NUMERICAL INTEGRATION OF NEARLY-HAMILTONIAN SYSTEMS

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ABSTRACT

Consideration is given to the solution by numerical integration of systems of differential equations that are derived from a Hamiltonian function in the extended phase space plus additional forces not included in the Hamiltonian (that is, nearly-Hamiltonian systems). An extended phase space Hamiltonian which vanishes initially will vanish on any solution of the system differential equations. Furthermore, it vanishes in spite of the additional forces, and defines a surface in the extended phase space upon which the solution is constrained.

Direct numerical comparisons are made between (1) nearly-Hamiltonian systems having vanishing Hamiltonians and (2) those having nonvanishing Hamiltonians. It is seen that for some problems, numerical solutions are more stable when computed from systems of the type (1). The problems considered are the harmonic oscillator with the van der Pol perturbation and perturbed Keplerian motion.

1. INTRODUCTION

This paper considers the solution by numerical integration of systems of differential equations that are derived from a Hamiltonian function in the extended phase space plus additional forces that are not included in the Hamiltonian. An extended phase space Hamiltonian which vanishes initially will vanish on any solution of the system differential equations. Furthermore it vanishes in spite of the additional forces, and defines a surface in the extended phase space upon which the solution is constrained.

Nacozy (1971) uses the idea of solutions of differential equations being constrained to lie on surfaces in phase space to develop a formula for corrections that, when added to the numerical solution, cancel the errors made during the preceding integration step, forcing the solution

V. Szebehely (ed.), Dynamics of Planets and Satellites and Theories of Their Motion, 159-173.

back to the surface. Baumgarte (1972) suggests for this purpose the use of a control term that is theoretically zero to be added to the differential equations of Keplerian motion. The control term which is the initial value of the energy minus the computed value at any step, vanishes on the exact solution and forces the solution back to the surface when it departs. These techniques require that there be an integral of the motion that defines a surface in the phase space. In case of nonconservative perturbed motion, these techniques are no longer strictly valid but may still be useful when the instantaneous surface is only changing slowly.

In Stiefel and Scheifele (1971) the idea of the Hamiltonian in extended phase space such that it will vanish on any solution in the space is discussed. This essentially says that even for nonconservative problems where no integral exists and which might have additional forces not included in the Hamiltonian, a surface in phase space may still be defined provided the new Hamiltonian in the extended phase space vanishes. Several formulations of Keplerian motion have recently appeared in the literature which are derived from Hamiltonians which vanish in the extended phase: Scheifele and Graf (1974) introduced Keplerian elements similar to the classical Delaunay elements; and Bond (1976) developed Keplerian elements similar to the classical Poincaré elements. These formulations use either the eccentric or the true anomaly as the independent variable. In the last paper numerical integration results were presented which showed that the elements similar to the Poincaré elements with eccentric anomaly as the independent variable (henceforth called Poincaré-Similar elements or PSu elements) showed unusually good stability.

In order to interpret these numerical results, the approach taken in this paper is to obtain two formulations - one with a vanishing Hamiltonian in the extended phase space and one with a nonvanishing Hamiltonian in the extended phase space - for a much simpler problem. The problem chosen is the one-dimensional perturbed harmonic oscillator. The particular example chosen for investigation was the van der Pol equation

$$\ddot{x} + x = \varepsilon(1 - x^2)\dot{x} \tag{1.1}$$

This equation has an exact asymptotic value for its amplitude, which is convenient in making error comparisons with numerical results.

This paper will make comparisons between a numerical solution and a known analytical solution rather than comparing a numerical solution computed by one method to a numerical solution computed by another method. In addition to the van der Pol problem, known solutions in the restricted problem of three bodies will be used as examples in perturbed Keplerian motion. One of these solutions is the stable Lagrangian libration point in the Earth-Moon system and the other is the unstable collinear libration point between the Earth and the Moon. The numerically integrated results from the PSu system of elements will be locally transformed and compared with the known solutions.

