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Geometric Integration

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1 Introduction

"The last decade has seen such a deluge of papers on the numerical solution of the initial value problems for ordinary differential equations that it is quite impracticable to list, far less to summarize, all the contributions." These are the opening words of J. D. Lambert's paper [54] in the State of the Art 1976 Conference Proceedings. In spite of such a disclaimer, the paper succeeds in presenting, in less than fifty large-print pages, a unified view of all that, at the time of its writing, was known on numerical initial-value problems (IVP) for ordinary differential equations (ODEs). Ten years later, the subject was just too big and although the State of the Art 1986 Conference [50] featured three ODE speakers (J.D. Lambert, A.R. Curtis and G. Wanner), their combined contributions are very far from surveying all the numerical ODE field. After another decade of growth in the subject, the present paper must limit itself to the presentation of an individual topic, geometric integration, without any ambition of being exhaustive. We have tried to convey to the reader a feeling for what we see as a new way of doing numerical ODEs. We have also tried to direct him or her to the relevant literature, but we have not considered it possible to present detailed mathematical arguments.

Before defining geometric integration let us place ourselves in the classical, 1976 State of the Art Conference point of view. Considered then were two situations, "general" and "stiff". For general problems, Lambert [54] perceived a "consensus of opinion on what are the 'best' methods" and reported that "some highly tuned and thoroughly tested packages" were available. The stiff field was not nearly as mature with "new methods ... continually being proposed", and, as a consequence, we were not "yet at the stage of being able firmly to recommend 'best' packages."

Given an initial value problem

$$\dot{y} = f(y), \quad y(0) = \alpha \in \mathcal{R}^D \tag{1.1}$$

(a dot represents differentiation with respect to time t), in 1976 we had

- *A well defined goal.* This was to find as cheaply as possible within the desired accuracy the vectors $y(t_i)$ at some prescribed output locations.
- *A tool to achieve the goal.* This was a package, or rather a couple of them, general/stiff, in which to plug the subroutine evaluating f. The general package dealt with all general f's and the stiff package dealt with all stiff f's.
- *A theoretical framework to design/understand the tool.* This included two main groups of ideas (i) consistency, local error, error constants, (ii) stability, error propagation, stability region.

The second of the items above deserves some comments. Surely, twenty years ago people were aware of the limitations of solving everything with two packages. Lambert mentioned "special classes of IVPs ... such as problems with periodic solutions" and regretted that they "received relatively little attention." (Was "relatively" a slight understatement when only one paper on special classes was quoted in [54]?) While Lambert aptly concluded that "where there is structure, we ought to be able to use it in the numerical method" for the numerical analyst, the field of special problems was a large, completely uncharted land.

The classical approach outlined above has clearly made an outstanding contribution to the solution of scientific problems. But, as all human things, it has limitations. These will be illustrated in two examples.

In July 1992, the pretigious journal Science featured in its Research News section [52] the announcement that "From Mercury to Pluto, Chaos pervades the solar system", as borne out by a numerical integration by Sussman and Wisdom [102] of the planetary equations of motion over a time span of nearly 100 million years. Does this widely publicized numerical ODE integration fall within the classical paradigm?

- The aim was not to compute accurately the state of the solar system after a long time; it was rather a matter of deciding whether the motion is regular or chaotic. When comparing results of different integration techniques in this sort of study, it was observed [115] that "the plots are remarkably similar", a clear indication that the authors had no illusions of having achieved any accuracy in a conventional sense, i.e. of having achieved small global errors.
- The tool was a special purpose splitting method, tailored to the problem at hand.
- The tool was designed through considerations that went a long way beyond the classical consistency/stability approach.

The second example concerns the simulation of the dynamics of biomolecules [10], a matter of integrating Newton's second law for the motion of the atoms in the molecule (the number of atoms could be as high as 10,000 or 100,000 and there are six differential equations per atom).

- The aim is to obtain information on things like average energies, conformational distributions, large-scale protein bending, etc. There is no hope of computing the solution with any accuracy: perturbations to the system being integrated typically double in size every picosecond and current simulations may cover time intervals of 1000 picoseconds. Furthermore the initial velocities are unknown and *assigned randomly*. Also the expressions currently used for the interatomic forces are only approximations that involve fitting parameters semiemperically.
- The current method of choice, leapfrog (known in molecular dynamics as Verlet [3]), is far away from the notion of package of the classical paradigm. Even if conventional packages could be applied to such a large problem, it is unlikely that they would outperform the simple leapfrog method.
- The success of the leapfrog method cannot be explained via the traditional ideas of stability and consistency. The scheme is only second order accurate. Being only marginally stable for linear forces and small time-steps, one would fear that the smallest nonlinearity could make it unstable (see [87,95] for a discussion).

2 Mathematical preliminaries

In this section we present the notation that will be used throughout the paper. We also include some background material that will later simplify the discussions.

2.1 Vector fields, flows and Lie operators

Each system of differential equations $\dot{y} = f(y)$, $y \in \mathcal{R}^D$ is defined by a *vector field* f [2,79]. With each system/vector field we associate its *flow* $\phi_{t,f}$ [2,6,79]. For each value of the real parameter t, $\phi_{t,f}$ maps $\mathcal{R}^D$ in $\mathcal{R}^D$ in such a way that $\phi_{t,f}(\alpha)$ is the value at time t of the solution of the system with initial value α at time 0. Thus, for fixed α and varying t, $\phi_{t,f}(\alpha)$ is the solution of the initial value problem Equation 1.1.

