SURVEY ON SYMPLECTIC INTEGRATORS

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1. Introduction

Non-dissipative phenomena in classical physics, chemistry and other sciences are often modeled by hamiltonian systems of differential equations. The name *symplectic integrator* is usually attached to a numerical scheme that intends to solve such a hamiltonian system approximately, while preserving its underlying symplectic structure. It is a guiding principle defended by some that "an algorithm which transforms properly with respect to a class of transformations is more basic than one that does not. In a sense the invariant algorithm attacks the problem and not the particular representation used." (from [20]).

It is the objective of this paper to present a brief survey of the theory and performance of symplectic integrators. In Section 2 we introduce symplectic integrators, and consider an important class of examples. In Section 3 we study some qualitative properties of symplectic methods, focusing on their relation to conservation of energy and the backward error interpretation. Finally, in Section 4 we present a summary of the performance exhibited by these methods in a variety of numerical experiments. But, before we plunge into the subject of symplectic integrators per se, it seems worthwhile to describe at least one problem that requires efficient numerical solving techniques.

The stability problem of celestial mechanics refers to the question of determining whether our planetary system will keep the same general form in the (distant) future as it has now, or whether some planets might leave the system or collide with another one, in such a way that radical changes would ensue. This famous question has moved the subject since the times of Laplace, Lagrange and Poisson, and it can be described mathematically in terms of the so called n-body problem: n mass points which move in three dimensional space according to Newton's laws. Inspired by the case in point, one also assumes, usually, that n-1 of the mass points are much smaller that the remaining one (playing the Sun's rôle), and then we are interested in the behavior

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of the system for all time. While the beautiful result of Kolmogorov, Arnold and Moser on perturbation of completely integrable systems threw new light on the subject, showing that stability is possible at least in principle, recent numerical integration of the movement of the outer planets (from Jupiter outward) seems to imply that this is not the case(see [21], [37], [40] and references therein, as well as [3], [28], [29]). Here symplectic integration, alongside more established and perhaps more trusted methods, has played an important role, and recently there have been some claims as to a theoretical reason explaining and confirming these numerical experiments (see [21]).

2. Symplectic Integrators

Let Ω be a domain in $\mathbb{R}^{2d}$, endowed with the canonical symplectic structure $\omega = \sum dq_i \wedge dp_i$. A smooth function $H \in C^\infty(\Omega)$ gives rise to the hamiltonian system of ODE's

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \quad i = 1, \ldots, d. \tag{1}$$

In physics, Ω usually corresponds to phase space, and H to a hamiltonian for the system.

Let $h > 0$ be fixed. A (single-step) numerical scheme to solve such a system consists of a function $\psi_{h,H} : \Omega \to \Omega$ depending smoothly on the step-size h and the hamiltonian H. Given an initial condition (p_0, q_0), the approximate solution at time nh defined as (q_n, p_n) can be computed iteratively by

$$(q_{n+1}, p_{n+1}) = \psi_{h,H}(q_n, p_n)$$

It is important to remark that this definition is a temporary simplification, and that frequently the function $\psi_{h,H}$ cannot be defined on the whole domain Ω. Implicit integrators are examples of this phenomenon, as we will see shortly, but this map still makes sense locally, much in the same way as flows of vector fields on a manifold.

Now let ϕ_t be the flow of (1). The method $\psi_{h,H}$ is said to be of order $r \in \mathbb{N}$ if, as $h \to 0$,

$$\|\phi_h(x) - \psi_{h,H}(x)\| = O(h^{r+1}), \quad x \in \Omega$$

At least heuristically, the source of the idea of order is that, to approximate $\phi_t(x)$ by dividing $[0, t]$ into N parts and iterating $\psi_{h,H}$ with a step-size $h = t/N$ we would perform $O(h^{-1})$ computations, so as to expect that

$$\|\phi_t(x) - \psi_{h,H}^N(x)\| = O(h^{r+1}) \cdot O(h^{-1}) = O(h^r)$$

Definition 1. *A map $\psi_{h,H}$ is called a symplectic integrator if it preserves the symplectic form, i.e. $\psi_{h,H}^{*}\omega = \omega$.*

Historically, symplectic integrators appeared for the first time in the pioneering work of de Vogelaere in the 50's [39], and in the 80's Ruth [30], Channell [8], Menyuk [27], and Feng [12, 13, 14] introduced methods arising from Hamilton-Jacobi Theory. We start, however, with the serendipitous independent discovery by Lasagni [23], Sanz-Serna [31] and Suris [36] that some implicit Runge-Kutta methods are symplectic for an appropriate choice of parameters.

