Global Error Control in the Runge-Kutta Solution of a Hamiltonian System using the RKQ Algorithm

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Abstract

We study the effect of global error control in the numerical solution of Hamiltonian systems. In particular, we apply the RKQ algorithm in the numerical solution of a Hamiltonian system. This algorithm is designed to provide stepwise control of both local and global error. A test problem demonstrates the error control features of RKQ. Good results are obtained, despite the fact that explicit Runge-Kutta methods have been used in RKQ, rather than symplectic Runge-Kutta methods. This simply emphasizes the value of stepwise global error control, as per the RKQ algorithm.

1 Introduction

Global error control in numerical solutions of initial-value problems is of paramount importance. In this paper, we consider the effect of global error control on the numerical solution of Hamiltonian systems. We solve a test problem using the RKQ algorithm, which is designed to achieve stepwise global error control. Significantly, we use explicit Runge-Kutta methods in RKQ, as opposed to implicit symplectic Runge-Kutta methods, which are often preferred for Hamiltonian systems.
2 Relevant Concepts, Terminology and Notation

2.1 Hamiltonian Systems

If the total energy of a physical system is given in the form of the Hamiltonian

\[ H(p, q) , \]

where the canonical coordinates \( p \) and \( q \) are the momentum and position, respectively, then the evolution of the system is given by

\[
\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q} .
\]

(1)

The Hamiltonian \( H(p, q) \) is a first integral of (1), meaning that it is constant for all \( t \). For an appropriate set of initial values, (1) is an initial-value problem (IVP). Since Hamiltonian systems are nonlinear, their solution is usually obtained numerically - using, for example, a Runge-Kutta (RK) method.

For ease of presentation we consider here a two-dimensional Hamiltonian, rather than the more general case

\[ H(p_1, \ldots, p_n, q_1, \ldots, q_n) , \]

but this restriction will not affect our discussion.

2.2 Runge-Kutta Methods

Runge-Kutta methods are very well-known, and the reader is referred to the extensive literature. For our purposes, an RK method applied to (1) has the form

\[
\begin{bmatrix}
\tilde{q}_{i+1} \\
\tilde{p}_{i+1}
\end{bmatrix}
= \begin{bmatrix}
\tilde{q}_i \\
\tilde{p}_i
\end{bmatrix} + h_{i+1} F \left( t_i, \begin{bmatrix} q_i \\ p_i \end{bmatrix}, h_{i+1} \right) .
\]

(2)

In (2), \( i \) denotes discrete points along the \( t \)-axis, so that \( \tilde{q}_i \) and \( \tilde{p}_i \) are numerical solutions at \( t_i \); the stepsize \( h_{i+1} \equiv t_{i+1} - t_i \); and \( F \) is a vector function associated to the RK method under consideration. Initial values of \( p \) and \( q \) are specified at \( t_0 \).

We define the local and global errors of an RK method as

\[
\text{local error: } \epsilon_{i+1} \equiv \left( \begin{bmatrix} q_i \\ p_i \end{bmatrix} + h_{i+1} F \left( t_i, \begin{bmatrix} q_i \\ p_i \end{bmatrix}, h_{i+1} \right) \right) - \begin{bmatrix} q_{i+1} \\ p_{i+1} \end{bmatrix}.
\]
and

$$\Delta_{i+1} = \left[ \begin{array}{c} \delta_{q,i+1} \\ \delta_{p,i+1} \end{array} \right] \equiv \left[ \begin{array}{c} \tilde{q}_{i+1} \\ \tilde{p}_{i+1} \end{array} \right] - \left[ \begin{array}{c} q_{i+1} \\ p_{i+1} \end{array} \right]. \quad (3)$$

Note the use of the exact values of $q$ and $p$ in the definition of the local error.

