

A Survey of Open Problems in Symplectic Integration

Robert I. McLachlan

Mathematics Department
Massey University
Palmerston North
New Zealand

Clint Scovel

Computer Research Group, C-3, MS-B265
Los Alamos National Laboratory,
Los Alamos, NM USA 87545
Dedicated to Feng Kang

Abstract. We present a personal view of the most important open problems and areas for research in symplectic integration and in the more general study of geometric structure in numerical methods.

1 Introduction

In the past few years there has been a substantial amount of research on symplectic integration. The subject is only part of a program concerned with numerically preserving a system's inherent geometrical structures, such as volume preservation, reversibility, differential constraints on PDEs such as those involving *div* and *curl*, and integral invariants. In many cases one requires a numerical method to stay in the smallest possible appropriate group of phase space maps. It is not the authors' opinion that symplecticity, for example, automatically makes a numerical method superior to all others, but it is our opinion that it should be taken seriously and that a conscious, informed decision be made in that regard.

We present here a survey of open problems in symplectic integration, including other problems from the larger program. This is not intended as a review of symplectic integration (see [36, 121, 122]) and is naturally derived from the authors' own research interests. Many of the problems mentioned here call for numerical experimentation, some for application of suggested but untested methods, some for new methods, and some for theorems. We hope that this survey helps to communicate the outstanding problems in this rapidly growing field to the research community.

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In most of the paper we have in mind that one is trying to solve initial value problems for known, fixed ODEs; PDEs are considered separately in Section 11 and other computational tasks in Section 14. The flavor of this subject is a mixture of numerical analysis and geometric mechanics, but a necessary aim of all this work is to produce algorithms. Coordinates must be used and all functions must be computable; coordinate-free geometry can be at most an intermediate step.

2 Composition methods

2.1 High-order methods It is now a standard practice in structure-preserving integration to compose one or more low-order methods (usually first or second order) with appropriately chosen time steps to obtain a higher-order method. If one has a differential equation $\dot{x} = X(x) = A(x) + B(x)$ such that $\dot{x} = A$ and $\dot{x} = B$ can both be solved analytically, with flows $\exp(tA)$ and $\exp(tB)$, then one may use the compositions

$$\dots \exp(a_2 t A) \exp(b_1 t B) \exp(a_1 t A) \quad (2.1)$$

or

$$\dots S(w_2 t) S(w_1 t) \quad (2.2)$$

where $S(t) = \exp(\frac{1}{2}tA)\exp(tB)\exp(\frac{1}{2}tA)$ is the leapfrog method. The time-step map is then in the Lie group whose Lie algebra is generated by the vector fields A and B . If they were Hamiltonian vector fields, for instance, this group would be a subgroup of the group of symplectic maps. If their flows had identical integrals such as angular momentum, then so would the composition. In particular, for an invariant of the full system to be preserved by this method, each component of the decomposition must preserve that invariant. Some invariants appear to be easier than others to preserve under decomposition. For example, symplecticity is easily preserved, but integrability and energy conservation are destroyed in general.

To analyze such methods, one may expand the compositions (2.1, 2.2) as $\exp(\sum_{i=1}^{\infty} t^i X_i)$ where $X_i \in L^n(A, B)$, the vector space spanned by the n -fold Lie brackets of A and B . This space is a subspace of the free Lie algebra generated by A and B [12, 111] whose dimension is known. There are thus $\sum_{n=1}^p \dim L^n(A, B)$ determining equations which must be satisfied for a method to have order at least p . It is traditional to compare different solutions of the determining equations based on an *effective error constant*—some measure of the first term in the local truncation error, adjusted for the complexity of the method. In this section we compare methods only in this limited sense.

Thus, this avenue leads in primarily algebraic rather than geometric directions. We also need to study curves through the identity in Lie groups, here with parameter t , rather than points and one-parameter subgroups.

Various symmetries can be imposed on (2.1) and (2.2) which turn out to reduce the number of determining equations, i.e., which in the language of Runge-Kutta methods act as simplifying assumptions. A family of maps $\varphi(t)$ is said to be *symmetric* (also self-adjoint, reversible, or revertible) if $\varphi(t)\varphi(-t) = 1$. Note that in (2.2), the individual stages $S(t)$ are themselves symmetric. Roughly, it has been found that the higher the order, the more symmetry it is worth imposing. Some borderline cases remain [84]:

- Is there a symmetric sixth-order method which is better than those composed of symmetric steps?

Now consider the case of “simple mechanical systems,” which are Hamiltonian with the standard symplectic structure, and have Hamiltonians of the form $H = H_A(p) + H_B(q)$ where H_A is quadratic in p . (Composition methods based on this splitting are instances of “Runge-Kutta-Nyström” methods.) Let A be the Hamiltonian vector field corresponding to the Hamiltonian H_A , etc. One can check that now $[B, [B, [B, A]]]$ (which we abbreviate as $B^{(3)}$) is identically zero, so the determining equations corresponding to this term, and to all its Lie brackets, may be dropped. This has been shown to lead to a definite advantage for nonsymmetric fourth-order and for symmetric sixth-order methods. Some eighth-order methods of this type have been found by Okunbor [97].

- Is there a symmetric eighth-order Runge-Kutta-Nyström method which is better than general methods of type (2.2)?
- Describe the Lie algebra generated by the vector fields A and B when $B^{(3)} = 0$.
- Describe the Lie algebra generated by the Hamiltonian functions p^2 and $H_B(q)$.

There are no differences between these two cases $B^{(3)} = 0$ and $H = p^2 + H_B(q)$ for $n \leq 7$, so the popular Runge-Kutta-Nyström methods of order 7 or less [84] apply in the more general case $B^{(3)} = 0$, which has some applications in nonlinear wave equations [83]. However, one can check that the eighth-order term $[B^{(2)}, [B^{(2)}, B^{(1)}]]$ is zero under the $p^2 + H_B(q)$ splitting, but is not explicitly a bracket of $B^{(3)}$.

There are some other cases of particular A s and B s which are advantageous to consider separately. For example, if $B \ll A$ so that the vector field is near-integrable, then the Lie brackets of A and B are of differing orders—e.g., $[B, [B, A]] \ll [A, [A, B]]$ and can be profitably ignored [85]. In a related case, Saha and Tremaine [115] and Wisdom, Holman, and Touma [142] take advantage of the relationships between the particular A and B occurring in solar system dynamics. On the other hand, the separable case with arbitrary $A = A(p)$ and $B = B(q)$ has been shown *not* to be a special case, in the sense that a composition method which works (has a certain order) in this case will also work for all A and B [1]. Therefore, the same is true for the case that A and B have linear flows (i.e., $\exp(tA) = 1 + tA$), as they do in the separable case and elsewhere [36].

- Are there other useful special cases, subspaces of particular Lie algebras, or kinds of compositions, which lead to better methods?

2.2 Existence of splittings What is special about the class of Hamiltonian systems—or of all vector fields—which possess splittings $X = \sum_i X_i$ for which the pieces can be integrated exactly? Even many non-canonical systems can be split in this way, such as those Lie-Poisson systems in which the Hamiltonian only couples variables within the Lie algebra’s abelian subalgebras [82]. This class includes, for

example, the moment algebra with separable energy function, the rigid body, and the sine-bracket truncation of the 2D Euler equations (see Section 11.1).

For most splittings used in practice, the pieces X_i are either linear or have linear flows. One can leave this class and ask,

- which Hamiltonian vector fields X can be written as $X = \sum_{i=1}^n X_i$ where each X_i is completely integrable?

