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LA-UR--89-3465

DE90 002380

TITLE Symplectic Numerical Integration of Hamiltonian Systems

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SUBMITTED TO MSRI Workshop on Geometry of Hamiltonian Systems

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Received by OSTI

11 10 1989

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Symplectic Numerical Integration of Hamiltonian Systems

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September 11, 1989

1 Introduction

The classical integration and transformation theory of Hamiltonian systems always considered canonical transformations, and to generate these transformations a generating function was used. However, with the advent of high speed digital computers it seems the importance of canonical transformations has been forgotten as the standard numerical technique is to consider the system as a vector field and to integrate it's trajectory by some ODE integrator. In 1956, De Vogelaere [24] attempted to publish concerning symplectic methods, and it wasn't until 1983 that Ruth [66] and Channell [15] developed the notion of a symplectic integration algorithm (SIA). It should be mentioned that it seems well known that the first order integrators

$$Q = q + tP \quad (1)$$

$$P = p - t * \nabla V(q) \quad (2)$$

and

$$Q = q + tp$$

$$P = p - t * \nabla V(Q)$$

for the Hamiltonian $H = p^2/2 + V(q)$ are symplectic. The computational importance of the symplectic condition has been understood in Celestial Mechanics [22],[51],[74], Accelerator Physics [27], and recent investigations

into the ergodic behavior of the Fermi-Pasta-Ulam system [10],[57], and Arnol'd diffusion [75], [76].

Recently, SIA's have received much attention [9], [13],[16],[20], [26],[30],[31], [33],[34],[35],[37],[39],[40],[41],[48],[49],[50],[52],[56],[60],[61], [63],[68],[71],[72], and have been shown to produce global phase space structures, commonly found in Hamiltonian mechanics. Since there is a KAM theorem for mappings [5], SIA's can be expected to simply distort all nondegenerate incommensurate invariant tori of the original system, and to possess exponentially slowly deviating adiabatic invariants according to the theory of Nekhoroshev [62]. Equivariant SIA's will enjoy a different class of generic bifurcation phenomena as discussed in Golubitsky et al. [43], and be subject to topological restrictions according to the recent developments of Ekeland and Hofer [28]. Numerical evidence suggests that symplectic integration might reveal hidden symmetries which analytically, at present, are mere fantasy. See Fomenko [32] for example. This, by no means, implies that the symplectic condition is the ultimate invariant, since preserving the energy may have strong compactification properties [52]. Feng and Qin [31] show that energy conservation is possible in a symplectic scheme but that the symplectic structure would have to be altered. In addition, Ge[39] has shown that, for a system which has no other first integrals, a SIA which preserves the energy exactly is a reparameterization, in time, of the real flow. This implies that the energy is the correct monitor of accuracy for SIA's which preserve all invariants but the energy. Indeed, numerical calculations [16] show that SIA's tend to preserve the energy extremely well over long integration times. On the other hand, Jimenez and Vazquez [52] show that SIA's may have blowup where an energy conserving scheme does not, and the latter's flow is volume preserving, and possibly symplectic, in the mean. It is clear that the dual relationship between energy and symplectic structure should be understood.

Many SIA's preserve integral invariants related to symmetries of the system to within roundoff error [16]. In particular, Feng [30] shows that there are SIA's that preserve all quadratic first integrals. Using the relationship between generating functions and Hamilton-Jacobi theory [30],[31], Ge and Marsden [39] have shown that the Hamilton-Jacobi equation reduces when the system has symmetry, and that this reduced Hamilton-Jacobi equation can be used to integrate symplectically, or by Poisson maps, on the reduced spaces. In addition, Ge[40],[41] has demonstrated a generating function for the Poisson map in the setting of Poisson Groupoids [73]. This opens up the possibility of Lie-Poisson integration of systems of Lie-Poisson type: the rigid body [2],[55], Euler fluids[2], the Maxwell-Vlasov and Vlasov-Poisson

equations of plasma physics [59], and many more (cf. Marsden et al. [59] and Marsden (these proceedings)). It should be emphasized that a consistent finite dimensional truncation will be required on present finite state machines (cf. Holm et al. [50]). Lie-Poisson integration of the rigid body [17] and a truncated moment description of the Vlasov equation [17] based upon [21] show that Lie-Poisson integrators possess the same stability characteristics as the symplectic integrators demonstrated in [16]. When the setting is the dual of a Lie algebra [59], [45], Lie-Poisson integration preserves the coadjoint orbits and defines a symplectic map on the coadjoint orbit with respect to it's Kirillov-Kostant-Souriau symplectic structure. Therefore, the stability of these integrators is related to the fact that they keep the dynamics on the correct coadjoint orbit and on it the dynamics is Hamiltonian.

