual since it is calculated for one full step. Since it is useful to have higher order maps for savings in computation time and for improved accuracy of the phase space behavior, in the next section this method is extended to third order.

Third Order Maps

There are many possible generalisations to extend the procedure described in the previous sections to higher order. The first approach that comes to mind is to include more intermediate steps or additional force evaluations. A second approach is to begin from the second order Hamiltonian and make yet another canonical transformation to eliminate another order in the t dependence of H. Both of these approaches are possible in principle and will work; however, there is one difficulty. The functional dependence in x and p of the terms which are of higher order in t can be quite complicated. Because of the nature of canonical transformations, one is forced to invert an equation $p_1(p_0)\to p_0(p_1)$. This can be done explicitly only in the simplest cases. In more complicated cases the functional form is implicit, and thus the utility of such an approach can be extemely diminished due to the lack of explicit formulae.

Fortunately, for the simple Hamiltonian in Equation (1) there is a method of avoiding this. The key to avoiding implicit expressions lies in two points. The first is that an exact expression relating new to old variables is only necessary in transformation equations. It is fine to substitute approximate perturbative expressions into the Hamiltonian (this has been done already). The second point is that only one half of the equations from the generating function need to be inverted. In our case this is the momentum equation. With this in mind a combination of the two approaches mentioned above will be used in order to generate a third order map. First write a somewhat more general two step transformation given by:

$$(x,p)\to(x_1,p_1): \quad F(x_1,p,t) = -x_1 p - \frac{ap^2 t}{2} - btV(x_1,ct)$$
$$p_1 = p - btf(x_1,ct) \qquad x = x_1 + apt,$$
$$(x_1,p_1)\to(x_2,p_2): \quad F = -x_2 p_1 - \frac{(1-a)}{2}p_1^2 t - (1-b)tV(x_2,dt) \tag{19}$$
$$p_2 = p_1 - (1-b)tf(x_2,dt) \qquad x_1 = x_2 + (1-a)p_1 t$$

Subsituting into the Hamiltonian in Equation (1) and expanding in the small parameter, t, we find (after some algebra)

$$H_2 = tp_2 f(x_2,0)\left[2b(1-a) - 1\right] + tV_t\left[1 - 2bc - 2(1-b)d\right]$$
$$+t^2 p_2^2 f_x\left[3(1-a)^2 b/2 - 1/2\right] + t^2 V_{tt}\left[1/2 - 3bc^2/2 - 3(1-b)d^2/2\right]$$
$$+ t^2 f_t p_2\left[3cb(1-a) - 1\right] \tag{20}$$
$$+ t^2 f^2\left[2(1-a)(1-b)b + b^2(1-a)/2 - ab - (1-b)\right] + O(t^3).$$

The philosophy of selecting the free parameters in this case is the same as in previous sections with one exception. Since there are more equations than unknowns, it is impossible to eliminate all second order terms at this step. However, another transformation can remove the remaining terms, provided that the equation for the momentum transformation is trivial to invert. Anticipating this problem, first eliminate all terms in Equation (20) with powers of p_2. This yields 3 equations for 3 unknowns with the solutions,

$$b = 3/4 \quad a = 1/3, \quad c = 2/3. \tag{21}$$

In addition the terms with time derivatives both vanish with the choice

$$d = 0. \tag{22}$$

With this choice of parameters H_2 becomes

$$H_2 = - t^2 f^2(x_2,0)/16 + O(t^3). \tag{23}$$

The transformation to eliminate the last $O(t^2)$ term is

$$F(x_3,p_2) = - x_3 p_2 + t^3 f^2(x_3,0)/48$$
$$p_3 = p_2 - t^3 f f_x(x_3,0)/24 \qquad x_2 = x_3 \tag{24}$$

However, since x is changed, we can simply combine the previous transformation with the second one in Eq (19).

Therefore, if we rewrite with the change of notation $x_2 \to x_0$, generalise to the multidimensional case, and rewrite the transformations in the opposite order, we find a third order symplectic map given by the following scheme:

Third Order

$H = \vec{p}^2/2 + V(x,t)$, $\quad \vec{f} = - \partial V/\partial \vec{x}$

time step = h; initial conditions = $(\vec{x}_0,\vec{p}_0,t_0)$

Map; $(\vec{x},\vec{p}) = M_3(h)\ (\vec{x}_0,\vec{p}_0)$, given by two step process: (25)

1) $\vec{p}_1 = \vec{p}_0 + \frac{1}{4} h\vec{f}(\vec{x}_0,t_0) + \frac{h^3}{48}\vec{\nabla}\left[\vec{f}(\vec{x}_0,t_0).\vec{f}(\vec{x}_0,t_0)\right]$

$\vec{x}_1 = \vec{x}_0 + 2h\vec{p}_1/3$

2) $\vec{p} = \vec{p}_1 + \frac{3}{4} h\ \vec{f}(\vec{x}_1,t_0+\frac{2}{3}h)$ $\quad \vec{x} = \vec{x}_1 + \frac{h}{3}\vec{p}$

