Validation of Accuracy and Efficiency of Long-Arc Orbit Propagation Using the Method of Manufactured Solutions and the Round-Trip-Closure Method

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ABSTRACT

For conservative systems, a common method for validating accuracy is that the Hamiltonian or a similar energy integral of a converged solution maintains constancy to a desired tolerance. While a Hamiltonian metric is a very useful for conservative systems, for non-conservative systems a Hamiltonian check is not applicable and other methods for validating solution accuracy must be employed. While we can utilize various ad-hoc methods for comparing the state history from a new integrator with some other well-tested code, or compare solutions using various accuracy tunings for a given method, there always remains uncertainty since rigorous convergence conclusions are difficult when comparing approximate solutions.

Two independent measures of solution accuracy are considered in this paper, based on the Method of Manufactured Solutions (MMS) and the Round-Trip-Closure Method (RTC). These metrics have the attractive property that they are both theoretically exactly zero if the integrator introduces zero error. For RTC, the convergence test is applied directly to the original differential equations and boundary conditions, whereas for MMS, a close neighbor of the unknown exact solution is established, with a known small perturbing force. The neighboring solution is the exact solution of the original differential equations with the known small perturbing force. Application of the solution methodology to this slightly perturbed problem permits strong conclusions on the algorithm’s accuracy of convergence.

MMS and RTC metrics are useful for virtually any numerical process for solving differential equations. MMS and RTC are useful in evaluating the relative merits of competing algorithms; the utility of these ideas are demonstrated in an accuracy study for three numerical integrators: Modified Chebyshev Picard Iteration (MCPI), an 8th order Gauss Jackson (GJ8) algorithm and Runge-Kutta-Nystrom (RKN12(10)). We utilize an intermediate order spherical-harmonic gravity (40,40) model. Since this problem is conservative, we check the Hamiltonian constancy with MMS and RTC. Results demonstrate the consistency of the two metrics and high efficiency vs accuracy of MCPI relative to the other integrators, for long-arc orbit propagation. MMS is readily applied to MCPI, since the solution process produces automatically an interpolating polynomial for the state variables. However, for most methods, one must introduce an auxiliary interpolation process, as discussed herein. We show MMS and RTC errors for these state of the art algorithms.

1. INTRODUCTION

A common method for validating the accuracy of numerical integrators is confirming that the Hamiltonian of an apparently converged solution maintains constancy to a desired tolerance for the time interval over which the computation was performed. This Hamiltonian metric is a useful test for conservative systems. For non-conservative systems, for example a Low Earth Orbit (LEO) that is under the influence of aerodynamic drag, the Hamiltonian check is not applicable and other methods for validating the accuracy of the solution must be employed. While we can utilize various ad hoc methods of comparing the state history (ephemeris) from a new integrator with some other well-tested integrator, or compare solutions using a given method with itself, there always remains uncertainty since neither solution is exact.