Such a situation is surely not generic, but there are many such vector fields to call on, for both canonical [105] and noncanonical [29, 39] systems. In this problem one is supposed to *start* with X , not with the X_i . A recent example arose in celestial mechanics, where the first post-Newtonian correction, previously supposed to be not splittable, has been neatly split [116].

Naturally one does not want n to be too large. Consider, for example, “Euler equations.” These are Poisson systems with Lie-Poisson structure, i.e., linear brackets, and quadratic Hamiltonians. In coordinates, $\dot{x}_i = \sum_{jkl} c_{ij}^k x_k a_{jl} x_l$. The Hamiltonian $\sum_{jl} \frac{1}{2} a_{jl} x_j x_l$ may be diagonalized and each term integrated [109], and this is often the best approach. But in one case, the $N \times N$ sine-bracket truncation of the 2D Euler fluid equations discussed in Section 11.1, it leads to an $\mathcal{O}(N^5)$ algorithm, as opposed to the $\mathcal{O}(N^3 \log N)$ possible with a different splitting [82].

Canonical systems with polynomial Hamiltonians are another important case. Channell ([19]) splits them into monomials, but Feng and Wang ([36]) split them into polynomials with linear flows. These different approaches have not been compared.

Of course $\exp(tX_i)$ should not be too difficult to evaluate—there is a big difference between proving a system integrable and actually computing its solution. For example, the Hamiltonian for the motion of n point vortices is $H = \sum_{i < j} V(x_i, x_j)$, where vortex i is located at $x_i \in \mathbb{R}^2$. The two-vortex interaction term $V(x_1, x_2) = -\frac{1}{4\pi} \log |x_1 - x_2|$ has a simple flow (in translating coordinates, the vortices rotate about their center of vorticity [114]), leading to an explicit symplectic integrator of any order for this problem. It is not at all clear that the integrability of the three-vortex problem can be exploited here. Another example is due to Wisdom and Holman [141], who successfully integrated the n -planet solar system with such a method. In Jacobi coordinates, they wrote $H = K(q, p) + V(q)$ where K represents n Sun-planet two-body Kepler problems (all mutually commuting, and easily solved) and V represents the $n(n-1)/2$ planet-planet interaction terms, whose flow is a shear. Because it preserves the near-integrability of the problem, this splitting is much more accurate than the $H_A(p) + H_B(q)$ splitting. However, it is only accurate for solar system-like configurations; it is not uniformly accurate in the planet-planet distances. We therefore pose the problem:

- Develop a symplectic integrator for the Newtonian n -body problem which is uniformly accurate near two-body collisions.

A promising approach is to use a partition of unity on the Hamiltonian so that each close pair is integrated exactly, with smooth transitions in the splitting as pairs break up.

2.3 Symplecticity for free Take a Hamiltonian differential equation $\dot{x} = X(x)$. Let $\varphi(t) = 1 + tX$ be Euler’s method, which is not symplectic. It has been noticed independently by Iserles and by Sanz-Serna (unpublished), that $\varphi(t/2)\varphi^{-1}(-t/2)$ is the midpoint rule, $x' = x + tX((x+x')/2)$, which explains the good long-time behavior of the nonsymplectic composition $\varphi^{-1}(-t/2)\varphi(t/2)$, which is the second-order Adams-Moulton method: $x' = x + t(X(x) + X(x'))/2$. Namely, it is conjugate to the midpoint rule by the map $\varphi(t/2)$, and thus preserves the perturbed symplectic form $\varphi(t/2)^*\omega$, where ω is the standard symplectic 2-form. Generalizing this cute example would give a huge new class of symplectic integrators.

A direct calculation shows that

$$\varphi(t)^*\omega = \varphi(-t)^*\omega,$$

is a necessary and sufficient condition for $\varphi(t/2)\varphi^{-1}(-t/2)$ to be symplectic. That is, $\varphi(t)^*\omega$ must be even in t . When $\varphi(t)$ is Euler’s method, $\varphi(t)^*\omega$ is even because it is quadratic and the linear terms vanish when the vector field is Hamiltonian. Other methods based on this idea have not been constructed.

- Give a general construction of methods $\varphi(t)$ such that $\varphi(t)^*\omega$ is even in t .
- Construct integrators which are conjugate to symplectic maps for each t .

3 Multiderivative methods

For some systems, such as those of molecular dynamics, the marginal cost of evaluating the *derivative* of the forces is small [126]. Therefore one should

- Investigate all possible ways of including extra derivative information in a symplectic integrator.

In fact, the earliest symplectic integrators, based on the Taylor series solution of the Hamiltonian-Jacobi equation [34, 20], *did* use derivatives, but these methods are not considered competitive today. An exception is the Stofer ansatz [133, 122], which achieves fourth order in one stage using only the second derivative of the Hamiltonian. There are also explicit multiderivative symplectic schemes available for some systems [86, 68]. Unfortunately, *linear* multiderivative symplectic schemes (those linear in $d^n x/dt^n$) do not exist [50].

4 No-derivative methods

Sometimes the Hamiltonian is so complicated that one does not wish to calculate its derivative by hand, or even by a symbolic manipulator.

- How efficient can symplectic integrators be, given only the Hamiltonian function?

One approach is to form the vector field using automatic differentiation, which is now a mature technique [37, 64]. Another is to use a fixed lattice in phase space to define an interpolated piecewise-polynomial Hamiltonian. A symplectic map $f(x)$ can be defined by taking the lattice points nearest x and using the vector field corresponding to that piece of the interpolating Hamiltonian. (Or can one finite-difference the Hamiltonian about x ?—see Section 12.2.) There is no cost associated

with making the interpolation error as small as desired, but care must be taken to make the $f(x)$ as smooth as possible, so that, e.g., the map will preserve invariant tori (see Section 12.1).

5 Implicit methods

Some vector fields cannot be split. Then one has the generating function and Gauss-Legendre Runge-Kutta methods. Note that as the order increases, the latter do not suffer combinatorial explosion as composition methods do—so they can sometimes be more efficient anyway [84]. Several authors [61, 117] have considered different symplectic Runge-Kuttas, but these have not been tested yet. If one is willing to form and invert Jacobians then Runge-Kuttas with real roots may be superior.

- Find the best symplectic Runge-Kuttas at each order.

When solving the implicit equations, the authors have always been content to extrapolate x^{n+1} from previous time steps, and then solve $x^{n+1} = x^n + f(x^n, x^{n+1})$, say, by iteration to roundoff error—probably unbeatable as $\Delta t \rightarrow 0$, but high-order methods were not made for this. In tests, one should consider large, strongly-coupled systems such as those of molecular dynamics and discretizations of PDEs (see Section 11). In any event, iterating to roundoff is wasteful; would prefer to only solve the equations to within the local truncation error.

- Develop iterations for the standard implicit symplectic methods which are symplectic and preserve equivariances of the original method after any number of iterations.

6 Generating functions

On a linear symplectic space there are many different kinds of generating functions. In addition to the four traditional types, Feng [34, 35] has provided a general discussion and described several non-conventional examples. These different types of generating functions may have different applications. For example, to generate the identity map from a generating function of the first (“ q, Q ”) kind requires a singular generating function [20].

- What are the advantages of the specific types of generating functions? In particular, what are the advantages or disadvantages of using a singular generating function?

Ge [42] has shown that generating functions of the first kind respect symmetries well for cotangent bundles of nonlinear configuration spaces. Namely, they can be used to generate integrators which preserves the momentum corresponding to *all* cotangent lift symmetries, not just linear ones as for generating functions of the third (“ q, P ”) kind. This leads to the Ge-Marsden [46] generating function for Lie-Poisson systems. Indeed, Ge [43] has generalized this construction to show that there is a generating function theory and a Hamilton-Jacobi equation, which in theory can be used to construct symplectic integrators for arbitrary Poisson manifolds. This construction uses the symplectic groupoid which exists locally over

every Poisson manifold [23]; the attendant groupoid structures give rise naturally to a generating function for the Poisson map.

