## PHYSICAL REVIEW LETTERS

VOLUME 71

8 NOVEMBER 1993

NUMBER 19

## Explicit Lie-Poisson Integration and the Euler Equations

Robert I. McLachlan

Program in Applied Mathematics, Campus Box 526, University of Colorado at Boulder, Boulder, Colorado 80309 (Received 28 April 1993)

We give a wide class of Lie-Poisson systems for which explicit, Lie-Poisson integrators, preserving all Casimirs, can be constructed. The integrators are extremely simple and have widespread applicability. Examples are the free rigid body, a moment truncation, and a new, fast algorithm for the sine-bracket truncation of the 2D Euler equations.

PACS numbers: 02.60.Cb, 02.20.Tw, 03.40.Gc, 11.10.Ef

Hamiltonian systems are fundamental, and symplectic integrators (SI's) have been increasingly used to do useful extremely long-time numerical integrations of them. Wisdom and Holman [1] have used fast SI's to integrate the solar system far more efficiently than with standard methods; there are numerous examples illustrating the superior preservation of phase-space structures and qualitative dynamics by SI's [2–4]. A philosophy has emerged of attempting to preserve as much geometric structure as possible in numerical treatments.

However, many Hamiltonian systems are not in canonical form but are most naturally written as *Poisson* systems, which generally arise as reductions from canonical formulations in more variables. The most common type, and the only one we shall deal with here, are Lie-Poisson systems [5]. These are distinguished by having a Poisson bracket which is linear in the phase-space coordinates. Each such bracket is associated with a Lie algebra which reflects the symmetry of the system at hand. For example, for the motion of a free rigid body, the Lie algebra is  $\mathfrak{so}(3)$ , the algebra of infinitesimal rotations in  $\mathbb{R}^3$ . Another area in which Lie-Poisson systems play a major role is the study of fluid-particle-field systems such as ideal hydrodynamics, magnetohydrodynamics, or the Vlasov-Poisson equations of plasma physics [5,6]. In these cases the Lie algebra in question is associated with the particlerelabeling symmetry of the Eulerian (spatial) form of the equations.

Integrating Lie-Poisson partial differential equations (PDE's) first requires a truncation to finite dimensions of the noncanonical Poisson bracket. This is equivalent to finding a finite-dimensional approximation of the underlying Lie algebra, and is a major research challenge at this time. Only two successful approaches have emerged at all, and some Poisson brackets appear to have *no* truncation. The two approaches are the sine bracket [7], associated with  $\mathfrak{su}(N)$  and applying to various 2D ideal in-' compressible fluids, and, for PDE's describing the evolution of localized distributions, the moment truncation of Scovel and Weinstein [8]. To integrate in time, there are general methods which preserve both the discrete Poisson bracket and its conserved quantities called Casimirs [9,10]. They are not only implicit but require evaluating functions like " $e^{ad_{\xi}}$ " via Taylor series; hence they can be very slow.

If Lie-Poisson integrators are to be as practical as standard symplectic integrators, they should be simple and fast. To this end we describe the widest general class of such systems for which explicit methods are available. Examples of such methods were first found by Ruth [11] for canonical systems, and by Channell and Scovel [9] for Lie-Poisson systems. Our class includes the sinebracket truncation of the 2D Euler equations, the *sine-Euler* equations. It seems appropriate that the miracle that the sine bracket exists at all should be followed up by a series of coincidences: Not only does an explicit method exist, because of the special form of the Euler Hamiltonian, but the beautiful structure of the sine-Euler bracket allows the new method to be  $O(N/\ln N)$  times faster than the standard implicit method.

