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ABSTRACT

Group theoretical concepts are applied to the numerical integration of the equations of motion of a conservative dynamical system. Rather than obtain the solution by one of the standard methods of numerical analysis a transformation group is derived which maps the state of system at time t_i onto the state of the system at time $t_{i+1} = t_i + \Delta t$. Because of the group property in conservative systems, time is reversable. That is, the readily obtained inverse to the transformation, maps the state of the system at time t_{i+1} onto the state at time $t_i = t_{i+1} - \Delta t$ so that given a desired terminal condition for a trajectory the problem may be worked backwards to determine the required initial conditions. Truncation error is arbitrary so that the programmer may trade off function evaluation for step size to optimize computer running time.

This memoranda is a preliminary report and the development is heuristic. A brief review of classical Hamiltonian theory is included.

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FROM: H. A. Helm

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TECHNICAL MEMORANDUM

Introduction

This memorandum is a preliminary report on one aspect of an investigation into the geometrical properties of dynamical systems. The numerical technique introduced below is derived from the canonical transformation theory of conservative systems. For this reason, a succinct (and, hopefully, readable) account of such transformation theory is included for reference and review.

The technique is interesting in several ways. In the first place, instead of solving the differential equations of motion numerically, an approximation to an "infinitesimal transformation" is used to map the state of the dynamical system at time t_i onto the state of the system at time $t_{i+1} = t_i + \Delta t$. Secondly, these transformations have the group property. In this connection, (and for conservative systems in general) this means that time is reversible; i.e. the inverse transformation maps the state of the system at time t_{i+1} onto the state of the system at time $t_i = t_{i+1} - \Delta t$. This is of obvious utility in the targetting problem where one desires the initial conditions of a trajectory given arbitrary terminal conditions. However, it should be remembered that the above does not apply to powered flight nor to flight in the atmosphere where dissipative drag forces are present. Finally, considered only from the point of view of numerical analysis the idea of approximating a transformation which leaves invariant an appropriate function, functional, or differential form would appear to be worthy of further investigation.

A Brief Review of Transformation Theory

We restrict our attention to conservative, holonomic systems. That is to say there are no dissipative forces acting and that in a system of n position coordinates there are n degrees of freedom.

Let the dynamical system be specified by n position coordinates $(q_1, q_2, \cdots q_n)$, where the q_i depend implicitly upon time. The restriction to holonomic systems may be more precisely stated as there shall be no functions $a_i(q)$ not identically zero such that

$$\sum_i a_i(q)\, dq_i = 0.$$

This of course also precludes constraints of the form $f(q_1, \cdots q_n) = 0$ since this implies

$$\sum_i \frac{\partial f}{\partial q_i} \, dq_i = 0.$$

In such a system the kinetic energy T is a positive semi-definite quadratic form in the $\dot{q}_i = \frac{dq_i}{dt}$. It is homogeneous of degree 2 in the variables $\dot{q}_i$. That is:

(1) $$T(q_1,\cdots q_n, s\dot{q}_1,\cdots,s\dot{q}_n) = s^2 T(q_1,\cdots q_n, \dot{q}_1,\cdots,\dot{q}_n)$$

The potential energy $V(q_1,\cdots q_n)$ is a function of the position coordinates alone. The Lagrangian is by definition:

(2) $$L(q_1,\cdots q_n, \dot{q}_1,\cdots,\dot{q}_n) = L(q_i, \dot{q}_i) = T-V$$

Hamilton's principle then says that the functional

(3) $$A = \int_{t_o}^{t_1} L \, dt$$

shall be an extremal. That is, the first variation $\delta A = 0$. The necessary condition that (3) shall be extremal is that the Euler's equations:

$$(4) \qquad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

shall hold. These n equations are the equations of motion of the system. In general, they are not immediately integrable. The object of transformation theory is to make a change of variable in a systematic way which will simplify the equations sufficiently so that a solution can be effected.

