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SYMPLECTIC NUMERICAL METHODS FOR HAMILTONIAN PROBLEMS

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We consider symplectic methods for the numerical integration of Hamiltonian problems, i.e. methods that preserve the Poincaré integral invariants. Examples of symplectic methods are given and numerical experiments are reported.

1. Introduction

We are concerned with autonomous Hamiltonian systems

$$\dot{p}^i = -\partial H/\partial q^i, \qquad \dot{q}^i = \partial H/\partial p^i, \qquad 1 \le i \le d, \tag{1}$$

where a dot represents differentiation with respect to t (time), d is the number of degrees of freedom and $H = H(\mathbf{p},\mathbf{q}) = H(p^1,\ldots,p^d,q^1,\ldots,q^d)$ denotes the Hamiltonian. The time t flow of (1) will be denoted by $\phi_{t,H}$; thus, for fixed $(\mathbf{p}_0,\mathbf{q}_0)$ and varying t, $(\mathbf{p}(t),\mathbf{q}(t)) = \phi_{t,H}(\mathbf{p}_0,\mathbf{q}_0)$ is the solution of (1) with initial condition $\mathbf{p}(0) = \mathbf{p}_0$, $\mathbf{q}(0) = \mathbf{q}_0$. For each fixed value of t, $\phi_{t,H}$ is a transformation in phase space that has the property of symplecticness or canonicity, i.e. for any bounded two-dimensional surface D in phase space the sum of the two-dimensional oriented areas of the d projections of D onto the planes (p^i,q^i) is the same as the sum of the two-dimensional oriented areas of the d projections of $\phi_{t,H}(D)$ onto the planes (p^i,q^i). In other words $\phi_{t,H}$ preserves the differential form $\omega = dp^1 \wedge dq^1 + \ldots + dp^d \wedge dq^d$. This implies the conservation of the exterior powers $\omega^2,\ldots,\omega^d$ (Poincaré integral invariants). The conservation of ω^d is the conservation of the $2d$-dimensional volume in phase space (Liouville's theorem). The symplectic property of the flow is the characteristic feature of Hamiltonian systems: a differential system with a symplectic flow must be a Hamiltonian system. Hamiltonian dynamics possess a number of properties (absence of attractors, recurrence, ...) not shared by 'general' dynamics. All those properties directly derive from the symplecticness of Hamiltonian flows.

A one-step method[1] for (1) used with step length h is of the form $(\mathbf{p}_{n+1}, \mathbf{q}_{n+1}) = \psi_{h,H}(\mathbf{p}_n, \mathbf{q}_n)$, where $(\mathbf{p}_n, \mathbf{q}_n)$ is the numerical solution at time level $t_n = nh$. For instance, for Euler's method $\psi_{h,H}(\mathbf{p}, \mathbf{q}) = (\mathbf{p} - h\,\partial H/\partial \mathbf{q}, \mathbf{q} + h\,\partial H/\partial \mathbf{p})$. Therefore the numerical solution at t_n is given by $(\mathbf{p}_n, \mathbf{q}_n) = \psi^n_{h,H}(\mathbf{p}_0, \mathbf{q}_0)$, while for the true solution $(\mathbf{p}(t_n), \mathbf{q}(t_n)) = \phi^n_{h,H}(\mathbf{p}_0, \mathbf{q}_0)$. Hence $\psi_{h,H}$ should be an approximation to $\phi_{h,H}$. If $\psi_{h,H} = \phi_{h,H} + O(h^{r+1})$ as $h \to 0$, the numerical method is said to be of order r. It then follows that $(\mathbf{p}_n, \mathbf{q}_n) = (\mathbf{p}(t_n), \mathbf{q}(t_n))$ as $h \to 0$ and $n \to \infty$ with t_n fixed. For classical methods such as explicit Runge-Kutta methods, the transformation $\psi_{h,H}$ turns out not to be symplectic. Then the numerical method misses the important features associated with symplectic transformations. However there are symplectic methods, i.e. methods for which $\psi_{h,H}$ is guaranteed to be a symplectic transformation.

