Rigorous Integration of Flows and ODEs using Taylor Models

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ABSTRACT

Taylor models combine the advantages of numerical methods and algebraic approaches of efficiency, tightly controlled recourses, and the ability to handle very complex problems with the advantages of symbolic approaches, in particularly the ability to be rigorous and to allow the treatment of functional dependencies instead of merely points. The resulting differential algebraic calculus involving an algebra with differentiation and integration is particularly amenable for the study of ODEs and PDEs based on fixed point problems from functional analysis. We describe the development of rigorous tools to determine enclosures of flows of general nonlinear differential equations based on Picard iterations. Particular emphasis is placed on the development of methods that have favorable long term stability, which is achieved using suitable preconditioning and other methods. Applications of the methods are presented, including determinations of rigorous enclosures of flows of ODEs in the theory of chaotic dynamical systems.

Categories and Subject Descriptors

I.1.2 [**Symbolic and Algebraic Manipulation**]: Algorithms; G.1.7 [**Numerical Analysis**]: Ordinary Differential Equations—*initial value problems, multistep and multivalue methods, error analysis*

General Terms

Algorithms

Keywords

Taylor model, rigorous ODE integration, rigorous flow integration, nonlinear flow of ODE, initial value problem, Taylor polynomial, error bound, interval arithmetic, double pendulum

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1. INTRODUCTION

An n-th order Taylor model of a multivariate function f that is $(n+1)$ times continuously partially differentiable on the domain D consists of the n-th order multivariate Taylor polynomial P, expanded around a point $x_0 \in D$ and representing a high order approximation of the function f, and a remainder error bound interval I for verification, the width of which scales in $(n+1)$-st order [5]. P and I satisfy

$$f(x) \in P(x - x_0) + I \text{ for all } x \in D.$$

In the following we will assume $x_0 = 0$ for notational convenience. Details of the background of the methods is given in a companion paper and will not be presented here. In the following we study the performance of methods of rigorously verified solutions of v dimensional differential equations

$$r' = f(r(t), t).$$

Specifically, we study the dependence of the final solution r_f at the time t on the initial conditions r_i in terms of Taylor models via

$$r_f = P(r_i, t) + I \text{ for all } r_i \in D.$$

An algorithm is developed that will allow the treatment of such problems, and examples about the performance of the method will be given.

2. AN EFFICIENT TAYLOR MODEL BASED FLOW SOLVER

2.1 The Reference Trajectory

The first step of obtaining a rigorously verified solution for the next time step is to determine the Taylor expansion in time of the solution of the ODE for the center point c_0, called the reference trajectory, i.e. to obtain the solution in the form

$$c(t) = c_0 + c_1 \cdot (t - t_0) + c_2 \cdot (t - t_0)^2 + ... + c_n \cdot (t - t_0)^n.$$

Methods to obtain this solution have been well known from the very beginning of the use of interval methods and automatic differentiation, see for example [7]. We follow a method that is particularly convenient and elegant, based on the Picard operator representation of the ODE

$$c(t) = c_0 + \int_0^t f(r(t'), t) dt'$$

The approach is based on the differential algebraic structure of the space ${}_nD_{(v+1)}$ of Taylor polynomials in $(v+1)$

variables and order n with truncation multiplication [2]. Utilizing the equivalence relation

$$f =_n g$$

on the space of smooth functions to denote agreement of all derivatives from 0 to n at the origin, and denoting the class of f by $[f]$, we can introduce addition, multiplication and scalar multiplication on the classes based on the corresponding operations on functions. The resulting structure forms an algebra. An algebra is a differential algebra if there is an operation ∂, called a derivation, that satisfies

$$\partial(s \cdot a + t \cdot b) = s \cdot \partial a + t \cdot \partial b \text{ and}$$
$$\partial(a \cdot b) = a \cdot (\partial b) + (\partial a) \cdot b$$

for any vectors a and b and scalars s and t. The natural partial derivative operations $[f] \to [\partial_i f]$ does not introduce a differential algebra because the loss of the highest order, a problem that is remedied in the next subsection. However, the corresponding inverse operation, the anti-derivation, allows porting of the Picard equation into the equivalence class of polynomials, and obtaining a solution in finitely many steps by mere iteration. Indeed, each iteration raises the order to which the solution is known by one. This approach is inexpensive since it only involves one-dimensional Taylor arithmetic.

