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METHODS OF INTEGRATION WHICH PRESERVE THE CONTACT TRANSFORMATION PROPERTY OF THE HAMILTON EQUATIONS

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RENE DEVOGELAERE

DEPARTMENT OF MATHEMATICS

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Methods of integration which preserve the contact transformation property of the Hamilton equations.

René DeVogelaere* 26 ...

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0. Summary. Hamilton equations are such that the relation, between the coordinates and momenta at time t and at time t_o, is a contact transformation. Methods of integration of Hamilton equations, which do preserve the contact transformation property are given here. These methods are of first and second order. They are given, for the equation $\dot{x}= f(x,t)$, then for the case of one degree of freedom, then for the general case. Some of the formulae are implicit.

1. Introduction. In recent years the construction of high powered accelerators has led to vast programs of computations involving the solution S_1 over a very long time range of Hamiltonian systems describing approximately the motion S of a proton in the accelerator. Errors between the computed solution S_2 and S_1 are introduced because of the method of integration (finite step of increase of t and because of round-off (finite number of binary or decimal digits). Their worst effect is probably to destroy the contact transformation property of S. Hence the suggestion of using a method of integration which, if there was no round-off error, would give a solution S_3 with the contact transformation property. Moreover, if the error, due to the finiteness of increase of t_1 is not too large, one may even expect that the error between S_3 and S will be of the same order of

magnitude as the error between S_1 and S. How good the solution S_2 has to be, will depend on a study of the physical system and its Hamilton approximation. One should also ~~to check if~~ make sure that the discontinuities in the derivatives introduced at each step, by the method of integration do not alter significantly the results.

One may expect that second order methods may lead to significant results even with step increments which are not too small.

The contact transformation property does reduce to area conservation when the Hamiltonian has one degree of freedom. We feel that it is not surperfluous to treat first this case in detail, it did lead us to the general case and we hope that the procedure used may give a lead to the construction of higher order methods. Two known first order methods are given for the special case

$$\ddot{x} = f(x,t), \tag{1.1}$$

they are extended to the case

$$\dot{x} = \frac{\partial H}{\partial y} \tag{1.2}$$

$$\dot{y} = -\frac{\partial H}{\partial x} .$$

Second order methods are described. The error term for one step is given, it may also provide a lead to higher order methods. The error after n steps is not given. (7.4) and (7.5) are probably the most important formulae in this paper.

2. Some basic properties. We will first recall a certain number of basic properties relevant to this paper, although their generalization is well known.

Definition 2.1 If $x_1 = f(x_o, y_o)$ and $y_1 = g(x_o, y_o)$ are two functions, continuous in x_o, y_o as well as their first partial derivatives,

$$J = \frac{d(x_1, y_1)}{d(x_o, y_o)} = \begin{vmatrix} \frac{\partial x_1}{\partial x_o} & \frac{\partial x_1}{\partial y_o} \\ \frac{\partial y_1}{\partial x_o} & \frac{\partial y_1}{\partial y_o} \end{vmatrix}$$

is called the Jacobian of x_1, y_1 with respect to x_o, y_o.

Property 2.1 If $x_1 = x_o$ and $y_1 = f(x_o, y_o)$,

$$\frac{d(x_1, y_1)}{d(x_o, y_o)} = \frac{\partial y_1}{\partial y_o} .$$

Property 2.2 If $x_2 = F(x_1, y_1)$ and $y_2 = G(x_1, y_1)$, then

$$\frac{d(x_2, y_2)}{d(x_o, y_o)} = \frac{d(x_2, y_2)}{d(x_1, y_1)} \cdot \frac{d(x_1, y_1)}{d(x_o, y_o)} .$$

Property 2.3 If $\frac{d(x_1, y_1)}{d(x_o, y_o)} \neq 0$, then

$$\frac{d(x_o, y_o)}{d(x_1, y_1)} = \left[\frac{d(x_1, y_1)}{d(x_o, y_o)}\right]^{-1} .$$

Property 2.4 The element of area $dx_o dy_o$ and $dx_1 dy_1$ are related by

$$dx_1 . dy_1 = dx_o . dy_o$$

provided $J = 1$.

(For the proofs one may consult de la Vallée Poussin, (1), I, p.360-364).