There has been much recent interest in the numerical integration of (1) by means of symplectic methods, starting with the work of Ruth, Channell and Feng. An extensive list of references can be seen in the survey[2].

2. Some Symplectic Methods

Broady speaking, symplectic methods can be divided into two categories. Firstly there are methods that are derived via the Hamiltonian formalism (generating functions[3], Lie transforms[4], etc.). These methods are only applicable to Hamiltonian problems. A second group of symplectic integrators consists of formulas that belong to well-known families of methods and just 'happen' to be symplectic when applied to Hamiltonian problems. For instance Lasagni[5], Sanz-Serna[6] and Suris[7] showed independently that Runge-Kuta formulas whose coefficients satisfy some relations are automatically symplectic. However symplectic Runge-Kutta methods are necessarily *implicit*. The class of Runge-Kutta-Nyström (RKN) methods[1] contains integrators that are both explicit and symplectic. RKN methods are applicable to systems of the special form

$$\dot{\mathbf{p}} = \mathbf{f}(\mathbf{q}), \qquad \dot{\mathbf{q}} = \mathbf{p} \tag{2}$$

i.e. to second order systems $\ddot{\mathbf{q}} = \mathbf{f}(\mathbf{q})$. If $\mathbf{f}$ is the gradient of a scalar function $-V(\mathbf{q})$, then (2) is a Hamiltonian system with $H = (1/2)\mathbf{p}^T\mathbf{p} + V(\mathbf{q})$. An explicit RKN method is specified by an integer s (the number of stages) and real constants α_{ij}, b_i, β_i, γ_i, $1 \le i \le s$, $1 \le j < i \le s$. A step from time t_n to time t_{n+1} with an RKN formula begins by computing the internal stages $\mathbf{Q}_i$

$$\mathbf{Q}_i = \mathbf{q}_n + h\gamma_i\mathbf{p}_n + h^2\sum_{j<i}\alpha_{ij}\,\mathbf{f}(\mathbf{Q}_j), \quad 1 \le i \le s. \tag{3}$$

Then

$$\mathbf{p}_{n+1} = \mathbf{p}_n + h\sum_{i=1}^{s} b_i\,\mathbf{f}(\mathbf{Q}_i), \tag{4}$$

and

$$\mathbf{q}_{n+1} = \mathbf{q}_n + h\mathbf{p}_n + h^2 \sum_{i=1}^{s} \beta_i \mathbf{f}(\mathbf{Q}_i). \tag{5}$$

The function $\mathbf{f}$ must be evaluated at each of the s stages $\mathbf{Q}_i$. These s function evaluations per step represent the bulk of the computational work of the method.

The method (3)–(5) is symplectic[7] if

$$\beta_i = b_i(1 - \gamma_i), \qquad 1 \le i \le s, \tag{6}$$

and

$$\alpha_{ij} = b_j(\gamma_i - \gamma_j), \quad 1 \le j < i \le s. \tag{7}$$

For symplectic methods with s stages we have s coefficients b_i and s coefficients γ_i as free parameters; the coefficients β_i and α_{ij} are given by (6) and (7) respectively.

Okunbor and Skeel[8] point out that when (6)–(7) hold, (3)–(5) can be rewritten as

$$\begin{aligned}
\mathbf{Q}_i &= \mathbf{Q}_{i-1} + h(\gamma_i - \gamma_{i-1})\mathbf{P}_{i-1}, \quad 1 \le i \le s, \\
\mathbf{P}_i &= \mathbf{P}_{i-1} + hb_i\mathbf{f}(\mathbf{Q}_i), \quad 1 \le i \le s, \\
\mathbf{q}_{n+1} &= \mathbf{Q}_s + h(1 - \gamma_s)\mathbf{P}_s \\
\mathbf{p}_{n+1} &= \mathbf{P}_s
\end{aligned}$$

with $\mathbf{Q}_0 = \mathbf{q}_n$, $\mathbf{P}_0 = \mathbf{p}_n$, $\gamma_0 = 0$. This alternative formulation reveals that (3)–(7) only requires the storage of two d-dimensional vectors; one of these successively contains $\mathbf{q}_n, \mathbf{Q}_1, \ldots, \mathbf{Q}_s, \mathbf{q}_{n+1}$; the other is used for $\mathbf{p}_n, \mathbf{P}_1, \ldots, \mathbf{P}_s, \mathbf{p}_{n+1}$.