If the RK method is of order $r$ (denoted $\text{RK}_r$), we have

$$\varepsilon_{i+1} \propto h_{i+1}^{r+1}$$

and

$$\Delta_{i+1} \propto h^r,$$

where $h$ is representative of the stepsizes (for example, $h$ could be taken as the average stepsize along the discretized $t$-axis).

Usually, symplectic RK methods are used to solve Hamiltonian systems [1]. Such methods have the property that the Hamiltonian arising from the numerical solution is bounded in the sense that it does not drift away from the exact value; rather, it exhibits small oscillations in the vicinity of the exact value. Also, symplectic RK methods reproduce closed orbits in the $(q, p)$ phase space, as expected when periodic solutions are present. The symplectic property of Hamiltonian systems refers to the invariance of the differential 2-form $dp \wedge dq$, a feature that is respected by symplectic RK methods (hence their name). Practically speaking, however, it is the first two properties listed here - essentially constant numerical Hamiltonian and closed phase space trajectories - that are of primary interest.

The disadvantage of symplectic RK methods is that they are implicit (a particular characteristic of the function $F$), and this requires the solution of a nonlinear system of equations at each node $t_i$, which can be computationally expensive. Explicit RK methods do not require the solution of such a nonlinear system, but neither are they symplectic.

### 2.3 The $\text{RK}_{rvQz}$ Algorithm

We will not discuss $\text{RK}_{rvQz}$ in detail here; the reader is referred to our previous work where the algorithm has been discussed extensively [2, 3]. It is sufficient to state that $\text{RK}_{rvQz}$ uses $\text{RK}_r$ and $\text{RK}_v$ to control the local error via so-called local extrapolation, while simultaneously using $\text{RK}_z$ to keep track of the global error in the $\text{RK}_r$ solution (we have $z \gg r, v$). Such global error arises from the propagation of the $\text{RK}_v$ global error in the $\text{RK}_r$ method, as a consequence of local extrapolation. $\text{RK}_{rvQz}$ is designed to estimate the various components of the global error in $\text{RK}_r$ and $\text{RK}_v$ at each node $t_i$ and, when the global error exceeds a user-defined tolerance, a quenching procedure is carried out. This simply involves replacing the $\text{RK}_r$
and RKv solutions with the much more accurate RKz solution, whenever necessary, so that the RKr and RKv global errors do not accumulate beyond the desired tolerance.

3 The Effect of Global Error Control

From (3) we have

\[ \tilde{q}_{i+1} = q_{i+1} + \delta_{q,i+1} \]
\[ \tilde{p}_{i+1} = p_{i+1} + \delta_{p,i+1}. \]

This gives

\[ H(\tilde{p}_{i+1}, \tilde{q}_{i+1}) = H(p_{i+1} + \delta_{p,i+1}, q_{i+1} + \delta_{q,i+1}) \]
\[ = H(p_{i+1}, q_{i+1}) + \frac{\partial H(p_{i+1}, q_{i+1})}{\partial p} \delta_{p,i+1} + \frac{\partial H(p_{i+1}, q_{i+1})}{\partial q} \delta_{q,i+1} + \ldots \]
\[ \approx H(p_{i+1}, q_{i+1}) + \frac{dq}{dt} \delta_{p,i+1} - \frac{dp}{dt} \delta_{q,i+1} \]

where we have ignored higher-order terms. Now, say \( \delta \) is an upper bound on the magnitude of the global errors. Hence,

\[ |H(\tilde{p}_{i+1}, \tilde{q}_{i+1}) - H(p_{i+1}, q_{i+1})| \leq \left( \frac{dq}{dt} \right) + \left( \frac{dp}{dt} \right) \delta. \]

We see that the bound on the error in the numerical Hamiltonian is proportional to the bound \( \delta \).