Poisson systems and integrators.—A Lie-Poisson system consists of (i) a phase space  $\mathbb{R}^n$  with coordinates x; (ii) a noncanonical Poisson bracket  $\{F, G\} = \frac{\partial F}{\partial x_i} J_{ij} \frac{\partial G}{\partial x_j}$  where  $J_{ij} = c_{ij}^k x_k$  with  $c_{ij}^k$  the structure constants of a

0031-9007/93/71(19)/3043(4)\$06.00 © 1993 The American Physical Society 3043

Lie algebra; (iii) a Hamiltonian  $H: \mathbb{R}^n \to \mathbb{R}$ ; and (iv) dynamics  $\dot{x} = \{x, H\} = J\nabla H$ . We write the solution of these differential equations as  $x(t) = \exp(tJ\nabla H)[x(0)]$ . Poisson systems can have certain conserved quantities C, called *Casimirs*, that depend only on the Poisson bracket and not on H: they satisfy  $\{C, F\} = 0 \forall F$ .

The dynamics preserve the Poisson bracket; a Poisson integrator is one whose time-step map  $x \to x'(x)$  also preserves the Poisson bracket. Symplectic splitting methods apply when the Hamiltonian is a sum of terms each of which can be explicitly integrated—for example, in a canonical Hamiltonian system, H = T(p) + V(q), which leads to standard explicit symplectic integrators [4,11]. For Lie-Poisson systems, our methods depend on the following observation.

 $Observation.{--Let}$ 

$$\Sigma = \{ \sigma \subset \{1, \ldots, n\} : J_{ij} = 0 \quad \forall \ i, j \in \sigma \}.$$

Let the Hamiltonian depend only on the variables  $x_i$  for  $i \in \sigma$ , which we denote by  $H = H(\sigma)$ . Then the dynamics of the Lie-Poisson system with Hamiltonian  $H(\sigma)$ ,  $\sigma \in \Sigma$ , are linear with constant coefficients.

In other words, a set of indices  $\sigma$  is in  $\Sigma$  if the corresponding coordinates Poisson commute with one another:  $\{x_i, x_j\} = 0 \forall i, j \in \sigma$ . In fact,  $\Sigma$  is the set of all Abelian subalgebras of the Lie algebra associated with J. The key point is that the dynamical equations now have  $\dot{x}_i = [J(x)\nabla H(\sigma)]_i = 0$  for  $i \in \sigma$ . This in turn implies that the differential equations for the remaining  $x_k, k \notin \sigma$ , although coupled linearly amongst themselves, depend only parametrically on  $x_i$  for  $i \in \sigma$ .

Usually the resulting linear systems, although depending in a complicated way on the parameters  $x_i$ ,  $i \in \sigma$ , can be solved explicitly. This will be illustrated in the examples below. Then an explicit, first-order, Lie-Poisson integrator for a Hamiltonian with p terms  $H = \sum_{k=1}^{p} H_k(\sigma_k)$ is

$$\varphi(t) = \exp(\Delta t X_1) \cdots \exp(\Delta t X_p)$$
, (1)

where  $\Delta t$  is the time step and  $X_k = J\nabla H_k$ ; that is, just integrate each piece of the Hamiltonian in turn. A second order symmetric method ("leapfrog") is  $\varphi(\frac{1}{2}\Delta t)\varphi^{-1}(-\frac{1}{2}\Delta t)$ . Methods of any order can be constructed by composing several such steps [12–15].

The above observation may appear somewhat specialized; however, we shall show by means of examples that it has widespread applicability, not only to elementary systems such as the free rigid body, but also to both of the known finite-dimensional truncations mentioned in the introduction.

First, note that  $\Sigma$  certainly includes the singleton subsets, because antisymmetry of J implies  $J_{ii} = 0$ . So we can immediately integrate Hamiltonians of the form  $H = \sum_{k=1}^{n} H_k(x_k)$ :

The free rigid body.—Recall the standard description of the free rigid body, as in [5]. Here  $\mathbf{m} \in \mathbb{R}^3$  is the angular momentum in body coordinates,  $H = \frac{1}{2}(m_1^2/I_1 + m_2^2/I_2 + m_3^2/I_3)$ , and the Lie algebra is  $\mathfrak{so}(3)$  so

$$J = egin{pmatrix} 0 & -m_3 & m_2 \ m_3 & 0 & -m_1 \ -m_2 & m_1 & 0 \end{pmatrix}.$$