Calvo and Sanz-Serna[9] have derived an optimized, fourth-order, explicit, symplectic RKN method. They set $\gamma_1 = 0$, $\gamma_s = 1$; this guarantees that the last stage $\mathbf{Q}_s$ of the current step coincides with the first stage of the next step, thus saving a function evaluation per step. Their method has $s = 5$ (four evaluations per step) and hence there are eight free parameters $\gamma_2, \gamma_3, \gamma_4, b_1, \ldots, b_5$. To ensure order four, the method coefficients must satisfy six equations[10], which leaves two free parameters. These were chosen so as to minimize the error constants in the $O(h^5)$ truncation error $\psi_{h,H} - \phi_{h,H}$. The result is

$\gamma_1 = 0$	$b_1 = 0.061758858135626325$
$\gamma_2 = 0.205177661542286386$	$b_2 = 0.338978026553643355$
$\gamma_3 = 0.608198943146500973$	$b_3 = 0.614791307175577566$
$\gamma_4 = 0.487278066807586965$	$b_4 = -0.140548014659373380$
$\gamma_5 = 1$	$b_5 = 0.125019822794526133$

For higher order symplectic RKN methods see Calvo and Sanz-Serna[11].

3. Backward Error Interpretation

An appealing feature of symplectic integrators is that they make it possible to perform a backward error analysis. In numerical analysis, backward error analysis

means interpreting the numerical result of a problem $\mathcal{P}$ as an *exact* solution to a problem $\tilde{\mathcal{P}}$ close to $\mathcal{P}$. Let $\psi_{h,H}$ be a symplectic integrator of order r, so that $\psi_{h,H} - \phi_{h,H} = O(h^{r+1})$. Then[2] for each integer $\rho > r$, no matter how large, it is possible to construct a perturbed Hamiltonian function $H_\rho(h) = H + O(h^r)$ in such a way that $\psi_{h,H} - \phi_{h,H_\rho(h)} = O(h^{\rho+1})$. Thus, if we ignore the small remainder $O(h^{\rho+1})$, we can say that the numerical method $\psi_{h,H}$ is the h-flow of a perturbed Hamiltonian problem with Hamiltonian $H_\rho(h)$.

An illustration is given in Fig. 1. The system being integrated is the pendulum system $\dot{p} = -\sin q$, $\dot{q} = p$; the dotted line depicts the true solution with initial value $q = 2$, $p = 0$; the stars correspond to the numerical solution obtained for $h = 2$ with the symplectic first-order RKN method specified by $s = 1$, $\gamma_1 = 1$, $b_1 = 1$. When $\rho = 2$, $H_\rho(h)$ turns out to be $(1/2)p^2 + (1 - \cos q) + (h/2)p \sin q$; the dash-dot line represents the level set of this Hamiltonian thorugh the point $q = 2$, $p = 0$. It is clear that the computed points that were meant to approximate the pendulum motion are in fact describing the motion of the perturbed problem.