A More General Hamiltonian

The previous sections have considered the Hamiltonian in Equation (1). In this section we treat a somewhat more general case given by

$$H = g(\vec{p}) + V(\vec{x},t). \tag{26}$$

Notice that a special case of Equation (26) is the Hamiltonian for relativistic motion. In that case

$$g(\vec{p}) = c\sqrt{\vec{p}.\vec{p} + m^2c^2}. \tag{27}$$

In addition Equation (26) can be used for the case of motion in a magnetic field which is described by only one component of the vector potential (say A_z). In this case the independent variable is z rather than t.

For the Hamiltonian in Equation (26), the "leap-frog" algorithm yields results correct through second order provided that it is modified as follows:

More General Second Order

$H = g(\vec{p}) + V(\vec{x},t)$, $\quad \vec{f} = -\partial V/\partial \vec{x}$

time step = h, initial conditions $(\vec{x}_0,\vec{p}_0,t_0)$

Map: $(\vec{x},\vec{p}) = M_2(h)(\vec{x}_0,\vec{p}_0)$ (28)
given by two step process:

1) $\vec{p}_1 = \vec{p}_0$ $\quad \vec{x}_1 = \vec{x}_0 + \frac{h}{2}\frac{dg(\vec{p}_1)}{d\vec{p}}$

2) $\vec{p} = \vec{p}_1 + h\vec{f}(\vec{x}_1,t_0+h/2)$ $\quad \vec{x} = \vec{x}_1 + \frac{h}{2}\frac{dg(\vec{p})}{d\vec{p}}$

Again, this method is expressed for one full time step and thus may appear somewhat different than the typical implementation in a computer code.

In addition, it is possible to obtain a third order map for the more general Hamiltonian. In this case it is necessary to perform a three step canonical transformation in order to avoid implicit expressions. Using the methods developed in the previous sections, the third order map can be written as

More General Third Order

$H = g(\vec{p}) + V(\vec{x},t)$, $\quad \vec{f} = -\partial V/\partial \vec{x}$

time step = h, initial conditions $(\vec{x}_0,\vec{p}_0,t_0)$

Map: $(\vec{x},\vec{p}) = M_3(h)(\vec{x}_0,\vec{p}_0)$ (29)
given by three step process:

1) $\vec{p}_1 = \vec{p}_0 + c_1 h\vec{f}(\vec{x}_0,t_0)$ $\quad \vec{x}_1 = \vec{x}_0 + d_1 h\frac{dg}{d\vec{p}}(\vec{p}_1)$

2) $\vec{p}_2 = \vec{p}_1 + c_2 h\vec{f}(\vec{x}_1,t_0+d_1h)$ $\quad \vec{x}_2 = \vec{x}_1 + d_2 h\frac{dg}{d\vec{p}}(\vec{p}_2)$

3) $\vec{p} = \vec{p}_2 + c_3 h\vec{f}(\vec{x}_2,t_0+(d_1+d_2)h)$, $\vec{x} = \vec{x}_2 + d_3 h\frac{dg}{d\vec{p}}(\vec{p})$

The c's and d's must satisfy the following equations,

$$c_1+c_2+c_3=1\ ,\ d_1+d_2+d_3=1\ ,\ c_2d_1+c_3(d_1+d_2)=1/2$$
$$c_2d_1^2+c_3(d_1+d_2)^2=1/3\ ,\ d_3+d_2(c_1+c_2)^2+d_1c_1^2=1/3 \tag{30}$$

Notice that there are five equations for six unknowns; thus, there are many solutions. One particularly simple solution is obtained by setting $d_3=1$[4].

$$c_1 = 7/24 \quad c_2 = 3/4 \quad c_3 = -1/24$$
$$d_1 = 2/3 \quad d_2 = -2/3 \quad d_3 = 1 \tag{31}$$

Notice that this three step third order map has no derivative of the force. In that sense it is the simplest (as well as the most general) obtained here.

Conclusions and Speculations

The purpose of this note has been two-fold; firstly to present results for third order symplectic maps, and secondly to illustrate, in some detail, the method in order to point the way to higher order maps. The third order maps obtained are not unique.

The general Hamiltonian will probably always lead to implicit equations for the final state in terms of the initial conditions; however, there is one other interesting Hamiltonian which may have an explicit high order map,

$$H = [\vec{p}-\vec{A}(\vec{x},t)]^2/2 \tag{32}$$

where A is just the vector potential for an electromagnetic field. In this case the troublesome term is

$$\vec{p}\ .\ \vec{A}. \tag{33}$$

This leads to matrix inversion even in the first order case and for order higher than two, it may be difficult to obtain explicit formulae. However, it is probably possible to write down a second order map and may be possible to find an explicit third order map.

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