In this paper, I describe some general techniques available for symplectic or Lie-Poisson integration and illustrate the results with some numerical computations. In this spirit, I also discuss reversible integration, equivariant integration, integration of volume preserving flows, and symplectic cellular automata. My intention is not to be exhaustive but to give a representative review.

2 The Techniques

2.1 Generating Functions

A general technique for the construction of symplectic maps is the use of a generating function [3],[12]. Let S be any scalar function. Then the map $(q, p) \rightarrow (Q, P)$ determined by solving the implicit system of equations

$$q = \frac{\partial S(Q, p, t)}{\partial p} \quad (3)$$

$$P = \frac{\partial S(Q, p, t)}{\partial Q} \quad (4)$$

is symplectic. Consider a Hamiltonian system

$$\begin{aligned} \dot{q} &= \frac{\partial H(q, p)}{\partial p} \\ \dot{p} &= -\frac{\partial H(q, p)}{\partial q} \end{aligned}$$

To approximately integrate it's trajectories via a generating function we need to determine the generating function in terms of the Hamiltonian.

There is no unique way to do this, so I will illustrate with the following simple example. The actual formulae can be found in [31],[16]. Expand the solution of the initial value problem in a Taylor series:

$$Q = F_1(q, p, t) \quad (5)$$

$$P = F_2(q, p, t). \quad (6)$$

Inverting the first equation for q and plugging into the second equation gives

$$q = F_1^{-1}(Q, p, t) \quad (7)$$

$$P = F_2(F_1^{-1}(Q, p, t), p, t). \quad (8)$$

which must be of the form of equations (1) and (2):

$$F_1^{-1}(Q, p, t) = \frac{\partial S(Q, p, t)}{\partial p} \quad (9)$$

$$F_2(F_1^{-1}(Q, p, t), p, t) = \frac{\partial S(Q, p, t)}{\partial Q} \quad (10)$$

for some scalar function S .

However, to compute, a truncation of F_1 and F_2 to some approximations f_1 and f_2 will be required giving, generally, a nonsymplectic result for the map (1) and (2). Consider the approximate inapping

$$Q = f_1(q, p, t)$$

$$P = f_2(q, p, t).$$

This mapping is assumed to be accurate to within some order. Determine f_1^{-1} to that same order. Consequently,

$$f_1^{-1}(Q, p, t) = \frac{\partial \tilde{S}(Q, p, t)}{\partial p} \quad (11)$$

$$f_2(f_1^{-1}(Q, p, t), p, t) = \frac{\partial \tilde{S}(Q, p, t)}{\partial Q} \quad (12)$$

is approximately correct for some computable function $\tilde{S}$.

Solving

$$q = \frac{\partial \tilde{S}(Q, p, t)}{\partial p} \quad (13)$$

$$P = \frac{\partial \tilde{S}(Q, p, t)}{\partial Q} \quad (14)$$

to within some prescribed tolerance (close to roundoff error) determines a symplectic map, within that tolerance, which approximately integrates the flow. Determination of the timestep by requiring Picard iteration to converge close to roundoff error within 3 to 7 iterations after a nonsymplectic predictor such as Runge-Kutta, seems to work well [16], but alternative methods (e.g. Newton's method) have not been explored with respect to additional computational effort being balanced by an increase in possible timestep size.

Classical generating functions are of four types [42] depending on mixing old and new variables. Feng [30], and Feng and Qin [31] generalize the mixing of old and new variables in the setting of Lagrangian submanifolds and construct SIA's which preserve all quadratic integral invariants: those related to linear Lie group actions. Channell and Scovel [16] use generating functions which are invariant under symmetry groups and observe that the corresponding integral invariants are preserved to within roundoff error, and show that for linear systems, the general SIA's preserve quadratic integral invariants close to those of the original system. Which generating function to use depends upon the symmetries of the problem, the ease in computing matrix inverses, and the form and size of the Hamiltonian.