The first step is to put the equations into the Hamiltonian or canonical form. The generalized momenta are defined by:

$$(5) \qquad p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial T}{\partial \dot{q}_i}$$

In Hamiltonian theory the generalized momenta are treated as independent coordinates. They have the same status as the position coordinates. One now makes a change of variable which converts the Lagrangian, L, to a new function H, the Hamiltonian. Thus:

$$(6) \qquad H = \sum_i p_i \dot{q}_i - L.$$

Computing the differential dH from the defining equation (6) one has

$$(7) \qquad dH = \sum_i p_i \, d\dot{q}_i + \sum \dot{q}_i \, dp_i$$

$$- \sum_i \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i - \sum_i \frac{\partial L}{\partial q_i} \, dq_i$$

Substitution of the definition of p_i into (7) leads to:

$$(8) \qquad dH = \sum_i \dot{q}_i \, dp_i - \sum_i \frac{\partial L}{\partial q_i} \, dq_i \, .$$

Expressing H now as a function of only $(q_1, \cdots q_n, p_1, \cdots p_n)$ and computing the differential dH by the chain rule in the usual manner

$$(9) \qquad dH = \sum_i \frac{\partial H}{\partial p_i} \, dp_i + \sum_i \frac{\partial H}{\partial q_i} \, dq_i \, .$$

Since a differential is independent of the coordinate system in which it is computed (8) and (9) are equivalent so that:

$$\frac{\partial H}{\partial p_i} = \dot{q}_i$$

$$\frac{\partial H}{\partial q_i} = - \frac{\partial L}{\partial q_i}$$

But from Euler's equation (4) we have

$$\frac{\partial L}{\partial q_i} = \frac{d}{dt}\left[\frac{\partial L}{\partial \dot{q}_i}\right] = \dot{p}_i \, .$$

Thus, the equations of motion in the Hamiltonian form are

(10)
$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

In the case of a conservative system it is possible to give a physical interpretation of H so that equations (9) are something more than a mere notational simplification.

As noted before the kinetic energy, T, is a positive definite quadratic form in the velocities $\dot{q}_i$ which is homogenious of degree 2. Hence, by Euler's theorem [1]:

(11)
$$2T = \sum_i \dot{q}_i \frac{\partial T}{\partial \dot{q}_i} = \sum_i p_i \dot{q}_i = H + L$$

---

[1] Taylor, A. E. Advanced Calculus, Ginn and Co., 1955, p 184

From which:

(12) $$H = 2T - L = 2T - (T-V) = T + V .$$

Thus, the Hamiltonian is the total energy of the system, and since the only systems under consideration are conservative, by definition the total energy, the Hamiltonian, must be a constant.

First Order Transformations

The canonical equations of motion (10) are immediately suggestive of an algorithm for their numerical solution. Thus, by approximating the derivative with the difference quotient equations (10) become:

(13)
$$\dot{q}_i = \frac{\partial H}{\partial p_i} \cong \frac{\Delta q_i}{\Delta t} = \frac{q_i(t_{k+1}) - q_i(t_k)}{t_{k+1} - t_k}$$
$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \cong \frac{\Delta p_i}{\Delta t} = \frac{p_i(t_{k+1}) - p_i(t_k)}{t_{k+1} - t_k}$$

which lead to:

(14)
$$q_i(t_{k+1}) \cong q_i(t_k) + \Delta t \left. \frac{\partial H}{\partial p_i} \right|_{t = t_k}$$
$$p_i(t_{k+1}) \cong p_i(t_k) - \Delta t \left. \frac{\partial H}{\partial q_i} \right|_{t = t_k}$$

where $t_{k+1} = t_k + \Delta t$. Equations (14) may be regarded as a change of variable, and the numerical solution as obtained by iteration of the change. However, in general, changing variables will change the form of the Hamiltonian, H, and computation will therefore be more complicated. It will now be shown that the particular transformation (14) leaves the Hamiltonian invariant to first order terms in Δt. In evaluating the variation of the Hamiltonian it is convenient to use matrix notation. From Taylor's formula with remainder for $H(q + \Delta q, p + \Delta p)$ one has:

$$(15) \quad H(q+\Delta q, p+\Delta p) = H(q,p) + \left[\frac{\partial H}{\partial q_1}, \cdots \frac{\partial H}{\partial q_n}, \frac{\partial H}{\partial p_1}, \cdots \frac{\partial H}{\partial p_n}\right] \begin{bmatrix} \Delta q_1 \\ \vdots \\ \Delta q_n \\ \Delta p_1 \\ \vdots \\ \Delta p_n \end{bmatrix}$$