Two independent measures of solution accuracy are introduced, based on the Method of Manufactured Solutions (MMS) and the Round-Trip-Closure Method (RTC). These metrics have the attractive property that they are both zero if the integrator introduces zero error. Healy and Berry [1] used a number of different tests to study the accuracy of two numerical integrators, Runge-Kutta 45 and an 8th order Gauss-Jackson. Both MMS, or Zadunaisky’s test as they refer to it, and RTC, or Reverse Test, are mentioned in their work.
An additional benefit for using MMS and RTC metrics over the Hamiltonian metrics when determining the accuracy of numerical solutions is specifically important for symplectic integrators. Symplectic integrators, such as the Implicit Runge-Kutta methods, enforce the accuracy of the Hamiltonian at each iteration and thus reduce the ‘‘purity’’ of the Hamiltonian when it is used as a final independent check of accuracy of the converged solution. We utilize a recently developed path approximation method: the Modified Chebyshev Picard Iteration (MCPI). MCPI differs from the symplectic methods in that the constancy of the Hamiltonian is not explicitly enforced during the numerical integration process, but MCPI relies instead on the property that the Picard iteration process is theoretically a contraction mapping attracted to the exact solution under the conditions of the Picard convergence theorem. The conditions under which Picard is proven to be a contraction to the solution is that the acceleration function be smooth and at least once differentiable, and that the time interval over which the solution is sought belongs to a bounded interval (typically, less than three orbit periods) and finally, that the starting orbit approximation must have a bounded error relative to the unknown true solution. Typically, convergence is achieved over large time intervals, even with a straight line starting approximation, however a “warm start” closer to the solution is needed for efficient convergence. MMS and RTC lead to “exact” metrics for performing accuracy checks and comparisons between different numerical integrators. In the case of RTC, the convergence test is directly on the original differential equations and boundary conditions. In the case of MMS, a close neighbor of the sought solution is established with a small perturbing force for which a given smooth approximate solution exactly satisfies the slightly perturbed differential equations. The metrics associated with MMS and RTC are easily computed. These “external” validation/accuracy checks are not to be confused with adaptive tuning of the solution segments and the number of nodes when orthogonal function approximations are fused with Picard iteration to maintain accuracy of acceleration approximation and numerical quadratures that are a part of the implementation of MCPI. Furthermore, the MSS and RTC metrics are useful for virtually any method for numerical solution of differential equations and therefore has utility in evaluating the relative merits of competing algorithms.

2. METHOD OF MANUFACTURED SOLUTIONS

The Method of Manufactured Solutions [2, 3, 4] computes an analytical function near to the actual problem of interest. A new system of differential equations, that is slightly different from the original problem, is constructed and solved. The solution to this problem has an analytical solution, which if compared to the numerical solution will allow the numerical accuracy of the integrator to be tested.

Consider the nonlinear differential equation, with specified initial conditions:

\[ \dot{x}(t) = f(t, x(t)), \quad x(t_0) = x_0, \quad t_0 \leq t \leq t_f \]  

(1)

Suppose that the differential equation of Eq. (1) does not have an analytical solution. Further suppose that an approximate solution \( x_r(t) \) is available that does not satisfy Eq. (1) exactly but is believed to satisfy it with “small” but unknown errors. Suppose that \( x_r(t) \) is smooth and at least once differentiable. On substituting \( x_r(t) \) into Eq. (1), we can obtain an explicit algebraic solution for the error as

\[ d_r(t) = \dot{x}_r(t) - f(t, x_r(t)) \]  

(2)

or

\[ \dot{x}_r(t) = f(t, x_r(t)) + d_r(t) \]  

(3)

We can compute the norm \( \|d_r(t)\| \) to see if it is sufficiently small to consider \( x_r(t) \) a good starting approximation. Comparing Eqs (3) and (1) and reflecting for a moment, it is clear that \( x_r(t) \) is the exact analytical solution of the slightly disturbed differential equation

\[ \dot{x}(t) = f(t, x(t)) + d_r(t), \quad x(t_0) = x_r(t_0), \quad t_0 \leq t \leq t_f \]  

(4)

Since we have a candidate solution with a small \( \|d_r(t)\| \), Eq (4) can be considered a very close neighboring problem to the original one of Eq. (1), but with the important advantage that we know the exact analytical solution
One can argue that whatever numerical method is under evaluation for solving Eq. (1), can be evaluated on the perturbed system of Eq. (4), which should prove slightly more difficult for the numerical solver than solving the original unforced system of Eq. (1). Whatever numerical solution process under study can be used to solve the perturbed system of Eq. (4) and obtain an approximate solution \( \tilde{x}(t) \), however we know the exact solution of Eq. (4) is \( x_r(t) \), so we can compute the exact solution error \( \tilde{x}(t) - x_r(t) \) at any/all times. If the numerical method we are studying to solve Eq. (1) gives, for example, a 15 digit solution of the more difficult perturbed problem of Eq. (4), then we can be justifiably optimistic that it will solve Eq. (1) with similar precision. In particular, if

\[
\left\| \frac{d}{dt} (x_r(t)) \right\| < \varepsilon, \text{ say } (10^{-14}),
\]

then it is virtually certain that the numerical method used to generate \( \tilde{x}(t) \), when applied to Eq. (1), will produce a solution with 14 or more significant figures.