For regular quadratic Lie algebras (those with a nondegenerate Ad -invariant quadratic form), there is a generating function which generates the identity transformation on the dual of the Lie algebra. However, it uses the coadjoint action, not of the identity group element, but of a family of group elements $g(\mu)$ such that each $g(\mu)$ is in the coadjoint isotropy group of μ . Namely, $Ad_{g(\mu)}^* \mu = \mu$. Reconstruction of this identity map to the cotangent bundle will give nontrivial group motions that we feel are unnecessary. Consequently, although numerical experiments shows that the method works well [21], we feel it desirable to construct a generating function for the identity map using $g(\mu) \equiv 1$.

- Is there a generating function for Lie-Poisson maps which generates the identity map via the coadjoint action of the identity group element?

A possible solution lies in the more general construction of Lagrangian submanifolds by Morse families [74]. Bear in mind that such a technique will not be of much use if it entails a substantial increase in computational complexity, as generating function methods already have inadequate efficiency [9].

For matrix Lie groups, the group can be thought of as a submanifold of a linear space which is acted on linearly by the group. One can integrate in the linear space with constraints to the submanifold, and one such algorithm [87, 107] has a generating function of the third kind. Indeed, there is a generating function that generates the identity map by the coadjoint action of the identity group element in this case. See Section 10 for further discussion of symplectic constraint algorithms.

7 Multistep methods

The failure of symplectic methods to use information from past time steps leads to their needing more function evaluations than nonsymplectic methods, particular at orders more than four. Unfortunately, the most useful definition of symplecticity for multistep methods has not yet been arrived at. Some experimentation with actual systems is called for.

Start with a Hamiltonian system on a symplectic manifold M . An n -step method on M may be written as a one-step method on M^n . The continuous system can also be extended to one on M^n with the product symplectic structure. Ge and Feng [41] have investigated the circumstances under which one can preserve the product symplectic structure on M^n . Eirola and Sanz-Serna [32] and Ge [44] have investigated more general symplectic structures on M^n , and Bochev and Scovel [11] have shown that the symplecticity of their methods follows from preservation of quadratic invariants.

But not every ODE on M^n arises from one on M in this way, so preserving the product symplectic structure cannot be expected to lead to good results. For example, the two-step method $x_{i+1} = x_{i-1} + 2tX(x_i)$ preserves the product symplectic structure on M^2 [35, 32], but has none of the nice properties one associates with symplecticity. Applied to integrable m -degree-of-freedom systems, the method does preserve invariant tori, but they have dimension $2m$ in the $4m$ -dimensional space M^2 , and do not project to subsets of M close to the original tori, even as the time step tends to zero. What is needed are some extra integrals in the new directions, so that the invariant tori have dimension m and do project nicely.

Feng [136] has proposed the completely different criterion that the induced one-step method (the map $m: M \rightarrow M$ satisfying the multistep method) should be symplectic in the usual sense. This sounds extremely appealing, but unfortunately Tang [136] has shown that no linear multistep methods can satisfy such a stringent criterion. Of course *some* general linear methods satisfy this criterion, namely, those derived from the composition of symplectic one-step methods; are there any others?

- Which multistep methods satisfy Feng's criterion?

One also needs to consider how multistep methods are functionally dependent on the initialization technique. Consider a two-step method for simplicity, in which x_3 is given as a function of x_1 and x_2 by combining the formulas for two identical one-step methods m . If the initial conditions are selected by $x_2 = m(x_1)$, the sequence of points is that determined by the symplectic map m . However, if the initial conditions are selected by another mapping $x_2 = f(x_1)$, this is not the case. We took the composition of two midpoint rules in the form

$$x_3 = x_1 + t \left(X \left(\frac{x_1 + x_2}{2} \right) + X \left(\frac{x_2 + x_3}{2} \right) \right),$$

which is symplectic in Feng's sense: its equivalent one-step method is the midpoint rule. Applied to the pendulum, we observed that as f is perturbed from the midpoint rule, each invariant curve bifurcates into two curves, with successive iterates alternating between the two. This suggests that the map corresponding to two time steps might be symplectic for all f .

MacKay [76] has proposed the criterion that if ξ^i and η^i are vectors such that $\omega(\xi^1, \eta^1) = \dots = \omega(\xi^n, \eta^n) = c$, where ω is the symplectic two-form, then one should have $\omega(\xi^{n+1}, \eta^{n+1}) = c$ also.

- Find a criterion for symplecticity of multistep methods, and methods satisfying it, that leads to methods with nice properties for Hamiltonian systems.

8 Preservation of integrals

To preserve integrals one generally appeals to the theorem of Ge [42] that to do so up to a constant it is necessary and sufficient for the algorithm to be equivariant with respect to the symmetries generating the integrals. (See also [79], where conditions are given under which the constant can be removed.) But there may be other approaches. Suris [134] has shown how making the Hamiltonian depend parametrically on the time step can lead to completely integrable versions of the standard map (i.e., $x_{j+1} - 2x_j + x_{j-1} = t^2 f(x_j, t)$). Moser and Veselov [94] showed that a Lagrangian discretization of the free rigid body on $T^*SO(n)$ is not only completely integrable but has all the same integrals as the continuous system, except the usual momentum is not conserved. On the other hand, Lewis and Simo [71] have constructed an energy-momentum-preserving symplectic integrator. Curiously, viewing the free rigid body as a free particle constrained to lie in $T^*SO(n) \subset T\mathbb{R}^{n \times n}$ and applying the symplectic constraint algorithm of Reich [107] gives the same integrator as Lewis and Simo [87], and on the reduced space, the same integrator as Moser and Veselov. We do not know if this is more than a

coincidence. Because the integrals do not depend on the time step, they are still preserved by higher-order maps formed by composition.

There are also the integrable discrete versions of integrable evolution equations such as the nonlinear Schrödinger equation and the Korteweg-de Vries equation. Some have integrable time discretizations too, although these are not usually spatially local [3]. Such equations are derived by discretizing the scattering problem of the continuous system, an approach which could be investigated from the point of view of symplectic integration. They usually preserve not the original symplectic structure, but a nearby one—an understandable price to pay for conserving energy exactly. The QR eigenvalue method can be viewed as a symplectic integrator conserving all integrals of the Toda lattice in Lie-Poisson form [135]. This, and the Moser-Veselov matrix factorization techniques [94], should be understood from the point of view of symplectic integration.

If a system were sensitive to errors in a known integral, it might be worth enforcing it implicitly. One would add the integral as a constraint, satisfied by a Lagrange multiplier, which would naturally be zero for the time-continuous problem. One needs an integrator which leaves invariant all the level sets of the integral, and is still symplectic in the usual sense—a slightly different criterion than that used in integration with constraints (see Section 10).

- In which ways can integrals be conserved? Is it worth weakening the symplectic condition by requiring only preservation of a perturbed symplectic structure, if it enables conservation of more integrals?

Many implementors of symplectic schemes have noticed that the energy, although not conserved exactly, does not drift secularly. A theorem of Ge [46] shows that for systems with no integrals apart from the energy, a map preserving both the energy and the symplectic structure would have iterates lying on the true orbit. Such a map is unlikely to be computable. The nice energy behavior of symplectic schemes has been explained by Neishtadt [96], who proves (among other things) that if the perturbation due to the integrator is of size ε , then the energy error will be bounded by $\mathcal{O}(\varepsilon)$ for time $\mathcal{O}(e^{c/\varepsilon})$.