$$+\frac{1}{2}[\Delta q_1, \cdots, \Delta q_n, \Delta p_1, \cdots, \Delta p_n] \begin{bmatrix} \frac{\partial^2 H}{\partial q_1^2} & \frac{\partial^2 H}{\partial q_1 \partial q_2} \cdots & \frac{\partial^2 H}{\partial q_1 \partial q_n} & \frac{\partial^2 H}{\partial q_1 \partial p_1} \cdots & \frac{\partial^2 H}{\partial q_1 \partial p_n} \\ \frac{\partial^2 H}{\partial q_2 \partial q_1} & \frac{\partial^2 H}{\partial q_2^2} & \cdots & \cdots & \cdots \\ \vdots & & & & \vdots \\ \frac{\partial^2 H}{\partial p_1 \partial q_1} & & \cdots \frac{\partial^2 H}{\partial p_1^2} & \cdots & \frac{\partial^2 H}{\partial p_1 \partial p_n} \\ \vdots & & & & \vdots \\ \frac{\partial^2 H}{\partial p_n \partial q_1} & & \cdots & \cdots & \frac{\partial^2 H}{\partial p_n^2} \end{bmatrix} \begin{bmatrix} \Delta q_1 \\ \vdots \\ \Delta q_n \\ \Delta p_1 \\ \vdots \\ \Delta p_n \end{bmatrix}$$

$$+ R$$

where R is the remainder. Substitution of $\Delta p_i = -\frac{\partial H}{\partial q_i}\Delta t, \Delta q_i = \frac{\partial H}{\partial p_i}\Delta t$ into (26) shows after a trivial computation that the variation of the Hamiltonian under this transformation consists only of terms proportional to powers of Δt higher than the first, which is as desired.

Some very difficult problems have relatively simple Hamiltonians; viz. the three body problem. Thus, the algorithm will be computationally practical since the functional evaluation of the partials at = t_k will usually be quite simple. The problem of determining a transformation which leaves the Hamiltonian invariant to higher orders of Δt is considered below. The first order transformation just introduced which is not a really good approximation will be seen to play a key role in the derivation of a more accurate method.

Group Theoretic Aspects

Without giving a formal definition of an abstract algebraic group, we shall describe its properties in terms of the transformation (14). Thus, if p and q are such that:

$$H(q, p) = E \tag{16}$$

where E is the total energy, then (15) shows that for

$$\tilde{q}_i = q_i + \frac{\partial H}{\partial p_i}\Delta t$$

and

$$\tilde{p}_i = p_i - \frac{\partial H}{\partial q_i} \Delta t$$

$H(\tilde{q},\tilde{p}) = E$ to within first order terms in Δt. Hence, the set of q_i, p_i such that (16) holds is closed under the transformation (14). Now, for simplicity, let $\Delta t = \tau$ and let T_τ be the transformation defined by (14). That is:

(17) $$T_\tau: \; q_i(t_k) \to q_i(t_k + \tau) = \tilde{q}_i$$

$$T_\tau: \; p_i(t_k) \to p_i(t_k + \tau) = \tilde{p}_i$$

Since the effect of T_τ on p_i is obvious once its effect on q_i has been given we will only consider the q_i for the present. The product of two transformations T_{τ_1}, T_{τ_2} is their composition. That is first apply T_{τ_1} and then apply T_{τ_2} to the result. Formally:

(18) $$T_{\tau_2} T_{\tau_1}: q_i(t) = T_{\tau_2}: q_i(t+\tau_1) \to q_i(t+\tau_1+\tau_2)$$

Clearly,

$$T_{\tau_3}(T_{\tau_2}T_{\tau_1}) = (T_{\tau_3}T_{\tau_2})\,T_{\tau_1} \tag{19}$$