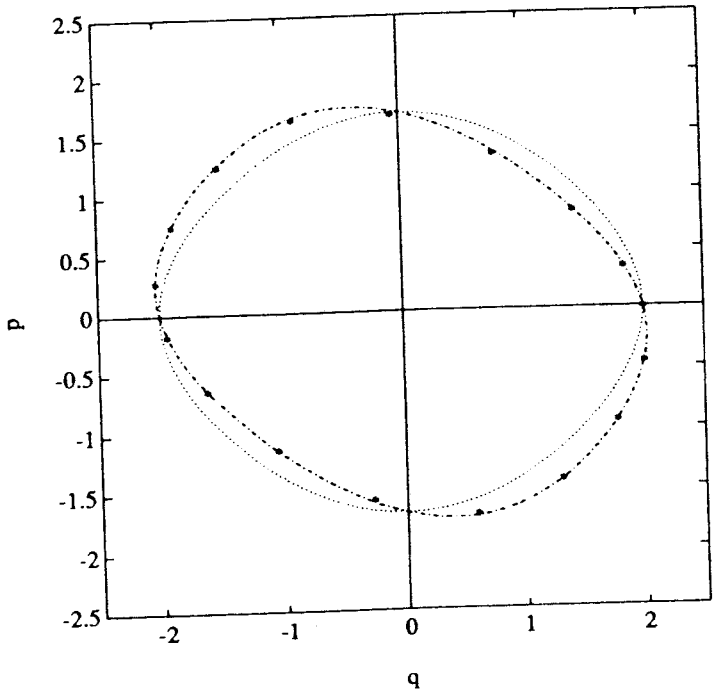

Fig. 1. Backward error interpretation.

In a modelling situation where the exact form of the Hamiltonian may be in doubt, the fact that integrating the model numerically introduces perturbations in the Hamiltonian comparable to the uncertainty in H inherent in the model is the most that can be hoped for.

On the other hand, when a nonsymplectic algorithm is used the differential

system really solved by the method is not Hamiltonian. For instance in Fig. 1 Euler's method would produce a spiral, something that cannot be matched by a Hamiltonian system. Here the process of numerical integration perturbs the model in such a way as to take it out of the Hamiltonian class.

4. Numerical Illustrations

We first consider the Newton potential $V(q^1, q^2) = -1/\|\mathbf{q}\|$ (Kepler's problem) with initial condition $p^1 = 0$, $p^2 = \sqrt{(1+e)/(1-e)}$, $q^1 = 1 - e$, $q^2 = 0$. Here e is the eccentricity of the orbit, that in the experiments to be reported is chosen to be $e = 0.5$. (The value of e does not significantly influence the outcome of the experiments.) The solution is 2π-periodic. Errors are measured in the Euclidean norm of $\mathcal{R}^4$. The problem was integrated for 21870 periods with the fourth order RKN method described in Section 2, implemented with constant step sizes and also with an efficient variable step size, nonsymplectic fourth order RKN code due to Dormand *et al.*[12]. It should be pointed out that while variable step sizes enhance the performance of conventional codes, they are detrimental to symplectic integrators[10].

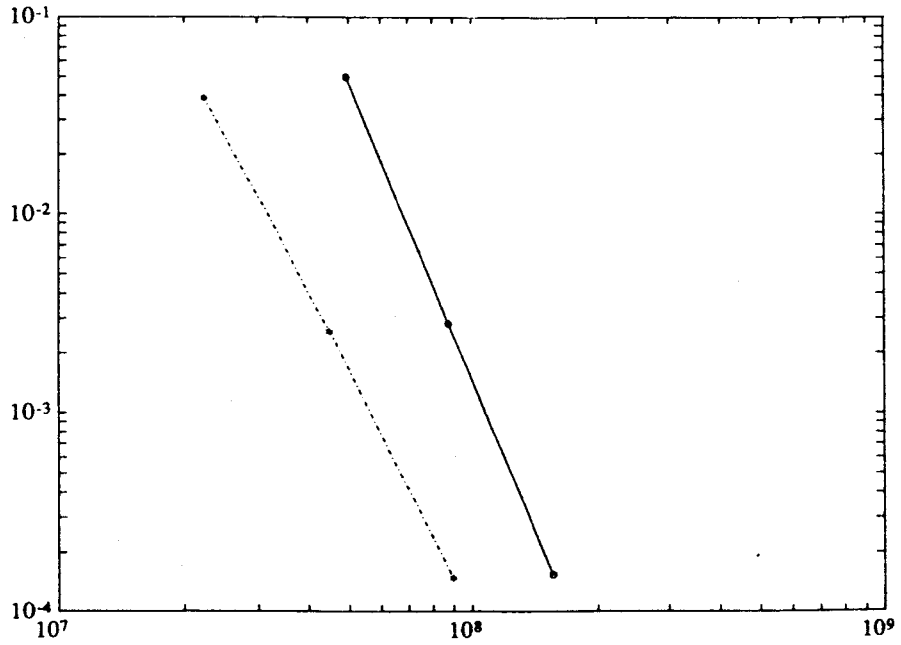

Fig. 2. Kepler's problem. Error against computational cost.