The main weakness with the MMS test is that that acceleration, \( \dot{x}_r(t) \), must be obtained by differentiating an approximation to the converged velocity solution. The quality of the approximation limits the ability of MMS to test the quality of the integrator. This is a drawback for the step integrators, but for MCPI the coefficients of the acceleration fit are already available due to the path approximation nature of the algorithm. No differentiation of the state trajectory approximation of the velocity is necessary, thus allowing MMS to honestly test the accuracy of the integrator, without the necessity of introducing other approximations.

### 3. ROUND-TRIP-CLOSURE

Round Trip Closure (RTC) is a test that measures the accumulative error that results during numerical integration. Consider the nonlinear differential equation, with specified initial conditions:

\[
\dot{x}(t) = f(t, x(t)), \quad x(t_0) = x_0, \quad t_0 \leq t \leq t_f
\]

(5)

Suppose that the differential equation of Eq. (5) does not have an analytical solution. An approximate solution may be obtained through numerical integration. As a specific example, consider propagating the trajectory of a spacecraft about the Earth, with specified initial conditions and final time. The gravitational acceleration experienced by the spacecraft varies as a function of position along the trajectory.

Having computed the trajectory, the final position is used as the new initial position, and the final time as the new initial time, as shown in Eq. (6).

\[
\dot{x}(t) = f(t, x(t)), \quad x(t_f) = x_f, \quad t_f \leq t \leq t_0
\]

(6)

The new initial conditions are propagated backwards in time along the trajectory in order to recover the initial conditions used for the forward integration. The error metric is evaluated as follows:

\[
J = 0.5 \left( \left\| \frac{r_0 - r_f}{r_0} \right\| + \left\| \frac{v_0 - v_f}{v_0} \right\| \right)
\]

(7)

For MCPI, which is a path approximation integrator, slightly varying the node locations along the reverse trajectory allows the solution to be computed using a slightly different gravity field, thus eliminating possible bias and/or aliasing issues that may arise due to performing the reverse calculations at the exact same node locations as the forward solution. Healy and Berry [1] mention this as being a disadvantage when testing step integrators in a perturbed environment. They comment that it does not measure any reversible integration error as it will be cancelled on the reverse trip when the sign of the step changes. However, the RTC method has been used extensively for performing numerical integration accuracy checks [5]. A high fidelity numerical integrator should recover the initial conditions with an accuracy of 14 significant figures, however, this will begin to decrease with long-term propagation and is a good measure of the achievable long-term propagation range of a numerical integrator.
4. MODIFIED CHEBYSHEV PICARD ITERATION

Modified Chebyshev Picard Iteration (MCPI) is an attractive numerical method for solving linear or non-linear differential and integral equations. MCPI combines the discoveries of two great mathematicians: Emile Picard (Picard Iteration) and Rafnuty Chebyshev (Chebyshev Polynomials), and recent developments in the associated linear algebra by Bai, Junkins, Feagin, et al. [6-15]. The original fusion of orthogonal approximation theory and Picard iteration was apparently introduced by Clenshaw and Norton in 1963 [16].

Picard observed that any first order differential equation
\[ \dot{x}(t) = f(t, x(t)), \] (8)
with an initial condition \( x(t_0) = x_0 \), and any integrable right hand side may be rearranged, without approximation, to obtain the following integral equation:
\[ x(t) = x(t_0) + \int_{t_0}^{t} f(\tau, x(\tau))d\tau. \] (9)

This re-arrangement, at first glance, does not appear to have made any progress, since the unknown trajectory \( x(t) \) is contained in the integrand on the right hand side. A sequence of approximate solutions \( x^{i}(t) \), \((i = 1, 2, 3, ..., \infty)\), of the true solution \( x(t) \) that satisfies this differential equation may be obtained through Picard iteration using the following Picard sequence of approximate paths \( \{x^{0}(t), x^{1}(t), x^{2}(t), x^{3}(t), \ldots \} \):
\[ x^{i}(t) = x(t_0) + \int_{t_0}^{t} f(\tau, x^{i-1}(\tau))d\tau, \quad i = 1, 2, \ldots . \] (10)