If $\tau = 0$ one has

$$T_o\colon\ g_i(t) \rightarrow g_i(t+0) = g_i(t) \tag{20}$$

and T_o is the identity transformation, I. From (18) one has:

$$T_{-\tau}\ T_{\tau} = T_o$$

hence

$$T_{\tau}^{-1} = T_{-\tau} \tag{21}$$

or the inverse of T_τ is $T_{-\tau}$. Now the above holds true, for the transformation given by (14) only when τ is very small so that the error resulting from the dropping of higher order terms is negligible. Thus for τ sufficiently small we may write:

$$p_i(t+\tau) = p_i(t) - \tau \left.\frac{\partial H}{\partial q_i}\right|_t = T_\tau(p_i)$$

$$q_i(t+\tau) = q_i(t) + \tau \left.\frac{\partial H}{\partial p_i}\right|_t = T_\tau(q_i)$$

The group T_τ depends continuously upon the parameter τ and is a one parameter continuous group or Lie Group. The problem now is to derive a continuous one parameter group so that the group relations hold for finite τ instead of only for an infinitesimal.

<u>Infinitesimal Transformations Associated with a Continuous One Parameter Group</u>

Below we shall use the notational convention that q_i shall stand for the 2n variables p_i and q_i. Thus, a function f(q) shall be understood to be a function of 2n variables

$$f(q_1, q_2, \cdots, q_n, p_1, \cdots p_n).$$

Furthermore, the function f shall be understood to be analytic at the point q. This means that we have placed restrictions upon allowable q. However, these restrictions for the problems of interest will generally occur naturally such as, for instance the Kepler problem being restricted to orbits with non-zero radii. Thus, on the set of analytic functions one can define[2] a <u>tangent</u> <u>vector</u> at the point $q = q^*$ as an operator of the form

$$X_{q^*} = \sum_i \xi^i(q^*) \frac{\partial}{\partial q_i}$$

---

[2]. Cohen, P. M., <u>Lie Groups</u>, Cambridge University Press, 1961, p. 11 ff.

where since the functions $\xi^i(q)$ are evaluated at point $q = q^*$ they are real constants. It is readily seen that for functions of one variable $y = f(q_1)$ one has as a tangent vector

$$X_{q^*}f = \frac{\partial f}{\partial q_1}\bigg|_{q_1=q^*} = \frac{df}{dq_1}\bigg|_{q_1=q^*}$$

the usual definition. One now has the following definition[3]:

Definition: An <u>infinitesimal transformation</u> is a collection of tangent vectors X_{q^*} one at each allowable point $q = q^*$; i.e.

$$X = \sum_i \xi^i(q) \frac{\partial}{\partial q_i} .$$

These transformations are closely related to the first order transformation groups discussed above. Their relationship to these groups will be discussed in terms of a particular transformation arising in dynamics. The approach is admittedly heuristic and justified only by the desire for brevity since a full treatment would require the development of the inter-relations between a Lie Group and its Lie Algebra.

Let us first consider the infinitestimal transformation associated with a first order transformation, remembering that

3. Ibid p. 16.

we will neglect terms in Δq higher than the first. Thus, rewriting (15) and dropping the remainder term one has:

$$(22) \qquad f(q+\Delta q) = f(q) + \sum_i \frac{\partial f}{\partial q_i} \Big|_{q_i} \Delta q_i$$

But allowing q in (22) to vary is precisely an infinitesimal transformation as defined, since Δq_i as given by (14) is in general a function and may be considered to be the $\xi^k(q)$ of the definition and if we define X as $\sum_i \Delta q_i \frac{\partial}{\partial q_i}$ one may write (22) (to first order terms) as

$$(23) \qquad f(q+\Delta q) = (I + X)\, f$$

where I is the identity operator. Now supposing $f = q_i$. Thus,

$$(24) \qquad q_i(q+\Delta q) = (I+X)\, q_i = q_i + \sum_i \Delta q_i \frac{\partial q_i}{\partial q_i} = q_i + \Delta q_i .$$

But for $\Delta q_i = \tau \frac{\partial H}{\partial p_i}$ this is just the first order transformation group which we derived as an approximation to the equations of motion of a dynamical system. In regard to the function f in (23), if $Xf = 0$, then (24) is the transformation group which leaves f invariant to the first order.

