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Magnus series expansion method for solving nonhomogeneous stiff systems of ordinary differential equations

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Abstract

In this paper, Magnus Series Expansion Method, which is based on Lie Groups and Lie algebras is proposed with different orders to solve nonhomogeneous stiff systems of ordinary differential equations. Using multivariate Gaussian quadrature, fourth (MG4) and sixth (MG6) order method are presented. Then, it is applied to nonhomogeneous stiff systems using different step sizes and stiffness ratios. In addition, approximate and exact solutions are demonstrated with figures in detail. Moreover, absolute errors are illustrated with detailed tables.

Keywords: Geometric integration; lie group method; linear differential equations; magnus series expansion method; stiff systems.

1. Introduction

Stiff differential equation systems emerge in the fields of chemical reactions, electrical networks, fluid mechanics, control theory and nuclear reactors (Bui & Bui, 1979; Flaherty & OMalley, 1997; Butcher, 2003; Ixar *et al.,* 2000).

In 1952, Curtis and Hirschfelder examined explicit methods that failed for the numerical solutions of stiff ordinary differential equations. They were the pioneers for determination of stiffness in differential equations (Curtiss & Hirschfelder, 1952). Dahlquist showed the difficulties of solving stiff differential equations with standard differential equation solvers (Dahlquist, 1963). Many authors joined in independent research for tackling the problems created by stiff differential equations. Gear is one of the most important authors in the field (Gear, 1971).

An exponential representation ($y(t) = e^{\Omega(t)}y_0$) of the solution of a first order linear differential equation for a linear operator was introduced by Wilhelm Magnus in 1954 (Magnus, 1954). However, W. Magnus has not proved convergence and he has not illuminated the general form of the $\Omega(t)$ expansion. In recent years, Iserles and Norsett have successfully completed both the tasks (Iserles & Norsett, 1997). Magnus Series have taken attention in the theory of differential equations (Chen, 1957), mathematical physics (Wilcox, 1972) and control theory (Brockett, 1976).

Iserles and Norsett analyzed the solution of linear differential equations in Lie groups (Iserles & Norsett, 1999). This method generated better results compared to classical methods. This situation was valid for both the recovery of qualitative features and stability (Iserles & Norsett, 1999; Iserles *et al.,* 1999; Iserles *et al.,* 1998). In addition, they demonstrated the advantages of the Magnus Series (Iserles & Norsett, 1999). An important advantage of the Magnus Series Expansion is that Magnus Series is truncated, but it is maintaining geometric properties of the exact solution.

Moreover, Blanes and Ponsoda applied Magnus Series Expansion Method to nonhomogeneous linear ordinay differential equations with a simple transformation (Blanes & Ponsoda, 2012). In 2013, it is demonstrated the analytical solution of reaction-diffusion equation by Garg and Manohar (Garg & Manohar, 2013).

In this paper, our aim is to show the efficiency of MG4 and MG6 on numerical solutions of nonhomogeneous stiff systems of ordinary differential equations with different step sizes and stiffness ratios.

The plan of this paper is as follows. In section 2, we present MG4 and MG6 by using Multivariate Gaussian Quadrature. Section 3 is concerned with the stiff differential equation systems. In section 4, we introduce a number of computational results which demonstrate the power of Magnus Series Expansion Method. Finally, Section 5 contains our conclusion.

2. The magnus series expansion method

Consider the following equation

$$y'(t) = A(t)y(t), \qquad t \geq 0 \tag{2.1}$$

subject to initial conditions $y(0) = y_0 \in G$, where G is the Lie group and $\mathfrak{g}$ is the Lie algebra of the corresponding to G. Here $A(t): \mathbb{R}^+ \longrightarrow \mathfrak{g}$ is coefficient matrix. This type of equations are called to as Lie group equations. As W. Magnus introduced, the analytical solution of Eq.(2.1) can be written as follows:

$$y(t) = e^{\Omega(t)}y(0), \quad t \geq 0 \tag{2.2}$$

where $\Omega(t): \mathbb{R}^+ \longrightarrow \mathfrak{g}$. Iserles and Norsett improved a general technique called the Magnus Series Expansion Method (Iserles & Norsett, 1997). Then, $\Omega(t)$ is referred to as Magnus Series Expansion.