2. THE EXTENDED PHASE SPACE HAMILTONIAN

Discussions on the extended phase space Hamiltonian may be found in the book by Szebehely and in the book by Stiefel and Scheifele. This latter reference also considers the case of additional forces which are not derivable from the Hamiltonian, referring to the additional forces as "canonical forces." The paper by Murdock (1975) refers to Hamiltonian systems of differential equations which are augmented by additional forces as "nearly-Hamiltonian systems." In this paper the terms "additional forces" and "nearly-Hamiltonian systems" will be used.

In Stiefel and Scheifele (1971) the following theorem is proved: Consider the nearly-Hamiltonian system

$$\frac{d\bar{x}_k}{ds} = \frac{\partial \bar{F}}{\partial \bar{p}_k} - \bar{X}_k$$

$$k = 0, 1, 2, \ldots n \qquad (2.1)$$

$$\frac{d\bar{p}_k}{ds} = -\frac{\partial \bar{F}}{\partial \bar{x}_k} + \bar{P}_k$$

where $\bar{X}_k$ and $\bar{P}_k$ are the additional forces and where $\bar{F}$ is the Hamiltonian in the extended phase space

$$\bar{F} = \mu(H + p_o)$$

H is the old Hamiltonian; and

$$p_o = -H$$

$$x_o = t \text{ (the time)}$$

and the new independent variable s is found from

$$\frac{dt}{ds} = \mu(x_o \ldots x_n;\ p_o \ldots P_n) \qquad (2.2)$$

On any solution of the system (2.1) satisfying the initial conditions

$$x_o(0) = 0;\ s = 0$$

$$p_o(0) = -H\big(x_o(0), \ldots x_n(0);\ p_1(0), \ldots p_n(0)\big) \qquad (2.3)$$

the Hamiltonian $\bar{F}$ vanishes for any value of the independent variable s.

https://doi.org/10.1017/S0252921100062242 Published online by Cambridge University Press

The new Hamiltonian $\bar{F}$ is thus equivalent to an integral of the system in the extended phase space. (It should be obvious that this integral is not always invariant under further transformation. In particular if a generating function is chosen which depends upon the independent variable s, then it is possible for the Hamiltonian to lose the property of vanishing.) Since $\bar{F} = 0$ it defines a surface in the phase space upon which the solution remains for all values of s. That is

$$\frac{d\bar{F}}{ds} = \sum_{k=0}^{n} \left[\frac{\partial \bar{F}}{\partial \bar{x}_k} \frac{d\bar{x}_k}{ds} + \frac{\partial \bar{F}}{\partial \bar{p}_k} \frac{d\bar{p}_k}{ds} \right] = 0 \tag{2.4}$$

or in vector notation, where $z = (\bar{x}_k, \bar{p}_k)$

$$\frac{\partial \bar{F}}{\partial z} \cdot \frac{dz}{ds} = 0 \tag{2.5}$$

The normal to the surface at any point is defined by the components of $\partial \bar{F}/\partial z$; any change in the coordinates or momenta must lie in the surface.

3. TWO CANONICAL FORMULATIONS OF THE PERTURBED HARMONIC OSCILLATOR

The Hamiltonian for the perturbed oscillator with a perturbing potential V and frequency of one may be written as

$$H = \frac{1}{2} p^2 + \frac{1}{2} x^2 + V(x,t) \tag{3.1}$$

A perturbing force f which includes perturbations which may not be derivable from a potential may be systematically included in the equations of motion. The equations of motion are

$$\dot{x} = \frac{\partial H}{\partial p} = p \tag{3.2}$$

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[1]Throughout this paper,

$$\dot{(\ )} = \frac{d(\ )}{dt} \text{ and } (\ )' = \frac{d(\ )}{d\tau}$$

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$$\dot{p} = -\frac{\partial H}{\partial x} + f = -x - \frac{\partial V}{\partial x} + f \tag{3.3}$$

Now a new Hamiltonian in the extended phase space, H_h, will be developed that will vanish on any solution of the equations of motion. This is done by introducing a new momenta, p_o, which is the negative of the Hamiltonian (eq. 3.1) and is therefore the total energy of the system. The new coordinate x_o that is canonically conjugate to p_o is the time, t. The new momenta, p_o, is

$$p_o = -H \tag{3.4}$$

and the extended phase space (x, p, x_o, p_o) Hamiltonian is

$$H_h = H + p_o = 0 \tag{3.5}$$

The independent variable may be changed from t to τ according to

$$\mu = \frac{dt}{d\tau} = t' = 1 \tag{3.6}$$

In the more general case, μ may be a function of all x_k and p_k. In the present case, the new independent variable τ is related to time by a constant.