Returning now to the 2n variables p_i, q_i, the infinitesimal transformations will be applied to the original problem. First (22) becomes:

(25) $$f(q+\Delta q,p+\Delta p) = f(p,q) + \sum_i \Delta q_i \frac{\partial f}{\partial q_i} + \sum_i \Delta p_i \frac{\partial f}{\partial p_i} + R$$

From (14) one has (letting $t = \tau$) for Δq_i and Δp_i

$$\Delta q_i = \frac{\partial H}{\partial p_i} \tau$$

$$\Delta p_i = - \frac{\partial H}{\partial q_i} \tau$$

From which we have an infinitesimal transformation:

(26) $$X_H = \sum_i \frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i}$$

Furthermore, it is obvious that $X_H H = 0$. Hence, for first order terms (15) may be written:

(27) $$H(\tilde{q},\tilde{p}) = (I + X_H) H(q,p) = H(q+\Delta q, p+\Delta p)$$

and the transformation group (14) becomes:

$$\tilde{q}_i = (I + X_H)\, q_i \tag{28}$$

$$\tilde{p}_i = (I + X_H)\, p_i \; .$$

In the next section we will consider the problem of obtaining a transformation group which leaves the Hamiltonian invariant for finite τ rather than truly infinitesimal τ.

The Exponential Map

The development below is essentially due to Cohn[4]. What is desired is to find the group T_τ mapping $q(t)$ onto $q(t+\tau)$ which leaves the Hamiltonian invariant. Again, for the moment, let q_i stand for both q_i and p_i. The action of T_τ on $q(t)$ can be written.

$$T_\tau(q(t)) = q(t+\tau) \tag{29}$$

Now the group T_τ not only depends continuously upon τ but is also a Lie Group. In the case under consideration here this means that there is an analytic function T such that

$$q_i(t+\tau) = T_i(q(t),\tau) = T_i\;(\tau) \tag{30}$$

---

[4] Ibid., p. 79 ff.

or as a vector $q(t+\tau) = T(q(t),\tau) = T(\tau)$. From the definition of the group T_τ one has that T_0 is the identity, hence

$$q(t) = T(q,0) = T(0)$$

For f an analytic function of q it is desired to evaluate.

$$f(T(q,\tau)) = f(T(\tau)) \tag{31}$$

Now by the chain rule:

$$f' = \frac{df}{d\tau} = \sum_i \frac{\partial f}{\partial q_i} \frac{\partial T_i}{\partial \tau} = X f \tag{32}$$

where X is the infinitesimal transformation corresponding to T_τ. It can be shown[5] that given an X there corresponds to it a unique T_τ. Therefore since we already have an infinitesimal transformation X_H and a translation group T_τ which is valid for τ truly infinitesimal the problem is to extend the method for a finite τ.

Since f in (31) is analytic, Taylor's series may be applied in the following way. Let

$$f(T_1(q,\tau),\cdots, T_n(q,\tau)) = F(\tau)$$

---

5. Ibid, Theorem 3.5.1 p. 70

re $F(\tau)$ is again analytic and hence expending about $\tau = 0$ ... has:

(33) $$F(\tau) = F(0) + \tau F'(0) + \frac{\tau^2}{2!} F''(0) + \frac{\tau^3}{3!} F'''(0) + \cdots$$

By (32) one has for $F'(0) = f'(T(q,0))$

$$F'(0) = f'(T(q,0)) = Xf \Big|_{\tau=0}$$

Thus, (33) becomes

(34) $$F(\tau) = f(T(q,\tau)) = f(q) + \tau Xf \Big|_{\tau=0} + \frac{\tau^2}{2!} X^2 f \Big|_{\tau=0} + \frac{\tau^3}{3!} X^3 f \Big|_{\tau=0} + \cdots$$

The series on the right of (34) may be taken as the definition of the exponential of the transformation X. (34) may therefore, be written concisely as

(35) $$f(T(q,\tau)) = [\exp(\tau X) f]_{\tau=0}$$

Remembering that $T(q,\tau) = q(t+\tau)$, $T(q,0) = q(t)$ one has for (35)

(36) $$f(T(q,\tau)) = f(q(t+\tau)) = \exp(\tau X)\, f(q(t))$$

It is now possible to evaluate $T(q,\tau)$ and thus obtain T_τ. First one considers that q_i itself is an analytic function of all the q_j. That is,

$$q_i(t) = q_i(q_1(t),\cdots,q_n(t))$$

and

$$q_i(T(q,\tau)) = q_i(T_1(q,\tau),\ T_2(q,\tau),\cdots,T_n(q,\tau)) = q_i(t+\tau).$$

Substitution of this q_i for f in (36) therefore leads to

$$(37)\qquad q_i(t+\tau) = q_i(T(q,\tau)) = \exp(\tau X)q_i(q(t)) = \exp(tX)q_i(t)$$

which is the desired formula. An example is now in order.