The relationship of generating functions to Hamilton-Jacobi theory seems implicitly understood (cf. Goldstein [42], p. 279) but is made explicit by Feng and Qin [31], and is summarized as follows: the graph of a symplectic map is a Lagrangian submanifold in the product space with the standard product symplectic structure. A Lagrangian submanifold which projects diffeomorphically to the configuration space (as in maps near the identity) is locally the graph of an exact one-form dS . S is called the generating function and the evolution of S as the map evolves by a Hamiltonian system is the Hamilton-Jacobi equation.

The works of Ge and Marsden [39] on Lie-Poisson Hamilton-Jacobi theory and Ge [40], [41] on the generating function for the Poisson map are fundamental in the development of Lie-Poisson integrators (LPI's) for systems of Lie-Poisson type. For Hamiltonian systems on T^*G , where G is a Lie group, and the Hamiltonian is invariant under G , Ge and Marsden [39] reduce the Hamilton-Jacobi equation to one for the reduced Hamiltonian on the dual of the Lie algebra $\mathfrak{g}^*$. This reduced Hamilton-Jacobi equation can be used to approximately integrate the Lie-Poisson flow on $\mathfrak{g}^*$ by Poisson maps. That is, the LPI constructed preserves the coadjoint orbits and the Poisson bracket. It should be pointed out that these algorithms preserve many additional symmetries that may be present. For example, left reduced

systems with right invariances, as in a rigid body with symmetry.

2.2 The Baker-Campbell-Hausdorff Formula

Consider a Hamiltonian of the form $H(q, p) = F(p) + V(q)$. Each part, F and V , of this Hamiltonian can be solved explicitly: The solution with Hamiltonian $F(p)$ is the map $m_1(t)$ defined by

$$\begin{aligned} Q &= q + t * \nabla F(p) \\ P &= p \end{aligned}$$

and for the Hamiltonian $V(q)$ is the map $m_2(t)$ defined by

$$\begin{aligned} Q &= q \\ P &= p - t * \nabla V(q). \end{aligned}$$

Write e^{tH} as the solution map for the Hamiltonian H . Then, $m_1(t) = e^{tF}$ and $m_2(t) = e^{tV}$. It is easy to see that both $m_1(t) \circ m_2(t)$ and $m_2(t) \circ m_1(t)$ equal e^{tH} plus $O(t^2)$. Therefore they both determine first order SIA's. Note that they are the SIA's mentioned in the introduction.

This is the essence of Ruth's method [67]. To obtain higher order integrators, concatenate m_1 and m_2 many times using different time steps to match the coefficients of e^{tH} (cf. [33], [34], [63], [13]) . . . For example, as found in Forest and Berz [34],

$$m_1(s_1) \circ m_2(d_1) \circ m_1(s_2) \circ m_2(d_2) \circ m_1(s_2) \circ m_2(d_1) \circ m_1(s_1) = e^{tH} + O(t^5),$$

is symplectic. The constants are $\beta = \sqrt[3]{2}$ and

$$\begin{aligned} s_1 &= t/(2 * (2 - \beta)) \\ s_2 &= t * (1 - \beta)/(2 * (2 - \beta)) \\ d_1 &= t/(2 - \beta) \\ d_2 &= -\beta * t/(2 - \beta). \end{aligned}$$

Both m_1 and m_2 are symplectic and explicit and if the system is large with local interaction, as in some molecular dynamics calculations, it is also local. Therefore, SIA's constructed this way are very fast and may be used for very large systems. However, they tend to neglect symmetries of the system which are not simultaneously symmetries of F and V . As mentioned in Neri [63], and Forest and Berz [34], this method generalizes to an arbitrary

Lie group and is applicable when the element of the Lie algebra, which one wants to exponentiate, is a linear combination of elements for which their exponentials can easily be computed, or approximated within the group.

One parameter subgroups are characterized by their linearization at the identity and the fact that they are groups. Therefore, the approximation of such a group can be accomplished by the correct linearization and preserving as much of the group property as possible. One application of this is the following: Suppose $\varphi(t)$ is a one parameter family of elements approximating a one parameter subgroup $\Phi(t)$ which is the identity at $t = 0$ and has the correct linearization there. Φ satisfies $\Phi^{-1}(t) = \Phi(-t)$ but $\varphi(t)$ may not. However, since $\varphi(t)$ is an approximation near $t = 0$, so is $\varphi^{-1}(-t)$ and the composed map $\psi(t) = \varphi^{-1}(-t/2) \circ \varphi(t/2)$ is manifestly the same order approximant but now satisfies $\psi^{-1}(t) = \psi(-t)$. This implies that ψ is of even order accuracy. This provides a way of turning a first order integrator into a second order one, and a third order integrator into a fourth order one, etc. Plus, to integrate backwards, simply change t to $-t$. As an example, consider the first order SIA $m_1(t) \circ m_2(t)$. Since both m_1 and m_2 are one parameter subgroups, a second order SIA is $m_1(t/2) \circ m_2(t) \circ m_1(t/2)$, giving a result of Neri's [63].