One may check that  $\dot{\mathbf{m}} = J\nabla H$  are the usual equations of motion of the free rigid body,  $\dot{m}_1 = (1/I_3 - 1/I_2)m_2m_3$ , etc. This J has a Casimir  $C = |\mathbf{m}|^2$ , the total angular momentum, so  $\hat{H} = H - C/2I_1$  generates the same dynamics as H; this leaves only two terms in  $\hat{H}$ . With  $\omega_k = m_k(1/I_k - 1/I_1)$  and  $R_k(\theta)$  being rotation by an angle  $\theta$  around the axis  $m_k$ , the map corresponding to (1) is

$$\mathbf{m}' = R_3(\Delta t \omega_3) R_2(\Delta t \omega_2) \mathbf{m}$$

—a "standard map" of the rigid body. The Casimir  $|\mathbf{m}|^2$  is clearly conserved. This is a new, explicit Lie-Poisson map approximating the flow of the free rigid body, and we found it to be 60 times faster (for the same accuracy) than the implicit Lie-Poisson method of [9]. Non-Poisson methods, such as the midpoint rule, have been considered in [16], but showed poor performance.

A moment algebra.—The following example of a Poisson bracket arises in problems involving the advection of a scalar field f(q, p) by Hamiltonian vector fields in the (q, p) plane, such as the 2D Euler equations or the 1D Vlasov-Poisson equations of plasma physics [9]. For the derivation of J, see [9]; however, we introduce it here as an illustration of our integration technique.

The finite-dimensional representation considered here retains only the second and fourth order moments of the field f(q,p). Coordinates are  $\langle q^{\alpha}p^{\beta}\rangle \equiv \int q^{\alpha}p^{\beta}$  $\times f(q,p) dq dp$  which we collect in a vector

$$x = \left(\langle q^2 \rangle, \langle qp \rangle, \langle p^2 \rangle, \langle q^4 \rangle, \langle q^3 p \rangle, \langle q^2 p^2 \rangle, \langle qp^3 \rangle, \langle p^4 \rangle 
ight)^T.$$

We have

	( 0	$2x_1$	$4x_2$	0	$2x_4$	$4x_5$	$6x_6$	$8x_7$
J =	$-2x_{1}$	0	$2x_3$	$-4x_{4}$	$-2x_{5}$	0	$2x_{7}$	$4x_8$
	$-4x_{2}$	$-2x_{3}$	0	$-8x_{5}$	$-6x_{6}$	$-4x_{7}$	$-2x_{8}$	0
	0	$4x_4$	$8x_5$	0	0	0	0	0
	$-2x_{4}$	$2x_5$	$6x_6$	0	0	0	0	0
	$-4x_{5}$	0	$4x_7$	0	0	0	0	0
	$-6x_{6}$	$-2x_{7}$	$2x_8$	0	0	0	0	0
	$-8x_7$	$-4x_{8}$	0	0	0	0	0	0/

As pointed out in [9], if H were separable in p and q as in the Vlasov-Poisson equations, i.e.,  $H = T(x_3, x_8) + V(x_1, x_4)$ , then an explicit Poisson integrator is possible, just as in the canonical case. But from the above observation, noting the positions of the zeros in J shows that

$$egin{aligned} H &= H_1(x_1,x_4) + H_2(x_2,x_6) + H_3(x_3,x_8) \ &+ H_4(x_4,x_5,x_6,x_7,x_8) \end{aligned}$$

also admits an explicit Poisson integrator.