Fig. 2 is an efficiency plot that shows errors at the end of the integration against computational cost measured in number of function evaluations. The runs depicted

correspond to the symplectic algorithm with $h = 2\pi/256$, $h = 2\pi/512$, $h = 2\pi/1024$ (stars joined by a dash-dot line) and the standard code with tolerances 10^{-9}, 10^{-10}, 10^{-11} (circles joined by a solid line). It is apparent that the symplectic algorithm is more efficient by a factor of two. This is in spite of the fact that the symplectic algorithm requires four function evaluations per step and the standard algorithm uses only three. The gains in efficiency associated with symplecticness are due to the fact that in symplectic algorithms the error grows linearly with t, while in general methods that growth is quadratic[10]. This is illustrated in Fig. 3 that shows error as a function of t for both methods.

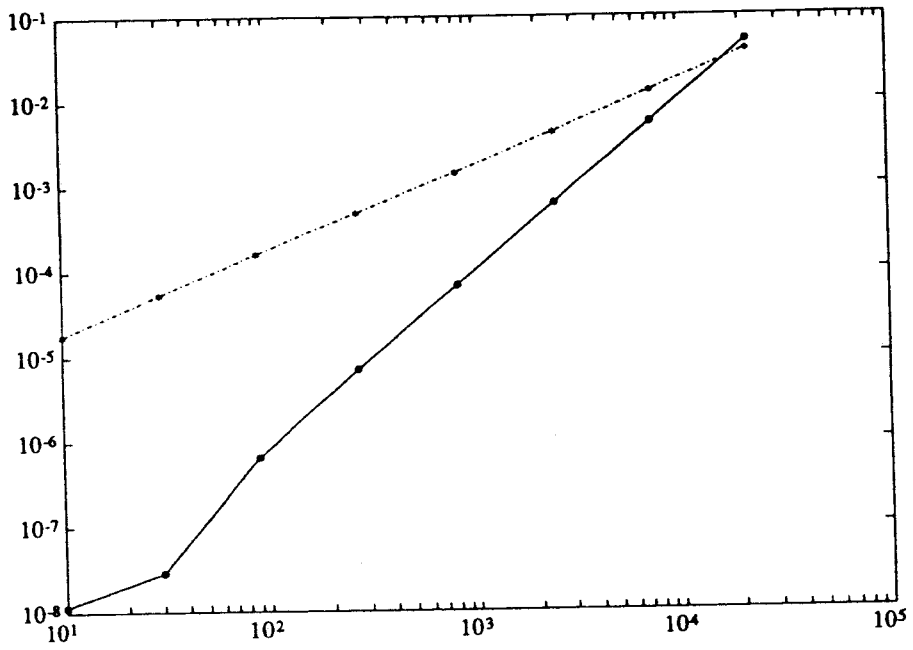

Fig. 3. Kepler's problem. Error against t measured in periods.

The second test problem is taken from Herbst and Ablowitz[13]. It originates from the sine-Gordon equation

$$u_{tt} - u_{xx} + \sin u = 0, \quad 0 < x < L = 2\sqrt{2}\pi, \quad t > 0, \tag{8}$$

subject to periodic boundary conditions and to the initial conditions

$$u(x,0) = \pi + 0.1\cos(2\pi x/L), \quad u_t(x,0) = 0. \tag{9}$$

The equation (8) may be thought of as describing the motion of a family of pendula. At each value of x, $0 < x < L$ we have one pendulum. The term u_{xx} provides coupling between the motions of neighboring pendula. It represent a force that