Explicitly, Magnus Series Expansion $\Omega(t)$ can be demonstrated as an infinite sum of terms $H_i(t)$, where each H_i is a linear combination of terms that involved exactly i commutators (Iserles *et al.,* 2000).

$$\Omega(t) = \sum_{i=0}^{\infty} H_i(t), \tag{2.3}$$

where the first few terms in Eq.(2.3) are given as follows:

$$H_0(t) = \int_0^t A(\xi_1)d\xi_1, \tag{2.4}$$

$$H_1(t) = -\frac{1}{2}\int_0^t [\int_0^{\xi_1} A(\xi_2)d\xi_2, A(\xi_1)]d\xi_1, \tag{2.5}$$

$$H_2(t) = \frac{1}{12}\int_0^t [\int_0^{\xi_1} A(\xi_2)d\xi_2, [\int_0^{\xi_1} A(\xi_2)d\xi_2, A(\xi_1)]]d\xi_1$$

$$+\frac{1}{4}\int_0^t [\int_0^{\xi_1} [\int_0^{\xi_2} A(\xi_3)d\xi_3, A(\xi_2)]d\xi_2, A(\xi_1)]d\xi_1, \tag{2.6}$$

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Here, commutator or Lie bracket is a map form $[*,*]: \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ with following properties,

- $[*,*]$ is $\mathbb{R}$ - bilinear.
- $[a\,,b] = -[b\,,a]\,,\ a, b \in \mathfrak{g}\ (antisymmetric)$
- $[a\,,[b,c]] + [b\,,[c,a]] + [c\,,[a,b]] = 0$ which is knownas Jacobi identity (Iserles & Norsett, 1999).

Now, it is researched the way of computing all the terms in the Magnus Series Expansion for the coefficients matrix *A(t)*. The approach of solving multiple integrals is known as Multivariate Quadrature.

Firstly, each integral in the Magnus Series Expansion is in the form of

$$I(h) = \int_S \ L\big(A(\xi_1), A(\xi_2), \dots, A(\xi_s)\big)d\xi_s \dots d\xi_1 \tag{2.7}$$

where *L* is a multiple variable function, *S* is the number of integrals in the expression, and *h* is stepsize discretisation of the multiple integral. It has been given in Iserles & Norsett, 1999 to use the quadrature formula as

$$I(h) = \int_S \ L\big(A(\xi_1), A(\xi_2), \dots, A(\xi_s)\big)d\xi_s \dots d\xi_1 \approx h^m \sum_{k\in C_S^v} b_k L(A_{k_1}, A_{k_2}, \dots, A_{k_s}) \tag{2.8}$$

where *v* are choosen as distinct quadrature points $c_1, c_2, \dots, c_v \in [0,1]$. b_k can be found explicitly by the formula

$$b_k = \int_S \ \prod_{i=1}^{s} l_{k_i}(\xi_i)d\xi_i. \tag{2.9}$$

Recall that the function $l_j(x)$ is the Lagrange interpolation polynominal at the nodes $c_1, c_2, \dots, c_v$ and

$$l_j(x) = \prod_{\substack{i=1 \\ i\neq j}}^{v} \frac{x-c_i}{c_j-c_i}, \qquad j = 1,2,\dots,v. \tag{2.10}$$

For each-step of stepsize *h* from t_n to t_{n+1}, with $y(t_n) = y_n$

$$A_1 = A\left(t_n + \left(\frac{1}{2} - \frac{\sqrt{3}}{6}\right)h\right) \tag{2.11}$$

$$A_2 = A\left(t_n + \left(\frac{1}{2} + \frac{\sqrt{3}}{6}\right)h\right) \tag{2.12}$$

$$\Omega_4 = \frac{1}{2}h(A_1 + A_2) + \frac{\sqrt{3}}{12}h^2[A_2, A_1] \tag{2.13}$$

$$y_{n+1} = \exp(\Omega_4)\, y_n. \tag{2.14}$$

This method is called as MG4 in (Iserles *et al.,* 1999).