2.2 The Nonlinear Flow

The second step is to obtain the Taylor expansion in time to order n **and** initial conditions to order k. This is usually the most expensive step, since it necessarily requires the use of $(v+1)$ dimensional Taylor arithmetic. In previous work[4][3][6], this has been accomplished also by iteration of the Picard operator on the multidimensional initial condition. While this approach is straightforward and elegant, it is not necessarily efficient, since it requires a re-evaluation of the right hand side f in each step of the solution process. We note that methods to solve the problem for $k = 1$ have been known for a long time, based on the derivation of adjoint differential equations for the partial derivatives of the flow.

We pursue a novel method here that represents a generalization of a method originally introduced in beam physics [1][2]. We introduce new "perturbation" variables $\tilde{r}$ such that

$$r(t) = c(t) + A \cdot \tilde{r}(t)$$

where the matrix A provides a preconditioning of the ODE for $\tilde{r}(t)$ via

$$\tilde{r}' = A^{-1} \left[f(c(t) + A \cdot \tilde{r}(t)) - c'(t) \right].$$

The next step involves evaluating the ODE for $\tilde{r}'$ in Taylor arithmetic, and thus to obtain a Taylor expansion of the ODE, i.e.

$$\tilde{r}' = P(\tilde{r}, t)$$

up to order n in time and k in $\tilde{r}$, where $k \le n$. It is very important for the further discussion that the polynomial P will have no constant part, i.e.

$$P(0, t) = 0.$$

The subsequent procedure is based on the concept of the Lie derivative. Let $r' = f(r, t)$ be a dynamical system. Let g be a variable in state space, and let us study $g(r(t))$, i.e. along a solution of the ODE. From the chain rule we apparently have

$$\frac{d}{dt} g(t) = f \cdot \nabla g + \frac{\partial g}{\partial t}.$$

Introducing the Lie derivative $L_f = f \cdot \nabla + \partial/\partial t$, we have

$$\frac{d^n}{dt^n} g = L_f^n g \text{ and } g(t) \approx \sum_{i=0}^{n} \frac{(t-t_0)^i}{i!} \, L_f^i g \Big/_{t=t_0}$$

utilizing the Lie derivative, and it is now possible to remedy the difficulty that the natural derivation operation introduced above loses order. However, consider the modified operation ∂_f with

$$\partial_f g = f \cdot \nabla g.$$

It follows that if f is origin preserving, i.e. $f(0) = 0$, then ∂_f is a derivation on the space ${}_nD_{(v+1)}$. Indeed, while each derivative operation in the gradient ∇g loses the highest order, the subsequent multiplication with f and the fact that $f(0) = 0$ entails that the missing order in ∇g does not matter. This is the case since in the operations to compute $f \cdot \nabla g$, the unknown highest order terms of ∇g are multiplied with the (vanishing) zeroth order terms of f

Utilizing the concept of the Lie derivative, we can now obtain the polynomial solution $\tilde{r}(t)$ depending on time to order n and initial conditions to order k of the flow simply by evaluating

$$\tilde{r}(t) = \sum_{i=0}^{n} \frac{(t-t_0)^i}{i!} \cdot \left(P \cdot \nabla + \frac{\partial}{\partial t} \right)^i \tilde{r}_0 \Big/_{t=t_0}$$

where the fact that $P(0, t) = 0$ restores the derivatives lost in the operation ∇. On the other hand, the term $\partial/\partial t$ that appears without origin-preserving factor limits the expansion order in time t to order n.

2.3 Performance of Lie Derivative Flow Methods

For complicated right hand sides f, the method presented here has several advantages. In fact, each term in the Lie derivative sum requires $v+1$ derivations, which are very cheap and amount to merely a re-shuffling of Taylor coefficients, and it requires v multiplications. However, only a single evaluation of the right hand side of f in ${}_nD_{(v+1)}$ is needed in the step of obtaining P.

On the other hand, in the conventional algorithm utilized in [6] and earlier methods, an evaluation of f is required in each iteration of the Picard operation, for a total of n such evaluations. Thus, the new method performs superior if the evaluation of f requires more than v multiplications. Since f depends on $(v+1)$ variables which have to enter the right hand side, in practice this is very often the case.