Lasagni [56], and Sanz-Serna [68] show that implicit Runge-Kutta, where the quadrature matrices satisfy a quadratic relation, are symplectic. In particular, those with Gauss-Legendre quadrature rules are symplectic [68].

2.3 Modified Midpoint Rule

Feng [30], Feng and Qin [31], and Stofer [71] show that the time centered Euler scheme is symplectic. They generalize to obtain SIA's of arbitrary order. Let $z = (q, p)$ and it's image under the map be $Z = (Q, P)$. Using the notation of [71], let $g(z) = J\nabla H(z)$ be the Hamiltonian vectorfield, where J is the symplectic matrix. The time centered Euler or implicit midpoint rule is the map determined by the implicit set of equations

$$Z - z = t * g((z + Z)/2)$$

which determine a second order SIA. To obtain higher order SIA's construct a function $\tilde{g}(z) = J\nabla \tilde{H}(z)$ so that the solution of

$$Z - z = t * \tilde{g}((z + Z)/2)$$

determines a fourth order (for example) SIA. This modified midpoint rule is automatically symplectic since $\tilde{g}$ is a Hamiltonian vector field. Typically,

these SIA's require one more derivative of the Hamiltonian for each order of accuracy desired. However, Stofer's ansatz for the form of $\tilde{g}$ provides a fourth order SIA which requires only second derivatives of H . Write

$$\begin{aligned} z^+ &= z + \alpha t * g(z) \\ z^- &= z - \alpha t * g(z) \\ \tilde{g}(z) &= (1 - 2\beta)g(z) + \beta(g(z^+) + g(z^-)) - \alpha\beta t Dg(z)[g(z^+) - g(z^-)], \end{aligned}$$

where $\alpha^2\beta = 1/24$. The new Hamiltonian is

$$\tilde{H}(z) = (1 - 2\beta)H(z) + \beta(H(z^+) + H(z^-)).$$

If g is equivariant under a symmetry group, then the modified midpoint rule is shown to be equivariant. In addition, Stofer shows that if g is reversible (as discussed in the next section), then the modified midpoint rule is also reversible.

2.4 Reversible Integration

Birkhoff [12] used the fact that the involution $(q, p) \rightarrow (q, -p)$ reverses the direction of the flow in the restricted three body problem to prove the existence of and classify periodic orbits. De Vogelaere [25] has also utilized this technique. Devaney [23] has proved the analogues of the closed orbit, Liapunov, and homoclinic orbit theorems for reversible systems independent of any existing Hamiltonian structure. Sevryuk [69] has demonstrated a KAM theorem for reversible systems and so it seems that numerical integration of reversible systems should be accomplished by reversible integrators. See also [8],[54],[66]. Bennett [11] discusses the reversibility of computation, not exactly in the present sense, with regards to defeating dissipative mechanisms in the computational process. Relegating reversibility to the present context, Fredkin and Toffoli [36], and Margolus [58], investigate it's implications in Physics computations.

Let R be an involution of phase space. A map φ on the phase space is said to be R reversible if $\varphi^{-1} = R^{-1}\varphi R = R\varphi R$. This implies that the inverse map is obtained by applying the forward map in the changed coordinates determined by R . A vector field χ is said to be R -reversible if $-\chi = R\chi R$.

For an R reversible dynamical system, the modified midpoint rule produces an R -reversible integration algorithm in addition to being symplectic [71].