In brief, for s a positive integer, an s-stage (implicit) Runge-Kutta method for the ODE

$$y' = f(t,y), \quad y(0) = y_0 \quad t \geq 0 \tag{2}$$

starts with a choice of a tableau

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{ss} \\ \vdots & \vdots & \vdots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

and setting

$$y_{n+1} = y_n + h\sum_{j=1}^{s} b_j f(t_n + c_j h, \xi_j)$$

where

$$c_j \geq 0, \quad \sum_{j=1}^{s} c_j = 1$$

$$\sum_{i=1}^{s} a_{ji} = c_j, \quad j = 1, \ldots, s$$

$$\sum_{j} b_j = 1$$

$$t_n = nh$$

and where the ξ_j's are given implicitly by

$$\xi_j = y_n + h\sum_{i=1}^{s} a_{ji} f(t_n + c_j h, \xi_i)$$

Remark 1. *The fact that the ξ_j's are given implicitly implies that to find them uniquely (with some other numerical scheme, e.g. Newton's*

method), one needs some conditions on f and h. For example, the inverse function theorem is often the theoretical result behind such uniqueness, and one requires f to be smooth, appropriately non-singular, and h to be small. In fact, generally $\psi_{h,H}$ can be defined only for small h, depending on the starting point. This implies that frequently there is no uniform choice of h, and $\psi_{h,H}$ cannot be defined on all of Ω. (For less strict conditions, see [19]*).*

It is clear that there is great freedom in the choice of parameters in the Runge-Kutta (abbreviated RK) method. This means that much of the art of RK methods rests on the ability to choose the remaining parameters wisely. First and foremost, one should make sure that such a method is convergent, i.e. that as the step-size shrinks to zero one actually recovers the exact solution. This is crucial, and realizable while still leaving free choices for the parameters, but we choose to refer the reader to [19] for the details. Secondly, one searches for the best possible combination of accuracy and speed, which involves choices of step-size, and order for the method. Regarding order, it is possible to show that for an s-stage RK method an appropriate choice of tableau gives rise to a $2s$-order method, so that there are RK methods of arbitrarily high order available. (for more details see [19] and [16])

Now let $M = (m_{ij})_{i,j=1}^{s}$ be the real $s \times s$ matrix given by

$$m_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j$$

for $i, j = 1, \ldots, s$. The matrix M comes up frequently in the study of RK schemes and nonlinear stability (see [11]) and moreover Lasagni, Sanz-Serna and Suris showed that

Theorem 2.1. *If $M = 0$, then the corresponding implicit Runge-Kutta method is symplectic.*

Remark 2. *According to Sanz-Serna* [33]*, Lasagni has shown that, for RK methods without redundant stages (that is, when the stages cannot be sub-partitioned into equivalent ones), this condition is actually necessary for the method to be symplectic. I could not find a (direct) proof for this result in the literature, however Abia and Sanz-Serna in* [1] *prove the analogous result for Partitioned Runge-Kutta methods.*

Of course, the next issue is whether there are symplectic Runge-Kutta methods of arbitrarily high order (having a very high order is not necessarily useful in applications, due to increase in computations per step, error propagation and so on, but it is desirable that these be available). In fact, the classical s-stage Gauss-Legendre Runge-Kutta methods are of $2s$-order, and moreover

Theorem 2.2. *The Gauss-Legendre Runge-Kutta methods are symplectic.*

We direct the reader to [19] for the tableaux corresponding to the Gauss-Legendre methods. Given these, the verification that $M = 0$ is immediate. For example, the 2-stage Gauss- Legendre method has tableau

$$\begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & 0.5 & 0.5 \end{array}$$

and it is clear that $M = 0$ by inspection.