Also associated with the field f is the *Lie operator* L_f [2,6,79]. This maps each real-valued function F defined in $\mathcal{R}^D$ into the real-valued function $L_f \cdot F$ such that, for $y \in \mathcal{R}^D$,

$$(L_f \cdot F)(y) = f_1(y)\frac{\partial F}{\partial y_1}(y) + \cdots + f_D(y)\frac{\partial F}{\partial y_D}(y).$$

(Subscripts denote components.) Clearly, for each $\alpha \in \mathcal{R}^D$ and each real t,

$$(L_f \cdot F)(\phi_{t,f}(\alpha)) = \frac{d}{dt}F(\phi_{t,f}(\alpha)). \tag{2.1}$$

By recursively applying Equation 2.1 with $L_f^{k-1} \cdot F$, $k = 2, 3, \ldots$, in lieu of F, we conclude

$$(L_f^k \cdot F)(\phi_{t,f}(\alpha)) = \frac{d^k}{dt^k}F(\phi_{t,f}(\alpha)),$$

and evaluating these derivatives at time $t = 0$ we arrive at the following formula [79]

$$F(\phi_{t,f}(\alpha)) = \left(\left(\sum_{k=0}^{\infty} \frac{t^k L_f^k}{k!}\right) \cdot F\right)(\alpha) = (\exp(tL_f) \cdot F)(\alpha), \qquad (2.2)$$

for the Taylor expansion of F along the solution of the IVP Equation 1.1. Particularization of Equation 2.2 to the case where F is the mapping that associates with each y its ith component y_i, $i = 1, \ldots, D$, provides the Taylor expansion of each of the components of the solution $\phi_{t,f}(\alpha)$.

Given two Lie operators L_f and L_g, their *commutator* $[L_f, L_g] = L_f L_g - L_g L_f$ turns out to be the Lie operator associated with a third vector field called the Lie or Lie-Poisson bracket [2,6,79] of f and g and denoted by $[f, g]$. The jth component of $[f, g]$ is given by

$$\sum_i f_i \frac{\partial g_j}{\partial y_i} - g_i \frac{\partial f_j}{\partial y_i}.$$

2.2 The Baker-Campbell-Haussdorff formula

The Baker-Campbell-Haussdorff (BCH) formula [113] has recently played an important role in the analysis of numerical methods.

Let X and Y be "symbols". (We later think of these as Lie operators, but this is not necessary for the present.) We form the exponentials

$$\begin{aligned} \exp(X) &= I + X + \frac{1}{2}X^2 + \frac{1}{6}X^3 + \cdots \\ \exp(Y) &= I + Y + \frac{1}{2}Y^2 + \frac{1}{6}Y^3 + \cdots \end{aligned}$$

and we multiply them out

$$\begin{aligned} \exp(X)\exp(Y) &= I + X + Y + \frac{1}{2}X^2 + XY + \frac{1}{2}Y^2 \\ &\quad + \frac{1}{6}X^3 + \frac{1}{2}X^2Y + \frac{1}{2}XY^2 + \frac{1}{6}Y^3 + \cdots \end{aligned}$$

According to the BCH formula, the product $\exp(X)\exp(Y)$ can be written as the exponential $\exp(Z)$ of a new symbol

$$\begin{aligned} Z &= X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}([X,X,Y] + [Y,Y,X]) \\ &\quad + \frac{1}{24}[X,Y,Y,X] - \frac{1}{720}([Y,Y,Y,Y,X] + [X,X,X,X,Y]) \\ &\quad + \frac{1}{360}([Y,X,X,X,Y] + [X,Y,Y,Y,X]) \\ &\quad + \frac{1}{120}([X,X,Y,Y,X] + [Y,Y,X,X,Y]) + \cdots \end{aligned} \qquad (2.3)$$

Here $[X, Y]$ is the commutator $[X, Y] = XY - YX$ and we use iterated commutators $[X, X, Y] = [X, [X, Y]]$, $[X, Y, Y, X] = [X, [Y, [Y, X]]]$, etc. It is remarkable that Z only consists of X, Y and commutators. In particular, if X and Y are Lie operators L_f, L_g, then Z is a new Lie operator: the operator associated with the vector field $f + g + (1/2)[f, g] + \cdots$, where now the brackets represent the Lie-Poisson bracket of vector fields as discussed above.

2.3 Numerical methods

Throughout the paper we ignore multistep numerical methods. This is due to the fact that the literature we try to survey has almost exclusively dealt with one-step integrators (see [30] however). Each one-step numerical method induces [92] a one-parameter family $\psi_{h,f}$ of maps in $\mathcal{R}^D$ in such a way that $\psi_{h,f}(\alpha)$ is the numerical solution after one step of length h starting from the initial condition α; for instance Euler's method has $\psi_{h,f}(y) = y + hf(y)$. For a numerical method to make sense it is necessary that $\psi_{h,f}$ approximates $\phi_{h,f}$ for small h; the order of the method is defined as the (highest) positive integer r such that $\psi_{h,f}(y) - \phi_{h,f}(y) = O(h^{r+1})$ as $h \to 0$ for each $y \in \mathcal{R}^D$ and each smooth f. A method is consistent if $r \geq 1$.