In the canonical case one often has a nonlinear term in H, not a function of q alone, which can nevertheless be integrated explicitly in terms of elementary functions. One such is  $H(q_1, q_2^2 + p_2^2)$ , which arises in the nonlinear Schrödinger equation and in the Zakharov equations [2] and which gives rise to the well-known splitting method for the nonlinear Schrödinger equation. This phenomenon is less common in Lie-Poisson systems because of the more complicated evolution of those  $x_j$ not appearing in H. But it can happen: for example, with a little work one can solve the linear, timedependent ordinary differential equations (ODE's) generated by  $H = H(x_1x_3)$  with the above J.

The sine-Euler equations.—Here we consider the motion of an inviscid incompressible fluid governed by the 2D Euler equations. The field variable is the vorticity  $\omega(x, y)$ , which is  $2\pi$  periodic in x and y. We have

$$J = \omega_y \partial_x - \omega_x \partial_y , \qquad (2)$$

$$H=-rac{1}{2}\int\psi\omega\,dx\,dy$$

 $abla^2 \psi = -\omega$ 

where

$$\dot{w} = J(\omega) \frac{\delta H}{\delta \omega} = J(\omega)\psi = -\omega_x \psi_y + \omega_y \psi_x$$
. (3)

For a geometric derivation of the above formulation, see [6]. This J has an infinite number of Casimirs, which we may take as  $C_n = \int \omega^n dx \, dy$ , reflecting the fact that the vorticity is simply advected by the fluid flow. In Fourier space Eqs. (2),(3) become

$$J_{\mathbf{mn}} = \mathbf{m} \times \mathbf{n} \, \omega_{\mathbf{m}+\mathbf{n}} ,$$
  

$$H = \frac{1}{2} \sum_{\mathbf{n} \neq \mathbf{0}} \frac{\omega_{\mathbf{n}} \omega_{-\mathbf{n}}}{|\mathbf{n}|^2} ,$$
  

$$\dot{\omega}_{\mathbf{m}} = \sum_{\mathbf{n} \neq \mathbf{0}} \frac{\mathbf{m} \times \mathbf{n}}{|\mathbf{n}|^2} \omega_{\mathbf{m}+\mathbf{n}} \omega_{-\mathbf{n}} ,$$

where  $\mathbf{m} \times \mathbf{n} = m_1 n_2 - m_2 n_1$  and for real  $\omega$ ,  $\omega_{-\mathbf{n}} = \omega_{\mathbf{n}}^*$ . There is a finite-dimensional truncation of (2) [7], the sine bracket

$$J_{\mathbf{mn}} = \frac{1}{\varepsilon} \sin(\varepsilon \mathbf{m} \times \mathbf{n}) \omega_{\mathbf{m}+\mathbf{n} \bmod N} , \qquad (4)$$

where  $\varepsilon = 2\pi/N$  and all indices are henceforth reduced modulo N to the periodic lattice  $-M \leq m_1, m_2 \leq M$ where N = 2M + 1. We shall take N prime for convenience; extension to nonprime N is straightforward. Figure 1 illustrates the lattice of modes retained in this



FIG. 1. Mode splitting in the sine-Euler equations. Here N = 7 and M = 3.  $\bigcirc$  shows modes in one term  $H_{\mathbf{k}}$  in the Hamiltonian  $[\mathbf{k} = (1, 1)]$ .  $\blacksquare$  shows modes which are coupled together in the linear system  $\dot{\omega} = J\nabla H_{\mathbf{k}}$  [here  $\mathbf{j} = (2, 0)$ ];  $\square$  shows modes whose values are the complex conjugate of the  $\blacksquare$  modes.

truncation. This J has N-1 Casimirs which approximate  $C_n$  for  $2 \le n \le N$ . Equations (4) specify the structure constants of  $\mathfrak{su}(N)$  in an appropriate basis [7,17], although we shall not use this rich structure here.