Modifications of the idea of looking for symplectic integrators among already established algorithms have been of course carried much further. As an example, in many practical situations (e.g. the integration of the movement of the outer planets), one has a separable hamiltonian

$$H(q, p) = T(p) + V(q)$$

and the system (1) decouples into two simpler ones, suggesting the use of different schemes for each variable. RK methods of this type are called Partitioned Runge-Kutta schemes (abbreviated PRK), and one can still show that there are symplectic PRK algorithms ([33]). Moreover, in this very special case one can choose the two components of the PRK method to be explicit (which is not possible in the general case), and thus makes the overall method more straightforward.

Other methods exist in the Runge-Kutta class. There are for instance Runge-Kutta-Nyström, and combinations of all of the above employing the so-called Yoshida trick ([43]), which one could perhaps describe as a clever application of the Baker-Campbell-Hausdorff formula to the Lie algebra of symplectic vector fields. We will take on this subject in a later section.

Finally, it is important to remark that there exists a very different class of symplectic integrators that comes from the theory of generating functions and the Hamilton-Jacobi equation, and these have found their way to important applications. However, we will not be able to look into this subject, for the sake of briefness.

3. Properties of Symplectic Integrators

3.1. **Conservation of Energy.** Perhaps following the guiding principle of looking for algorithms that preserve the structure inherent to a

problem, it is reasonable to inquire whether it is possible to augment further a symplectic algorithm so that it also preserves the energy (i.e. the hamiltonian) of the underlying system. As an example of a situation where this is possible, Sanz-Serna proved

Theorem 3.1. [31] *A symplectic Runge-Kutta method leaves all quadratic first integrals of a hamiltonian system invariant, i.e. if* $y_n = (q_n, p_n)$ *and* $G = G^t \in M_{2d}(\mathbb{R})$*, then* $y_{n+1}^t\, G\, y_{n+1} = y_n^t\, G\, y_n$ *for all* n*.*

In particular, if a linear autonomous system is integrated with a symplectic RK method, than the energy will be conserved exactly (up to truncation errors, of course).

This setting, however, is very restricted. Indeed, Z. Ge[1] and J. Marsden proved

Theorem 3.2 (Ge and Marsden[15])**.** *Let* $K \subseteq C^\infty(\Omega)$ *be a Poisson sub-algebra and assume that* $\forall F \in K$*,* $\{F, H\} = 0 \Rightarrow F(z) = F_0(H(z))$ *for some smooth function* F_0 *and let* ψ_h *be a smooth symplectic method defined for small* $h > 0$ *from a generating function in* K*. If* ψ_h *conserves* H *exactly, then it is the time advance map for the hamiltonian up to a reparametrization of time.*

Remark 3. *The assumption that* $\psi_{h,H}$ *comes from a generating function is not restrictive. Locally every symplectomorphism arises from such a function, and in that case the theorem has to be modified accordingly.*

The requirement on this theorem, that there be no first integrals of the given hamiltonian system independent of H in K, might seem very strong at first sight. However, given a symplectic manifold M, it is known that, under certain conditions, the set $R(M)$ of all hamiltonian systems of M that have *no* first integrals independent of the energy is rather large. For example, L. Markus and K. Meyer [24] have shown that when M is compact and 4-dimensional, $R(M)$ is actually generic (in the sense of Baire category) in the set of all C^∞ hamiltonian systems.

Of course, the strong negative result of Ge and Marsden can be turned into a tool, in at least three different ways: 1) by enlisting the energy variation with respect to the real solution as a measure of the deviation from it, 2) as an active way of "projecting" the symplectic solution to the appropriate energy level and so try to increase accuracy (which can cause difficulties with convergence and order estimates), or 3) adding the additional conserved quantities as constraints

[1] while Zhong Ge appears with this name in [15], in the literature and in Mathscinet he is also listed as G. Zhong.

via Lagrange multipliers, and other *ad hoc* techniques (see for example [4, 18, 19]).