Consider the case of two variables q_1, q_2 with

$$X = \xi_1(q)\ \frac{\partial}{\partial q_1} + \xi_2(q)\ \frac{\partial}{\partial q_2}$$

Then, including only 2nd order terms,

$$q_i(t+\tau) = [q_i + \tau(\xi_1(q)\frac{\partial}{\partial q_1} + \xi_2(q)\frac{\partial}{\partial q_2})\, q_i + \frac{\tau^2}{2!}(\xi_1(q)\frac{\partial \xi_1}{\partial q_1}\frac{\partial}{\partial q_1}$$

$$+ \xi_1^{\,2}(q)\frac{\partial^2}{\partial q_1^{\,2}} + \xi_1(q)\frac{\partial \xi_2}{\partial q_1}\frac{\partial}{\partial q_2} + \xi_1(q)\,\xi_2(q)\frac{\partial^2}{\partial q_1 \partial q_2}$$

$$+ \xi_2(q)\frac{\partial \xi_1}{\partial q_2}\frac{\partial}{\partial q_1} + \xi_2(q)\,\xi_1(q)\frac{\partial^2}{\partial q_2 \partial q_1} + \xi_2(q)\frac{\partial^2}{\partial q_2\,\partial q_2}$$

$$+ \xi_2^{\,2}(q)\frac{\partial^2}{\partial q_2^{\,2}})\, q_i + \cdots]$$

Thus:

$$q_1(t+\tau) = [q_1 + \tau\xi_1(q) + \frac{\tau^2}{2!}(\xi_1(q)\frac{\partial \xi_1}{\partial q_1} + \xi_2(q)\frac{\partial \xi_1}{\partial q_1}) + \cdots]$$

or

$$q_1(t+\tau) = [q_1 + \tau\xi_1(q) + \frac{\tau^2}{2!}(X\ \xi_1) + \cdots]$$

$$q_2(t+\tau) = [q_2 + \tau\xi_2(q) + \frac{\tau^2}{2!}(X\ \xi_2) + \cdots]$$

Specializing now (and returning to the p, q, notation) for the case X_H as given by (26) one has from (36) when f = H

$$H(q(t+\tau),\ p(t+\tau)) = H(\tilde{q},\tilde{p}) = \exp(\tau X_H)\ H(q,p) = H(q(t),p(t))$$

since $X_H\ H = 0$.

Suppose now one applies (36) twice in succession. That is one computes $T(q,\tau_1)$ and then extrapolates on this point by $T(q(t+\tau_1), \tau_2)$. Formally, one has for $q_i^* = q_i(t+\tau_1)$

$$(38) \quad q_i^*(t+\tau_2) = \exp(\tau_2 X)\, q_i^* = \exp(\tau_2 X)[\exp(\tau_1 X) q_i] = q_i(t+\tau_1+\tau_2)$$

Now X is an operator not a number, and the usual rules of manipulation for exponentials do not necessarily hold. That is to say (exp X) (exp Y) for X and Y operators does not in general equal exp(X+Y). However, in the case of interest above $\tau_1 X$ and $\tau_2 X$ commute; i.e. $\tau_2 X(\tau_1 X\ f) = \tau_1 X(\tau_2 X\ f)$. It can be shown that for commuting operators.

$$(39) \quad \exp(\tau_2 X)\ \exp(\tau_1 X) f = \exp(\tau_1 X)\ \exp(\tau_2 X) f = \exp(\tau_1 X+\tau_2 X) f.$$