On the other hand, if the function f does not satisfy this, for example in the purely linear case involving only scalar multiplications, this is not the case; but in this case, also the resulting P will show much sparsity (in the linear case, all higher order terms vanish), and in any implementation of the Taylor model operations supporting sparsity, the multiplication with P in the Lie derivative is inexpensive.

Table 1: Comparison of the performance for the double pendulum initial value problem by VNODE, ValEncIA, and COSY-VI. *Data based on a Matlab-Intlab implementation / a C++ interval library.

ODE Time t	CPU VNODE	CPU ValEncIA	CPU COSY-VI
0.5	15.4 sec	5880 sec / 94 sec *	0.51 sec
1.0	(breakdown $t < 0.6$)	(breakdown $t < 0.6$)	2.04 sec

2.4 Rigorous Error Treatment via Defect Integrals

In the third step of the rigorous method, we need to provide a rigorous estimate for the error made in the integration. For this purpose, we now introduce a set of variables $\tilde{e}$, the error variables, such that the flow rigorously satisfies

$$r(t) = c(t) + A \cdot \tilde{r}(t) + \tilde{e}.$$

Apparently the differential equation for $\tilde{e}(t)$ satisfies

$$\tilde{e}' = f(c(t) + A \cdot \tilde{r}(t) + \tilde{e}) - c'(t) - A \cdot \tilde{r}'(t).$$

However, evaluating the differential equation of $\tilde{e}'$ in Taylor arithmetic leads to the remarkable result

$$\tilde{e}' = 0$$

up to order $n-1$ in time and k in initial conditions. Of course this is not the real ODE, since we are missing the remainder errors of the function f. However, evaluating the ODE for $\tilde{e}'$ in Taylor model arithmetic[5] with a remainder interval I allowing for a maximal value of $\tilde{e} \in I$, we obtain a very small interval remainder term R. The value of $\tilde{e}'$ is then limited by R, i.e.

$$\tilde{e}' \in R.$$

Using a linear bounding cone for the evolution of $\tilde{e}'$ thus given, we obtain a fully verified solution for step sizes Δt that satisfy $R \cdot \Delta t \subset I$.

The above summarizes the behavior of the Lie derivative based rigorous flow integrator for the single step. A full discussion requires the understanding of longer term error propagation, which in turn rests on a proper choice of preconditioning matrices A, as well as efficient methods of step size control.

3. A PERFORMANCE EXAMPLE

In the following we will study some properties of the performance of the methods for the case of the double pendulum, a system that is known to exhibit chaoticity and is difficult to integrate precisely for long periods of time. The pendulum satisfies the ODEs

$$\begin{aligned}
\frac{d^2}{dt^2}\psi_1 &= \frac{l_1 m_2 \left[l_2(\dot{\psi}_1+\dot{\psi}_2)^2 + l_1\dot{\psi}_1^2\cos\psi_2\right]}{l_1^2\left[m_1+m_2\sin^2\psi_2\right]}\sin\psi_2 \\
&\quad + g\cdot\frac{-l_1(m_1+m_2)\sin\psi_1 + l_1 m_2\cos\psi_2\sin(\psi_1+\psi_2)}{l_1^2\left[m_1+m_2\sin^2\psi_2\right]} \\
\frac{d^2}{dt^2}\psi_2 &= -\frac{(l_1(m_1+m_2)+l_2 m_2\cos\psi_2)l_1\dot{\psi}_1^2}{l_1 l_2(m_1+m_2\sin^2\psi_2)}\sin\psi_2 \\
&\quad - \frac{l_2 m_2(l_2+l_1\cos\psi_2)(\dot{\psi}_1+\dot{\psi}_2)^2}{l_1 l_2(m_1+m_2\sin^2\psi_2)}\sin\psi_2 \\
&\quad + g\cdot\frac{(m_1+m_2)(l_2+l_1\cos\psi_2)\sin\psi_1}{l_1 l_2(m_1+m_2\sin^2\psi_2)} \\
&\quad - g\cdot\frac{(l_1(m_1+m_2)+l_2 m_2\cos\psi_2)\sin(\psi_1+\psi_2)}{l_1 l_2(m_1+m_2\sin^2\psi_2)}.
\end{aligned}$$