For a point on the trajectory in phase space, we have

\[ \| (\tilde{q}_{i+1}, \tilde{p}_{i+1}) - (q_{i+1}, p_{i+1}) \| = \| (\delta_{q,i+1}, \delta_{p,i+1}) \| \leq \| (\delta, \delta) \| \]

where \( \| \cdots \| \) is any norm suitable for determining distances in the phase space. Hence, the bound on the trajectory error is proportional to \( \delta \). For the Euclidean norm and the two-dimensional case considered here, we have

\[ \| (\tilde{q}_{i+1}, \tilde{p}_{i+1}) - (q_{i+1}, p_{i+1}) \| \leq \sqrt{2}\delta. \]

The implication of the above analysis is obvious: if we apply RKrvQz to the problem, with a suitable tolerance of \( \delta \), then we would generate solutions \( \tilde{p} \) and \( \tilde{q} \) for which the error bounds on the numerical Hamiltonian and the phase-space trajectories are acceptably small. Furthermore, this can be achieved using explicit RK methods in the RKrvQz algorithm, as opposed to the more computationally intensive symplectic RK methods.
4 Numerical Example

As an example, we consider the Hamiltonian

\[ H(p, q) = \frac{p^2}{2} - \left(1 - \frac{p}{6}\right) \cos q \]

which yields

\[ \frac{dq}{dt} = p + \frac{\cos q}{6} \]
\[ \frac{dp}{dt} = \left(\frac{p}{6} - 1\right) \sin q. \]

This is the same example considered in Hairer et al [1]. We use initial values

\[ q(0) = \arccos(-0.8) \]
\[ p(0) = 0 \]

and we integrate over \( t \in [0, 4000] \).

We solve the system using RK34Q8 \((r = 3, v = 4, z = 8)\), with a tolerance of \( \delta = 10^{-6} \) on both the local and global error. For comparison, we solve the system via local extrapolation only with RK3 and RK4, also subject to a tolerance (on the local error) of \( \delta = 10^{-6} \). Results are shown in the figures following the references. The various explicit RK methods used here are the same as those referenced in [2],[3]. We use the notation RK34 to indicate the local extrapolation algorithm using RK3 and RK4.

In Figure 1, the top two plots show the first few periods of the solution numerical \( \tilde{p}(t) \) and \( \tilde{q}(t) \), demonstrating their periodic character. Consistent with this periodicity is the closed trajectory in phase space, shown in the third plot in Figure 1. The numerical Hamiltonian is shown in the fourth plot, for RK34Q8 and RK34. Clearly, the latter exhibits a generally monotonic drift from the exact value of 0.8, while the former is essentially constant with slight oscillations. For the sake of clarity we have not shown all the data points in this plot; there are some 96000 nodes on \([0, 4000]\) in the computation, and we show relatively few - sufficient, nonetheless, to exhibit the salient features of the calculation (this also holds for subsequent plots in Figures 2-4). The drift in \( H \) is slight - only about \( 3 \times 10^{-6} \) over the entire interval of integration - but it is definite. Given that \( H \) should be invariant, however, the result obtained with RK34Q8 should be preferred.

Figure 2 shows global errors in \( \tilde{p}(t) \) and \( \tilde{q}(t) \), determined from the difference of the RK34 solution and the RK8 solution. Clearly, the errors in the RK34 algorithm grow as the integration proceeds, achieving maximal
values of $\sim 0.02$. On the other hand, the RK34Q8 algorithm, thanks to the high-order quenching device, gives a solution that is bounded by $\delta = 10^{-6}$, as desired. This bound is indicated by the horizontal line labelled ‘tolerance’. The maximal errors in this case are $9.998 \times 10^{-7}$ in $\tilde{q}(t)$, and $8.54 \times 10^{-7}$ in $\tilde{p}(t)$.

In Figure 3 we show the trajectory error, determined using the Euclidean norm, for both algorithms. Clearly, the trajectory error grows for RK34, consistent with growth of global error in the solutions seen in Figure 2. For RK34Q8, the trajectory error is bounded by $\sqrt{2} \times 10^{-6}$, as expected. This bound is indicated by the horizontal line labelled ‘upper bound’.