Picard proved an important convergence theorem that essentially states that for smooth, differentiable, single-valued nonlinear functions \( f(t, x(t)) \), there is a time interval \( |t_f - t_0| < \delta \) and a starting trajectory \( x^{0}(t) \) satisfying \( \|x^{0}(t) - x(t)\|_\infty < \Delta \), for suitable finite bounds \( (\delta, \Delta) \), the Picard sequence of trajectories represents a contraction operator that converges to the unique solution of the initial value problem. What was not apparently appreciated until the work of Bai et al. [6-8], is that these bounds are surprisingly large for the main initial value problem in celestial mechanics (\( \delta \) exceeds an orbit period, and the starting approximation for the trajectory can be a straight line osculating initial position and velocity).

In the first step toward the MCPI method, orthogonal Chebyshev polynomials are used as basis functions to approximate the integrand in Eq. (10) along the previous approximate trajectory \( x^{i-1}(t) \). Unlike traditional step-by-step integrators, for example the Runge-Kutta methods, MCPI is a path iteration method in which long state trajectory arcs are approximated and updated at all time instances on each iteration. Under usually satisfied and known theoretical circumstances, we can show [6] that the Picard sequence is a contraction mapping guaranteed to converge to the solution of Eq. (8). The system dynamics are normalized such that the timespan of integration is projected onto the domain \( \{-1 \leq \tau \leq +1\} \) of the Chebyshev polynomials, so the system states can be conveniently approximated using the Chebyshev basis functions. The orthogonal nature of the basis function means that the coefficients that linearly scale the basis functions can be computed independently as simple ratios of inner products with no matrix inversion. Since the Chebyshev polynomials are a complete set, we can achieve machine precision (if desired) approximation of any smooth integrand in Eq. (10) on each iteration and the resulting converged trajectory can approach a machine precision solution of the differential equation over large time spans. In Bai’s dissertation [6], she found that the actual time interval over which convergence is obtained for problems in celestial mechanics is over 3 orbits (for the case of an initial value problem and the usual Cartesian coordinate formulation of the equations of motion). For the two-point boundary value problem in Cartesian coordinates, however, she found that the time interval for which Picard iteration converges is reduced to about 0.38 of an orbit period.
As a consequence of the independence and orthogonality of the basis functions, the coefficients multiplying the Chebyshev basis functions may be computed, as an inner product of the basis functions with the integrand, in parallel by separate independent threads with no matrix inversion required. This independently computable integrand approximation coefficients is the first of two available layers of parallelization in the MCPI method. The second layer of parallelization is much more important and is enabled by the fact that acceleration over the entire state trajectory $x^{-1}(t)$ permits us to compute independently and simultaneously. Thus the calculation of the integrand functions (which must be computed as a function of the system states along the current approximate trajectory, at the nodes, as required for the discrete inner products leading to the approximation coefficients) can be performed at all nodes simultaneously in parallel processor threads. Using MCPI, over an order of magnitude speedup from traditional methods is achieved in serial processing, and an additional one-to-two orders of magnitude, are achieved in parallel architectures, depending on the specifics of the parallel implementation.

A key feature of MCPI is a non-uniform cosine sampling of the $[-1 \leq \tau \leq 1]$ domain of the called Chebyshev-Gauss-Lobatto (CGL) nodes: $\tau_j = -\cos(j \pi / N), j = 0, 1, 2, \ldots, N$. This set of samples has higher nodal density near the $\pm 1$ domain boundaries, which enables a higher accuracy solution near the boundaries to compensate for the Runge phenomena (a common concern whereby larger oscillatory errors may occur near the edges of the domain due to lack of support for the approximation outside the boundaries of the domain). The coefficients that linearly combine the Chebyshev basis functions are approximated by the method of least squares, which generally requires a matrix inversion. A consistent choice of basis functions, weights, and node locations to ensure orthogonality means that the matrix required to be inverted in the Normal Equations of least squares is diagonal, thus the inverse is trivial and the coefficient computation is independent.