For parameters and initial conditions, we consider the values

$$(l_1, l_2, m_1, m_2, g) = (1, 1, 1, 1, 9.81)$$

and

$$\begin{aligned}
\psi_1(t=0) &\in \frac{3\pi}{4} + \frac{1}{100}\frac{3\pi}{4}[-1,+1] \qquad (1)\\
\psi_2(t=0) &= -1.726533538 \\
\dot{\psi}_1(t=0) &= 0.4138843714 \\
\dot{\psi}_2(t=0) &= 0.6724072960
\end{aligned}$$

which lie in the chaotic regime. In order to assess the performance of the COSY-VI code utilizing the above integrator based on Taylor models, we study the case of integration from $t=0$ to $t=0.5$ and $t=1.0$. We compare it with the performance of two other verified integration codes, VNODE and ValEncIA as reported by Rauh [8].

The two data for CPU times in Table 1 by ValEncIA are based on a Matlab-Intlab implementation, and a C++ interval library offering better performance. Apparently the COSY implementation is superior to the two other codes both in terms of actual execution time, as well as the ability to integrate over a longer time span, while both other codes already fail for the ODE time $t < 0.6$.

An interesting test for the performance of a Taylor model based method lies with the fact that the double pendulum preserves energy. Evaluating energy in Taylor model arithmetic over the entire flow at any two points in the integration, and subtracting the results, must result in a tight enclosure of zero. The total Energy E is given as

$$E = m_1\cdot g\cdot y_1 + m_2\cdot g\cdot y_2 + \frac{1}{2}m_1\left(\dot{x}_1^2+\dot{y}_1^2\right) + \frac{1}{2}m_2\left(\dot{x}_2^2+\dot{y}_2^2\right).$$

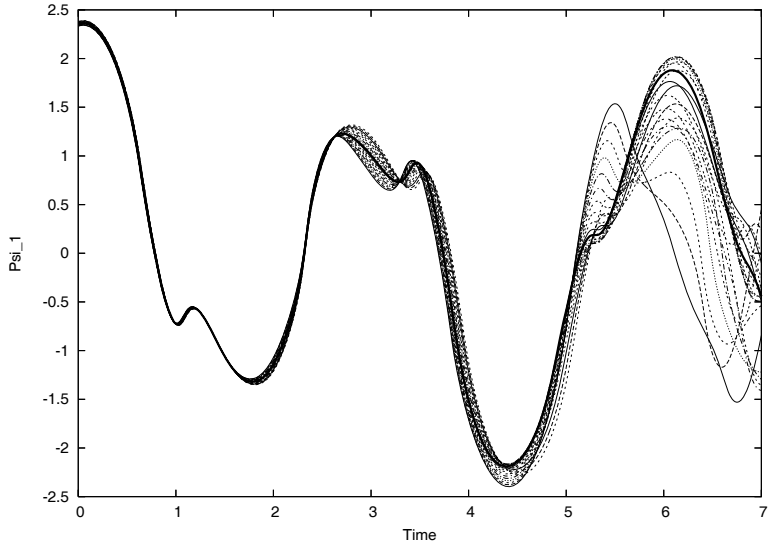

Figure 1: Evolution of ψ_1 of the double pendulum problem. The center orbit (solid) and 20 different orbits originating in the initial condition box are shown. The initial condition box is given by $\psi_1(0) \in 3\pi/4 + 1/100 \cdot 3\pi/4 \cdot [-1, +1]$, $\psi_2(0) = -1.726533538$, $\dot{\psi}_1(0) = 0.4138843714$ and $\dot{\psi}_2(0) = 0.6724072960$.

Elementary arithmetic shows that

$$
\begin{aligned}
x_1 &= l_1 \cdot \sin\psi_1 \\
x_2 &= x_1 + l_2 \cdot \sin(\psi_1 + \psi_2) \\
y_1 &= -l_1 \cdot \cos\psi_1 \\
y_2 &= y_1 - l_2 \cdot \cos(\psi_1 + \psi_1) \\
\dot{x}_1 &= \dot{\psi}_1 \cdot l_1 \cdot \cos\psi_1 \\
\dot{x}_2 &= \dot{x}_1 + (\dot{\psi}_1 + \dot{\psi}_2) \cdot l_2 \cdot \cos(\psi_1 + \psi_2) \\
\dot{y}_1 &= \dot{\psi}_1 \cdot l_1 \cdot \sin\psi_1 \\
\dot{y}_2 &= \dot{y}_1 + (\dot{\psi}_1 + \dot{\psi}_2) \cdot l_2 \cdot \sin(\psi_1 + \psi_2).
\end{aligned}
$$