Iserles *et al.* developed a sixth-order Magnus method based on Gauss-Legendre points (Iserles *et al.,* 1999).

$$A_1 = A\left(t_n + \left(\frac{1}{2} - \frac{\sqrt{15}}{10}\right)h\right) \tag{2.15}$$

$$A_2 = A\left(t_n + \frac{1}{2}h\right) \tag{2.16}$$

$$A_3 = A\left(t_n + \left(\frac{1}{2} + \frac{\sqrt{15}}{10}\right)h\right). \tag{2.17}$$

where,

$$D_0 = A_2, \qquad D_1 = \frac{\sqrt{15}}{3}(A_3 - A_1), \qquad D_2 = \frac{20}{3}(A_3 - 2A_2 + A_1). \tag{2.18}$$

The method can be expressed as,

$$\Omega_6 = h\left(D_0 + \frac{1}{24}D_2\right) + h^2\left(\frac{1}{12}[D_1, D_0] - \frac{1}{480}[D_2, D_1]\right)$$

$$+h^3\left(\frac{1}{240}[D_1,[D_1,D_0]] - \frac{1}{720}[D_0,[D_2,D_0]] - h^4\frac{1}{720}\Big[D_0,\big[D_0,[D_1,D_0]\big]\Big]\right. \tag{2.19}$$

$$y_{n+1} = \exp(\Omega_6)\, y_n. \tag{2.20}$$

This method is called as MG6 in (Iserles *et al.,* 1999).

3. Stiff differential equation systems

There are different kinds of problems that are said to be stiff. It is very difficult to write a precise definition of stiffness in relation with ordinary differential equations, but the main theme is that for a given system of ordinary differential equations, stiffness means a big difference in the time scales of the components in the vector solution.

For a general formulation for stiff problems,

$$y'(t) = \lambda_s y(t) + \phi(t) \tag{3.1}$$

where $\lambda_s \in R^{n\times n}$ are the eigenvalues of the Jacobian matrix of the system for $s = 1,2,\dots,n$.

Definition 3.1

$y \in R^n$ is said to be stiff if and only if the eigenvalues λ_s of the Jacobian matrix satisfy the following conditions:

a) $Re(\lambda_s) < 0,\ \ s = 1,2,\dots,n.$

b) stiffness ratio $R = \frac{max|Re(\lambda_s)|}{min|Re(\lambda_s)|} \gg 1$, s=1,2,…,n (Fatunla, 1978).

4. Numerical experiments

In this section, Magnus Series Expansion Method is applied to nonhomogeneous stiff systems of ordinary differential equations.

Example 4.1. Consider the two-dimensional nonhomogeneous stiff ordinary differential equation (Lee *et al.,* 2002)

$$y'_1(t) = 9y_1(t) + 24y_2(t) + 5cost - \tfrac{1}{3}sint,$$

$$y'_2(t) = -24y_1(t) - 51y_2(t) - 9cost + \tfrac{1}{3}sint, \tag{4.1}$$

subject to initial condition

$$y_1(0) = \tfrac{4}{3},\ \ y_2(0) = \tfrac{2}{3}.$$

Its exact solution is $y_1(t) = 2e^{-3t} - e^{-39t} + \frac{1}{3}cost$, $y_2(t) = -e^{-3t} + 2e^{-39t} - \frac{1}{3}cost$.

We consider the stiff differential equation system (4.1) with three different case for MG4 and MG6.