There is a projection to R -reversible maps. Let $\varphi(t)$ be an approximation to a reversible system. Then, $R\varphi^{-1}(t)R$ is also an approximate of the same system and the composition $\psi(t) = R\varphi^{-1}(t/2)R\varphi(t/2)$ is R -reversible. Since R is anti-symplectic, ψ is symplectic if φ is. The Hamiltonian system with Hamiltonian $H = p^2/2 + V(q)$ is reversible with respect to the involution $(q, p) \rightarrow (q, -p)$. However, the first order SIA

$$\begin{aligned} Q &= q + tP \\ P &= p - t * \nabla V(q) \end{aligned}$$

is not reversible with respect to this involution. The projection discussed above could be used to make it reversible or notice that, as in Kook and Meiss [54], it is reversible with respect to the involution $(q, p) \rightarrow (-q, p - t\nabla V(q))$ when V is an even function. It is important to notice that this involution is parametrized by time so that the involution changes depending on the time step. This reversing involution can be explained as follows: Let R be the involution $(q, p) \rightarrow (q, -p)$. The symplectic maps m_1 and m_2 , defined in section 2.2 are both R -reversible. Consequently, $R \circ m_1$, $R \circ m_2$, $m_1 \circ R$, and $m_2 \circ R$ are all involutions. The set of reversible maps does not form a group, in fact, it is easy to show that the composition of two reversible maps is reversible if and only if the two maps commute. The SIA defined above is $\varphi = m_1 \circ m_2$, and the non-commutativity of m_1 and m_2 explains why their composition φ is not R -reversible. Consider the involution $\tilde{R} = R \circ m_2$. Compute

$$\tilde{R}m_1m_2\tilde{R} = Rm_2m_1m_2Rm_2.$$

Since $Rm_2 = m_2^{-1}R$, this becomes

$$m_2^{-1}Rm_1m_2m_2^{-1}R = m_2^{-1}Rm_1R = m_2^{-1}m_1^{-1} = (m_1m_2)^{-1}$$

showing that φ is $\tilde{R}$ -reversible. Likewise, it is also Rm_1^{-1} -reversible. The other two involutions can be used for the SIA $m_2 \circ m_1$. In the event that V is an even function, $-I$ commutes with m_1 , m_2 , and R , and all reversing involutions may be multiplied by $-I$. The reversing involution of Kook and Meiss is $-R \circ m_2$.

2.5 Volume Preserving Integration

Divergence free vectorfields determine volume preserving transformations and it is known that such flows possess a non-canonical Hamiltonian structure which could be used to integrate them [14],[18],[19], [76]. However,

these structures are singular at fixed points of the vector field, and the Hamiltonian and the canonically conjugate variables might be complicated functions so that it seems desirable to integrate them directly as volume preserving maps. Volume preserving maps preserve the helicity: a topological invariant important in magnetic field line problems [7],[4]. Such flows are also important in fluid mechanics [2],[6].

It is interesting to note that the substitution of a nongradient term $F(q)$ for $\nabla V(q)$ in (1) and (2) deems the integrator non-symplectic. However, it is exactly volume preserving, and comparison of it with the symplectic version will be reported on in a future publication. Construction of volume preserving integrators(VPI's) for divergence free vector fields is not quite so simple. Following Thyagaraja and Haas [72], mix old and new variables to obtain generating functions for the volume preserving map. Let $v = (v_1, v_2, v_3)$ be a divergence free vector field in R^3 . Consider a map $(x, y, z) \rightarrow (X, Y, Z)$ represented implicitly by the equations

$$X = f(x, y, Z) \quad (15)$$

$$Y = g(x, y, Z) \quad (16)$$

$$z = h(x, y, Z). \quad (17)$$

A simple calculation shows that this map is volume preserving if and only if

$$\frac{\partial h}{\partial Z} = \frac{\partial f}{\partial x} \frac{\partial g}{\partial y} - \frac{\partial f}{\partial y} \frac{\partial g}{\partial x}.$$

This determines h as a partial integral of a function of the two generating functions f and g . Let $v = (v_1, v_2, v_3)$ be a divergence free vector field in R^3 . The determination of the generating functions f and g in terms of v can be accomplished in the same manner as in section 2.1. I will give the first and second order results. Let

$$f(x, y, Z) = x + f_1(x, y, Z)t^1 \quad (18)$$

$$g(x, y, Z) = y + g_1(x, y, Z)t^1 \quad (19)$$

$$h(x, y, Z) = Z + h_1(x, y, Z)t^1 \quad (20)$$

be the Taylor series of f, g , and h , in t , where the map is determined to be the identity at $t = 0$. A first order VPI is obtained from