As ε increases, this time decreases, and can eventually limit the feasible time-span of the simulation. Often a critical step size is observed beyond which the energy behavior suddenly worsens. (Related phenomena are seen in Arnold diffusion.) The energy can even blow up in finite time [130]. To avoid this, it seems that the step size must be small compared to the shortest period of the system, a severe restriction if the system is a discretization of a PDE [130, 131].

- Quantify this observed energy breakdown, and find ways to avoid it.

An alternative route is to abandon symplecticity, and require instead strict energy conservation. This approach has been explored by (among others) Simo and coworkers [79, 129, 130, 131]. It is possible to simultaneously conserve momentum, and such “energy-momentum” integrators are very promising. At first sight, however, the resulting map on the energy-momentum level set is not constrained in any way. It might not preserve a volume form, for example, and it might possess attractors, so the implications for long-time simulations are not clear. They are

very effective, though, in providing unconditionally stable methods for conservative PDEs [129]: the usual methods for improving stability introduce large dissipation.

9 Variable time steps

Standard methods can sometimes beat symplectic methods for pointwise accuracy, even at low order, if the system contains widely varying time scales in different parts of phase space. The reason is that the standard methods can adaptively change the time step. If one tries to, say, halve the time-step in a symplectic integration when $\|H''\|$ exceeds a certain threshold, the resulting map is not even continuous at the threshold hypersurface, and hence not symplectic. KAM tori are broken and good long-time behavior is lost [15].

Just as the time- t map of a canonical Hamiltonian system is symplectic, so its time- $t(q, p)$ is symplectic with respect to a non-canonical symplectic form. This suggests that this latter form should be preserved by a numerical method, and that $t(q, p)$ should depend locally and smoothly on q and p . This approach has not been developed to our knowledge. Another, similar, approach would be to integrate $JdH/\|JdH\|$, which also preserves a non-canonical symplectic form. It has been suggested that the ultimate criterion is that the numerical method should be the time- $t(q, p)$ flow of a Hamiltonian system close to the original one. For this and further discussions, see [121, 127].

In the integration of Hamiltonian systems with a nonstandard symplectic structure, such as the integrable discrete nonlinear Schrödinger equation [2], Darboux charts are useful to bring the system to the standard canonical form. Our preliminary investigations show that often the mapping to symplectic variables is explicit but its inverse is not; the inverse is required to specify the Hamiltonian in the new variables. This presents algorithmic difficulties that require further investigation.

To date the only successful approach is that of Skeel and Biesiadecki [128] and MacEvoy and Scovel [75]. They partition the Hamiltonian so that it is a sum of fast and slow terms, the fast terms being zero outside some region of phase space. The slow terms are integrated with a large time step unless that step puts that orbit in the fast region, in which case it must be retaken with a smaller time step. MacEvoy and Scovel [75] join the two regions smoothly by a partition of unity. To date these algorithms have not been developed to the point where one can make a fair comparison with standard variable time step schemes. Simó [125] has suggested taking the Kepler problem (a particle in $\mathbb{R}^2$ under a central inverse-square force) with eccentricity 0.999999 as a good test of a variable time step method.

- Develop variable time step symplectic integrators so that they are competitive for pointwise accuracy with standard methods for the Kepler problem, while retaining the good long-time behavior of constant time step symplectic methods.

10 Constrained systems

10.1 Dirac constraints Suppose that we are given a Hamiltonian on a symplectic manifold M and a submanifold $N \subset M$ to which we would like to constrain the dynamics. Suppose that we have found a set of constraint functions $\phi : M \rightarrow V$ (where V is a linear space) such that $N = \{x \in M : \phi(x) = 0\}$ and the matrix $\{\phi_i, \phi_j\}$ is nonsingular. The problem is to construct a map from N to N approximating the constrained dynamics and preserving the induced symplectic

structure on N . Frequently the system is invariant under a symmetry group, in which case the integrator should preserve the corresponding momenta.

This has been addressed and solved only in the case of *holonomic* constraints [63, 69, 87, 107, 108], and when the symmetry group acts by cotangent lifts of *linear* transformations. That is, when $M = T^*Q$ is a cotangent bundle, Q is a linear space, and the constraints are divided into two sets, the primary constraints $R = \{q \in Q : \phi_1(q) = 0\}$, and the secondary constraints $\phi_2(q, p) = d\phi(q)\partial_p H(q, p) = 0$. The constraint methods induce a symplectic map on T^*R .

The problem for the more general class of non-holonomic constraints is still open, as is the question of the correct analogue of symplectic integration for non-holonomically constrained Lagrangian systems.

- Develop momentum-preserving constrained symplectic integrators for general constraints and for general symmetry groups.

For Hamiltonian ODEs, Dirac constraints are equivalent to the intrinsic procedure of constraining a Hamiltonian vector field by merely restricting both the Hamiltonian and the symplectic form to the desired submanifold (call this vector field X_N). Is there an analogous procedure for maps? (call the constrained map φ_N). (Reich [110] has shown that for holonomic constraints, an arbitrary symplectic integrator for the unconstrained problem can be projected to a symplectic map on the constraint space.) The operation should at least commute with the previous procedure under the operation of taking flows, that is, $\exp(tX_N) = \exp(tX)_N$.

At present, the general theorems concerning momentum preservation require the constraint functions to be group invariant. However, in the case of the Lagrange top, McLachlan and Scovel [87] found only degenerate invariant constraint functions. Since nondegeneracy is essential for the constraint algorithm, they dropped one of the invariances; but it turned out that the integrator preserved its momentum anyway.

- What special properties are required of the constraint function in order that a momentum-preserving symplectic integrator may be determined?

10.2 Fewer implicit steps The currently recommended algorithms for holonomically constrained separable Hamiltonian systems [4, 63, 69, 87, 107] involve solving a set of implicit equations to enforce the primary constraints each time q is updated. For a higher-order method formed by composition, this means many implicit steps. (The secondary constraints can be enforced with an explicit step.) Is it possible to do better by only enforcing the constraints at the end of each complete time-step?

- Are there constrained symplectic integrators with fewer implicit steps than those currently in use?

10.3 Generating functions It is easy to determine the exact Lagrange multipliers for the continuous system, but at the cost of more derivatives and matrix inversions. In return, the number of iterations on the implicit step is reduced. At present we are using Lagrange multipliers extrapolated from previous time steps, combined with simple or Newton-chord iteration to roundoff error.

- Can one modify the Hamiltonian or predict the value of the Lagrange multipliers to make the implicit step more efficient? Are there methods which are symplectic after a finite number of iterations on the multipliers?

Indeed, the generating function picture is far from complete.

- Understand the symplectic geometry of the generating function method for holonomic constraints.

It is hoped that a full understanding of this problem will lead to a method for nonholonomic constraints.

10.4 Automatic preservation of quadratic constraints In many physical systems, such as rigid body and molecular dynamics, the constraints are quadratic functions, being based on preservation of Euclidean lengths. Because symplectic Runge-Kutta methods, such as the midpoint rule, preserve quadratic integrals [22, 26, 120], these seem to be good candidates to integrate such quadratically-constrained systems.

Specifically, the constraints on the configuration variables are quadratic and the secondary constraints $\phi(q, p)$ have quadratic extensions to the full space. In some examples [87], we have successfully modified the Hamiltonian away from the constraint surface so that the flow of the Hamiltonian leaves the level sets of the primary constraints invariant and the zero level set of the secondary constraint invariant. However, we were unable to determine a modification such that all the level sets of the secondary constraints are invariant. Therefore, the quadratic invariant preserving methods will not automatically preserve the secondary constraints.