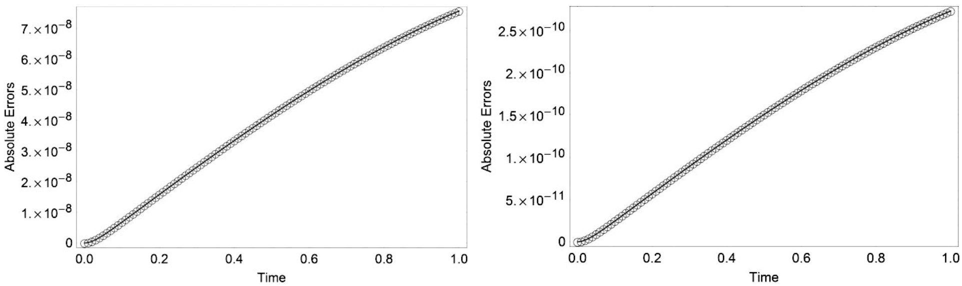

Fig. 1. Absolute errors of Example 4.1 wtih MG4 (left) and MG6 (right) for $t \in [0,1]$ and $h = 0.01$

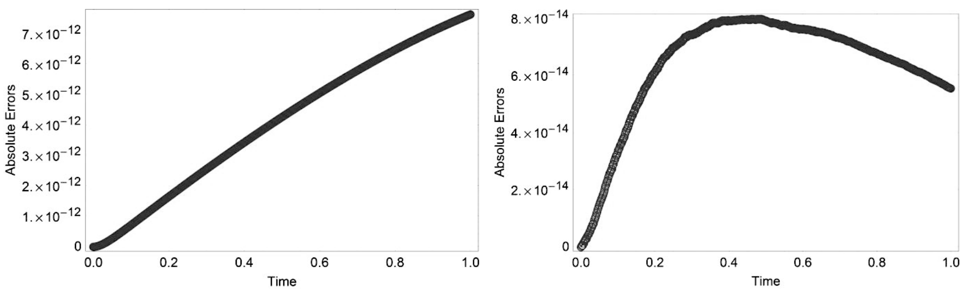

Fig. 2. Absolute errors of Example 4.1 wtih MG4 (left) and MG6 (right) for $t \in [0,1]$ and $h = 0.001$

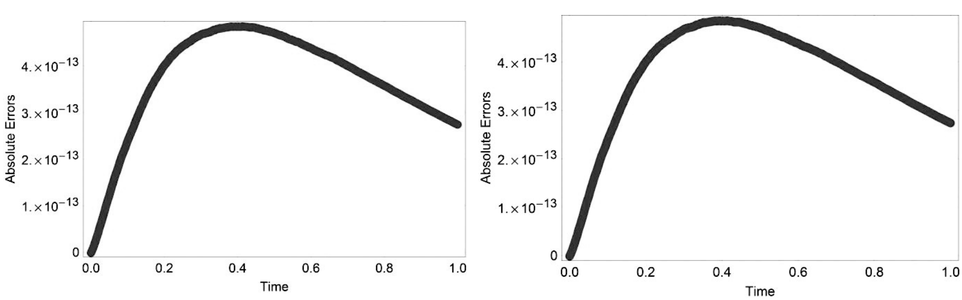

Fig. 3. Absolute errors of Example 4.1 wtih MG4 (left) and MG6 (right) for $t \in [0,1]$ and $h = 0.0001$

Table 1. Numerical values of exact and approximate solutions obtained from fourth-order Magnus Expansion Method (MG4) for Example 4.1.

t	*y(t)* *(Exact)*	*y(t)* *(Approx. for h=0.01)*	*y(t)* *(Approx. for h=0.001)*	*y(t)* *(Approx. for h=0.0001)*
0.1	1.7930625850103068	1.7930625782067209	1.7930625850095876	1.7930625850105464
0.2	1.4239023964894868	1.423902380674598	1.4239023964878361	1.4239023964898885
0.3	1.1315765220372396	1.1315764973215359	1.131576522034681	1.1315765220377074
0.4	0.9094085872759461	0.9094085539043321	0.909408587272514	0.9094085872764311
0.5	0.738787837528716	0.7387877958337838	0.7387878375244491	0.7387878375291873
0.6	0.6057096480109452	0.605709598408684	0.6057096480058877	0.6057096480113842
0.7	0.49986025226606756	0.49986019525163333	0.49986025226027	0.4998602522664684
0.8	0.41367147636118523	0.41367141250391104	0.41367147635470586	0.4136714763615437
0.9	0.34161434823638703	0.34161427817406453	0.34161434822929115	0.3416143482367031
1.0	0.2796749053584411	0.2796748297909253	0.2796749053507996	0.27967490535871603