Now introduce a new Hamiltonian in the extended phase space by

$$F_h = H_h\mu = \frac{1}{2} p^2 + \frac{1}{2} x^2 + p_o + V(x,x_o) = 0 \tag{3.7}$$

The system given by the Hamiltonian (3.7) will now be transformed into two new canonical systems. The first new system corresponds to the oscillator solution of the form

$$x = \alpha \sin \beta \tag{3.8}$$

where α is a constant and β is a linear function of time. The second new system corresponds to the equivalent solution,

$$x = a \cos t + b \sin t \tag{3.9}$$

where a and b are constants. It is well known that the last two equations are equivalent solutions to the unperturbed oscillator.

The procedures for developing the two transformations are similar: generating functions will be used to transform from the old canonical variables (x, p, x_o, p_o) to the new sets ($\bar{x}$, $\bar{p}$, $\bar{x}_o$, $\bar{p}_o$) and ($\tilde{x}$, $\tilde{p}$, $\tilde{x}_o$, $\tilde{p}_o$). The new Hamiltonians will then be presented. The two transformations are elementary and presented without details.

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(A) First New System

The generating function:

$$\bar{S}(x_o, x, \bar{p}_o, \bar{p}) = \int (2\bar{p} - x^2)^{1/2} \, dx + \bar{p}_o x_o \tag{3.10}$$

where

$$p = \frac{\partial \bar{S}}{\partial x}, \quad p_o = \frac{\partial \bar{S}}{\partial x_o}, \quad \bar{x} = \frac{\partial \bar{S}}{\partial \bar{p}}, \quad \bar{x}_o = \frac{\partial \bar{S}}{\partial \bar{p}_o}$$

The transformation $(x, p, x_o, p_o \rightarrow \bar{x}, \bar{p}, \bar{x}_o, \bar{p}_o)$:

$$\begin{aligned} x &= \sqrt{2\bar{p}} \sin \bar{x} \\ p &= \sqrt{2\bar{p}} \cos \bar{x} \\ x_o &= \bar{x}_o \\ p_o &= \bar{p}_o \end{aligned} \tag{3.11}$$

The new Hamiltonian:

$$\bar{F}_h = \bar{p} + \bar{p}_o + V(\bar{x}, \bar{p}, \bar{x}_o) = 0 \tag{3.12}$$

The differential equations for the elements

$$\begin{aligned} \bar{x}' &= 1 - \frac{x}{2\bar{p}} \left(f - \frac{\partial V}{\partial x} \right) \\ \bar{p}' &= p \left(f - \frac{\partial V}{\partial x} \right) \\ \bar{x}_o' &= 1 \\ \bar{p}_o' &= - \frac{\partial V}{\partial x_o} - pf \end{aligned} \tag{3.13}$$

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(B) Second New System

The generating function:

$$\tilde{S}(p_o,\ p,\ \tilde{x}_o,\ \tilde{x},\ \tau) = \frac{1}{\sin\tau}\left[\frac{1}{2}(p^2 + \tilde{x}^2)\cos\tau - p\tilde{x}\right] - p_o\,\tilde{x}_o \tag{3.14}$$

where

$$x = -\frac{\partial\tilde{S}}{\partial p},\quad x_o = -\frac{\partial\tilde{S}}{\partial p_o},\quad \tilde{p} = -\frac{\partial\tilde{S}}{\partial\tilde{x}},\quad \tilde{p}_o = -\frac{\partial\tilde{S}}{\partial\tilde{x}_o}$$