tries to keep a common value of the angle u for all the pendula. From the initial condition (9) we see that all pendula are initially left near the unstable equilibrium $u = \pi$. The pendula in $0 < x < L/4$ or $3L/4 < x < L$ start *above* the value $u = \pi$ and hence will increase u in order to approach the stable equilibrium at $u = 2\pi$. The pendula in $L/4 < x < 3L/4$ start *below* the value $u = \pi$ and will decrease u to approach the stable equilibrium at $u = 0$. This causes the term u_{xx} to become important. The effect of the restoring force is that the pendula are prevented from reaching the lowest $u = 2\pi$ or $u = 0$ positions and rather start going upwards back to the initial positions, leading to a periodic motion. The solid line in Figure 4 represents u as a function of t, $0 < t < 16L$ for the pendulum at $x = L/2$.

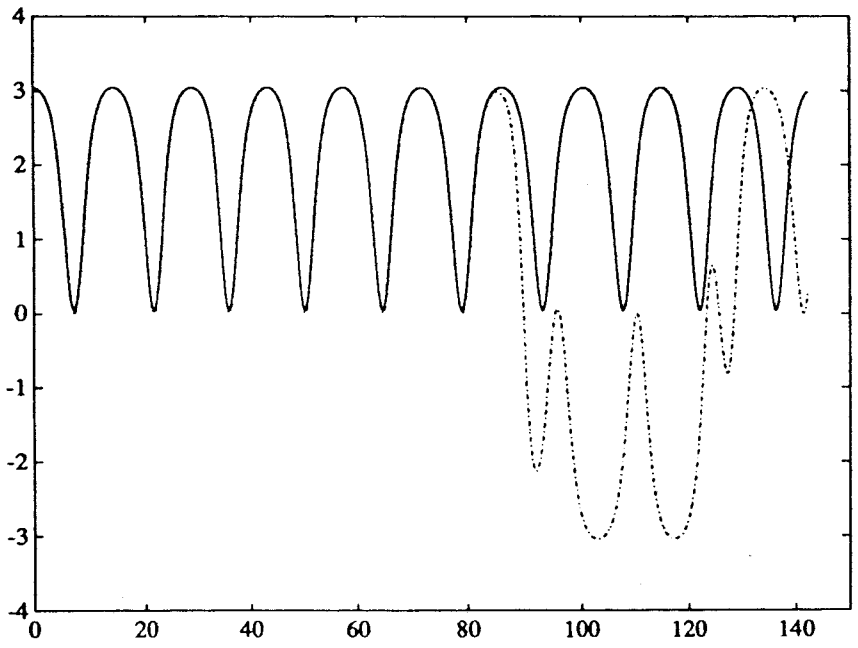

Fig. 4. Sine-Gordon problem. Solution at $x = L/2$ against t.

As in[13], the equation (8) is discretized in space by the standard pseudospectral technique, with a mesh-length $\Delta x = L/32$. This leads to a Hamiltonian system of the form (2) where the dependent variables $\mathbf{q}$ are the 32 discrete Fourier coefficients of the solution. This system of ordinary differential equations was integrated for $0 < t < 16L \approx 142.17$, both with the fourth order symplectic method and with an eighth order RKN code with variable step sizes due to Dormand *et al.*[14]. The standard method was run with absolute error tolerances in the range 10^{-8} to 10^{-13}. Smaller tolerances were not tried because we felt they would be too close to the size of the round-off error associated with the evaluation of the force $\mathbf{f}$ (this requires a couple of discrete Fourier transforms). None of the values of the tolerance we tried

led to a successful integration and the conventional method was not able to come up with the right qualitative behavior of the solution. The dash-dot line in Fig. 4 corresponds to the tolerance 10^{-13}, $x = L/2$, the computed solution is completely wrong for $t > 80$. For this value of the tolerance the code uses 32810 function evaluations. On the other hand with $h = 1/32$ (18200 evaluations) the fourth order symplectic method correctly identifies the right qualitative behavior (solid line in Fig. 4).

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