Remark 4. *The numerical analysis community has devoted a great deal of attention to energy conserving methods, which are sometimes applicable even to non-hamiltonian situations. The Ge-Marsden Theorem points to a very important question, then: given a specific hamiltonian system, should one use symplectic or energy conserving methods to integrate it? Energy conservation guarantees, a priori, only that the approximate solution is restricted to a codimension 1 submanifold of* Ω*. When this dimension is big there is no reason to expect that this information is very helpful. Nevertheless, energy conserving methods have been available for a longer time, and hence have gone through considerable enhancement. On the other hand, symplectic integrators take into account the symplectic form, and hence to a certain extent a more global and multi-dimensional behavior. Moreover, numerical experiments have shown that symplectic integrators have exhibited a bounded energy error. In practice, since many problems are worth their own tailored solutions, general judgments on efficiency cannot be expected.*

3.2. **Backward Error Interpretation.** The concept of backward error interpretation comes from numerical linear algebra, and it refers to the ability of reinterpreting the numerical solution of a problem in a certain class as the exact solution of a perturbation of the original problem, without leaving that class [17].

In our present context, this helps to explain the experimental observation that the energy deviation of the numerical solution of a hamiltonian system by a symplectic method remained bounded for long-time integrations (for a very interesting example of this fact, see [37]).

Before we consider this phenomenon more closely, recall that if G if a Lie group and $\mathfrak{g}$ is its Lie algebra,

Theorem 3.3 (Baker-Campbell-Hausdorff Formula)**.** *There is a neighborhood* $\mathcal{U}$ *of* 0 *in* $\mathfrak{g}$ *and an analytic map* $\theta : \mathcal{U} \times \mathcal{U} \to \mathfrak{g}$ *such that for all* $X, Y \in \mathcal{U}$*,*

$$\exp(X) \cdot \exp(Y) = \exp(\theta(X, Y))$$

For a proof, and more details, the reader is directed to [38]. One can compute the first terms of $\theta(X, Y)$ to find

$$\theta(X, Y) = X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}([X, [X, Y]] + [Y, [Y, X]]) + \dots$$

Returning to hamiltonian systems, we have observed before that often in practical situations the hamiltonian is H separable, that is to

say, $H(p,q) = T(p) + V(q)$, and one can integrate each variable with different methods (namely, integrating first the hamiltonian equations for T with an RK method, and then doing the same for V, which can be done even exactly if these are especially simple). In terms of the hamiltonian vector fields $X = X_T$ and $Y = X_V$ (i.e. $\imath_X\omega = dT$ and $\imath_Y\omega = dV$, following Yoshida [44] we can express this as

$$\psi_{h,H} = \exp(hX) \cdot \exp(hY)$$

So that, by the BCH formula,

$$\psi_{h,H} = \exp(\theta(hX, hY))$$

for h small enough. Of course this argument is formal, since here the underlying 'Lie group' is the group of symplectomorphisms of the manifold, and one cannot expect that $\theta(X,Y)$ corresponds to a hamiltonian vector field. To have

$$\psi_{h,H} = \exp(hH^h_\infty)$$

it is necessary that

$$H^h_\infty(p,q) = T(p)+V(q)-\frac{h}{2}\{T,V\}+\frac{h^2}{12}(\{T,\{T,V\}\}+\{V,\{V,T\}\})+\dots$$

converges in some sense. Side-stepping this issue, however, we can clearly define for $r > 0$ the r-order truncation H^h_r by

$$H^h_\infty = H^h_r + O(h^{r+1})$$

and so we have that, for a fixed amount of time, up to an arbitrary order the given symplectic integrator preserves a perturbed hamiltonian. When the sum is convergent, the perturbed hamiltonian is preserved for all times.

It is interesting to observe that this hints at a potential problem for variable step-size symplectic integrators, for in this case one cannot expect to conserve a certain approximate hamiltonian (different h's and vector fields at each step prevent a profitable use of the BCH formula). In fact, experiments show ([6]) that an implementation of a symplectic method with variable step-sizes seems to destroy the advantages of symplectic integrators with respect to more classical ones. We refer the reader to [5, 6] for more information on this topic.

In the case when H^h_∞ can actually be defined, one can understand mathematically the bounded oscillatory behavior of the energy in experiments with symplectic integrators. The powerful theory of Kolmogorov-Arnold-Moser on perturbations of completely integrable systems states that for a small perturbation of such a system the majority of orbits will be quasi-periodic (in the sense that the set of unstable orbits has small measure in phase space. See [3] for more details on KAM

theory). For the n-body problem, this accounts for the quasi-periodic behavior of the energy error in symplectic integrations.