Table 2. Numerical values of exact and approximate solutions obtained from sixth-order Magnus Expansion Method (MG6) for Example 4.1.

t	*y(t)* *(Exact)*	*y(t)* *(Approx. for h=0.01)*	*y(t)* *(Approx. for h=0.001)*	*y(t)* *(Approx. for h=0.0001)*
0.1	1.7930625850103068	1.793062585034908	1.793062585010273	1.7930625850105466
0.2	1.4239023964894868	1.4239023965466797	1.4239023964894257	1.4239023964898883
0.3	1.1315765220372396	1.13157652212662	1.1315765220371654	1.1315765220377079
0.4	0.9094085872759461	0.9094085873966254	0.9094085872758669	0.909408587276432
0.5	0.738787837528716	0.7387878376794886	0.7387878375286369	0.7387878375291872
0.6	0.6057096480109452	0.6057096481903044	0.6057096480108688	0.6057096480113843
0.7	0.49986025226606756	0.49986025247222116	0.49986025226599434	0.4998602522664691
0.8	0.41367147636118523	0.4136714765920734	0.41367147636111745	0.4136714763615445
0.9	0.34161434823638703	0.34161434848970246	0.341614348236325	0.3416143482367027
1.0	0.2796749053584411	0.2796749056316528	0.2796749053583856	0.2796749053587161

Example 4.2. Consider the two-dimensional nonhomogeneous stiff ordinary differential equation (Aminikhah & Hemmatnezhad, 2011)

$$y'_1(t) = -3y_1(t) + 2y_2(t) + 3cost - 3sint,$$

$$y'_2(t) = 2y_1(t) - 3y_2(t) - cost + 3sint, \tag{4.2}$$

with initial condition

$$y_1(0) = 1, \;\; y_2(0) = 0.$$

The exact solution of system is $y_1(t) = cost, y_2(t) = sint$.

We consider the stiff differential equation system (4.2) with three different case for MG4 and MG6.

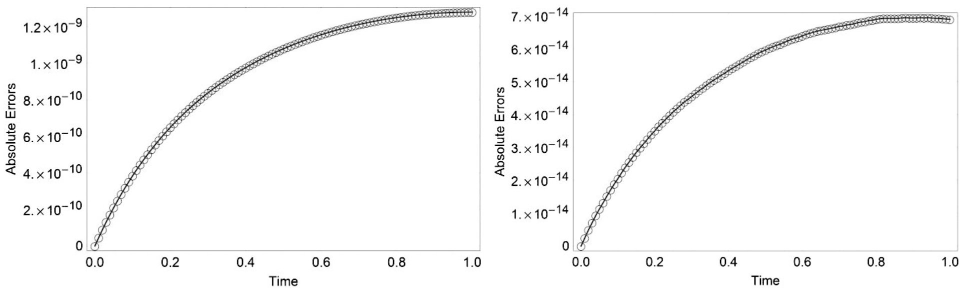

Fig. 4. Absolute errors of Example 4.2 wtih MG4 (left) and MG6 (right) for $t \in [0,1]$ and $h = 0.01$

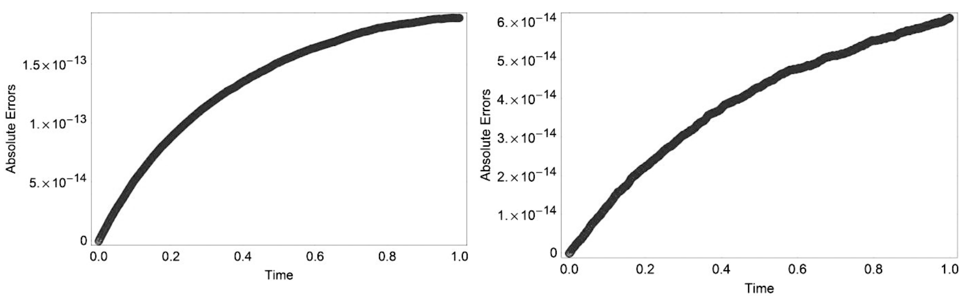

Fig. 5. Absolute errors of Example 4.2 wtih MG4 (left) and MG6 (right) for $t \in [0,1]$ and $h = 0.001$