- For which quadratically-constrained systems can the Hamiltonian and the constraint functions be extended to a neighborhood of the constraint surface such that the constraints are true quadratic integrals of the extended Hamiltonian system?

Another application involves Lie-Poisson systems. Many Lie groups can be written as submanifolds of linear spaces defined by quadratic constraints. For example, $SO(n) = \{q \in \mathbb{R}^{n \times n} : q^t q = 1\}$. In this case symplectic Runge-Kutta methods can be used to approximate the exponential map and compute group elements. For $\mathfrak{so}(n)$, the midpoint rule is the Cayley transform between $\mathfrak{so}(n)$ and $SO(n)$: for $A \in \mathfrak{so}(n)$, $(I - A)^{-1}(I + A) \in SO(n)$. It is tempting to use this fact in conjunction with the coadjoint action to construct Lie-Poisson integrators for matrix Lie groups determined by quadratic constraints. For example, consider the integrator $z \mapsto Z$ where

$$Z = Ad_{R(dH((z+Z)/2))}^* z,$$

and $R(x)$ is the Runge-Kutta integrator applied to the Lie algebra element x . The range of R is in the group, so that it is natural to ask if this integrator is Lie-Poisson. Our preliminary calculations indicate that it is not, but that does not mean that there is not some alternative Lie-Poisson form. There are many other integrators based on this idea; one should test them numerically first.

- Use quadratic-preserving Runge-Kutta methods to generate Lie-Poisson integrators.

11 Approximation of infinite-dimensional Poisson manifolds

For Hamiltonian field theories, the phase space is an infinite-dimensional Poisson manifold. For an introduction to this subject, see Olver [98]; for applications to fluid mechanics, see Salmon [119] and Arnold and Khesin [8]. To numerically simulate these equations a finite dimensional truncation is necessary.

- Should a finite dimensional truncation of an infinite dimensional Hamiltonian system be Hamiltonian?

Specifically, we want to be able to let $\Delta t = f(\Delta x)$ (f being determined by stability criteria) and study

$$\lim_{\Delta x \rightarrow 0} \lim_{t \rightarrow \infty} \quad (11.1)$$

Usually in numerical analysis these two limits are reversed, or t is held fixed. But most real computations use (11.1), because global errors can be kept small only for impractically short times. It is implicitly hoped that the qualitative and statistical behavior of the PDE is mimicked by the finite-dimensional model, Hamiltonian or not.

In the hope that there are positive answers to the above question, we now discuss the approximation of Poisson manifolds. After the truncation of the phase space, there is still the question of choosing the best Hamiltonian.

If the Poisson bracket is constant, i.e., independent of the field variables, truncation is trivial, because any antisymmetric matrix is Poisson. As in finite dimensions, this is the most common case. Thus we immediately get Hamiltonian truncations for nonlinear wave equations, the nonlinear Schrödinger equation, the Davey-Stewartson and Boussinesq equations, and so on. In fact, with periodic boundary conditions, all of these have a two-term splitting, so the design of the Hamiltonian method is finished. Some questions of numerical analysis are considered in [83]. If the resulting Courant-type stability restriction (roughly two time-steps per period of the fastest wave) are too severe, the fast modes should be removed in the Hamiltonian, not by the integrator.

For equations of the form $\dot{u} = \partial_x(\mathcal{L}u + f(u))$, where $\mathcal{L}$ is a linear operator, it is annoying that being able to solve $\dot{u} = \partial_x f(u)$ by characteristics is no help: we must solve the discretized equation $\dot{\mathbf{u}} = D\mathbf{f}(\mathbf{u})$. If D has bandwidth b above the diagonal, then we can do a $b+1$ -piece splitting (e.g., odd-even splitting for $b=1$), and $b/(b+1)$ of the unknowns evolve under a given piece. During a (first-order) time step, each unknown is stepped b times, which is unappealing—particularly if D is full, as for spectral methods. We have the paradoxical situation that an implicit method using FFTs would be asymptotically faster than an explicit method.

The simplest truncation for Hamiltonian systems on T^*Q , where Q is the configuration space, is to determine a Hamiltonian system on T^*N where N is a finite-dimensional submanifold of Q . This is done in the Lagrangian description by restriction to the tangent space $TN \subset TQ$. Then the Legendre transform gives a Hamiltonian system on T^*N . This is the technique proposed by Holm et al. [53].

However, it can destroy symmetries of the system such as the particle relabeling symmetries of fluid mechanics.

Many other evolution equations of physics—Eulerian inviscid fluids, the Vlasov-Poisson equation, the Korteweg-de Vries equation—can be written as Lie-Poisson systems. Their phase space is the dual of some infinite-dimensional Lie algebra. To spatially truncate such systems to a set of Lie-Poisson ODEs leads naturally to the question of finding finite-dimensional approximations of these Lie algebras. The approximation should converge to the infinite-dimensional algebra in some useful sense (perhaps its structure coefficients converge pointwise) and inherit as much structure as possible: all the discrete Casimirs (such as helicity in the 3D Euler equations), and an increasing number of the continuous ones (such as the generalized enstrophies in the 2D Euler equations) as the approximation improves. It is hoped that in this way statistical properties of the discrete system will approximate those of the continuous system, although this is little more than a hunch at present [10, 62, 145]. For example, how does symplectic integration of Zeitlin's truncation of the Euler equation converge to Joyce-Montgomery [60] states? Is there a Joyce-Montgomery equation for negative temperature states on $\mathfrak{su}(n)$? What is the effect of different Hamiltonians, such as the one presented in Dowker and Wolski [28]? How important is it to preserve the higher Casimirs in the numerical simulation?

Truncation of Poisson manifolds is a very difficult and fundamental problem, and little progress has been made. There is no general theory. Simple finite differences and spectral methods do not work, even elegant ones such as Arakawa's energy- and enstrophy-preserving schemes [5, 6]. We can only summarize the presently known approaches.

11.1 The sine bracket For the algebra of Hamiltonian vector fields on the torus $\mathbb{T}^2$, the Lie bracket in Fourier space takes the form

$$[\omega_{\mathbf{m}}, \omega_{\mathbf{n}}] = (\mathbf{m} \times \mathbf{n}) \omega_{\mathbf{m}+\mathbf{n}} \quad (11.2)$$

where $\mathbf{m} = (m_1, m_2)$ is a wavenumber and $\mathbf{m} \times \mathbf{n} = m_1 n_2 - m_2 n_1$. The sine-bracket truncation retains the modes with $-M \leq m_1, m_2 \leq M$ and perturbs the bracket to

$$[\omega_{\mathbf{m}}, \omega_{\mathbf{n}}]_{\sin} = \varepsilon^{-1} \sin(\varepsilon \mathbf{m} \times \mathbf{n}) \omega_{\text{mod}(\mathbf{m}+\mathbf{n})} \quad (11.3)$$

where $N = 2M + 1$, $\varepsilon = 2\pi/N$, and $\text{mod}(\mathbf{m})$ reduces $\mathbf{m}$ modulo N to the lattice $-M \leq m_1, m_2 \leq M$ [33, 54, 55]. Notice how the sine bracket converges to the continuous bracket as $N \rightarrow \infty$ for fixed $\mathbf{m}, \mathbf{n}$. (11.3) turns out to define the Lie bracket of $\mathfrak{su}(N)$, so this algebra has $N - 1$ Casimirs, the n th one of which tends to the n th Casimir of (11.2) as $N \rightarrow \infty$ for fixed n . Clearly the precise sense in which $SU(N)$ approximates the group of symplectic maps of $\mathbb{T}^2$ remains to be established!