Bai’s dissertation [6] extended the classical work of Clenshaw and Norton [16], and the more recent and related works of Feagin [15] Fukushima [17] and Shaver [18]. Bai established new convergence insights and optimized the solution of initial value problems utilizing vector-matrix formulations. Bai and Junkins applied MCPI to non-linear IVPs and orbit propagation in [7], and then showed promising results comparing MCPI to other higher order integrators such as Runge-Kutta-Nystrom 12(10). In reference [8] Bai and Junkins applied MCPI to efficiently solve Lambert’s orbit transfer problem in the usual Cartesian coordinates, and to solve an optimal control trajectory design problem, formulated in polar coordinates, more accurately and efficiently than the Chebyshev pseudospectral method. Notably, over intervals where the Picard iteration converges, there is no need to use a shooting method to solve Lambert problems and similar two point boundary value problems (TPBVPs). Furthermore, the MCPI algorithm renders the indirect (Pontryagin’s Principle) state, co-state differential equations solvable without a shooting method for a large class of problems. In [9] Bai and Junkins use MCPI in three-body station-keeping control problem for halo orbits, formulated as a sequence of TPBVPs. Subsequent publications by Junkins et al. [10], [11], and [12] further clarify the concept and derivation of MCPI and orthogonal approximation in general, and apply the method to various problems in astrodynamics. Reference [13] discusses an implementation of the MCPI algorithm for the IVP as an easily accessible library, mainly focused on the case of Cartesian coordinates.

A full derivation of MCPI is outside the scope of this paper. Instead we present flow charts in Fig. 1 that briefly summarize the algorithms represented in the compact vector/matrix formulation, which is computationally the most efficient way to implement the method. The above references provide detailed derivations, as well as examples and results that demonstrate the power of the MCPI algorithms with regard to efficiency and accuracy. Additionally, those references contain comparisons to other well-known integrators including high-order Runge-Kutta methods and the Gauss-Jackson method.
5. RESULTS AND DISCUSSION

Method of Manufactured Solutions

We consider three test cases (LEO, GEO, Molniya) and propagate each for 10 two-body orbital periods. The MMS error metric for determining the closeness of the analytical solution is computed as

$$\frac{\|d_i(t)\|}{\|f(t, x, (t))\|} < \varepsilon, \text{ say } (10^{-14}),$$

and the error metric for determining the closeness of the numerical approximation to the analytical solution is calculated as the maximum absolute difference between the position norms of the two trajectories (numerical and analytical).

In this paper we consider only MCPI and RKN(12)10. As mentioned earlier, a drawback for step integrators is that the velocity must be approximated and differentiated to obtain acceleration. This limits the ability of MMS to quantify the accuracy of the algorithm. For the MATLAB implementation of RKN(12)10 used for this analysis, it is possible to specify an input time array on a cosine distribution, thus allowing the velocity to be fit and approximated with Chebyshev polynomials, and then differentiated using Chebyshev polynomials of the second kind [6]. Interpolation with Chebyshev polynomials is very accurate compared with other methods such as power series approximation. The MATLAB Gauss-Jackson algorithm used for this analysis does not permit specification of a desired input time array, thus leading to a less accurate approximation. Until further investigation is performed with regard to better fitting techniques, we have decided to exclude it from the analysis.

Fig. 2 shows MMS error for MCPI and RKN(12)10 plotted as a function of increasing orbital distance. Both integrators are relatively stable, maintaining 12 digits of accuracy over this interval. For this GEO test case, MCPI appears to be more accurate that RKN(12)10. Fig. 3 shows how the MMS error for MCPI (LEO, GEO, Molniya) gradually increases over a range of decreasing Hamiltonian accuracies. The test is performed over 50 orbits.
Round Trip Closure

We consider 3 test cases (LEO, GEO, Molniya) and propagate each forward in time for 50 two-body orbital periods. The final states are then used as the initial conditions and time is reversed to propagate backwards and recover the initial conditions. Fig. 4 shows the Molniya test case integrated forward and backward in time with MCPI. The node locations on the return trajectory are intentionally selected to be at different positions from that on the forward trajectory. This is done to eliminate aliasing and error cancellation that may arise from performing the reverse calculation at the exact same node locations as the forward solution. A subtraction of the states is done over the entire trajectory and the difference is plotted in Fig. 4.