If one considers the differential equations

$$\dot{x} = f(x,y,t)$$
$$(2.1) \qquad \dot{y} = g(x,y,t)$$

where f and g are continuous functions in x, y and t and have first partial derivatives continuous in x and y; if x(t), y(t) are solutions of (2.1) with initial conditions x_o and y_o when $t = t_o$; then one has

Property 2.5

$$J = \frac{d(x,y)}{d(x_o,y_o)} = e^{\int_{t_o}^{t} dt\left(\frac{\partial f}{\partial x} + \frac{\partial g}{\partial y}\right)}$$

(See for instance de la Vallée Poussin II, p 146).

Property 2.6

A necessary and sufficient condition that

$$f\,dy - g\,dx$$

be an exact differential dH-when t is considered as a parameter-is

$$\frac{\partial f}{\partial x} + \frac{\partial g}{\partial y} = 0.$$

~~(de la Valée Poussin II, p 41).~~ (1, II, p.41).

Hence

Theorem 2.1 A necessary and sufficient condition that the equations (2.1)-under the above condition- be such that the area in the space of initial conditions at t = 0 be preserved for all t, is that there exists a function H(x,y,t) such that

$$f = \frac{\partial H}{\partial y}, \quad g = -\frac{\partial H}{\partial x}$$

or that (2.1) is a Hamiltonian system.

(See also Whittaker (2) Ch XI).

This theorem shows that the only systems of two equations of first order that we have to consider are of the form (1.2). The proceeding properties will enable us to prove that the given methods of integration have Jacobian one, hence are area preserving. These methods of integration are dependent upon a parameter h (time increment). If the solution of (2.1) has a continuous nth derivative for $o \leq t - t_o \leq h$, one can write

$$x(t_o+h) = x(t_o) + h\,\dot{x}(t_o) + \dots + \frac{h^n}{n!}\,[x^{(n)}(to) + \varepsilon],$$

where ε tends to zero with h.

<u>Definition 2.2</u> If the method of integration is such that the approximation $\overline{x}(t_o+h)$ expanded in terms of h coincides with the above Taylor expressions to the order $p \leq n$, one says that the method is of the <u>p^{th} order</u> and we will use the symbol $\{p\}$ besides the formulae of the method.

We have not included in this paper the algebraic manipulation which proves rigorously, by this identification method, that the formulae are correct to the given order. We refer to Ince ~~(1945)~~ (3) or Hildebrandt ~~(1956) or Kopal (1956)~~ (4) for the famous application of this method to obtain Runge-Kutta type formulae.

If $p = \leq n-1$, it is possible to give the error term of the formula, as the coefficient of h^{p+1} of $\overline{x}(t_o+h)-x(t_o+h)$ multiplied by h^{p+1}. This error will be given. The error after n steps where nh is fixed is of the order of h^p. It can be found, if necessary, by methods used in similar cases. See for instance Collatz (5) ~~(1951)~~ or Hildebrandt (4). ~~(1956)~~

3. <u>The known methods.</u> The following methods are well known when $\alpha = o$, but they are only first order and applicable to the special case (1.1):

$$(3.1) \qquad \begin{aligned} \bar{x}_1 &= x_o + h\,\dot{x}_8 \\ \dot{\bar{x}}_1 &= \dot{x}_o + hf(\bar{x}_1, t_o + \alpha h) \end{aligned} \qquad \{1\}$$

The error terms are

$$(3.2) \qquad \begin{aligned} \bar{x}_1 - x(t_o+h) &= \frac{-h^2}{2} f(x_o, t_o) \\ \dot{\bar{x}}_1 - \dot{x}(t_o+h) &= [\tfrac{1}{2}\,\dot{x}_o (\tfrac{\partial f}{\partial x})_o + (\alpha - \tfrac{1}{2})\,(\tfrac{\partial f}{\partial t})]\,h^2, \end{aligned}$$

the last equation suggests to take $\alpha = \frac{1}{2}$.
Also

$$(3.3) \qquad \begin{aligned} \dot{\bar{x}}_1 &= \dot{x}_o + hf(x_o, t_o + \alpha h) \\ \bar{x}_1 &= x_o + h\,\dot{x}_1 \end{aligned} \qquad \{1\}$$

the error terms are

$$(3.4) \qquad \begin{aligned} \bar{x}_1 - x(t_o+h) &= \frac{h^2}{2} f(x_o, t_o) \\ \dot{\bar{x}}_1 - \dot{x}(t_o+h) &= [-\tfrac{1}{2}\,\dot{x}_o (\tfrac{\partial f}{\partial x})_o + (\alpha - \tfrac{1}{2})(\tfrac{\partial f}{\partial t})_o]\,h^2, \end{aligned}$$

the last equation suggests to take $\alpha = \frac{1}{2}$.