The transformation $(x,\ p,\ x_o,\ p_o \to \tilde{x},\ \tilde{p},\ \tilde{x}_o,\ \tilde{p}_o)$:

$$\begin{aligned} x &= -\tilde{p}\cos\tau + \tilde{x}\sin\tau \\ p &= \tilde{p}\sin\tau + \tilde{x}\cos\tau \\ x_o &= \tilde{x}_o \\ p_o &= \tilde{p}_o \end{aligned} \tag{3.15}$$

The new Hamiltonian:

$$\tilde{F} = F_h + \frac{\partial\tilde{S}}{\partial\tau} = \tilde{p}_o + V(\tilde{x},\ \tilde{p},\ \tilde{x}_o) \neq 0 \tag{3.16}$$

The differential equations for the elements:

$$\begin{aligned} \tilde{x}' &= \left(f - \frac{\partial V}{\partial x}\right)\cos\tau \\ \tilde{p}' &= \left(f - \frac{\partial V}{\partial x}\right)\sin\tau \\ \tilde{x}_o' &= 1 \\ \tilde{p}_o' &= -\frac{\partial V}{\partial x_o} - pf \end{aligned} \tag{3.17}$$

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Note that equations (3.11) and (3.13) have only an implicit dependence on the independent variable τ, whereas equations (3.15) and (3.17) have an explicit dependence on τ. Also, the Hamiltonian equation (3.12) for the system A still vanishes after the transformation, whereas the Hamiltonian equation (3.16) for the system B has lost the vanishing characteristic.

The association of implicit differential equations with a vanishing Hamiltonian in extended phase space (system A) and explicit differential equations with a nonvanishing Hamiltonian in extended phase space (system B) is not entirely accidental. A generating function $\bar{S}$ which does not depend explicitly on τ generates implicit transformations between the new and old variables ($\bar{x} = \bar{x}(x,p)$, $\bar{p} = \bar{p}(x,p)$) in extended phase space and also maintains the vanishing property of the Hamiltonian. A generating function $\tilde{S}$ which does depend explicitly on τ generates explicit transformations ($\tilde{x} = \tilde{x}(x,p,\tau)$, $\tilde{p} = \tilde{p}(x,p,\tau)$) and in general does not maintain the vanishing Hamiltonian property. Since in either case the old variables are eliminated from the right hand side of the differential equations by these transformations, it follows that the implicit differential equations and the vanishing Hamiltonian stem from a generating function which does not depend upon τ. This of course does not imply that implicit differential equations must have a vanishing Hamiltonian.

4. A TEST PROBLEM (VAN DER POL EQUATION)

A van der Pol equation will be used as a test problem for the two Hamiltonian formulations of the perturbed harmonic oscillator. The van der Pol equation in its coordinate form, equation (1.1) is an oscillator with the perturbation.

$$f = \varepsilon(1 - x^2)\dot{x} \tag{4.1}$$

where ε is a small parameter, the potential V has been set to zero.

For the system (A) where $\bar{F}_h = 0$:

The perturbation, f, is;

$$f = \varepsilon p(1 + p^2 + 2\bar{p}_o)$$

The initial conditions ($x = 0$, $p = 2$, when $t = 0$) become;

$$\bar{x} = 0,\ \bar{p} = 2,\ \bar{x}_o = 0,$$

$$\bar{p}_o = -2$$

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The amplitude, A, of the oscillation is

$$A = \sqrt{2p}$$

where $A \to 2$ asymptotically.

By averaging in the asymptotic region over one cycle of the equations of motion

Equations (3.13) yield

$$\left\langle \frac{dA}{d\tau} \right\rangle = 0$$

Has no secular increase in amplitude.

For system (B) where $\tilde{F}_h \neq 0$:

The perturbation, f, is;

$$f = \varepsilon p(1 + p^2 + 2\tilde{p}_o)$$

The initial conditions ($x = 0$, $p = 2$, when $t = 0$) become;

$$\tilde{x} = 2, \ \tilde{p} = 0, \ \tilde{x}_o = 0, \ \tilde{p}_o = -2$$

The amplitude, A, of the oscillation is

$$A = \sqrt{\tilde{x}^2 + \tilde{p}^2}$$

where $A \to 2$ asymptotically.