Utilizing this, we obtain for a Taylor model evaluation of the energy at $t = 0$ the following polynomial coefficients and remainder bound:

```
 I  COEFFICIENT            ORDER EXPONENTS
 1   6.636304564436251       0   0 0  0 0  0
 2  0.4629982784681443       1   1 0  0 0  0
 3  -.1650152672869661E-02   2   2 0  0 0  0
 4  -.4284009231437226E-04   3   3 0  0 0  0
 5  0.7634228476230531E-07   4   4 0  0 0  0
 6  0.1189166522762920E-08   5   5 0  0 0  0
 7  -.1412752780648741E-11   6   6 0  0 0  0
 8  -.1571866492860271E-13   7   7 0  0 0  0
R [-.1538109061161243E-012,0.1517608952722424E-012]
```

Performing the same at $t = 0.5$, we obtain the following Taylor model:

```
 I  COEFFICIENT            ORDER EXPONENTS
 1   6.636304564436253       0   0 0  0 0  0
 2  0.4629982784681632       1   1 0  0 0  0
 3  -.1650152672942219E-02   2   2 0  0 0  0
 4  -.4284009217517837E-04   3   3 0  0 0  0
 5  0.7634212049420934E-07   4   4 0  0 0  0
 6  0.1189297979605227E-08   5   5 0  0 0  0
 7  -.1487493064301731E-11   6   6 0  0 0  0
 8  0.1498746352978318E-13   7   7 0  0 0  0
 9  -.8978311500296960E-14   8   8 0  0 0  0
10  0.1732136627097570E-14   9   9 0  0 0  0
11  -.1410358744591400E-15  10  10 0  0 0  0
12  -.3488804283416099E-16  11  11 0  0 0  0
13  0.1647113913603616E-16  12  12 0  0 0  0
R [-.6845903858358710E-010,0.7016561210090576E-010]
```

which leads to a Taylor model difference of

```
 I  COEFFICIENT            ORDER EXPONENTS
 1  0.2664535259100376E-14   0   0 0  0 0  0
 2  0.1881828026739640E-13   1   1 0  0 0  0
 3  -.7255849567011641E-13   2   2 0  0 0  0
 4  0.1391938932279908E-12   3   3 0  0 0  0
 5  -.1642680959724263E-12   4   4 0  0 0  0
 6  0.1314568423076692E-12   5   5 0  0 0  0
 7  -.7474028365299068E-13   6   6 0  0 0  0
 8  0.3070612845838590E-13   7   7 0  0 0  0
 9  -.8992317058282886E-14   8   8 0  0 0  0
10  0.1732136627097570E-14   9   9 0  0 0  0
11  -.1410358744591400E-15  10  10 0  0 0  0
12  -.3488804283416099E-16  11  11 0  0 0  0
13  0.1647113913603616E-16  12  12 0  0 0  0
R [-.6861710643018788E-010,0.7032572995835042E-010]
```

which is indeed a very tight enclosure of zero.

We now attempt to assess the long term behavior of the integration of the initial condition, utilizing COSY-VI's domain decomposition features. To assess the complexity of the problem, we first perform integration of the domain box above via an ordered sampling of point solutions originating in the initial condition box (1). We observe