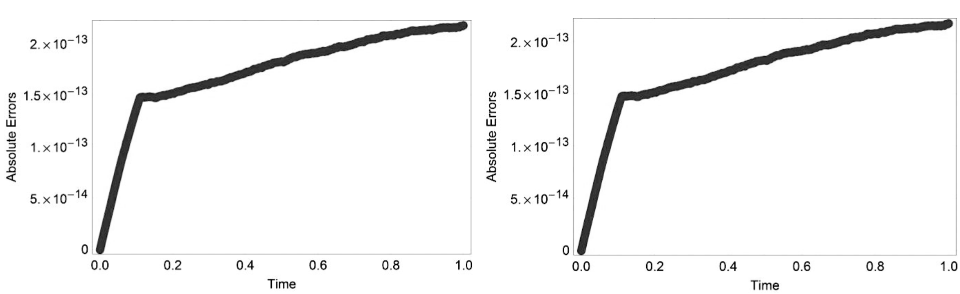

Fig. 6. Absolute errors of Example 4.2 wtih MG4 (left) and MG6 (right) for $t \in [0,1]$ and $h = 0.0001$

Table 3. Numerical values of exact and approximate solutions obtained from fourth-order Magnus Expansion Method (MG4) for Example 4.2.

t	*y(t)* *(Exact)*	*y(t)* *(Approx. for h=0.01)*	*y(t)* *(Approx. for h=0.001)*	*y(t)* *(Approx. for h=0.0001)*
0.1	0.9950041652780258	0.9950041648936438	0.9950041652779738	0.9950041652778887
0.2	0.9800665778412416	0.9800665771916226	0.9800665778411536	0.98006657784109
0.3	0.955336489125606	0.9553364882870825	0.955336489125491	0.9553364891254453
0.4	0.9210609940028851	0.9210609930261116	0.9210609940027498	0.921060994002713
0.5	0.8775825618903728	0.8775825608106744	0.8775825618902209	0.8775825618901901
0.6	0.8253356149096783	0.8253356137532794	0.825335614909514	0.8253356149094869
0.7	0.7648421872844884	0.7648421860722431	0.764842187284314	0.7648421872842888
0.8	0.6967067093471654	0.6967067080967697	0.6967067093469831	0.6967067093469571
0.9	0.6216099682706644	0.6216099669979467	0.6216099682704775	0.6216099682704511
1.0	0.5403023058681398	0.5403023045877927	0.5403023058679502	0.5403023058679219

Table 4. Numerical values of exact and approximate solutions obtained from sixth-order Magnus Expansion Method (MG6) for Example 4.2.

t	*y(t)* *(Exact)*	*y(t)* *(Approx. for h=0.01)*	*y(t)* *(Approx. for h=0.001)*	*y(t)* *(Approx. for h=0.0001)*
0.1	0.9950041652780258	0.9950041652780464	0.9950041652780135	0.9950041652778887
0.2	0.9800665778412416	0.9800665778412767	0.9800665778412192	0.98006657784109
0.3	0.955336489125606	0.9553364891256515	0.9553364891255754	0.9553364891254453
0.4	0.9210609940028851	0.9210609940029385	0.9210609940028475	0.921060994002713
0.5	0.8775825618903728	0.8775825618904324	0.8775825618903297	0.8775825618901901
0.6	0.8253356149096783	0.8253356149097423	0.8253356149096305	0.8253356149094869
0.7	0.7648421872844884	0.7648421872845552	0.7648421872844372	0.7648421872842888
0.8	0.6967067093471654	0.6967067093472343	0.6967067093471102	0.6967067093469573
0.9	0.6216099682706644	0.6216099682707338	0.6216099682706065	0.6216099682704513
1.0	0.5403023058681398	0.5403023058682087	0.5403023058680788	0.540302305867922

Example 4.3. Consider the two-dimensional nonhomogeneous stiff ordinary differential equation (Hojjati *et al.,* 2004)

$$y'_1(t) = -y_1(t) - 15y_2(t) + 15e^{-t},$$

$$y'_2(t) = 15y_1(t) - y_2(t) - 15e^{-t}, \tag{4.3}$$

subject to initial values

$$y_1(0) = 1, \;\; y_2(0) = 1.$$

The exact solution of system is $y_1(t) = e^{-t}, y_2(t) = e^{-t}$.