Given an IVP Equation 1.1 and a step-length $h > 0$, the numerical method obtains approximations y^n to the true solution values $y(t_n)$ corresponding to the gridpoints $t_n = nh$, $n = 0, 1, \ldots$. The numerical solution is recursively defined by $y^0 = \alpha$, $y^{n+1} = \psi_{h,f}(y^n)$, $n = 0, 1, \ldots$, (for the true solution $y(t_{n+1}) = \phi_{h,f}(y(t_n))$). For a method of order r, the global errors $y_n - y(t_n)$ are $O(h^r)$ uniformly in bounded time-intervals. The extension of these considerations to variable steplengths h_n is straightforward.

For Taylor, Runge-Kutta (RK) and multiderivative Runge-Kutta methods, the expansion of $\psi_{h,f}$ in powers of h is a B-series [11,46]

$$y + \sum_{n=1}^{\infty} h^n \sum_{\tau \in RT_n} \frac{1}{\sigma(\tau)} c(\tau) F(\tau)(y). \qquad (2.4)$$

Here RT_n denotes the set of rooted trees with n-vertices and, for each rooted tree τ, $\sigma(\tau)$ is the number of symmetries of τ, $F(\tau)(y)$ denotes the corresponding elementary differential evaluated at y and $c(\tau)$ is a real coefficient depending only on the numerical method. For an RK method with weights b_i and coefficients a_{ij}, the c's corresponding to the trees of orders one and two are $\sum_i b_i$, $\sum_{ij} b_i a_{ij}$. (The B-series Equation 2.4 has been normalized as in [11] or [72]; a different normalization is used in [46], cf. [12].)

The expansion Equation 2.4 is the key to writing the conditions for the corresponding method to have order r. Indeed the true solution has an expansion of the form Equation 2.4 with the coefficients $c(\tau)$ replaced by $1/\gamma(\tau)$, where $\gamma(\tau)$ is an integer called the density of τ. By imposing that the expansions of

the numerical method and the true solution coincide except for $O(h^{r+1})$, one concludes that a method is of order r if and only if

$$c(\tau) = \frac{1}{\gamma(\tau)}, \quad \tau \in RT_n, \quad n = 1, \ldots, r. \tag{2.5}$$

For an RK method these conditions read $\sum_i b_i = 1$, $\sum_{ij} b_i a_{ij} = 1/2$, etc.

For methods that partition the components of y and treat differently different components, including Partitioned Runge-Kutta (PRK) methods [92] and Runge-Kutta-Nyström (RKN) methods, B-series have to be generalized to P-series [46,72]. For methods based on decompositions of f into N parts, the relevant generalization is called NB-series [5].

3 New error analyses

In recent years it has become increasingly clear that there is a need for making sense of numerical results that have little or no accuracy in a conventional sense, i.e. whose global errors are large. As pointed out in the introduction, there are many instances where scientists have benefited from the use of numerical ODE solvers and yet it is impossible to get numerical results with small global errors. Similar situations have appeared before in numerical analysis and backward error analysis has been most useful. In a backward error analysis the question is not how big is the difference between the exact and computed solutions; one rather shows that the computed solution solves exactly a problem $\tilde{\mathcal{P}}$ that is a perturbation of the problem $\mathcal{P}$ one wants to solve and then tries to estimate the difference between $\tilde{\mathcal{P}}$ and $\mathcal{P}$. In our context, backward error analysis could show that the effect of using a numerical method is to change slightly the IVP being solved. Such a conclusion would be particularly useful in applications, as those mentioned in the introduction, where there is an inherent uncertaintity in the model, i.e. in the exact values of f and α.

Many recent papers in numerical ODEs have compared the numerical solution y^n of the IVP Equation 1.1 with the values $\tilde{y}(t_n)$ of the solution of a neighbouring IVP. One succeeds in obtaining bounds for $y^n - \tilde{y}(t_n)$ that are much smaller than those that can be derived for the conventional global error $y^n - y(t_n)$. While several of those papers use the terminology "backward error analysis", one is in fact dealing with a mixed forward/backward error analysis strategy; there is a backward component because a perturbed problem is introduced and there is a forward component because the numerical solution and the exact solution of the perturbed problem are not quite the same and one has to estimate their difference.

Since the IVP Equation 1.1 is specified by two items f and α, one may perturb it by changing either the vector field f or the initial condition α. The two possible perturbations respectively lead to the ideas of modified equations and shadowing.

An early important reference on the "backward" approach is Eirola [29].

3.1 Modified equations

For partial differential equations, the method of modified equations has been known for a long time as a valuable tool to investigate the behaviour of numerical solutions. A classical reference is [114] and a more rigorous approach may be seen in [42].

In our context, a modified system (of order N) $\dot{y} = \tilde{f}_N(y)$ for a method $\psi_{h,f}$ is a system for which $\psi_{h,f} - \phi_{h,\tilde{f}_N} = O(h^{N+1})$. For the solution flow of the system $\dot{y} = f(y)$ to which the method is being applied, $\psi_{h,f} - \phi_{h,f} = O(h^{r+1})$, with r the order of the method and therefore, if $r < N$, the flow of the modified system provides a better description of $\psi_{h,f}$ than the true flow does. In fact, if $\tilde{y}(t)$ denotes the solution of the modified system with initial condition α (see Equation 1.1), then the numerical solution satisfies $y^n - \tilde{y}(t_n) = O(h^N)$.