This algebra provides a Lie-Poisson truncation of, among other systems, the 2D Euler equations with periodic boundary conditions [10, 28, 89, 145]. It seems to be the only such truncation, and is related to the Moyal bracket of quantum mechanics [38]. It allows truncations of the shallow water equations in Eulerian [47] and Lagrangian [113] formulations, although these have not been tested. Perhaps one should first study the sine-bracket independently of its application to fluid mechanics, for instance, by choosing Hamiltonians which give smoother flows.

- Is the sine bracket useful in numerical methods?

11.2 Moment truncations For Vlasov-Poisson-type systems whose phase space consists of densities f on a base symplectic manifold P , one can define the moments $f^\alpha = \int_P x^\alpha f dx$ and the induced Poisson bracket $\{f^\alpha, f^\beta\} = f^\gamma$, where $x^\gamma = \{x^\alpha, x^\beta\}_P$. (Here α is a multiindex.) There are two trivial truncations of this infinite-dimensional Poisson space which may be useful. Notice that $|\gamma| = \max(0, |\alpha| + |\beta| - 2)$ so that the algebra has two subalgebras, one consisting of moments of order 0, 1, and 2, and one of moments of orders 2 and higher. In the first case no truncation is required, and Rouhi [114] has used this to approximate elliptical vortex patches; one can also get the “next correction” to point vortices in this way. The second case has an elementary finite-dimensional truncation to moments of order 2 through n [21], discussed below. Such a truncation is useful for the localized distributions that arise in accelerator dynamics [17]. But if one wishes to retain moments of order 0 through n , perhaps with multiple base points, a more sophisticated approach leading to mixed Eulerian-Lagrangian schemes, outlined in Section 11.4, is needed.

More applications of these truncations should be explored, if only because truncations are rare.

- Apply moment truncations to fluid mechanics and to general Hamiltonian PDEs.

11.3 Other approaches Unfortunately, the sine bracket exists only for the algebra of Hamiltonian vector fields on the sphere, the $2n$ -torus, and possibly on other quotients of coadjoint orbits [54]. If one changes variables by the discrete Fourier transform, the sine bracket transforms to a bracket on functions on a lattice. However, this bracket is nonlocal.

- Is there a local Lie bracket on functions on a discrete representation of the plane approximating the usual Poisson bracket?

It is possible that there is none, due to the rigidity of Lie algebras. One cannot get rid of this problem by going to a nonlinear Poisson bracket since the Poisson structure transverse to the symplectic leaves is linearizable to a Lie-Poisson structure [139], so there must be Lie algebras present. However, if we could find a local Lie bracket, the next question would be how to deal with boundary conditions. For example, to do simulations of the Euler equations on the sphere it would be nice to have a Lie algebra which approximates the Poisson algebra of Hamiltonian functions which vanish on continents. This would also be useful for the boundary conditions imposed by the walls in an accelerator.

There is also the work of Dubrovin [30] on discrete Poisson brackets. For a certain bracket on the field variable $u : \mathbb{R} \rightarrow \mathfrak{g}$, where $\mathfrak{g}$ is a Lie algebra, he was able to replace the domain $\mathbb{R}$ by a discrete lattice only by deforming the range $\mathfrak{g}$ to a Poisson-Lie group. Workers in quantum groups have pointed out the similarity between the processes of quantization and discretization [101].

There is no known approximation for the algebra of divergence-free vector fields on $\mathbb{T}^3$, which would be needed to study the 3D Euler equations. To make the formulas easier one might study the algebra of vector fields on the circle, for which the Poisson operator is $u\partial_\theta + \partial_\theta u$ [84, 101].

However, one can leave the category of strict Poisson truncation. For the algebra of vector fields $u(\theta)$ on the circle, the change of variables $u = v^{1/2}$ makes the Poisson operator constant [83]. Similar changes of variables exist in other cases [91] but due to their hodograph nature may not be of practical use. One could search for canonical variables on particular symplectic leaves, or find symplectic (Clebsch) variables on the whole space [80, 144]. This latter approach is unappealing as the truncation will generally destroy the gauge symmetry of the symplectic variables, leading to an excessively large phase space. Lagrangian formulations of fluids can be canonical, so one should explore as many such formulations as one can find. The “velocity” method [14, 99] is interesting in this regard. See also Virasoro [137]. Lagrangian vorticity and velocity-vorticity formulations should be studied. The three-dimensional vortex methods currently in use do not appear to be canonical [140]; extending them to be so would be an important development. Symplecticity is important in stellar dynamics too [90], so Hamiltonian truncations of its Vlasov-Poisson formulation should be useful.

The method of Dirac constraints has proved useful in deriving simplified evolution equations [118]; is it possible to get a sensible Hamiltonian truncation by constraining the fluid motion to a finite-dimensional submanifold?

11.4 Augmentation and decoupling of semi-direct products Although there is no approximation of the group D of volume-preserving diffeomorphisms at present, there is a useful approximation of the dual of its Lie algebra as a Poisson manifold. Following Scovel and Weinstein [124] we augment to a slightly larger space and use an isomorphism to direct products of Poisson manifolds, each which have Poisson truncations.

Consider the subgroup D_0 consisting of those diffeomorphisms of the 3-torus $\mathbb{T}^3$ which preserve the origin. Let N_k denote the normal subgroup of D_0 whose elements d are such that the 1st through k th derivatives of $d(x) - x$ vanish at the origin. Then, $D_k = D_0/N_k$ can be thought of as an approximation to D_0 . It is the finite-dimensional group consisting of the k th-order jets of volume-preserving diffeomorphisms which preserve the origin. Likewise, the dual of the Lie algebra $\mathcal{D}_k$ is a space of vector moments up to k th order.

However, what we wish to approximate is $\mathcal{D}^*$. We do this by pulling back the Hamiltonian to the semidirect Poisson manifold $\mathcal{D}^* \otimes \mathbb{T}^3$ by the Poisson map consisting of projection onto the first factor. Then pull back by a Poisson isomorphism $T^*\mathbb{T}^3 \oplus \mathcal{D}_0^* \rightarrow \mathcal{D}^* \otimes \mathbb{T}^3$ which decouples the semidirect product Poisson manifold into the direct product of Poisson manifolds. This determines a Hamiltonian system on $T^*\mathbb{T}^3 \oplus \mathcal{D}_0^*$ for which the first factor is finite dimensional and the second is truncatable. The new phase space has the physical interpretation of the replacement of the momentum density by a single particle plus the 0th through n moments of the distribution about that particle [124]. The determination of a Hamiltonian on the truncated space would follow by pulling back by the Poisson map $T^*\mathbb{T}^3 \oplus \mathcal{D}_k^* \rightarrow T^*\mathbb{T}^3 \oplus \mathcal{D}_0^*$ which is the adjoint to the one induced by the projection $\mathcal{D}_0 \rightarrow \mathcal{D}_k$. However, the Hamiltonian is not usually well defined on this image since an image point consists of sums of delta functions and their derivatives, which we call a multipole. Consequently, we pull back by another map $\phi: T^*\mathbb{T}^3 \oplus \mathcal{D}_k^* \rightarrow T^*\mathbb{T}^3 \oplus \mathcal{D}_0^*$ such that when it is composed with a natural projection $T^*\mathbb{T}^3 \oplus \mathcal{D}_0^* \rightarrow T^*\mathbb{T}^3 \oplus \mathcal{D}_k^*$ should give the identity. Probably ϕ should be the identity in the first factor.

- What are the optimal ϕ 's for a specific physical system?