$$f_1 = v_1 \quad (21)$$

$$g_1 = v_2 \quad (22)$$

$$h_1 = -v_3 \quad (23)$$

$$h_2 = \int^Z \left[\frac{\partial v_1}{\partial x} \frac{\partial v_2}{\partial y} - \frac{\partial v_1}{\partial y} \frac{\partial v_2}{\partial x} \right]. \quad (24)$$

and a second order one from

$$f_1 = v_1 \quad (25)$$

$$f_2 = 1/2 \left(\frac{\partial v_1}{\partial x} v_1 + \frac{\partial v_1}{\partial y} v_2 - \frac{\partial v_1}{\partial Z} v_3 \right) \quad (26)$$

$$g_1 = v_2 \quad (27)$$

$$g_2 = 1/2 \left(\frac{\partial v_2}{\partial x} v_1 + \frac{\partial v_2}{\partial y} v_2 - \frac{\partial v_2}{\partial Z} v_3 \right) \quad (28)$$

$$h_1 = -v_3 \quad (29)$$

$$h_2 = 1/2 \left(\frac{\partial v_3}{\partial Z} v_3 - \frac{\partial v_3}{\partial x} v_1 - \frac{\partial v_3}{\partial y} v_2 \right) \quad (30)$$

$$h_3 = \int^Z \left[\frac{\partial f_1}{\partial x} \frac{\partial g_2}{\partial y} - \frac{\partial f_1}{\partial y} \frac{\partial g_2}{\partial x} + \frac{\partial f_2}{\partial x} \frac{\partial g_1}{\partial y} - \frac{\partial f_2}{\partial y} \frac{\partial g_1}{\partial x} \right] \quad (31)$$

$$h_4 = \int^Z \left[\frac{\partial f_2}{\partial x} \frac{\partial g_2}{\partial y} - \frac{\partial f_2}{\partial y} \frac{\partial g_2}{\partial x} \right]. \quad (32)$$

The lower limits of integration have not been specified but if chosen at a value of z for which there are zeros of the vector field, these points will remain fixed under the map. In concrete problems the first order can easily be implemented because the integral can be done by hand. However, the second order may require the use of a symbolic manipulation program such as SMP as discussed in [16].

Consider now a divergence free vector field such as the ABC flows [6]. They have the special form $v = (v_1, v_2, v_3) = v_1 + v_2 + v_3$, where v_1, v_2 , and v_3 are individually divergence free vector fields which can be integrated explicitly. Specifically,

$$v_1 = v_1(y, z) \quad (33)$$

$$v_2 = v_2(x, z) \quad (34)$$

$$v_3 = v_3(x, y) \quad (35)$$

so that exact integration of the flow corresponding to v_1 is accomplished by the the one parameter subgroup of volume preserving transformations $m_1(t)$ defined by

$$X = x + t v_1(y, z) \quad (36)$$

$$Y = y \quad (37)$$

$$Z = z \quad (38)$$

with corresponding subgroups $m_2(t)$ and $m_3(t)$ for the flows v_2 and v_3 .

Thus we can use Ruth's method (section 2.2) to construct VPI's for the flow. For example, composition of m_1 , m_2 , and m_3 , in any order, is a first order VPI. This is the so-called ABC map used by Feingold, Kadanoff, and Piro [29]. A second order VPI is given by

$$m_1(t/2)m_2(t/2)m_3(t)m_2(t/2)m_1(t/2)$$

and higher order VPI's can be constructed using the techniques discussed in Ruth [67], Forest and Ruth [33], Neri [63], and Forest and Berz [34]. Note that besides being explicit, these VPI's preserve all fixed points of the flow.

2.6 Symplectic Cellular Automata

Coupled map lattices have been studied with regard to the fundamental question of ergodicity and equipartition of energy in Hamiltonian systems with many degrees of freedom. Most of these studies numerically integrate using the first order SIA (1) and (2), and can be considered symplectic coupled map lattices. However, as of yet no studies have been performed concerning the importance of the symplectic condition, and none with respect to system symmetries and reversibility. I am presently investigating these issues and will report concerning them in a future publication.

Kaneko [53] generalizes a technique of Rannou [65] to more than one degree of freedom, and shows that finite state symplectic map lattices (cellular automata) can be constructed by requiring a symplectic map lattice to map integer states to integer states and to commute with a mod- q operation. De Vogelaere [26] has also developed a version of discrete Hamiltonian mechanics. Cellular automata require integer arithmetic and so have no roundoff error. Therefore, they promise to be important tools in the study of large systems. See also Hannay and Berry [46]. Kaneko studies (for mod-3) a complete list of models and classifies them according to their statistical behavior. Their relation to any physical system is yet undetermined but Frisch, Hasslacher, and Pomeau [38] show that cellular automata can successfully simulate certain regimes for the Navier-Stokes equation. In addition, Pomeau [64] computes an energy-like invariant for reversible cellular automata.