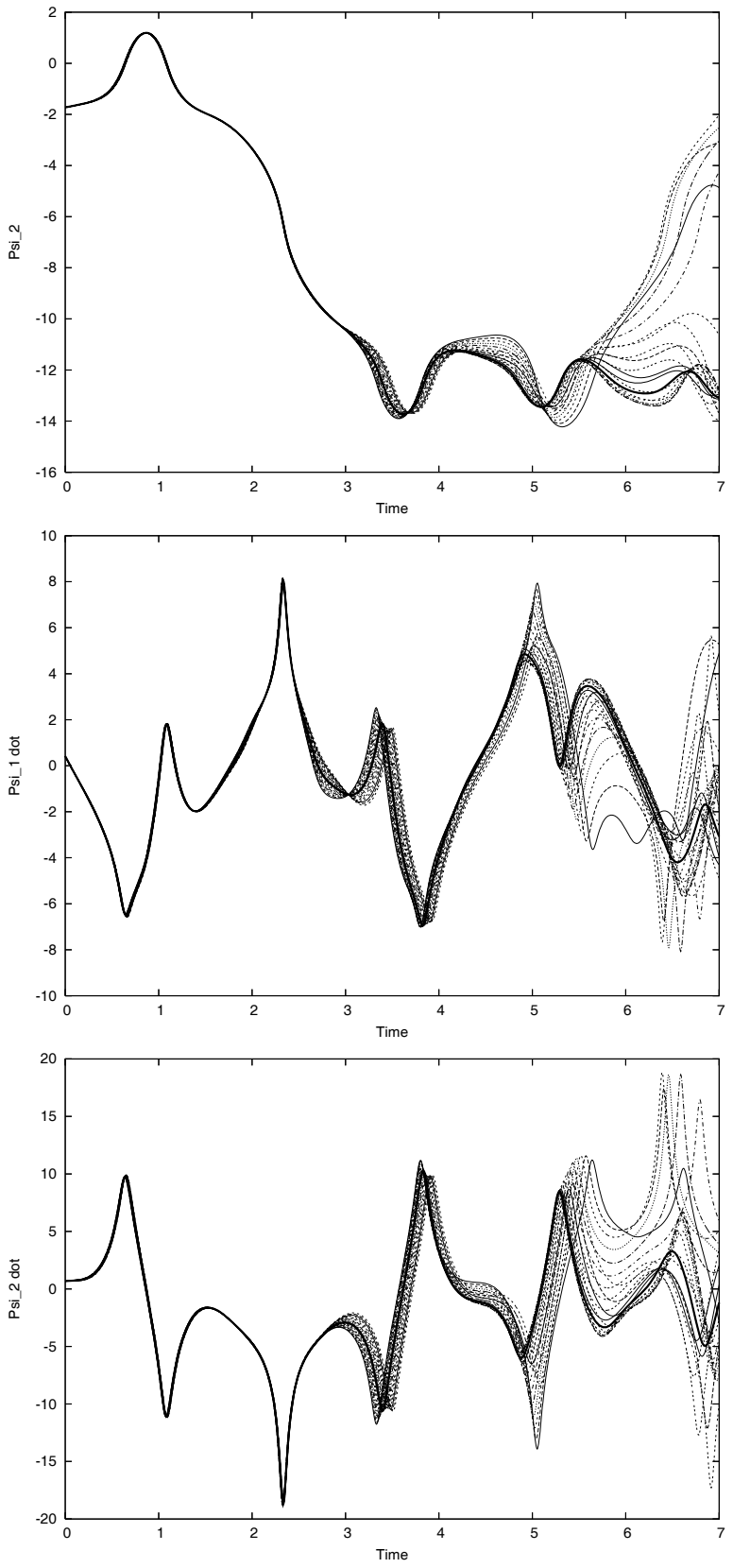

Figure 2: Evolution of ψ_2 (top), $\dot{\psi}_1$ (middle) and $\dot{\psi}_2$ (bottom) of the double pendulum problem. The center orbit (solid) and 20 different orbits originating in the initial condition box are shown. The initial condition box is given by $\psi_1(0) \in 3\pi/4 + 1/100 \cdot 3\pi/4 \cdot [-1, +1]$, $\psi_2(0) = -1.726533538$, $\dot{\psi}_1(0) = 0.4138843714$ and $\dot{\psi}_2(0) = 0.6724072960$.

- around $t = 2$ a noticeable broadening of ranges,
- around $t = 5$ an angle spread by $> 2\pi$, corresponding to different numbers of full revolutions,
- around $t = 30$ the accuracy limit of conventional non-verified integrators.

Figures 1 and 2 show the evolution of the four coordinates ψ_1, ψ_2, $\dot{\psi}_1$ and $\dot{\psi}_2$ of the problem for 20 different orbits and the center orbit originating in the domain box of interest for an integration time of $t = 7$, at which time solutions diverge so strongly that they occupy already approximately one quarter of the phase space available due to the energy constraints.

Performing a fully verified computation with COSY-VI utilizing domain decomposition methods allows integration to an integration time of about $t = 25$ using automatic domain decomposition methods. The number of boxes required grows exponentially owing to the chaotic nature of the system, requiring approximately 10^3 boxes for $t = 12$ and 10^6 boxes for $t = 25$.

4. ACKNOWLEDGMENTS

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