It is obvious that the modified vector field $\tilde{f}_N$ has to depend on the parameter h, but this dependence has not been incorporated to the notation. It is easy to construct, for any given N and method $\psi_{h,f}$, a modified vector field $\tilde{f}_N$ of order N. The easiest possibility is to look for $\tilde{f}_N(y)$ as a polynomial in h of degree N

$$\tilde{f}_N(y) = f^0(y) + hf^1(y) + \cdots + h^N f^N(y),$$

where the f^n do not depend on h. It is clear that a method is consistent if and only if f^0 coincides with the true f. In a similar manner, a consistent method is of order $r > 1$ if and only if $f^1, \ldots, f^{r-1}$ vanish. It is also easy to guess that the f^n do not change with the order of the approximation being sought. Then it is possible to construct a formal power series

$$f^0(y) + hf^1(y) + h^2 f^2(y) + \cdots \tag{3.1}$$

whose truncations coincide with the $\tilde{f}_N$'s.

When the method can be expanded in a B-series Equation 2.4, Hairer [43] shows that the f^n can be written of terms of the elementary differentials of f. Indeed Hairer shows that the formal power series Equation 3.1 is a B-series

$$\sum_{n=1}^{\infty} h^{n-1} \sum_{\tau \in RT_n} \frac{1}{\sigma(\tau)} b(\tau) F(\tau)(y). \tag{3.2}$$

and provides a systematic way to construct the coefficients $b(\tau)$ from the B-series coefficient $c(\tau)$ of the method Equation 2.4. An alternative derivation of Hairer's result was given in Murua's thesis [72] (see [15,90]). Note that the consistency of the method translates into the requirement that, for the tree with one vertex, $b(\tau) = 1$, and that, for consistent methods, order $r > 1$ is equivalent to $b(\tau) = 0$ for trees of orders $2, \ldots, r$. This provides an alternative to Equation 2.5 when writing the order conditions for the method.

Ideally one would like to have an "exact" modified system $\dot{y} = \tilde{f}(y)$, for which $\psi_{h,f} \equiv \phi_{h,\tilde{f}_\infty}$. For linear problems $\tilde{f}_\infty$ is easily constructed, see Beyn [8].

However for nonlinear situations, the solutions generated by the mapping $\psi_{h,f}$ may possess features that cannot be present in the solutions generated by flows of differential systems [87]. For instance, in two dimensions, a mapping ψ may generate chaotic orbits, while no solution flow is chaotic. For this reason it is impossible to exactly interpolate the numerical solution by a suitable ϕ_{h,f_∞}.

The problem of how close can a smooth invertible mapping $\psi_{h,f}$ be approximated by flows of differential equations is well known in dynamical systems [65]. We saw above that $O(h^{N+1})$ approximations are easily constructed for any N. Neishtadt [74] was the first in rigorously proving that an "optimal" h-dependent modified vector field $\tilde{f}$ for which the discrepancy between $\psi_{h,f}$ and $\phi_{h,\tilde{f}}$ is exponentially small (see also [28]). This optimal $\tilde{f}$ can be obtained by truncating the series Equation 3.1 (which in general diverges) after a suitably chosen number of terms that increases as $h \to 0$. Two recent papers [7,44] provide new proofs of the exponential smallness of the error with respect to the flow of the optimal modified vector field. These papers also present a number of valuable applications.

3.2 Shadowing

In shadowing, the computed solution y^n of the IVP Equation 1.1 is compared to the exact solution values $\bar{y}(t_n)$ of the IVP given by the differential equation being solved $\dot{y} = f(y)$ along with a perturbed initial condition $\bar{y}(0) = \tilde{\alpha}$. The idea of shadowing is well known in dynamical systems; its applications to numerical IVP in ODEs prior to 1993 are surveyed in the paper [93] and lack of space prevents us from repeating that material here. Recent references, not covered in [93], are [4,24–27,55,56,64,71,112].

4 Composition methods

Many of the methods used in geometric integration are *composition methods*, i.e. their associated mappings $\psi_{h,f}$ are a composition of simpler mappings.

- Sometimes one is given a method $\psi^{[B]}_{h,f}$ (the basic method) and constructs a new method

$$\psi_{h,f} = \psi^{[B]}_{b_s h,f} \circ \psi^{[B]}_{b_{s-1} h,f} \circ \cdots \circ \psi^{[B]}_{b_1 h,f}, \tag{4.1}$$

  where the b_i are suitable real constants chosen in such a way that $\psi_{h,f}$ is of higher order than $\psi^{[B]}_{h,f}$. In practice, the basic method has a favourable geometric property and low order. If the geometric property is preserved by composition, the new $\psi_{h,f}$ will share it.

- Often (see [5] for a discussion) the right-hand side function f can be written in a natural way as a sum of several, say two, contributions $f = f^{[1]} + f^{[2]}$, and one may construct an integrator $\psi_{h,f}$ by combining steps of a method $\chi_{h,f^{[1]}}$ for the system $\dot{y} = f^{[1]}(y)$ and steps of a method $\pi_{h,f^{[2]}}$ for the system $\dot{y} = f^{[2]}(y)$,

$$\psi_{h,f} = \pi_{b_s h,f^{[2]}} \circ \chi_{a_s h,f^{[1]}} \circ \cdots \circ \pi_{b_1 h,f^{[2]}} \circ \chi_{a_1 h,f^{[1]}}. \tag{4.2}$$

  An important particular case is that where the systems $\dot{y} = f^{[i]}(y)$ can be integrated in closed form and χ and π are taken to be the corresponding exact flows. Then the method reads

$$\psi_{h,f} = \phi_{b_s h,f^{[2]}} \circ \phi_{a_s h,f^{[1]}} \circ \cdots \circ \phi_{b_1 h,f^{[2]}} \circ \phi_{a_1 h,f^{[1]}}. \tag{4.3}$$

  These splitting integrators are of course well known; the different parts of f often correspond to physically different contributions, say different reactions in chemistry or different forces in mechanics.