We consider the stiff differential equation system (4.3) with three different case for MG4 and MG6.

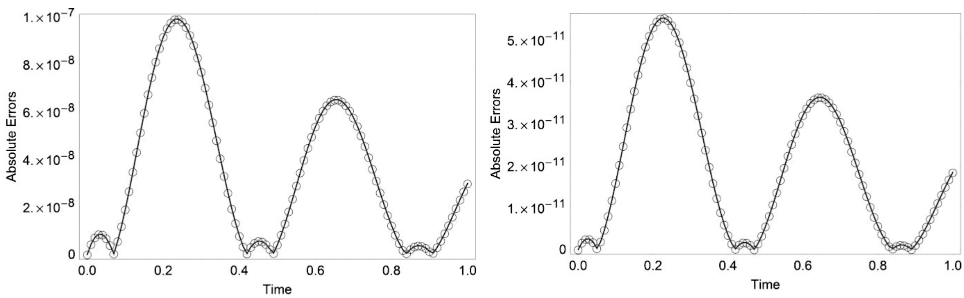

Fig. 7. Absolute errors of Example 4.3 wtih MG4 (left) and MG6 (right) for $t \in [0,1]$ and $h = 0.01$

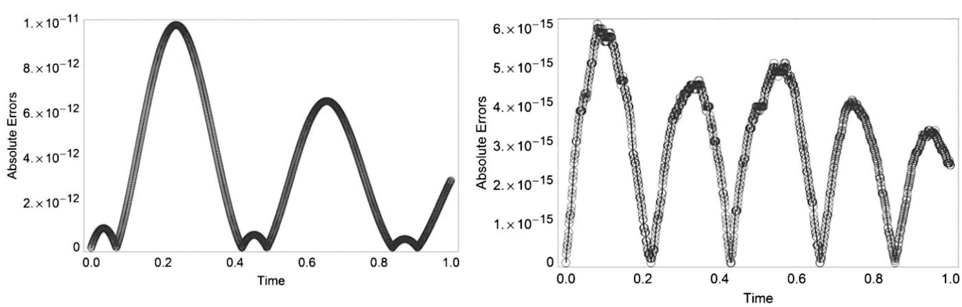

Fig. 8. Absolute errors of Example 4.3 wtih MG4 (left) and MG6 (right) for $t \in [0,1]$ and $h = 0.001$

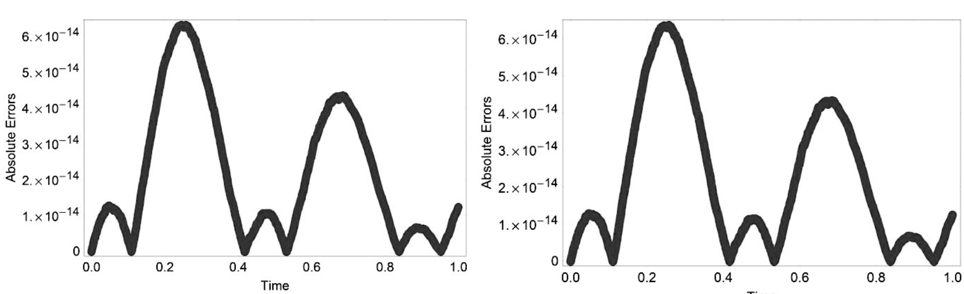

Fig. 9. Absolute errors of Example 4.3 wtih MG4 (left) and MG6 (right) for $t \in [0,1]$ and $h = 0.0001$

Table 5. Numerical values of exact and approximate solutions obtained from fourth-order Magnus Expansion Method (MG4) for Example 4.3.