3 Numerical Calculations

A SIA for some Hamiltonian system is a symplectic map (or 1-parameter family) which approximates the (symplectic) flow map of the system. This implies that the KAM theorem for mappings [5] and Nekhoroshev's theorem [62] on adiabatic invariants apply. This immediately implies long term stability results in near integrable, and non-resonance regimes ignoring the important topic of roundoff error. In addition, stochastic layers bounded by regular regions appear to be represented well since the regular regions will be strictly avoided by the SIA [16]. Symplectic integration of many systems shows that good energy preservation over extremely long runs is typical, and Figure 1. shows the comparison in energy deviation from being constant of of a second order SIA with the standard fourth order Runge-Kutta for the Fermi-Pasta-Ulam system as presented in Channell and Scovel [16]. The qualitative features of Figure 1 are the same for all systems I have coded except for the three body problem, due to close encounters.

Poor energy conservation has been observed for SIA's by Jimenez and Vazquez [52] and Forest [35]. A few comments are in order. In Channell and Scovel [16], the timestep was determined by several factors. Firstly, the total energy deviation over a fixed long time interval should scale according to the accuracy of the algorithm. This test should be performed at a variety of initial conditions. Secondly, The generating function equations should be solvable in less than 5 to 7 Picard iterations. The examples of Jimenez and Vazquez [52] and Forest [35] do not satisfy the first criterion. Numerically induced stochasticity is also investigated in [9],[37],[48], and [49].

For the Hénon-Heiles Hamiltonian at low values of the energy, the system appears completely integrable [47], but comparison of Poincaré sections of an SIA (Figure 2a.) with a RKI (Figure 2b.) for a long run shows the SIA to lie on a closed curve, where the RKI initially travels near this closed curve, but monotonically drifts (similarly to how it drifts in energy in Figure 1.).

Figure 3 shows four views of the results of a single initial condition. Figure 3a is the Poincaré section and Figure 3b is the projection of the three dimensional data onto this plane, while Figures 3c and 3d are the projection onto the other two coordinate planes.

Now consider a system of six Kirchhoff point vortices. The Hamiltonian

is

$$H = -1/4\pi \sum_{j \neq k}^6 \Gamma_j \Gamma_k \ln |z_j - z_k|$$

where Γ_j is the strength of the j -th vortex situated at the point z_j in the complex plane. Three point vortices are completely integrable and four vortices of the same strength are not [1]. The system has two integrals of center of mass $\sum \Gamma_j z_j = Q + iP$ and one of angular momentum $\sum \Gamma_j |z_j|^2$. Let the strengths all be 1, and let the position of the vortices be $(1,1), (1+dr,1), (2,2), (3,3), (4,3), (5,3)$ where the second vortex position is variable. For dr small, the first and second interact with the other vortices as a coherent vortex pair. The other vortices are typically a distance of order 1 from neighboring vortices. What happens to the vortex pair as dr is increased towards 1? I implemented the third order SIA as explained in [16], and monitored the energy of the isolated vortex pair (= minus the log of their separation). The total energy remained constant to one part in 10^{-6} , the integrals remained constant to within roundoff error and the time step was .03. When dr is less than .4, the pair remain coherent over extremely long runs ($t=20,000$), but for $dr=.46$, the pair undergoes separation but then apparently stable reattachment (Figure 4a). For $dr=.5$, the pair experiences a modulation to slightly larger separation, true separation, reattachment, and then finally, permanent separation (Figure 4b). For $dr=.5005$, permanent separation occurs very early (near $t=1000$), and somewhat earlier for larger values of dr .

My last example is the classical three body problem. I implemented a fourth order SIA for the full non-planar problem as found in [16], and all three integrals of center of mass were preserved correctly in terms of the three of center of velocity which remained constant to within roundoff error. The three integrals of angular momentum were also preserved to within roundoff error. However, due to the fact that too many fortran multiplications were needed, it was slow. Energy preservation was typical until a close encounter when the timestep was halved until the generating function equations could be satisfied in less than 7 Picard iterations. For mild encounters this worked well but strong encounters would change the energy drastically or require the time step to be reduced too many times. I terminated the run after 20 time step reductions. Presumably, a reduction in the order of the scheme is appropriate, and/or use of a scheme which requires less derivative information as in Stofer's algorithm in section 2.3, and a symplectic close encounter algorithm, following the two body regularization

procedure as found in Siegel and Moser [70], should be implemented.