When $\psi_{h,f}$ is a composition of simpler mappings, its properties may be investigated through the BCH formula Equation 2.3. The methodology is as follows.

- Construct modified systems $\tilde{f}_{N,i}$ of order N for the individual mappings being composed in Equation 4.1 or 4.2 (here the index i labels the mappings ψ_i being composed). Then (ignoring $O(h^{N+1})$ error terms), each ψ_i is the h-flow of the corresponding $\tilde{f}_{N,i}$.
- Write, by means of Equation 2.2, the flows of the $\tilde{f}_{N,i}$'s as exponentials.
- Use the BCH formula to combine all the exponentials into a single exponential $\exp(hL_{\tilde{f}_N})$; in doing so, care must be taken of the right order of the factors, see [92]. From the exponent $hL_{\tilde{f}_N}$, one recovers an (order N) modified system $\tilde{f}_N$ for the overall method. The properties of the method, including the order of consistency r, are then retrieved from $\tilde{f}_N$.

It can be shown [116] that, if in Equation 4.1 the basic method is of order two, then, for any prescribed r, it is possible to choose the number of stages s and the weights b_i so that the composition $\psi_{h,f}$ achieves order r.

Suzuki [103–111] was among the first in studying composition methods. Further useful references in connection with this approach are [41,60,68,69,81].

The discussion of composition methods will be continued later.

5 Symplectic integration

Symplectic methods for Hamiltonian problems have been the most studied family of geometric integrators. In the opening chapter of their 1987 collection of papers on Hamiltonian problems [66], MacKay and Meiss wrote: "Another neglected

problem is the development of computer algorithms which respect the symplectic nature of the Hamiltonian". That situation changed quickly. Only a few years later, the field of symplectic integration had grown large enough to deserve a section in the second edition of the treatise by Hairer, Nørsett and Wanner [46] and even a monograph [92].

5.1 Hamiltonian systems

Suppose that the dimension D of Equation 1.1 is even $D = 2d$ and write $y = (p, q)$ with $p, q \in \mathcal{R}^d$. Then the system in Equation 1.1 is a Hamiltonian problem [6,66] if and only if f is of the form

$$f(y) = J^{-1}\nabla H \tag{5.1}$$

for a suitable real-valued function $H = H(p, q)$ (the Hamiltonian function). In Equation 5.1 ∇ is the operator

$$\left(\frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2}, \ldots, \frac{\partial}{\partial p_d}, \frac{\partial}{\partial q_1}, \frac{\partial}{\partial q_2}, \ldots, \frac{\partial}{\partial q_d}\right)^T,$$

and J is the skewsymmetric matrix

$$J = \begin{bmatrix} 0_d & I_d \\ -I_d & 0_d \end{bmatrix}. \tag{5.2}$$

The quantity H is conserved along the solutions of the corresponding Hamiltonian system [92]. This often corresponds to the principle of conservation of energy.

If the vector fields f and g in $\mathcal{R}^{2d}$ are both Hamiltonian, i.e. $f = J^{-1}\nabla H$ and $g = J^{-1}\nabla G$, then the Lie-Poisson bracket $[f, g]$ is also a Hamiltonian vector field. The corresponding Hamiltonian function is given by $-\{H, G\}$ (note the sign!), where [6,92]

$$\{H, G\} = \sum_i \frac{\partial H}{\partial q_i}\frac{\partial G}{\partial p_i} - \frac{\partial H}{\partial p_i}\frac{\partial G}{\partial q_i}$$

is the Poisson bracket of Hamiltonian functions. There is a correspondence between fields+Lie-Poisson bracket, Lie operators+commutator and Hamiltonian functions+*negative* Poisson bracket. The reader should be warned that there is no agreement in the literature: sometimes, to avoid the *negative* Poisson bracket in the correspondence above, things are defined with signs that disagree with our choice here. For instance, Arnold [6] reverses the signs of our $[f, g]$ and $[L_f, L_g]$. In [92] commutators and Poisson brackets are defined as in the present paper but the sign of L_f is reversed.

Hamiltonian systems appear very frequently in the applications; virtually all phenomena where dissipation is absent or can be ignored may be modelled by a Hamiltonian system. In particular, Hamiltonian systems play a key role in classical, statistical and quantum mechanics, in optics and in plasma physics.

The property of $\dot{y} = f(y)$ being Hamiltonian, which refers to the vector field of the system differential equations, can be translated into a corresponding property of the flow $\phi_{t,f}$. In fact a system in $\mathcal{R}^{2d}$ is Hamiltonian if and only if its flow is, for each t, a *symplectic* transformation. By definition, a transformation Ψ in $\mathcal{R}^{2d}$ is symplectic if its Jacobian matrix $\Psi'(y)$ satisfies [92]

$$\Psi'^T(y) J \Psi'(y) \equiv J,$$

where J is the matrix Equation 5.2. An equivalent definition in terms of differential forms exists [6]. Differential forms lead to manipulations that are easier than those required when using Jacobians. More importantly, differential forms provide a geometric interpretation of symplecticness in terms of conservation of areas.

