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Comparative numerical solutions of stiff ordinary differential equations using Magnus series expansion method

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Abstract: In this paper, we investigated the effect of Magnus Series Expansion Method on homogeneous stiff ordinary differential equations with different stiffness ratios. A Magnus type integrator is used to obtain numerical solutions of two different examples of stiff problems and exact and approximate results are tabulated. Furthermore, absolute error graphics are demonstrated in detail.

Keywords: Linear Differential Equations, Magnus Series Expansion Method, Stiff Problems, Geometric Integration, Lie Group Method.

1 Introduction

Stiff ordinary differential equations are a very important special case of the systems taken up in initial value problems. Stiff systems arise in the fields of chemical kinetics, control theory, electrical circuit theory, vibrations, nuclear reactors, etc [4,11,5,17].

The earliest determination of stiffness in differential equations in the digital computer era, by the Curtiss and Hirschfelder was far in advance of their time [9]. In 1963, Dahlquist proved the difficulties that the standart differential equation solvers have faced with stiff differential equations [10]. It has exerted significant efforts to develop numerical intergration of stiff problems [24]. Stiff differential equations can be considered as those solutions evolve on very seperate time scales occuring. For example, consider a case where a component of the solution oscillates rapidly on a time scale much shorter than that associated with the other solution components [2].

An exponential representation of the solution of a first order linear homogeneous differential equation for a linear operator was introduced by Wilhelm Magnus in 1954 [18]. His study was called as ”Magnus Series Expansion”. Then many studies were conducted on this method. It has been successfully applied to linear differential equations since 1954.

Iserles and Norsett studied on the solutions of linear differential equations in Lie groups and they formally introduced the Magnus Series for Lie type equation [15]. Later on the Magnus Expansion as a tool for the numerical integration of linear matrix differential equations was analyzed. In addition, a certain number of practical issues related to Magnus

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based numerical integration methods were discussed [3]. Building on earlier works, Orel conducted Time-symmetry and high-order Magnus Methods in 2001 and he analyzed the use of extarpolation with Magnus method for the solution of a system of linear differential equations. The idea was a generalization of extrapolation with symmetric methods for the numerical solution of ODEs [21]. Celledoni et al. described a number of numerical algortihm designed with respect to Lie group structure such as Runge-Kutta-Munthe-Kaas Schemes, Fer and Magnus Expansions [7]. Casas investigated the sufficient conditions for the convergence of the Magnus Expansion [6]. Moan and Niesen [19] examined that convergence of Magnus Series was an infinite series which arises the study of linear ODE. In [8], the time-dependent Schrdinger equation was solved by using explicit Magnus Expansion. And also, several numerical results were given which were in good agreement with the theoretical ones to a good extent. New and more accurate analytic approximations based on the Magnus expansion involving only univariate integrals which also shares with the exact solution its main qualitative and geometric properties were introduced in [23].

2 The Magnus Expansion

The purpose of the study is to apply Magnus methods to different kinds of stiff linear ordinary differential equations of the form

$$y'(t) = A(t)y(t), \quad t \geq 0, \quad y(0) = y_0 \tag{1}$$

where $y_0 \in G$ and $A(t) \colon \mathbb{R}^+ \to \mathfrak{g}$ is the matrix function, G is the Lie group and $\mathfrak{g}$ is the Lie algebra of the corresponding to Lie group. The Eq.(1) is called as linear type Lie group equation. More detailed information can be found in [20].
The analytical solution of (1) is given by

$$y(t) = e^{\Omega(t)} y_0, \quad t \geq 0 \tag{2}$$

where the derivative of $\Omega(t)$ is defined as follows:

$$\Omega'(t) = dexp_{\Omega}^{-1}(A(t)), \quad \Omega(0) = 0 \tag{3}$$

where $dexp_{\Omega}^{-1}$ is the power series

$$dexp_{\Omega}^{-1}(A) = \sum_{j=0}^{\infty} \frac{B_j}{j!} ad_{\Omega}^{j}(A) = \frac{ad_{\Omega}}{exp(ad_{\Omega}) - I}(A) \tag{4}$$

with formula

$$\frac{x}{exp(x) - 1} = 1 - \frac{1}{2}x + \frac{1}{12}x^2 - \frac{1}{720}x^4 + \ldots \tag{5}$$

In the Eq.(4), $B_k (k \in \mathbb{Z})$ are Bernoulli numbers $(B_0 = 1, B_1 = -\frac{1}{2}, B_2 = \frac{1}{6}, B_3 = 0, \ldots)$. Note that all odd-indexed Bernoulli numbers except for B_1 are zero. In the Eq.(4), ad^k is the adjoint operator defined by $ad_{\Omega}^{0}A = A, \quad ad_{\Omega}^{k+1}A = [\Omega, ad_{\Omega}^{k}A]$ and $ad_{\Omega}(A) = [\Omega, A] = \Omega A - A\Omega$.
In the Eq.(3) can be expanded as follows:

$$\Omega'(t) = A(t) - \frac{1}{2}[\Omega(t), A(t)] + \frac{1}{12}[\Omega(t), [\Omega(t), A(t)]] + \ldots \tag{6}$$