Neither solution in Fig. 4 is correct because each is effected by numerical error that accumulates during the propagation. The left most values are most significant because these represent the error in the recovery of the initial conditions after propagating forward for 50 orbits and then backwards for 50 orbits. The error is smallest on the far right because this is where the final states at the end of 50 orbits of forward propagation are set as the initial conditions for the backward propagation. The general trend shows the error slowly accumulating over time. In addition to the general trend there are also variations that occur periodically as a function of position around the orbit. See the enlarge inset at the bottom left of the figure.
RTC errors are computed for each test case over a range of tolerances \((1 \times 10^{-7}, 1 \times 10^{-9}, 1 \times 10^{-11}, 1 \times 10^{-13}, 1 \times 10^{-15})\). The error metric, Eq. (12), is used to quantify the accuracy of each RTC solution. In Figs. 5 through 7, the RTC error is plotted as a function of Hamiltonian accuracy. As expected, the general trend shows the RTC error increasing as the accuracy of the solution decreases. In general, MCPI seems to perform better at higher solution accuracies than Gauss-Jackson. For the Molniya case at low Hamiltonian accuracies MCPI has a large RTC error. This is likely due to sub-optimal segmentation and node distribution. The algorithm was tuned by hand for the high accuracy cases, and the same segmentation is used for the low accuracy cases. We anticipate improved results for the low accuracy range once the optimal segmentation scheme is implemented [19]. Fig. 8 shows how the RTC error changes as the propagation time increases from 10 to 50 orbits. We note that the MCPI Molniya test case shows some variation (improved accuracy after 50 orbit RTC compared with 40 orbit RTC). This is likely depicting the variations observable in Fig. 4. In Fig. 9 we take the average of RTC error values on either side of the desired 50 orbit propagation distance. Considerable fluctuation is evident over this small range, thus highlighting the importance of computing an average value. Overall, the three integrators show relatively similar stability trends.

\[
J = 0.5 \left( \frac{|r_0 - r_f|}{|r_0|} + \frac{|v_0 - v_f|}{|v_0|} \right) \tag{12}
\]

**Fig. 5** LEO: Comparison of RTC errors over 50 orbits for Gauss-Jackson, MCPI and RKN(12)10, as a function of Hamiltonian accuracy.

**Fig. 6** GEO: Comparison of RTC errors over 50 orbits for Gauss-Jackson, MCPI and RKN(12)10, as a function of Hamiltonian accuracy.

**Fig. 7** Molniya: Comparison of RTC errors over 50 orbits for Gauss-Jackson, MCPI and RKN(12)10, as a function of Hamiltonian accuracy.
Fig. 8 Comparison of RTC errors for Gauss-Jackson, MCPI and RKN(12)10, as a function of orbital propagation distance. Top to bottom: LEO, GEO, Molniya.

Fig. 9 Variation of RTC error over two orbital periods in the vicinity of 50 orbits RTC.

6. CONCLUSION

A common method for validating the accuracy of numerical integrators is confirming that the Hamiltonian of the converged solution maintains machine precision for the time interval over which the computation was performed. This is a useful test for conservative systems, but for non-conservative systems the Hamiltonian check is no longer sufficient and other methods for validating the accuracy of the solution must be employed.

Two methods, the Method of Manufactured Solutions (MMS) and Round Trip Closure (RTC) are employed for comparing the accuracy of three numerical integrators: Modified Chebyshev Picard Iteration, Gauss-Jackson and Runge-Kutta-Nystrom. The two tests reveal all three integrators are comparably stable for long-term integration for LEO, GEO and highly eccentric orbits. Of the three MCPI is the most efficient for serial computation (see sister paper [20]) and is also ideally suited for parallel computation to enable further speedup.
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8. REFERENCES