Hamiltonian systems possess many features not shared by other systems of differential equations. Many properties that "general" systems possess only under exceptional circumstances appear generically in Hamiltonian systems. All these features and properties can be traced back to the symplecticness of Hamiltonian flows.

5.2 What is a symplectic integrator?

The failure of virtually all well-known methods in mimicking Hamiltonian dynamics suggested the consideration of schemes such that the mapping $\psi_{h,f}$ is symplectic whenever the field f is Hamiltonian. Such methods are called *symplectic* or *canonical*. Early references on symplectic integration are Ruth [83], Channel [22], Menyuk [70], Feng [31-33], even though the idea of symplectic integration apparently goes back to DeVogelaere in 1956 (cf. [23]).

Since a flow is symplectic if and only if the corresponding vector field is Hamiltonian, it is not difficult to see that a method is symplectic if and only if the corresponding formal modified vector field Equation 3.1 is Hamiltonian, or equivalently all the $\tilde{f}_N$ are Hamiltonian. Therefore, ignoring the $O(h^{N+1})$ remainder term, a symplectic discretization of a Hamiltonian problem changes the Hamiltonian system being solved into a nearby Hamiltonian problem. The discretization provided by a nonsymplectic method changes the Hamiltonian system into a nearby non-Hamiltonian perturbation. Thus for a symplectic method, the Hamiltonian vector field Equation 3.1, has an associated Hamiltonian function that we denote by

$$H^0(y) + hH^1(y) + h^2H^2(y) + \cdots. \tag{5.3}$$

As discussed above the properties of a method are encapsulated in the vector series Equation 3.1. In the Hamiltonian context we can rather use the simpler, scalar series Equation 5.3. More details will be given later.

For extensions of the idea of symplectic integration, including constrained systems, partial differential equations and nonstandard symplectic structures, see [37,38,58,59,67,89,92].

5.3 Families of symplectic integrators

There have been three main approaches to the construction of symplectic integrators.

5.3.1 Symplectic methods based on generating functions

Symplectic transformations can also be characterized in terms of so-called generating functions [6,92] and the early papers on symplectic integration resorted to this characterization. Most of the resulting methods were too involved for practical use. Those generating function methods that are practical are best analyzed as members of the classes of symplectic composition methods or symplectic Runge-Kutta methods. For instance, Ruth first derived his methods [83] through the generating function formalism, but later reinterpreted them as composition methods [36]. For these reasons this methodology will not be discussed further here and the interested reader is referred to [92].

5.3.2 Symplectic methods using compositions

Assume that the individual mappings being composed in Equation 4.1–4.3 are symplectic. This will automatically be the case for splitting methods Equation 4.3 if the parts $f^{[i]}$ are Hamiltonian. (Note that splitting f into *Hamiltonian* parts $f^{[1]} + f^{[2]}$ corresponds to splitting the Hamiltonian function H in *arbitrary* pieces $H = H^{[1]} + H^{[2]}$.) Under this assumption of symplecticness of the parts being composed, the resulting overall method $\psi_{h,f}$ will also be symplectic.

The methodology presented in Section 4 to analyze $\psi_{h,f}$ is particularly suitable in the symplectic case, because rather than working with vector fields and their Lie-Poisson brackets one works with Hamiltonian functions and their Poisson brackets, see [35,92,94].

Perhaps separable Hamiltonians

$$H = T(p) + V(q) \tag{5.4}$$

have provided the most common application of the composition approach. These Hamiltonians appear often in practice with T and V respectively giving the kinetic and potential energies. After the splitting $H = H^{[1]} + H^{[2]}$, $H^{[1]} = T(p)$, $H^{[2]} = V(q)$, the individual pieces are integrable in closed form; the solution flow of for $T(p)$ is $(p^0, q^0) \to (p^0, q^0 + t\nabla T(p^0))$ (sometimes referred to as a "drift") and the solution flow of for $V(q)$ is $(p^0, q^0) \to (p^0 - t\nabla V(q^0), q^0)$ (sometimes referred to as a "kick"). Then a step of the method Equation 4.3 is given by

$$Q_i = Q_{i-1} + a_i h \nabla T(P_i), \quad P_{i+1} = P_i - b_i h \nabla V(Q_i), \quad i = 1, \ldots, s, \tag{5.5}$$

where (P_1, Q_0) (respectively (Q_s, P_{s+1})) is the numerical solution at the beginning (respectively the end) of the step.

It is also possible [63] to modify the kicks by modifying the force $-\nabla V$ with a term involving the Hessian matrix of V. A pioneering paper is due to Rowlands [82]. Rowlands method is very efficient and achieves fourth order by a change of variables. The idea of changing variables to increase the order goes back to Butcher, see the discussion in [61-63].

Splittings of the Hamiltonian also arise when using multiple time-steps [9], so that different forces are sampled at different rates.