By averaging in the asymptotic region over one cycle of the equations of motion

Equations (3.17) yield

$$\left\langle \frac{dA}{d\tau} \right\rangle = 0(\varepsilon)$$

Has a secular increase in amplitude of the order $0(\varepsilon)$.

The averaging over one cycle of equations (3.13), system A, is done with respect to the angle $\bar{x}$ which is permissible since the independent variable τ does not appear explicitly on the right hand sides of the equations. The averaging results in no secular change in amplitude.

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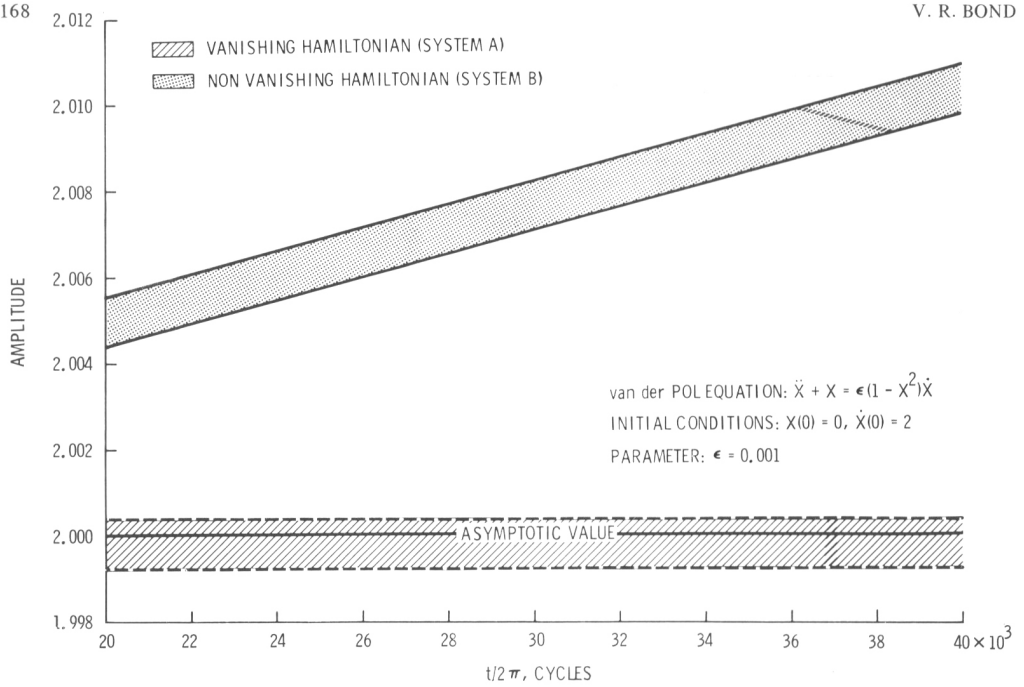

Figure 1.- Comparison of numerically computed solutions of the van der POL equation (Runge-Kutta 2nd order).

This problem was solved by averaging using a slightly different set of elements (non-canonical) by Cesari (1970). The averaging of equations (3.17), system B, is slightly more difficult since the independent variable appears on the right hand side and the average must be done over an imprecise period, $2\pi + O(\varepsilon)$. The averaging results in a secular change of order ε in the amplitude. This is an example of a physically stable problem which is made mathematically unstable because of the choice of the variables in which the problem is solved.

Both formulations of the van der Pol problem were numerically integrated. These results are shown in figures (1) and (2). In figure (1) the amplitudes were compared to the asymptotic value of two where the numerical integrator was a second order Runge-Kutta method; figure (2) shows a similar comparison using third order Runge-Kutta method. The computations were done using approximately 15 steps per cycle. It is obvious that the system B solution has linear deviation from the theoretical asymptotic amplitude of two, whereas the system A solution is quite stable oscillating slightly about two. For higher order Runge-Kutta methods, the difference between the two solutions is less pronounced.