It is easy to check the area conservation property using definition 2.1.

Alternately, one may also write the transformation as a product of two transformations and use the property 2.2. For instance (3.1) can be written

$$\bar{x}_1 = x_o + h\dot{x}_o \quad , \ \dot{x}_o = \dot{x}_o$$

$$\dot{\bar{x}}_1 = \dot{x}_o + hf(\bar{x}_1, t_o + \alpha h), \ \bar{x}_1 = \bar{x}_1 \ ;$$

the Jacobian of both transformations is one because of the property 2.1.

4. Second order methods for (1.1).

The following method can be used to solve (1.1):

$$
\begin{aligned}
&\dot{\bar{x}}_1 = \dot{x}_o + \frac{h}{2} f(x_o, t_o + \alpha h) \\
(4.1) \qquad &\bar{x}_2 = x_o + h\,\dot{\bar{x}}_1 \qquad \{2\} \\
&\dot{\bar{x}}_2 = \dot{\bar{x}}_1 + \frac{h}{2} f(\bar{x}_2,\ t_o + (1-\alpha)h)
\end{aligned}
$$

One can infer that the method is second order because the second equation uses the slope at the mid-point, and the last equation combined with the first uses the mean of the slopes of $\dot{x}$ at the extremities of the interval, indeed the error terms are

$$
\begin{aligned}
&\bar{x}_2 - x(t_o+h) = \left[-\frac{1}{6}\dot{x}\frac{\partial f}{\partial x} + \left(\frac{\alpha}{2}-\frac{1}{6}\right)\frac{\partial f}{\partial t}\right]_o h^3 \\
(4.2) \qquad &\dot{\bar{x}}_2 - \dot{x}(t_o+h) = \left[\frac{1}{12}\frac{\partial^2 f}{\partial x^2}\dot{x}^2 + \left(\frac{1}{6}-\frac{\alpha}{2}\right)\frac{\partial^2 f}{\partial x\,\partial t}\dot{x} + \right. \\
&\qquad \left. \left(\frac{\alpha^2-\alpha}{2} + \frac{1}{12}\right)\frac{\partial^2 f}{\partial t^2} + \frac{1}{12} f \frac{\partial f}{\partial x}\right]_o h^3
\end{aligned}
$$

The alternate method at the end of section 3, gives immediately the area conservation property. The first equation suggests that we ~~to~~ take $\alpha = \frac{1}{3}$.

A similar argument shows that we can also use

$$
\begin{aligned}
&\bar{x}_1 = x_o + \frac{h}{2}\dot{x}_o \\
(4.3) \qquad &\dot{\bar{x}}_2 = \dot{x}_o + hf(\bar{x}_1,\ t_o + \frac{1}{2}h) \qquad \{2\} \\
&\bar{x}_2 = \bar{x}_1 + \frac{h}{2}\dot{\bar{x}}_2
\end{aligned}
$$

with the error terms:

$$
\begin{aligned}
&\bar{x}_2 - x(t_o+h) = \left[\frac{\partial f}{\partial x}\dot{x} + \frac{\partial f}{\partial t}\right]_o \frac{h^3}{12} \\
(4.4) \qquad &\dot{\bar{x}}_2 - \dot{x}(t_o+h) = -\left[\frac{1}{2}\frac{\partial^2 f}{\partial x^2}\dot{x}^2 + \frac{\partial^2 f}{\partial x\,\partial t}\dot{x} + \frac{1}{2}\frac{\partial^2 f}{\partial t^2} + 2\frac{\partial f}{\partial x} f\right]_o \frac{h^3}{12}
\end{aligned}
$$

This second method has comparable error terms, but asks for only one computation of $f(x,t)$ per interval, hence is barely more complicated that the first order method.

5. First order method for (1.2).

The methods (3.1) and (3.3) are symmetrical ~~of~~ to each other and do suggest the following generalization:

$$(5.1)\quad \begin{aligned} \bar{x}_1 &= x_o + h\, f(\bar{x}_1, y_o, t_o + \alpha h) \\ \bar{y}_1 &= y_o + h\, g(\bar{x}_1, y_o, t_o + \alpha h) \end{aligned} \qquad \{1\}$$

with the error term

$$\bar{x}_1 - x(t_o+h) = \left[-\frac{1}{2}\frac{\partial}{\partial y} fg + \left(\alpha-\frac{1}{2}\right)\frac{\partial f}{\partial t}\right]_o h^2$$

$$\bar{y}_1 - y(t_o+h) = \left[\frac{1}{2}\frac{\partial}{\partial x} fg + \left(\alpha-\frac{1}{2}\right)\frac{\partial g}{\partial t}\right]_o h^2.$$

We suggest $\alpha = \frac{1}{2}$.