5.3.3 Symplectic Runge-Kutta methods

The standard class of implicit RK methods happens to contain symplectic integrators. This was shown independently by Lasagni [57], Sanz-Serna [86] and Suris [99]. For a method with coefficients (a_{ij}) and weights (b_i) the condition

$$\forall i, j, \quad b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \tag{5.6}$$

guarantees symplecticness. The Gauss methods (order $2s$ with s stages) are symplectic. There are also diagonally implicit, symplectic methods; with s stages they include s free parameters. These diagonally implicit methods are compositions of the midpoint rule (the lowest order Gauss method) and can be analyzed via the BCH formula. Other references on the construction of methods satisfying Equation 5.6 are [48,49,85].

The condition Equation 5.6 is also essentially necessary for symplecticness [92]. The first proof of the necessity of Equation 5.6 was given by Lasagni in an unpublished manuscript and is very delicate; a similar proof was published in [1].

A more modern approach to the symplecticness condition Equation 5.6 is via B-series [19]. First, a necessary and sufficient condition is derived on the coefficients $c(\tau)$ of a B-series Equation 2.4 for this series to define a symplectic transformation whenever the underlying vector field is Hamiltonian. In a second stage, the B-series coefficients are expressed in terms of the tableau elements (a_{ij}) and (b_i) and the symplecticness condition for the $c(\tau)$'s is shown to be equivalent to Equation 5.6. The proof of the necessity of Equation 5.6 via B-series is easier and more powerful than the original Lasagni proof. Furthermore the B-series technique is also more general, because it allows to deal with methods, other than RK methods, expressible as B-series. Hairer, Murua and Sanz-Serna, building on the B-series characterization of symplecticness, showed that there are not any nontrivial examples of symplectic multiderivative RK methods [45].

Another important contribution based on B-series is due to Hairer [43]. For Hamiltonian f, Hairer investigates the modified vector field Equation 3.2 and writes a necessary and sufficient condition on the coefficients $b(\tau)$ for this series to be symplectic, i.e. for the underlying method to be symplectic. He then shows that, when the $b(\tau)$'s are written as functions of the method coefficients $c(\tau)$ Equation 2.4, his symplecticness condition on the $b(\tau)$'s becomes the Calvo and Sanz-Serna [19] symplecticness condition on the $c(\tau)$'s. Furthermore when

Equation 3.2 is symplectic, Hairer gives an explicit formula for the modified Hamiltonian Equation 5.3. This is of the form

$$\sum_{n=1}^{\infty} h^{n-1} \sum_{\omega \in T_n^*} \frac{1}{\sigma(\omega)} d(\omega) H(\omega)(y), \tag{5.7}$$

where the meaning all the various symbols will be discussed presently. The inner summation extends to all *trees* with n-vertices, while in conventional B-series Equation 2.4, Equation 3.2 one deals with *rooted* trees. A rooted tree is a tree in which a vertex has been highlighted to play the role of the root; conversely a tree can be seen as an equivalence class of rooted tree obtained by grouping all rooted trees that only differ in the location of the root. Thus Equation 5.7 has *fewer* terms than Equation 3.2. The star in T_n^* means that not all trees are present in the summation: so-called superfluous trees [91] are not to be included. For each tree ω, $\sigma(\omega)$ represents the number of symmetries and $H(\omega)(y)$ is the corresponding elementary Hamiltonian, a real-valued function of y obtained by combining H and its partial derivatives. Elementary Hamiltonians were first introduced in [91] with the name canonical elementary differentials. Finally $d(\omega)$ is a real coefficient that can be computed in terms of the coefficients $b(\tau)$ in Equation 3.2. Murua [72] calls expressions like Equation 5.7 H-series and shows how to manipulate them.

It was first proved in [91] (see also [84]) that, for an RK method, the symplecticness condition Equation 5.6 acts as a simplifying assumption, i.e. when Equation 5.6 holds not all the order conditions Equation 2.5 are independent. Indeed when Equation 5.6 holds, to achieve order r it is enough to impose $c(\tau) = 1/\gamma(\tau)$ for *one* rooted tree τ in each nonsuperfluous tree of order $\leq r$. This is a consequence of two facts:

1. order r can be imposed by demanding that Equation 5.7 agrees with the true Hamiltonian H except for a remainder of order $O(h^r)$ and
2. in Equation 5.7 there is a term for each nonsuperfluous tree.

(In [91] generating functions were used instead of the modified Hamiltonians, but the argument is essentially the same.)

We finally discuss other classes of Runge-Kutta-like methods that contain symplectic integrators.

- Partitioned Runge-Kutta (PRK) methods for separable Hamiltonian systems Equation 5.4. These are Runge-Kutta methods with two tableaux; one is used for the p variables and the other for the q variables. A symplecticness condition analogous to Equation 5.6 was first presented by Sanz-Serna at the 1989 London ODE meeting [88], and discovered independently by Suris [101]. The order conditions were studied in [1]. This class of methods is useful because it contains *explicit* schemes that are symplectic. These turn out to be [77] of the form Equation 5.5 and may therefore be studied through the BCH formula, see [14]. Specific methods are constructed in [1,20,77,88].
- Runge-Kutta-Nyström (RKN) methods for Hamiltonian problems of the form $\dot{p} = -\partial V/\partial q$, $\partial q = M^{-1}p$, where $V = V(q)$ is the potential and M the mass matrix. The corresponding symplecticness conditions were first derived by Suris [99,100]. For the order conditions see [16]. Specific methods are constructed in [17,18,77,78]. See also [76].
- Partitioned Runge-Kutta methods for general (not necessarily separable) Hamiltonians. This family is methodologically useful because it includes the families of RK methods, PRK methods for separable Hamiltonians and RKN methods. It is the class considered in important recent theoretical papers such as [43]. Interesting references are [51,73].
- Additive Runge-Kutta methods [5]. This class applies to splittings of the Hamiltonian functions and contains all the others as particular cases.