5. TEST PROBLEMS IN KEPLERIAN MOTION

Two of the libration points in the restricted problem of three bodies are used as test cases for the Keplerian motion formulations.

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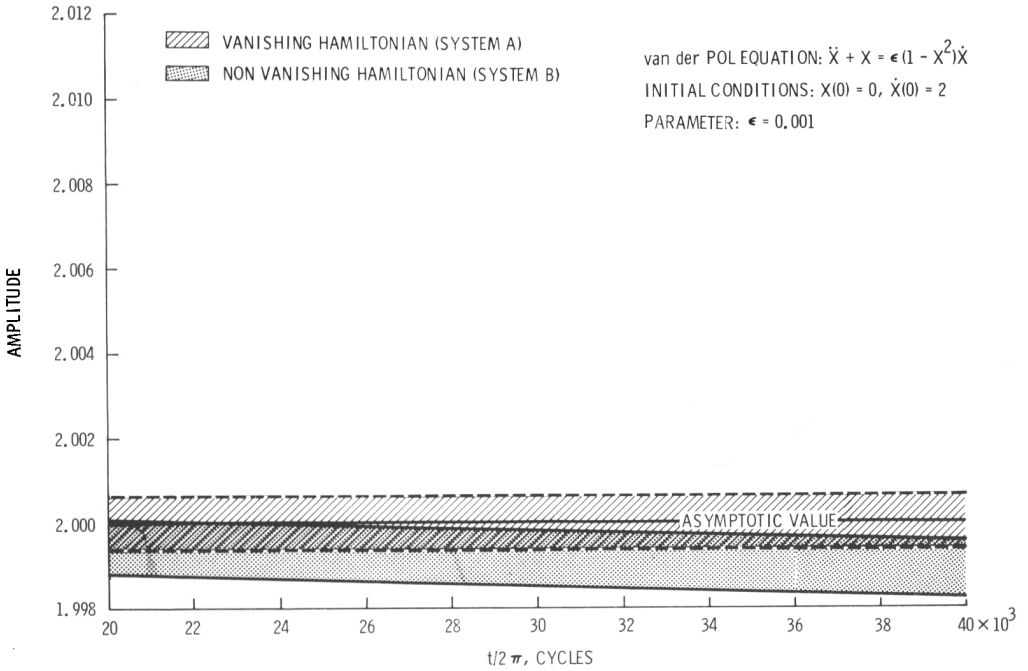

Figure 2. - Comparison of numerically computed solutions of the van der Pol equation (Runge-Kutta 3rd order).

These solutions are known solutions in the restricted problem and therefore make excellent test cases for perturbed Keplerian motion. The numerically integrated results are locally transformed and compared with the known solutions. The model for the Earth-Moon system used in this computation was taken from the book by Stiefel and Scheifele. The model and the initial conditions are provided for those who wish to make their own comparisons.

Gravitational parameters:

Earth: $GM_E = 398601.0\ KM^3\ SEC^{-2}$

Moon: $GM_M = 4902.66\ KM^3\ SEC^{-2}$

Earth-Moon distance: $R_{EM} = 384400.0\ KM$

Moon orbital rate: $\Omega = \sqrt{(GM_E + GM_M)/R_{EM}^3}$

The moon is considered to be initially on the x_1 axis.