Now all the group properties given by equations (17) through (21) follow from (39) and well known properties of the exponential. For instance the inverse is obtained by setting $\tau_2 = -\tau_1$ in (39) leading to:

$$\exp(-\tau_1 X)\ \exp(\tau_1 X) f = \exp(0) f = If = f.$$

As a more detailed example of the above let us consider the linear oscillator in one dimension; a simple spring and mass. For q the displacement of the mass, p its momentum, the Hamiltonian is

$$(40) \qquad H = T+V = \frac{p^2}{2m} + \frac{k\,q^2}{2} = \frac{p^2}{2} + \frac{q^2}{2} \text{ for } m = k = 1.$$

Obviously

$$X_H = \frac{\partial H}{\partial p}\frac{\partial}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial}{\partial p} = p\frac{\partial}{\partial q} - q\frac{\partial}{\partial p}$$

Our first order transformation is for $\Delta t = \tau$

$$p(t+\tau) = (I+X_H)\,p(t) = p(t) - \tau\frac{\partial H}{\partial q}\Big|_{p(t),q(t)} = p(t) - \tau q(t)$$

$$q(t+\tau) = (I+X_H)\,q(t) = q(t) + \tau\frac{\partial H}{\partial p}\Big|_{p(t),q(t)} = q(t) + \tau p(t)$$

as before.

Now we wish to correct our procedure at least to the second order by applying (37). Thus, we wish

$$q(t+\tau) = T(q,p,\tau)$$

$$p(t+\tau) = T(q,p,\tau)$$

Now

$$\exp(tX_H)\ p(t) = [I+(p\frac{\partial}{\partial q} - q\frac{\partial}{\partial p}) + \frac{1}{2}\tau^2(p^2\frac{\partial^2}{\partial q^2} - p\frac{\partial}{\partial p} - q\frac{\partial}{\partial q} + q^2\frac{\partial^2}{\partial p^2})$$

$$+ \cdots]\ p(t) = p(t) - \tau q(t) - \frac{\tau^2}{2}\, p(t) = p(t+\tau)$$

Similarly:

$$q(t+\tau) = q(t) + \tau p(t) - \frac{\tau^2}{2}\, q(t)$$

Substitution into (15) leads to the following upon neglecting terms higher than the second:

$$\Delta H = [\frac{\partial H}{\partial p}, \frac{\partial H}{\partial q}] \begin{bmatrix} \Delta p \\ \Delta q \end{bmatrix} + \frac{1}{2}[\Delta p, \Delta q] \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \Delta p \\ \Delta q \end{bmatrix} + \cdots$$

Substitution of $\Delta p = -\tau q(t) - \frac{\tau^2}{2} p(t)$, $\Delta q = \tau p(t) - \frac{\tau^2}{2} q(t)$ into the above gives:

$$H = \tau[-pq - \frac{\tau p^2}{2} + qp - \frac{\tau q^2}{2}] + \frac{\tau^2}{2}[q^2 + \tau pq + \frac{\tau^2}{4} p^2 + p^2 - \tau pq + \frac{\tau^2}{4} q^2]$$
$$+ \cdots$$

$$= -\frac{\tau^2}{2}(p^2+q^2) + \frac{\tau^2}{2}(p^2+q^2) + \frac{\tau^4}{4}(p^2+q^2) + \cdots$$

$$= \frac{\tau^4}{4}(p^2+q^2) + \cdots$$

so that $\Delta H = 0$ to second order at least.

Conclusion

The above numerical technique is now being programmed to evaluate whether it is indeed as good in practice as the above theory would indicate. Results will be reported in a later memorandum. However, the technique does in theory offer the following advantages:

a) Truncation error can be made as small as desired. This allows a programmer to trade off step size versus function evaluation to minimize running time.

b) The method applies to a clearly defined reasonably large class of problems. Although the partial derivatives must be recomputed if the problem changes the truncation error is always a function of the highest power of X_H used-not the problem.

c) Since the transformation used is a group it possesses an inverse. Hence, given the Hamiltonian and the terminal position and momenta, it is possible to work the problem backwards to obtain the initial conditions of the trajectory. This is of obvious utility in targetting problems. However, it must be remembered that this does not apply to powered trajectories or to trajectories in the atmosphere.

d) The concepts involved open up a new approach to the fundamental understanding of the geometry of dynamics problems themselves. This aspect will be explored in subsequent memoranda.

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