The easiest way to prove that the Jacobian is one is to write the transformation as a product of transformations and to use the properties 2.2, 2.3 (for the first transformation) and 2.6.

The first equation (5.1) gives x_1 by an implicit formula, hence the method is lengthier than the special case (3.1) obtained when $f(x,y,t) \equiv y$ or than the other special case when $f(x,y,t)$ is linear in x. In all other cases, the solution will be obtained by iteration; because y and t are fixed any accelerative process of iteration will furnish quickly the solution. The most obvious accelerating processes are Newton's and Aitken's methods.

The simple iteration method defined by the equation (5.1) will converge if

(5.3) $\quad \left| h \frac{\partial f}{\partial x} (x, y_o, t_o + \alpha h) \right| < 1.$

Because h must be taken small (to make the error terms small enough), this relation will not usually lead to an additional restriction and the rate of convergence will usually be fast.

It is clear that one may interchange x and y in (5.1), the form (3.3) is then a special case.

6. Second order method for (1.2).

The methods (4.1) and (4.3) did suggest to us the generalization

$$
(6.1) \qquad \begin{aligned}
\bar{x}_1 &= x_o + \frac{h}{2} f(\bar{x}_1, y_o, t_o + \alpha h) \\
\bar{y}_1 &= y_o + \frac{h}{2} g(\bar{x}_1, y_o, t_o + \alpha h) \\
\bar{y}_2 &= \bar{y}_1 + \frac{h}{2} g(\bar{x}_1, \bar{y}_2, t_o + (1-\alpha)h) \\
\bar{x}_2 &= \bar{x}_1 + \frac{h}{2} f(\bar{x}_1, \bar{y}_2, t_o + (1-\alpha)h)
\end{aligned} \qquad \{2\}
$$

with the error terms

$$
(6.2) \qquad \begin{aligned}
\bar{x}_2 - x(t_o + h) &= (\Phi f)_o h^3 \\
\bar{y}_2 - y(t_o + h) &= (\Phi g)_o h^3
\end{aligned}
$$

Where the operator Φ is given by

$$
\begin{aligned}
\Phi = &- \frac{1}{24} f^2 \frac{\partial^2}{\partial x^2} + \frac{1}{12} g^2 \frac{\partial^2}{\partial y^2} + \left(\frac{\alpha^2 - \alpha}{2} + \frac{1}{12}\right) \frac{\partial^2}{\partial t^2} \\
&+ \left(\frac{1}{6} \ \frac{\alpha}{2}\right) g \frac{\partial^2}{\partial y \partial t} - \frac{1}{12} f \frac{\partial^2}{\partial x \partial t} - \frac{1}{12} f g \frac{\partial^2}{\partial x \partial y} \\
&+ \frac{1}{4} \frac{\partial g}{\partial t} \frac{\partial}{\partial y} + \frac{\alpha}{2} \frac{\partial f}{\partial t} \frac{\partial}{\partial x} + \frac{1}{4} f \frac{\partial g}{\partial x} \frac{\partial}{\partial y} \\
&+ \frac{1}{4} f \frac{\partial f}{\partial x} \frac{\partial}{\partial x} + \frac{1}{4} g \frac{\partial g}{\partial y} \frac{\partial}{\partial y} - \frac{1}{6}\, g \frac{\partial f}{\partial y} \frac{\partial}{\partial x} .
\end{aligned}
$$

We suggest $\alpha = 0$.

The two first equations are analogous to (5.1) hence the Jacobian of $\bar{x}_1$, $\bar{y}_1$ with respect to x_o, y_o is one. The two last equations are analogous to (5.1) where x and y are interchanged, hence the jacobian of $\bar{x}_2, \bar{y}_2$ with respect to $\bar{x}_1$, $\bar{y}_1$ is one. The complete transformation preserves the area because of the property 2.2.

That the method is second order could have been inferred by remarking that

$$\bar{y}_2 = y_o + \frac{h}{2} g(\bar{x}_1, y_o, t_o + \alpha h) + \frac{h}{2} g(\bar{x}_1, y_2, t_o + (1-\alpha)h)$$

hence that if y did not appear in g the slope is taken at the mid-point for x and that if x did not appear in g one uses the mean of the slopes at the extremity of the interval for y.

