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Exponential integrators for coupled self-adjoint non-autonomous partial differential systems

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ABSTRACT

We consider the numerical integration of coupled self-adjoint non-autonomous partial differential systems. Under convergence conditions, the solution can be written as a series expansion where each of its terms correspond to solutions of linear time dependent matrix differential equations with oscillatory solutions that must be solved numerically. In this work, we analyze second order of Magnus integrators whose numerical error grows with the number of terms considered in the truncated series, n, at a rate that still allows us to guarantee convergence of the numerical series. In addition, the integrator can be implemented with a recursive algorithm such that the computational cost of the method grows only linearly with the number of terms of the series. Higher order Magnus integrators are also analyzed. Commutator-free Magnus integrators can be used with a similar recursive algorithm and can provide highly accurate results, but they show a faster error growth with n, and some caution must be taken if these methods are used. Numerical experiments confirm the performance of the proposed algorithm.

1. Introduction

Let us consider the numerical integration of self-adjoint partial differential equations of the type

$$(P(t)u_t(x,t))_t = Q(t)u_{xx}(x,t); \quad 0 \leqslant x \leqslant d, \quad t \geqslant 0, \tag{1}$$

with initial and boundary conditions given by

$$\left.\begin{array}{ll} u(0,t) = u(d,t) = 0, & t \geqslant 0, \\ u(x,0) = f(x), & 0 \leqslant x \leqslant d, \\ u_t(x,0) = g(x), & 0 \leqslant x \leqslant d, \end{array}\right\} \tag{2}$$

where $u(x,t),\ f(x),\ g(x) \in \mathbb{R}^r$. We consider the case where:

(I) $P(t),\ Q(t) \in \mathbb{R}^{r\times r}$ are symmetric positive definite matrices.
(II) $-P'(t)$ and $Q'(t)$ are both symmetric positive (or negative) semidefinite matrices.
(III) $f(x)$ is three times differentiable and $f^{(3)}(x)$ is piecewise continuous in $[0,d]$ with $f(0) = f(d) = f^{(2)}(0) = f^{(2)}(d) = 0$.
(IV) $g(x)$ is twice differentiable with $g^{(2)}(x)$ piecewise continuous in $[0,d]$ and $g(0) = g(d) = 0$.

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The system (1) appears frequently in the study of microwave heating processes, where the variations of the dielectric properties of the material with temperature, density, moisture content and other parameters make the system non-autonomous, see [10,13] for more details. Systems of type (1) can also be found on models for the study of electromagnetic processing of homogeneous materials at high power densities or in the analysis of multi mode microwave applicators, see [8,17]

Under conditions (I)–(IV), the problem (1),(2) has, at most, a twice continuously differentiable solution [16, Section 2]. We look for a numerical solution, and to this purpose we first consider separation of variables. In a bounded domain $D(d,T)=\{(x,t);\ 0\leqslant x\leqslant d,\ 0\leqslant t\leqslant T\}$, for a given $T>0$, the solution can be formally written as a convergent series

$$u(x,t)=\sum_{n\geqslant 1}\left\{Y_n(t)a_n+\widetilde{Y}_n(t)b_n\right\}\sin\left(\frac{n\pi x}{d}\right), \tag{3}$$

where $a_n,\ b_n\in\mathbb{R}^r$ are given by

$$a_n=\frac{2}{d}\int_0^d f(x)\sin\left(\frac{n\pi x}{d}\right)dx,\quad b_n=\frac{2}{d}\int_0^d g(x)\sin\left(\frac{n\pi x}{d}\right)dx. \tag{4}$$

The matrices $Y_n(t),\ \widetilde{Y}_n(t)\in\mathbb{R}^{r\times r}$ are given by

$$Y_n(t)=[I_r\quad 0_{r\times r}]V_n(t),\quad \widetilde{Y}_n(t)=[I_r\quad 0_{r\times r}]W_n(t), \tag{5}$$

with $V_n(t),\ W_n(t)\in\mathbb{R}^{2r\times r}$ verifying the initial value problems (IVPs)

$$V'_n(t)=M(t,n)V_n(t),\quad V_n(0)=\begin{bmatrix} I_r\\ 0_{r\times r}\end{bmatrix}; \tag{6}$$

$$W'_n(t)=M(t,n)W_n(t),\quad W_n(0)=\begin{bmatrix} 0_{r\times r}\\ P(0)\end{bmatrix}; \tag{7}$$

where

$$M(t,n)=\begin{bmatrix} 0_{r\times r} & P^{-1}(t)\\ -\left(\frac{n\pi}{d}\right)^2 Q(t) & 0_{r\times r}\end{bmatrix}\in\mathbb{R}^{2r\times 2r}, \tag{8}$$

see [16] for details. Here, $0_{r\times r},\ I_r\in\mathbb{R}^{r\times r}$ denotes the null and identity matrices, respectively. Note that, from our assumptions, $P(t),\ Q(t)$ are non-singular matrices for all $t\geqslant 0$.

Given a tolerance, it is possible to find n_0 such that the truncated series for $n\leqslant n_0$ has an error below than this tolerance. However, in general, the solution for the matrices $Y_n(t),\ \widetilde{Y}_n(t),\ n=1,2,\ldots,n_0$ can not be obtained in a closed form and must be computed numerically (typically on a mesh $0<t_1<t_2<\ldots<t_L$ where L also depends on n_0), being this the most costly part for the algorithm.

Since the performance of standard explicit integrators deteriorates, in general, as the value of n grows, implicit methods are usually required to numerically solve the equations. However, in general, one needs to take $L=\mathcal{O}(n_0^2)$, i.e. the mesh size has to be chosen inversely proportional to n_0^2 and, in each interval, the method has to be applied n_0 times (for $n=1,2,\ldots,n_0$). As a result, the matrices $Q(t)$ and $P^{-1}(t)$ need to be evaluated in a number of mesh points which grows as n_0^2, and the method has to be applied $\mathcal{O}(n_0^3)$ times.

On the other hand, most exponential integrators can deal efficiently with the numerical solution for relatively large values of n. Usually, one can take $L=\mathcal{O}(n_0)$ and on each mesh the exponentials have to be computed for each value of $n\leqslant n_0$.

The contributions (under convergence conditions) of $Y_n(t),\ \widetilde{Y}_n(t)$ to the solution (3) decrease with n, but the errors and computational cost of most numerical integrators increase with n. For this reason, we consider a class of exponential integrators based on the Magnus series expansion which provides sufficiently accurate solutions as n grows and the exponentials can be computed using a simple recursive relation such that the computational cost of each term is irrespective of the value of n. The numerical solutions obtained are also such that the series solution remains still convergent.

The paper is organized as follows. In Section 2, the convergence of the formal series solution (3) is established. In section 3, numerical methods based on Magnus expansion are proposed in order to solve the IVPs (6)–(8). Exploiting the structure of the matrices, we found that the computational cost of the proposed method is very advantageous with respect to standard numerical methods. The convergence of the series obtained by the numerical scheme is studied in Section 4. Section 5 deals with the presentation of numerical experiments in order to test the effectiveness of the proposed algorithm. Conclusions are presented in the last section.

Throughout this paper, $\|\cdot\|_2$, denotes the usual Euclidean norm of a vector in $\mathbb{R}^r$, and $\|\cdot\|$, denotes the 2-norm of a square matrix in $\mathbb{R}^{r\times r}$.

2. Convergence of the formal series solution

We first review the most relevant results on the convergence of the series solution (see [16] for more details). Under the assumptions (I)–(IV), existence solutions of (5)–(8) are guaranteed and, given $T>0$, there exists a constant δ such that