t	*y(t)* (*Exact*)	*y(t)* (*Approx. for h=0.01*)	*y(t)* (*Approx. for h=0.001*)	*y(t)* (*Approx. for h=0.0001*)
0.1	0.9048374180359595	0.9048374369597412	0.9048374180378442	0.9048374180359566
0.2	0.8187307530779818	0.8187308444870725	0.8187307530871168	0.8187307530780347
0.3	0.7408182206817179	0.7408182974080687	0.7408182206893917	0.7408182206817704
0.4	0.6703200460356393	0.6703200538741403	0.6703200460364238	0.6703200460356462
0.5	0.6065306597126334	0.6065306638207445	0.6065306597130387	0.6065306597126248
0.6	0.5488116360940265	0.5488116898518103	0.548811636099398	0.5488116360940533
0.7	0.49658530379140947	0.4965853612826954	0.4965853037971592	0.4965853037914511
0.8	0.44932896411722156	0.449328976300502	0.44932896411844053	0.4493289641172339
0.9	0.4065696597405991	0.4065696584197628	0.40656965974046344	0.4065696597405927
1.0	0.36787944117144233	0.3678794710118004	0.367879441174423	0.36787944117145477

Table 6. Numerical values of exact and approximate solutions obtained from sixth-order Magnus Expansion Method (MG6) for Example 4.3.

t	*y(t)* (*Exact*)	*y(t)* (*Approx. for h=0.01*)	*y(t)* (*Approx. for h=0.001*)	*y(t)* (*Approx. for h=0.0001*)
0.1	0.9048374180359595	0.9048374180518104	0.9048374180359539	0.9048374180359559
0.2	0.8187307530779818	0.818730753130921	0.8187307530779807	0.8187307530780348
0.3	0.7408182206817179	0.7408182207215819	0.740818220681722	0.7408182206817706
0.4	0.6703200460356393	0.670320046039081	0.6703200460356418	0.6703200460356457
0.5	0.6065306597126334	0.60653065971815	0.6065306597126295	0.606530659712624
0.6	0.5488116360940265	0.5488116361260384	0.5488116360940224	0.5488116360940531
0.7	0.49658530379140947	0.49658530382186616	0.49658530379141214	0.496585303791451
0.8	0.44932896411722156	0.4493289641228474	0.4493289641172245	0.44932896411723366
0.9	0.4065696597405991	0.40656965974166054	0.4065696597405966	0.4065696597405926
1.0	0.36787944117144233	0.36787944118984306	0.36787944117143984	0.3678794411714549

5. Conclusion

In this paper, we applied MG4 and MG6 to nonhomogeneous stiff systems of ordinary differential equations with different step sizes and stiffness ratios. When the figures and tables are examined, in comparison with results of MG4, we can see that the approximations obtained byMG6 are better than MG4 for smaller step sizes at the same interval for all nonhomogeneous problems. MG4 and MG6 are explicit methods, which can be used with variable time step and variable order. Also, they have similar stability to the implicit methods. Therefore, they are methods suitable for stiff sytems of ordinary differential equations. As a result, MG4 and MG6 are very effective for stiff ordinary differential equations with different stiffness ratios.

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طريقة ماغنوس المنشورة لحل أنظمة معادلات تفاضلية اعتيادية جامدة غير متجانسة

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خلاصة

نقترح في هذا البحث استخدام طريقة ماغنوس للمتسلسلات المنشورة، وبمرتبات مختلفة و ذلك لحل أنظمة معادلات تفاضلية اعتيادية جامدة غير متجانسة. كما نقوم بتقديم طريقة المرتبة الرابعة و طريقة المرتبة السادسة و ذلك باستخدام مكتمل غاوس متعدد المتحولات. ثم نقوم بتطبيق ذلك على الانظمة الجامدة غير المتجانسة مستخدمين مقاسات خطوية مختلفة و نسب جمود مختلفة . بالإضافة إلى ذلك نشرح بالتفصيل و بالأشكال كل من الحلول المضبوطة و الحلول التقريبية. كما نقوم أيضاً بتوضيح الأخطاء المطلقة بواسطة جداول مفصلة.