Two of the relations (6.1) are implicit, this seems to be the price we have to pay for the general equations, when one insists on a method which preserves the area.

Of course, ~~Indeed~~ one may interchange x and y in (6.1).

7. Generalization to n degrees of freedom

Let us now consider the Hamilton system

$$(7.1) \quad \begin{aligned} q_i' &= \frac{\partial H}{\partial p_i} \\ p_i' &= -\frac{\partial H}{\partial q_i} \end{aligned} \qquad H = H(q_i, p_i, t), \; i = 1,2,\ldots,n$$

and the solutions $q_i(\alpha_i, \beta_i, t)$, $p_i(\alpha_i, \beta_i, t)$ with initial conditions α_i, β_i when $t = t_o$.

The property J=1 generalizes into the Poisson brackets relations (See ~~Whittaker~~ (2) Ch XI):

$$[p_i,\ p_k] = o$$

$$(7.2)\quad [q_i,\ q_k] = o \qquad i,k = 1,2,\ldots,n$$

$$[p_i,\ q_k] = \delta_{ik}\ .$$

To check that a transformation is a contact one, one may either use (7.2) or prove that

$$\Sigma\ (p_i\ dq_i - \beta_i\ d\alpha_i)$$

is a total differential, when p and q are expressed in terms of α and β and when t is considered as a parameter.

The method

$$(7.3)\qquad \begin{aligned} q_i &= \alpha_i + h\ \frac{\partial H(q_i,\beta_i,t)}{\partial \beta_i} \\ p_i &= \beta_i - h\ \frac{\partial H(q_i,\beta_i,t)}{\partial q_i} \end{aligned} \qquad \{1\}$$

is first order. See (5.1), which suggests $t = t_o + \frac{1}{2}\ h$.

(7.3) is a contact transformation:

$$\Sigma(p_i dq_i - \beta_i d\ \alpha_i) = \Sigma(p_i dq_i + \alpha_i d\beta_i - d(\alpha_i\beta_i)$$

$$= \Sigma(\beta_i - h\ \frac{\partial H}{\partial q_i})\ dq_i + (q_i - h\ \frac{\partial H}{\partial \beta_i})\ d\beta_i - d(\alpha_i\beta_i)$$

$$= d\left\{\Sigma[\beta_i q_i - \beta_i\alpha_i - h\ H(q_i,\beta_i\ t)]\right\}$$

where t is considered as a parameter.

Similarly the method

$$(7.4)\qquad \begin{aligned} q_i &= \alpha_i + \frac{h}{2}\ \frac{\partial H(q_i,\beta_i,t_o+\alpha h)}{\partial \beta_i} \\ p_i &= \beta_i - \frac{h}{2}\ \frac{\partial H(q_i,\beta_i,t_o+\alpha h)}{\partial q_i} \end{aligned} \qquad \{2\}$$

$$p_i(t_o+h) \cong P_i = p_i - \frac{h}{2}\ \frac{\partial H(q_i,P_i,t_o+(1-\alpha)h)}{\partial q_i}$$

$$q_i(t_o+h) \cong Q_i = q_i + \frac{h}{2}\ \frac{\partial H(q_i,P_i,t_o+(1-\alpha)h)}{\partial P_i}$$

is second order as seen in section 6. (7.4) is a contact transformation because it is the product of two contact transformations. We suggest $\alpha = 0$.

In general two of the above relations are implicit. The special case

$$H = \frac{1}{2}\,[\Sigma p_i^2 + 2U(q_i, t)]$$

is worth mentioning. (7.4) reduces then to

$$q_{i1} = q_{io} + \frac{h}{2}\,\dot{q}_{io}$$

$$(7.5) \quad q_i(t_o + h) \cong q_{i2} = \dot{q}_{io} - h\,\frac{\partial U(q_{i1}, t_o + \frac{1}{2}h)}{\partial q_{i1}} \qquad \{2\}$$

$$q_i(t_o + h) \cong q_{i2} = q_{i1} + \frac{h}{2}\,\dot{q}_{i2}.$$

No detailed example or discussion is given. This will best be done by those working on these problems in the Brookhaven, Harwell, MURA or CERN group.

8. <u>Acknowledgement.</u> I wish to thank Professor J. Snyder of the University of Illinois and MURA for having brought this problem to my attention at the MURA meeting of April 14, 1956.

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