Consider now the planar problem. As in Graziani and Black [44], let the sun have mass 1 and two planets of equal mass m . Initially, the sun is at the origin and the two planets m_1 and m_2 are diametrically opposed on the x axis at radii r_1 and r_2 such that $r_2/r_1 = 1.567$ and $(r_1 + r_2)/2 = 10.4$. They are given initial momenta which starts them in almost circular orbits so that they both rotate counterclockwise. When $m=0$ the planets evolve in perfect circular orbits. Direct comparison with their result's is not possible at the present time since I chose my gravitational constant incorrectly. However, the qualitative phenomena is still of interest. The time step was one and the period of the outer planet m_2 was approximately 1000 and the inner 500. At $m = .015$ the system survives at least 70,000 orbits of the outer planet, keeping the energy constant to within one part in 10^{-6} over the whole run. At $m = .0155$ the outer planet completes 1200 regular orbits, attempts to switch places with the inner planet, but becomes unstable and ejects. r_1 is about 20 and r_2 is about 30 and I called a planet ejected if it's position was greater than 1000 from the center of mass. A cleaner version of the switch of the outer planet to the inner and the inner to the outer is shown in Figure 5. This switch terminates (apparently) in a very typical *mode* where the inner planet is undergoing a forced (by the outer planet) two body problem and the outer planet interacts with the inner-sun pair as in a two body problem except on its closest approach, when abrupt switches to other quasi-stable modes are possible. I refer to a mode as quasi-stable if it remained as in Figure 5. for more than 10 periods of the outer planet. Stability here is a funny thing. When the outer planet is in a highly eccentric elliptical orbit, this should be very unstable. However, the time it takes to travel this orbit is very large. Also, numerical calculations show that modes with highly eccentric outer planet orbits can be fairly stable. In particular, quasi-stable modes with the outer planet reaching 900 were not unusual. At $m = .0167$, the configuration space plots were extremely chaotic. However, Figure 6., plotting the mutual separation of the two planets, shows that they attach and form a stable satellite system revolving about the sun.

Acknowledgements

I would like to thank MSRI at Berkeley, and ETH - Zürich for their hospitality and support. Thanks go to Etienne Forest, Ge Zheng, Jerry Marsden, Tudor Ratiu, and Alan Weinstein, for many helpful conversations. I am very

grateful to Paul Channell for teaching me many things, including what an algorithm is.

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Figure Captions

Clint Scovel

September 8, 1989

Figure 1: Comparison of relative energy error of a second order SIA and fourth order RKI for the Fermi-Pasta-Ulam system. The time step was .001 for the SIA and .02 for the RKI and the final time was 7500.

Figure 2: Comparison of third order SIA (a) and fourth order RKI (b) for the H'enen- Heiles system. The initial condition was (.12,.12,.12,.12) with energy .029952. The time step was 1/6 and 1,200,000 timesteps were computed.

Figure 3: Four views of the results from a single initial condition, $(q_1, p_2, q_2) = (0., 0., -0.1)$, with energy 0.117835: (a) Two dimensional slice at the $q_1 = 0$ plane; (b) Projection of the three dimensional phase space onto the $q_1 = 0$ plane; (c) Projection of the three dimensional phase space onto the $p_2 = 0$ plane; (d) Projection of the three dimensional phase space onto the $p_2 = 0$ plane; 14000 timesteps were computed with timestep 0.3.

Figure 4: Plot of energy of vortex pair $= -1/4\pi\ln(r)$, where r is their separation. A third order SIA was used with timestep .03; (a) $dr=.16$; (b) $dr=.5$.

Figure 5: Configuration space (x,y) plots of trajectories computed by a fourth order SIA for the planar three body problem; (a) the sun; (b) initially inner planet m_1 ; (c) initially outer planet m_2 . Both planets have mass $m = .019$. The timestep was 1 and the final time 133270; (d) Configuration space plot for m_1 at $m = .0188$; (e) plot of the separation of the two planets as a function of time at $m = .0167$.

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