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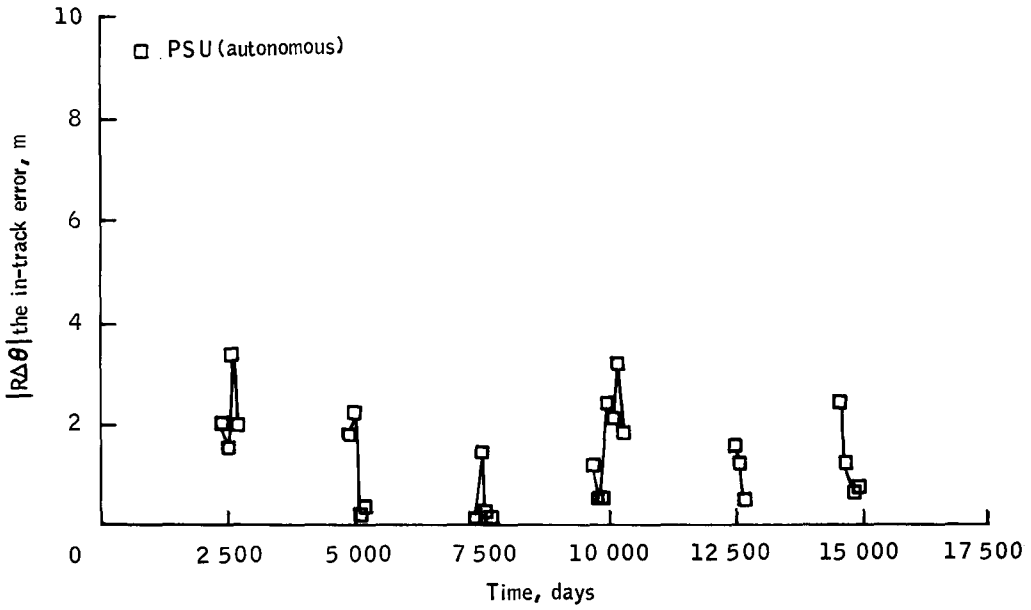

Figure 3.- The in-track error in the motion of a particle about the Lagrangian libration point in the Earth-Moon system over a period of 15 000 days.

Figure 3 shows the intrack error of the numerical solution versus the analytical solution for a particle at a stable libration point in the Earth-Moon system. This test case is given by Bond (1976). The initial conditions for the trajectory commencing at the stable point are:

$$x_1 = \frac{R_{EM}}{2} \; ; \; x_2 = \sqrt{3}\frac{R_{EM}}{2} \; ; \; x_3 = 0$$

$$\dot{x}_1 = -\Omega x_2 \; ; \; \dot{x}_2 = \Omega x_1 \; ; \; \dot{x}_3 = 0$$

The numerical solution was computed from the PSu formulation of perturbed Keplerian motion with a fifth order Runge-Kutta method at 20 steps per revolution. The solution shows no error growth over a period of 15,000 days. The equations of motion, in PSu elements, were averaged by quadrature for this case with the result that no secular change occurs in the elements. This process is rather lengthy and is omitted. But here as in the case of the system (A) formulation of the van der Pol problem the numerical solution and the first order analytical solution yield consistent results.

The next test case is that of problem of a particle at the collinear unstable libration point in the Earth-Moon system located between

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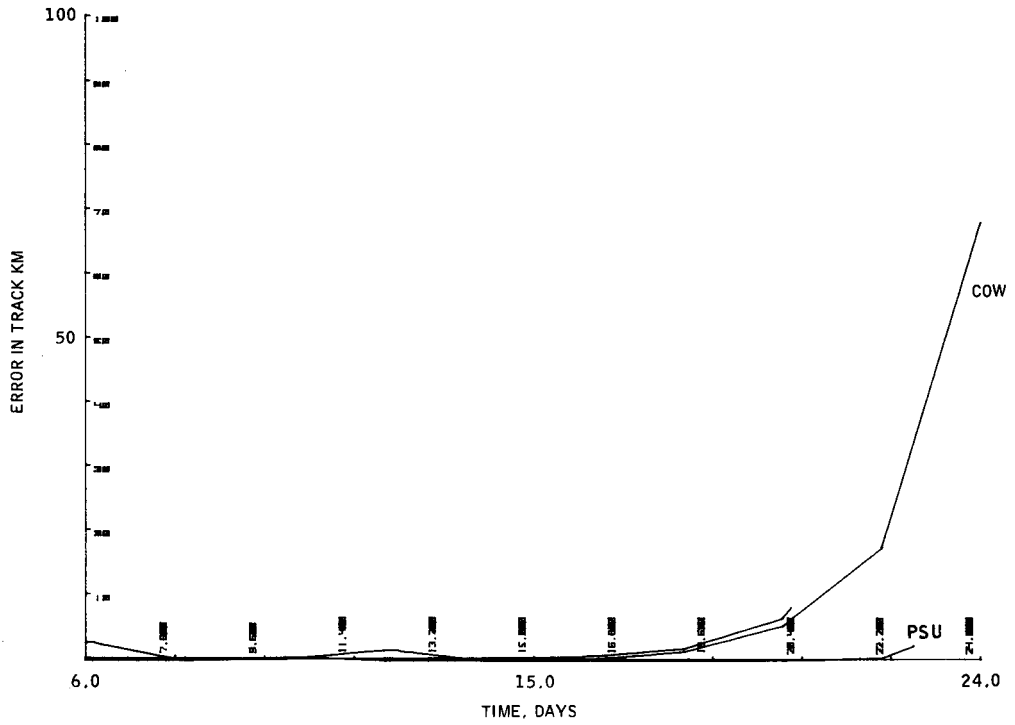