For completeness, we show the estimated global error in the RK8 solution in Figure 4 (errors for both $p$ and $q$ are shown). This has been computed with (see [2], [3], [4])

$$
\Delta_{i+1} = \varepsilon_{i+1} + (I_2 + h_{i+1}F_{q,p}) \Delta_i \\
\approx \varepsilon_{i+1} + (I_2 + h_{i+1}f_{q,p}) \Delta_i.
$$

Here, $F_{q,p}$ is the Jacobian of the function $F$ in (2), $f_{q,p}$ is the Jacobian of $f(q, p) \equiv \left[ \frac{\partial H}{\partial p} - \frac{\partial H}{\partial q} \right]$, $I_2$ is the $2 \times 2$ identity matrix, and we assume

$$
\Delta_0 = \left[ \begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array} \right].
$$

Also, we have used Richardson extrapolation to estimate the local error $\varepsilon_{i+1}$ in the RK8 solution [2, 5]. For a reasonably small stepsize ($\sim 0.05$ in this problem) and a high-order RK method, we expect this to be a good estimator. The largest error in either component of the RK8 solution was $1.86 \times 10^{-12}$. This means that any global error in the RK8 solution would not ‘contaminate’ the RK34Q8 error control procedure, since the tolerance of $\delta = 10^{-6}$ is considerably larger than $1.86 \times 10^{-12}$. We note here that it is feasible to use a method of higher order than RK8 to estimate the global error in the RK8 solution, even though this would probably increase the computational effort. At the time of writing, however, we did not have access to such a method. Nevertheless, in this regard one might consider transforming the problem into a second-order problem, making it suitable for Nyström integration, as we considered in [6]. This would enable the use of the $(10, 12)$ embedded Nyström pair due to Dormand et al [7].
4.1 Relative Error Control

In this paper, we have only considered absolute error control, since the magnitude of the solution was $\sim 1$. If the magnitude of the solution had been much larger than unity, it would have been better to implement relative error control. We will not discuss this in detail; a thorough account has been given in [3], wherein we generalized the RKQ algorithm. It suffices to say that at each node, for relative error control in the problem considered here, the tolerance would have the form

$$\delta = \min \{ \max \{ \delta_A, \delta_R |q_i| \}, \max \{ \delta_A, \delta_R |p_i| \} \},$$

where $\delta_A$ and $\delta_R$ are user-defined (the presence of $\delta_A$ caters for those situations where $q_i$ and/or $p_i$ are very close to zero).

5 Conclusion

We have explored global error control in the numerical solution of Hamiltonian systems. A theoretical analysis shows that if the error in the solution is bounded, then errors in quantities such as the numerical Hamiltonian and phase space trajectories are also bounded. We have considered the use of the RKQ algorithm, with explicit Runge-Kutta methods, as our choice of numerical integrator, since RKQ is specifically designed to achieve global error control. A test problem has demonstrated the expected results. In addition to the bounding of the error in the solution, we also observe an essentially constant numerical Hamiltonian and a bounded error in the numerical trajectory in phase space. This contrasts Hamiltonian drift and unbounded trajectory deviation normally associated with the use of explicit Runge-Kutta methods in solving Hamiltonian systems. It is our contention that, even though RKQ utilizes explicit Runge-Kutta methods, stepwise global error control via RKQ leads to results with a similar quality to those that would be obtained using symplectic methods.

References

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Fig. 1

Position $q(t)$

Momentum $p(t)$

Phase space trajectory $(q,p)$

Hamiltonian $H(p(t),q(t))$
Global error in $q(t)$ for RK34Q8 and RK34

Global error in $p(t)$ for RK34Q8 and RK34

Fig. 2
Fig. 3

Trajectory error for RK34Q8 and RK34

Trajectory error

RK34

upper bound

RK34Q8

$t$
Fig. 4

Estimated global error in RK8

Global error vs. time (t)

$2 \times 10^{-12}$ to $2$