This technique appears to work well when the distribution in $\mathcal{D}^*$ is concentrated about a point and can be well represented by its first few moments. One can incorporate many of these multipoles by first pulling back to the direct sum $\sum \mathcal{D}^*$ by the map $\sum \mathcal{D}^* \rightarrow \mathcal{D}^*$ that simply sums up the distributions. Since the Lie-Poisson structure on $\mathcal{D}^*$ is linear, this summation is a Poisson map. Consequently, we have a progression of Hamiltonian truncations, from one multipole with a large number of moments to a large number of multipoles with a small number of moments.

- For a specific problem, what is the optimal balance between the number of multipoles and the number of moments retained for each?

In the truncation of the shallow water equation, Ge and Scovel [47] use a Poisson isomorphism

$$T^*F^* \oplus \mathcal{D}_\mu^* \rightarrow \mathcal{D}^* \otimes F^*$$

where F^* is the space of positive mass densities, $\mathcal{D}^*$ is the space of momentum densities, and $\mathcal{D}_\mu^*$ the space of vorticities. The direct product space can be truncated by truncating F^* by a finite element method and approximating $\mathcal{D}_\mu^*$ by $\mathfrak{su}(n)$ for n large [33]. The difficulty here is that the isomorphism involves a map determined to exist by a theorem of Moser [95] on volume elements. Liao et al. [72] have been developing a numerical approximation of this map based on a deformation technique, and Cullen et al. [24] have successfully used the Monge-Ampere equation. The latter method appears to be more amenable to differentiation.

- Construct a numerical approximation to a map corresponding to Moser's [95] theorem on volume elements that makes the Ge-Scovel [47] shallow water approximation implementable.

12 Theoretical performance

12.1 The KAM theorem One of the strongest, and at the same time the most rigorous, explanations for the good performance of symplectic integrators is the KAM theorem. When it applies, one can be sure that for some orbits at least—the quasi-periodic ones—there are nearby numerical trajectories for which the orbital error is bounded for all time.

Consider a smooth autonomous Hamiltonian of the form

$$H_0 + \varepsilon H_1 + (\Delta t)^p H_2 \quad (12.1)$$

where H_0 is integrable, $H_0 + \varepsilon H_1$ is not, and H_2 is the first term in the perturbation due to a symplectic integrator. If $\varepsilon = 0$, KAM theory implies that most of the invariant tori of the system H_0 are preserved by the integrator, and that the fraction preserved tends to 1 as $\Delta t \rightarrow 0$. What can we do when $\varepsilon \neq 0$? A direct application of KAM theory only shows that most of the tori of $H_0 + \varepsilon H_1$ are still preserved when $\Delta t \neq 0$, by comparing back to H_0 . It seems that one should be able to get more; see for example the informal discussion in [84].

- Rigorously investigate Hamiltonians of the form (12.1) as $\Delta t \rightarrow 0$ for ε fixed but arbitrarily small.

12.2 Extensions of Hamiltonian stability theorems We discussed in Section 8 how symplectic integrators preserve energy well for long times. However, this result on the adiabatic invariance of the energy appears to have some validity outside the realm of Hamiltonian mechanics. We also suspect that the KAM and Nekhoroshev theorems have counterparts in larger categories than Hamiltonian systems. Let us be more precise.

Some proposed integrators are not actually symplectic but appear to have the same stability characteristics as symplectic methods. For example, consider the integrators of Channell and Scovel [20] based on generating functions determined from the Hamilton-Jacobi theory. They are not symplectic. This can be seen as follows. Pick an initial point z_0 . Then, determine the generating function about z_0 to generate the symplectic map from z_0 to the next point. Now consider another point z_1 near z_0 . In [20], its generating function is determined by a Taylor series about z_1 , not z_0 , so the generating functions do not match in general. Therefore, z_1 is advanced by a different symplectic map than z_0 . Consequently, the method does not necessarily determine even a local symplectic map. However, their numerical experiments show that this method has the typical superior performance of symplectic integrators.

The domain where this integrator exists is probably something like the action groupoid $G \times Z$ where G is the group of symplectic maps and Z is the phase space, instead of the symplectic group relevant for the usual symplectic integrator. Actually, G is more likely to be the local symplectic mappings, but we prefer not to confuse the issue any more than necessary here. For a review of groupoids and algebroids see MacKenzie [77]. The partially-defined multiplication in $G \times Z$ is $(g_2, z_2)(g_1, z_1) = (g_2 g_1, z_1)$ if $z_2 = g_1(z_1)$. This is natural, since if one starts at z_1 and determines a flow map g_1 , then on the next step one begins at $z_2 = g_1(z_1)$. This structure seems to be relevant for numerical analysis in general, not just for Hamiltonian mechanics. The analogue of the Lie algebra of Hamiltonians $\mathfrak{g}$ of G for the groupoid is the Lie algebroid $\mathfrak{g} \times Z$ which is a vector bundle with fibers $\mathfrak{g}$ and base Z . It is not a Lie algebra, but there is a Lie bracket on sections of this vector bundle. Now consider a Hamiltonian $H \in \mathfrak{g}$ and the constant section $Z \rightarrow \mathfrak{g} \times Z : z \mapsto (H, z)$.

- If the KAM or Nekhoroshev theorems are applicable to the Hamiltonian system determined by H , are there analogues of these stability theorems for sections of the action algebroid $\mathfrak{g} \times Z$ which are small perturbations of the constant section $z \mapsto (H, z)$? Is there an adiabatic invariance theorem for such an extension?

As mentioned above, there is numerical evidence to support the existence of these theorems. Further, since the evolution of H is by quasi-periodic motion, substitution of this motion into the z dependency of the perturbation gives a quasi-periodic time-dependent perturbation of H to use as a base motion.

12.3 Reversible adiabatic invariance theorem It is known that there is a KAM-type theorem for R -reversible systems (see also Section 14.2). However, in [75] and [83] it is observed that integrating an R -reversible Hamiltonian system by

an R -reversible nonsymplectic integrator preserves the energy well over long simulations. See [112] for a review of the interactions between reversible and Hamiltonian systems.

- Is there an adiabatic invariance theorem for reversible perturbations of reversible Hamiltonian systems?

When the original Hamiltonian system is integrable, one can ask whether all the integrals of motion are adiabatic invariants for R -reversible perturbations.

- Is there a Nekhoroshev theorem for reversible perturbations of reversible integrable Hamiltonian systems?

Reversibility extends naturally to multistep methods, and Saha and Tremaine [115] have developed and applied such methods usefully to the solar system. Presumably one only obtains good behavior near the symmetry plane. More generally we propose:

- Study R -reversible perturbations of R -reversible Hamiltonian systems.

12.4 Chaos It is impossible to track orbits whose Lyapunov exponents are of order one for long times. Typically, the chaotic and quasiperiodic orbits are intermingled in Hamiltonian systems; indeed, there are no known completely hyperbolic polynomial Hamiltonians. So, at least the boundaries of the chaotic regions will be better preserved in a symplectic than in a nonsymplectic integrator. But what about the flow in the chaotic region itself?

Because individual orbits cannot be tracked accurately, the chaotic case should be symplectic integrators' forte. But so little is known analytically that it is hard to know what kind of result one should aim for. Instead, there is a result which argues *against* the necessity of symplectic methods: for Anosov systems, *all* nearby flows are conjugate, not just the symplectic ones. Some numerical work might resolve the apparent contradiction.

- Measure statistical properties of chaotic orbits, and their dependence on symplectic and nonsymplectic perturbations.

13 Dissipative systems

- In the numerical simulation of slightly dissipative perturbations of Hamiltonian systems, does one simply give up the Hamiltonian structure?

There is evidence to the contrary. Unpublished work of the second author with D. Umbarger used the fact that the Duffing oscillator has a time-dependent coordinate transformation into a time-dependent Hamiltonian system. They compared a fourth-order symplectic integrator in this moving frame with a Bulirsch-Stoer variable time step method: the two appeared to be of comparable quality.