Figure 4.- Numerical solution at L2 RK45 200 SPR.

the Earth and the Moon. For example, after one lunar period (approximately 27 days) from figure 4 the error in the PSu solution was only 1 or 2 KM. The solution computed by the Cowell method had an error of about 70 KM. The integration was done with a Runge-Kutta fifth order method at 200 steps per revolution. The initial conditions for the trajectory commencing at the unstable point are:

$$x_1 = 326381.403878418380 \text{ KM}; \; x_2 = 0; \; x_3 = 0$$

$$\dot{x}_1 = 0, \; \dot{x}_2 = 0.869909506345283935 \text{ KM SEC}^{-1}; \; \dot{x}_3 = 0$$

This problem is extremely sensitive to the initial conditions, which were obtained by iteration using initial conditions obtained from the book by Szebehely. The full 18 digit initial conditions with the above model must be used in order to obtain results which are to compare with figure 4.

6. DISCUSSION

In the numerical solution of ordinary differential equations a distinction must be made between the stability of the physical problem

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which is to be solved and the stability of the mathematical formulation or choice of variables. The physical problem can be dynamically stable, as in the case of the van der Pol problem, but the mathematical formulation of the problem can be unsuited for the problem and induce instability. For example from section 4.0 the solution from the formulation of the van der Pol oscillator with a non-vanishing Hamiltonian (system B) has a secular error growth in the average amplitude, but the solution from the formulation with the vanishing Hamiltonian (system A) has no error growth in the average amplitude. These results are the same for both the analytically averaged and the numerical solutions. From section 5.0, the solution in PSu elements (vanishing Hamiltonian) of a particle at a stable libration point also shows no error growth in both the analytically averaged and the numerical solution.

It is not surprising that numerical solutions of differential equations should exhibit the same stability characteristics as their analytical solutions. From the definition of stability, stable solutions are affected only slightly by small errors in initial conditions while unstable solutions diverge for small errors in initial conditions. The numerical integration process introduces errors in the solution at a given step. Since the results of this step are used to initialize the next step, the errors in initial conditions are propagated forward in the same manner as they would be in their analytical solutions.

It is also possible that instabilities may be introduced due to the numerical method chosen to solve the problem. This paper has not emphasized this aspect, but the order of the integration method was shown to have an effect. For example, increasing the order of the Runge-Kutta method was shown to improve the stability of the numerical solution of the van de Pol when the system with the nonvanishing Hamiltonian was integrated, but the increase in the order made no difference in the stability of the numerical solution when the system with the vanishing Hamiltonian was used. That is, the latter formulation gave a stable solution even for the lowest order integrator.

Some excellent discussions of particular approaches to the problem of matching the numerical integration method to the mathematical formulation of a physical problem are given by Bettis (1970), Szebehely and Bettis (1971), Graf and Bettis (1973), Janin (1974), Velez (1974), Shampine and Gordon (1975), and Graf (1975).

ACKNOWLEDGMENTS

The author wishes to thank Dr. Victor Szebehely of the University of Texas at Austin for his helpful discussions concerning stability; and Dr. Dale Bettis of the University of Texas at Austin for providing the numerical integration programs for these applications.

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