The most natural truncated H is

$$H = \frac{1}{2} \sum_{\substack{n_1, n_2 = -M \\ \mathbf{n} \neq \mathbf{0}}}^{M} \frac{\omega_{\mathbf{n}} \omega_{-\mathbf{n}}}{|\mathbf{n}|^2}$$

giving the sine-Euler equations, first proposed by Zeitlin [17]:

$$\dot{\omega}_{\mathbf{m}} = \sum_{\substack{n_1, n_2 = -M \\ \mathbf{n} \neq \mathbf{0}}}^{M} \frac{1}{\varepsilon} \frac{\sin(\varepsilon \mathbf{m} \times \mathbf{n})}{|\mathbf{n}|^2} \omega_{\mathbf{m}+\mathbf{n}} \omega_{-\mathbf{n}} , \qquad (5)$$

where as in (4) all indices are taken modulo N. As a numerical approximation of (3), these equations are only  $\mathcal{O}(\varepsilon^2)$  accurate. Even if (5) is not very appealing on standard numerical grounds, it is hoped that the model's Hamiltonian structure and conserved quantities will bring compensating advantages, at least qualitatively. A discussion and numerical simulation of this model can be found in [18], and a derivation of a similar system in [19].

The approach outlined above now gives an explicit,  $\mathcal{O}(N^3 \ln N)$ , Poisson integrator of (5), preserving all N-1Casimirs to within round-off error—which is faster than the  $\mathcal{O}(N^4)$  needed just to evaluate the right hand side of (5). The first piece of luck is that the sets  $\sigma$ , describing the commuting coordinates, are very large. For any  $\mathbf{k} = (k_1, k_2)$ , we have

$$\sigma_{\mathbf{k}} = \{ n\mathbf{k} : 0 \le n < N \} \in \Sigma.$$

To split the Hamiltonian we need a set of modes K such that multiples of K cover the entire lattice. When N is prime,

$$K = \{(0,1)\} \cup \{(1,m) : 0 \le m < N\}$$

suffices. The second piece of luck is that the truncated



Hamiltonian only couples terms which are in the same set  $\sigma_{\mathbf{k}}$ . We have

$$H = \sum_{\mathbf{k} \in K} H_{\mathbf{k}}(\sigma_{\mathbf{k}}), \qquad H_{\mathbf{k}} = \frac{1}{2} \sum_{n=0}^{N-1} \frac{\omega_{n\mathbf{k}}\omega_{-n\mathbf{k}}}{|n\mathbf{k}|^2}.$$

The final miracle is that the resulting linear ODE's decouple into sets of equations which can be solved by the fast Fourier transform. We need to solve  $\dot{\omega} = J\nabla H_{\mathbf{k}}$ . Of course  $\dot{\omega}_{\mathbf{m}} = 0$  for  $\mathbf{m} \in \sigma_{\mathbf{k}}$ . From (5), the other modes decouple into 2M sets of N equations, of which we only need to solve M sets; the others are their complex conjugates (see Fig. 1). The variables in each set are a translation of  $\sigma_{\mathbf{k}}$ , say by **j**: let  $z_m = \omega_{\mathbf{j}+m\mathbf{k}}$ , then

$$\dot{z}_m = \sum_{n=-M}^M a_n z_{m-n},$$

where

$$a_n = -\frac{\sin(\varepsilon n\mathbf{j} \times \mathbf{k})}{\varepsilon |n\mathbf{k}|^2} \omega_{n\mathbf{k}}.$$

These ODE's are diagonalized by the discrete Fourier transform (DFT): let  $\tilde{z} = F\mathbf{z}$  where F is the DFT  $F_{jk} = \frac{1}{N} \exp(-2\pi i j k/N)$ , then

$$\widetilde{\mathbf{z}} = \Lambda \widetilde{\mathbf{z}}$$
 where  $\Lambda = \operatorname{diag}(F\mathbf{a})$ ,

so the equations can now be integrated explicitly.

Summary of algorithm: (i) for  $\mathbf{k} \in K$  do, (ii) for  $\mathbf{j} = 1$ st,..., Mth translation of  $\mathbf{k}$  do [may be done in parallel], (iii) with  $z_m = \omega_{\mathbf{j}+m\mathbf{k}}$ , set  $\mathbf{z}' = F^{-1}e^{\Delta t\Lambda}F\mathbf{z}$ , (iv) copy  $(\mathbf{z}')^*$  into  $\omega_{-(\mathbf{j}+m\mathbf{k})}$ , (v) end do, (vi) end do.