5.4 Properties of symplectic integrators

Hamiltonian flows exactly preserve the symplectic structure *and* the value of the Hamiltonian function (energy). It was proved by Ge and Marsden [40] that it is in general impossible for a symplectic integrator to exactly preserve energy. However in practice symplectic integrators do a very good job of preserving the value of the energy. This conservation is linked to the existence of a modified Hamiltonian function, as first noted by Lasagni in a set of unpublished notes mentioned in [57]. See also [7,44,65] and the discussion in [92].

Sometimes symplectic integrators have more favourable error-growth properties than their general counterparts. See [13,18,21,39]. It is interesting that those favourable properties are not shared [80] by schemes obtained by fitting the classical stability region of the method; this shows that we are dealing with methods that cannot be analyzed or obtained within the classical paradigm.

Unfortunately the advantages of symplecticness cannot be combined with variable stepsizes [17]. This is due to fact that with variable stepsizes the backward error interpretation breaks down, see [17,92].

6 Reversible integration

In this section the presentation emphasizes the analogies with symplectic integration.

6.1 Reversible systems

Let ρ be a linear involution, i.e., a linear mapping in $\mathcal{R}^D$ such that $\rho^2 = Id$. An example often found in mechanics has $y = (p, q)$ and $\rho(p, q) = (-p, q)$, where p is the collective vector of velocities of the system being studied and

q the corresponding collective vector of positions or coordinates. A system of differential equations $\dot{y} = f(y)$ is ρ-reversible if

$$f(\rho y) \equiv -\rho f(y).$$

This property, that operates at the vector field level, is equivalent to the requirement that the corresponding flow $\phi_{t,f}$ be, for each t, a ρ-reversible mapping. By definition, a mapping Ψ in $\mathcal{R}^D$ is ρ-reversible if

$$\rho^{-1} \circ \Psi \circ \rho = \Psi^{-1}. \tag{6.1}$$

Thus a mapping Ψ is ρ-reversible if it is transformed in its inverse Ψ^{-1} by the change of variables $y \to \rho y$. In the particular case of a flow, the reversibility condition becomes

$$\rho^{-1} \circ \phi_{t,f} \circ \rho = \phi_{t,f}^{-1} = \phi_{-t,f};$$

for a reversible system changing variables $y \to \rho y$ just reverses the sense of the arrow of time.

6.2 What is a reversible integrator

Methods for which $\psi_{h,f}$ is a ρ-reversible mapping for each h and each ρ-reversible vector field are called ρ-reversible. D. Stoffer has been one of the leading contributors to the area of reversible integration, starting with his thesis [96].

6.3 Families of reversible integrators

6.3.1 Reversible composition methods

By using Equation 6.1 it is easy to derive sufficient conditions for a composition method to be reversible. For instance a symmetric composition of reversible mapp $\Psi^{[1]}\Psi^{[2]}\Psi^{[1]}$ is reversible.

6.3.2 Reversible Runge-Kutta methods

For RK, PRK, RKN and other standard families of numerical methods, ρ-reversibility turns out to be equivalent to time-reversibility, i.e. to the requirement

$$\psi_{-h,f} = (\psi_{h,f})^{-1}. \tag{6.2}$$

This is because such methods are equivariant with respect to linear changes of variables

$$\rho^{-1} \circ \psi_{h,f} \circ \rho = \psi_{h,\rho f}$$

(changing variables by ρ in the computed solution is the same as applying the method to the differential equation resulting from changing variables).

Note that Equation 6.2 is independent of ρ. Time-reversible (also called selfadjoint [92]) methods were of course well known before the introduction of the notion reversible integration. Therefore there has been no need to study the classes of ρ-reversible RK, PRK and RKN method, as distinct from the situation for symplectic RK, PRK and RKN methods.

6.4 Properties of reversible integrators

Reversible integrators share many of the favourable properties of symplectic methods [13,21], with the advantage that they retain those properties even when applied with variable stepsizes, provided that the stepsize selection is carried out so as to preserve reversibility [47,97].

7 Volume preserving flows

A divergence-free $\nabla \cdot f = 0$ vector field gives rise to a volume-preserving flow $\phi_{t,f}$, i.e., to a flow whose Jacobian determinant is $\equiv 1$, leading to the property that, for any domain Ω in phase-space, Ω and $\phi_{t,f}(\Omega)$ possess the same volume. Volume-preserving integration has received some attention [34,65,75,98], but not nearly as much as symplectic or reversible integration.

8 Epilogue

We shall finish as we started: quoting Lambert. In his (1973) textbook [53], he writes: "Remarkably little is required by way of prerequisites for the study of computational methods for ordinary differential equations." In fact in the black-box subroutine mode of operation, the numerical analyst was screened from the specific structure of the problem being solved, from its mathematical singularities and from the application fields. Things have now changed and it is our feeling that they will change even more in the future. Contributors to *numerical* ordinary differential equations will need to be familiar with relevant developments in the *theory* of differential equations. Furthermore, many important developments are likely to arise when considering specific problems from the different application fields and therefore some degree of interdisciplinary work will be essential.

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