Lewis and Marsden [70] describe a Hamiltonian-dissipative normal form decomposition of a vector field and discuss how the Hamiltonian part provides an organizing center of the system. Kirchgraber et al. [67] observe that in a simple case

that if the integrator is symplectic when the dissipation is turned off, the numerical center manifold is stable under the dissipative perturbation. Mielke [88] describes the Hamiltonian structure inherited on center manifolds and Sleeman [132] shows that time-periodic solutions of reaction-diffusion equations can form Hamiltonian systems in the single spatial variable. Since the center manifold is a component of the system with the exponential decay factored out we ask the following questions.

- When is the flow on the center manifold of a dissipative system Hamiltonian? When is the flow on an inertial manifold Hamiltonian?

Such a situation is surely not true in general, but it would be interesting to know if there are any important special cases.

Grmela [48] and Morrison [92, 93] provide bracket formulations for Hamiltonian plus gradient systems and Vujanovic and Jones [138] have described a variational form for nonconservative systems. What is missing is an invariant structure whose preservation provides superior numerical simulations.

For a Hamiltonian system on M , the graph of the vector field is a Lagrangian submanifold of TM with respect to the tangent symplectic structure. This is the infinitesimal version of the fact that the graph of the flow map of a Hamiltonian system is Lagrangian in the symplectic manifold $M \times M_-$, where M_- is M with the negative of its symplectic form. Cantrijn [16] has shown that the graph of a gradient perturbation of a Hamiltonian system in TM is Lagrangian with respect to a symplectic form on TM which is close to the tangent one. Unfortunately, this symplectic formulation does not seem to produce invariants at the map level, so it is unclear what its implications are for numerical simulations.

- Which dissipative systems have flow invariants whose preservation produces superior numerical simulations?

For any dynamical system, one can double the dimension of the space and extend the ODE by cotangent lift to obtain a Hamiltonian system. This does no good numerically as invariant tori are typically half the dimension of the symplectic manifold, i.e., equal to the dimension of the original system. However, Nosé [100] shows that molecular dynamics formulations with constant temperature may be presented in Hamiltonian form by the addition of two more variables.

- What is the structure of a dynamical system which allows a Hamiltonian formulation by the addition of a small number of variables?

14 Assorted issues

The program of studying geometric structure in numerical methods has scarcely begun. We select just a few such structures for further comment.

14.1 The discrete Lagrangian method Discretization of the Lagrangian description appears to be very old. Maeda [78] and MacKay [76] outline formalisms for discrete Lagrangian methods and describe the corresponding symplectic method. Wu [143] illustrates the corresponding discrete variational problems corresponding to a large class of symplectic methods and applies shooting techniques to 2-point

boundary value problems. Moser and Veselov [94] discretize the Lagrangian description of the free rigid body and determine a completely integrable approximation preserving the rigid body integrals.

It is possible that in many cases either the Lagrangian formulation or the the Hamiltonian formulation might yield a superior numerical simulation.

- Investigate the quality of Lagrangian integrators, and their equivalent Hamiltonian forms.

14.2 Reversible systems Many authors have pointed out how easy it is to construct *reversible* integrators [83, 84, 107, 122], and how important it is *a priori*. Most applications are in Hamiltonian systems. However, one should also

- Perform numerical experiments to investigate the importance of preserving reversibility with respect to one or multiple involutions.

This is important since one may not know the involutions explicitly, or even if they exist. Scovel [122] projects an arbitrary map onto R -reversible maps; this doubles the amount of work, so one would like to know whether it is worth it. See [112] for a review of reversibility and Hamiltonian systems.

14.3 Volume preservation Volume-preserving flows arise in particle-tracking in incompressible fluids and in the standard spectral truncation of the 2D Euler equations. (Interestingly, this latter model also preserves energy and enstrophy—how well are they preserved by a volume-preserving scheme?) The space of divergence-free vector fields seems to be too large: no standard numerical methods, such as Runge-Kutta, are volume-preserving for all such vector fields [102]. There is a generating function for volume-preserving maps [103, 122], but it involves evaluating definite integrals of the vector field and does not preserve fixed points in general. In many systems such as the ABC flows a splitting technique works well [51, 52, 102, 103, 122].

- Are there general volume-preserving integrators which use only the vector field?
- Develop efficient, general volume-preserving methods.

14.4 Symplectic lattice maps Often roundoff accumulation can become a problem even with symplectic methods. Symplectic lattice maps have been studied [106, 66, 65] and are a possible resolution of this problem. Earn and Tremaine [31] show that the elimination of roundoff error in this way can effect the statistical behavior of the simulation. Scovel [123] shows that often a symplectic map can be altered to a nearby symplectic map which preserves a lattice. The lattice maps should get more accurate as the lattice is refined. However, as the lattice gets finer, the preservation of the lattice causes a high-frequency perturbation which may cause diffusion problems in the zero-lattice-spacing limit.

- For specific Hamiltonian systems, is there an optimal lattice spacing for a symplectic lattice map approximation?

14.5 Standard methods For some dynamical systems, very high order Cowell methods are so accurate and so inexpensive that the local truncation errors can be made comparable to roundoff errors. Then (to within roundoff error) it is a symplectic multistep scheme in Feng's sense. See Hyman et al. [58] for a discussion of this matter.

- For a specific Hamiltonian system, and a fixed degree of accuracy of some property of the system, develop a criterion to determine when it is worth the extra effort to use a symplectic integrator versus a traditional method.

14.6 Shooting methods One-dimensional quantum mechanics problems often involve computing the eigenvalues of a Schrödinger operator. Leaving the eigenvalue as a parameter to be determined one can use a shooting method from the left-hand boundary to the right. The differential equations are Hamiltonian and the shooting technique has been studied by Wu [143].

- What are the benefits of using a symplectic integrator in a shooting method?

14.7 Elliptic equations Can one devise numerical approximations of the *Div*, *Grad*, and *Curl* operators that satisfy the vector identities $\text{Div} \circ \text{Curl} = 0$, $\text{Curl} \circ \text{Grad} = 0$ exactly? The answer is yes [27, 57]. Triangulate the basic manifold by a chain complex. Then the coboundary operator δ is the discrete analogue of the exterior derivative d and the discrete vector identities $\delta \circ \delta = 0$ are consistent with the fact that the de Rham map from the de Rham complex to the cochain complex is a chain map. In a closely related strategy, Hyman et al. [59] develop and test finite volume approximations to differential operators on nonuniform grids based on Stokes's theorem.

If we impose a Riemannian structure, we can take adjoints and compute a Laplacian. In fact, Hyman and Scovel [57] show that the Hodge theorem still applies here in the sense that there is a discrete Hodge decomposition and the dimension of the kernel of the discrete version of the Laplacian on k -forms is the dimension of the k th cohomology group of the manifold. However, at present these Laplacians are not local since the induced Hodge star operator is not local.

- Is there a local discrete Hodge star operator which has a local inverse?
- Are there chain map approximations to the exterior derivative that are more than first-order accurate?
- Can one quantify the benefits of using these techniques?

14.8 Linear algebra Although we are not qualified to comment extensively, we would like to direct attention to the active field of structure-preserving algorithms in numerical linear algebra [13]. Such algorithms for finding the eigenvalues for Hamiltonian or symplectic matrices, for example, are both faster and more accurate (because the resulting eigenvalues have the right symmetries) than standard methods. Another application is to solving algebraic Riccati equations [104]. This work may also feed back to differential equations, as in work on differential Riccati equations [25] and on computing Lyapunov exponents [49, 73].

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