Remark 5. *By judiciously applying the BCH formula one can obtain methods of arbitrarily high order. Indeed, if H is a separable hamiltonian $H = T + V$ as before, with X, Y the hamiltonian vector fields corresponding to T, V respectively, then*

$$\exp(tX + tY) = \exp(tX/2)\exp(tY)\exp(tX/2) + O(t^3)$$

which is a second order symplectic integrator. One can proceed further, by good choices of partitions of the interval, to attain higher orders (see Yoshida in [43]*).*

4. Experimental Performance

In numerical analysis, actual speed and accuracy of computations provide the real measure of success of a method. Symplectic methods are usually implicit (even though for certain special hamiltonians explicit schemes do exist [33]), and, moreover, at least heuristically one would expect that the extra 'symplectic requirements' (for example $M = 0$ for symplectic Runge-Kutta) might render these less advantageous for short time computations. This is actually the case, and any advantages should be sought for in long-time integrations, where the built-in symplectic feature might for example have a favorable error-propagation behavior.

As we have mentioned in the introduction, one of the most interesting sources of numerical experiments employing symplectic integrators has been astrophysics. In particular, Holman, Sussman, Wisdom and others ([21, 37, 42]) have performed long time integrations in order to study the chaotic behavior of the outer planets. They have built on important previous work (see references in [37]), for example the 1-million-year integration of Cohen, Hubbard and Oesterwinter [10], the 5-million-year integration of Kinoshita and Nakai [22], and the 210-million-year integration performed on the Digital Orrery [2] to name just a few. In [41], for example, a symplectic method is introduced to tackle the movement of the outer planets for 1 billion years, and Wisdom and Holman were led to the conclusion (in accord with earlier experiments) that the motion of Pluto is chaotic. It is clear that while symplectic integrators seemed to behave satisfactorily in these experiments, in the sense that the gain in speed was not paid dearly with accuracy at least in comparison to the Digital Orrery computation, statements regarding chaotic behavior based on numerical integration are clearly worrisome. Nevertheless, trust in symplectic integrators

seems to have been vindicated: very recently Holman and Murray [21] have proposed a theoretical explanation for these results. This subject, however, is historically full of twists and turns, and the jury is certainly still out on such a recent development.

Other experiments can be found in molecular dynamics, where some good results have been achieved in the long-time integration of some complicated collisions or long-lived trajectories. In [34], for example, a comparison of many algorithms, including traditional top-of-the-line ones, is made, and the authors conclude that "the sixth-order [symplectic] integrator of Teloy is definitely better than all others, which we have now or earlier tested, and it has very good stability. We will use it henceforth for our routine calculations". For more popular symplectic algorithms applied in molecular dynamics, including the "leapfrog" method, see [35].

There are of course many other experiments (see [6, 7, 9, 27, 32, 33], the articles in [25] and references therein), but the conclusion appears to be that the application of symplectic methods to long-time integrations is very successful in identifying most relevant qualitative features of hamiltonian systems. In these experiments, often some comparison is made with more traditional methods of same order of accuracy, which frequently require smaller step-sizes (and hence more iterations) to identify the relevant dynamics. While this seems encouraging, it also comes through that symplectic integrators have often been brought to problems already understood, sometimes to great extent, via the application of other methods. Even the case of the chaotic behavior of the outer planets, one may rightfully defend, falls in this category. This might account for the apparent reluctance that the numerical analysis community has had to embrace these tools. (It does not help, unfortunately, that symplectic integrators are often compared with traditional methods of the same order, sometimes even with fixed step-sizes. This ignores the state-of-the-art mathematical technology for traditional methods, and the standing principle that one should use variable step-size techniques whenever possible. The argument on the side of symplectic integrators is that the fairness of comparing a newborn method with mature state-of-the-art ones that had years of enhancement is at least questionable).

Finally, it is appropriate to mention that although we have dealt mostly with systems of ODE's, there are more recent methods that apply geometric ideas to the numerical analysis of PDE's. For these developments, we direct the reader to [26].

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