The whole procedure requires  $3M(N+1) = \frac{3}{2}(N^2-1)$ DFT's of length N. As there are FFT's available for sequences of prime length N [20], the whole algorithm is  $\mathcal{O}(N^3 \ln N)$ . Figure 2 shows the relative energy error [H(t) - H(0)]/H(0) for  $10^5$  time steps with  $\Delta t = 0.05$ , N = 7,  $|\omega| = 1$ , and H(0) = 0.75. As is expected from an integrator which is a symplectic map on the level sets of the Casimirs, the energy error does not grow with time. The errors in the Casimirs, e.g.,  $C_2 = \sum \omega_{\mathbf{n}} \omega_{-\mathbf{n}}$ , are due only to roundoff error, and grow by about  $5 \times 10^{-15}$  per time step.

This explicit method exists because the only coupled terms in the Hamiltonian belong to the sets  $\sigma_{\mathbf{k}}$ ; it is fast because of the special form of the sine bracket in this basis. Preliminary simulations indicate that the evolution can be followed for arbitrarily long times. It will be interesting to see what the implications of this model are for the ergodicity and statistical steady state of the 2D Euler equations, which will be the subject of future work [21].

I would like to thank Clint Scovel for a careful reading of the manuscript, and for encouraging to me to persevere with Poissonology. I am grateful for the helpful comments of Harvey Segur.

- J. Wisdom and M. Holman, Astron. J. **102**, 1528–1538 (1991).
- [2] R. I. McLachlan (to be published).
- [3] D. I. Pullin and P. G. Saffman, Proc. R. Soc. London A 432, 481–494 (1991).
- [4] J. C. Scovel, in *The Geometry of Hamiltonian Systems*, edited by T. Ratiu (Springer-Verlag, New York, 1991).
- [5] J. E. Marsden, A. Weinstein, T. Ratiu, R. Schmid, and R. G. Spencer, Proc. IUTAM-ISIMM Symp. Mod. Dev. Anal. Mech. Torino 117, 289–340 (1983).
- [6] J. E. Marsden and A. Weinstein, Physica (Amsterdam)
   7D, 305–323 (1983).
- [7] D. B. Fairlie and C. K. Zachos, Phys. Lett. B 224, 101– 107 (1989).
- [8] C. Scovel and A. Weinstein (to be published).
- [9] P. J. Channell and J. C. Scovel, Physica (Amsterdam) 50D, 80–88 (1991).
- [10] Ge Zhong and J. E. Marsden, Phys. Lett. A 133, 134–139 (1988).
- [11] R. D. Ruth, IEEE Trans. Nucl. Sci. 30, 2669–2671 (1983).
- [12] S. Benzel, Ge Zhong, and C. Scovel, Phys. Lett. A 174, 229–232 (1993).
- [13] M. Suzuki, J. Math. Phys. 32, 400-407 (1991).
- [14] H. Yoshida, Phys. Lett. A 150, 262–269 (1990).
- [15] R. I. McLachlan (to be published).
- [16] M. Austin, P. S. Krishnaprasad, and L.-S. Wang, Report No. TR 91–45r1, Systems Research Center, University of Maryland at College Park, 1991 (unpublished).
- [17] V. Zeitlin, Physica (Amsterdam) 49D, 353-362 (1991).
- [18] J. S. Dowker and A. Wolski, Phys. Rev. A 46, 6417–6430 (1992).
- [19] J. Miller, P. B. Weichman, and M. C. Cross, Phys. Rev. A 45, 2328–2359 (1992).
- [20] C. M. Rader, Proc. IEEE 56, 1107-1108 (1968).
- [21] S. Benzel, R. I. McLachlan, and J. C. Scovel (to be published).