Applying the idea of Picard iterations [1], an explicit approximation to $\Omega(t)$ can be obtained. This approximation is known as Magnus Series Expansion [14]. Hence it can be written as a summation of terms

$$\Omega(t) = \sum_{k=0}^{\infty} H_k(t). \tag{7}$$

where each H_k is a linear combination of terms that include exactly $k+1$ integrals [14]. Thus,

$$H_0(t) = \int_0^t A(\xi_1)d\xi_1 \tag{8}$$

$$H_1(t) = -\frac{1}{2}\int_0^t [\int_0^{\xi_1} A(\xi_2)d\xi_2, A(\xi_1)]d\xi_1 \tag{9}$$

$$\begin{aligned} H_2(t) = \frac{1}{12}\int_0^t [\int_0^{\xi_1} A(\xi_2)d\xi_2, [\int_0^{\xi_1} A(\xi_2)d\xi_2, A(\xi_1)]]d\xi_1 \\ +\frac{1}{4}\int_0^t [\int_0^{\xi_1} [\int_0^{\xi_2} A(\xi_3)d\xi_3, A(\xi_2)]d\xi_2, A(\xi_1)]d\xi_1 + ... \end{aligned} \tag{10}$$

So, $\Omega(t)$ is showed as follows:

$$\begin{aligned} \Omega(t) = \int_0^t A(\xi_1)d\xi_1 - \frac{1}{2}\int_0^t \int_0^{\xi_1} [A(\xi_2), A(\xi_1)]d\xi_2 d\xi_1 \\ +\frac{1}{4}\int_0^t \int_0^{\xi_1} \int_0^{\xi_2} [[A(\xi_3), A(\xi_2)], A(\xi_1)]d\xi_3 d\xi_2 d\xi_1 \\ +\frac{1}{12}\int_0^t \int_0^{\xi_1} \int_0^{\xi_1} [A(\xi_3), [A(\xi_2), A(\xi_1)]]d\xi_3 d\xi_2 d\xi_1 + ... \end{aligned} \tag{11}$$

Note that, if $A(t)$ is a constant matrix, then all commutators in Eq.(6) are equal to zero. Thus, $H_k = 0$ for all $k > 0$, $H_0 = At$ and all orders of Magnus expansion should provide the same results for a constant matrix A. In this way, $H(t) = H_0(t) = At$ and $Y(t) = exp(At)$, which is the (exact) solution.

Now, we investigate the way of computing all the terms in the Magnus series expansion for the matrix function $A(t)$. The approach of solving multiple integrals is known as multivariate Gaussian quadrature, which will be explained briefly in following section.

3 Multivariate Gaussian Quadrature

Generally, calculations of multivariate quadrature is costly. In this section, by using Gauss-Legendre quadrature, the detail of applying multivariate quadrature to find the numerical values for terms in the truncated Magnus Series Expansion of order p will be explained.

Firstly, it can be noted that each integral in the Magnus series expansion is in the form

$$I(h) = \int_{hS} L(A(\xi_1), A(\xi_2), ..., A(\xi_s))d\xi_s ... d\xi_1 \tag{12}$$

where L is multiple variable function, S is the number of integrals in the expression and h is stepsize discretisation of the multiple integral. S is defined by

$$S = \{\xi_1, \xi_2, ..., \xi_s \in \mathbb{R} : 0 \le \xi_1 \le h, 0 \le \xi_l \le \xi_{m_l}, l = 2,3,...,s\} \tag{13}$$

where $m_l \in \{1,2,...,l-1\}$, for $l = 2,3,...,s$. It has been given in [15] to use the quadrature formula as

$$\begin{aligned} I(h) &= \int_S L(A(\xi_1), A(\xi_2), ..., A(\xi_s)) d\xi_s ... d\xi_1 \\ &\approx h^m \sum_{k \in C_S^v} b_k L(A_{k_1}, A_{k_2}, ..., A_{k_s}) \end{aligned} \tag{14}$$

where, v are choosen as distinct quadrature points $c_1, c_2, ..., c_v \in [0,1]$. v distinct quadrature points will be the roots of the legendre polynomial $P_v^*(x)$. Then, it is calculated that approximation $A_k = hA(c_k h)$, for $k = 1,2,...,v$ and the quadrature are as follows:

$$D(h) = \sum_{k \in C_S^v} b_k L(A_{k_1}, A_{k_2}, ..., A_{k_s}) \tag{15}$$

where, $k_1, k_2, ..., k_s \in k$ and C_S^v is the set of all combinations of s-tuples k from the set $\{1,2,...,v\}$. The weight b_k can be found explicitly by the formula

$$b_k = \int_S \prod_{i=1}^{s} l_{k_i}(\xi_i) d\xi_i \tag{16}$$

Note that the function $l_j(x)$ is the Lagrange interpolation polynominal at the nodes $c_1, c_2, ..., c_v$ and

$$l_j(x) = \prod_{i=1, i \ne j}^{v} \frac{x - c_i}{c_j - c_i}, \qquad j = 1,2,...,v. \tag{17}$$

The order of multivariate quadrature is precisely the same as of the classical univariate quadrature. Let us consider

$$A_1 = A((\frac{1}{2} - \frac{\sqrt{3}}{6})h), \quad A_2 = A((\frac{1}{2} + \frac{\sqrt{3}}{6})h) \tag{18}$$

the fourth-order Gauss-Legendre quadrature in $[0,1]$. Therefore,

$$I_1(t) \approx \frac{1}{2} h (A_1 + A_2) \tag{19}$$

$$I_2(t) \approx \frac{\sqrt{3}}{6} h^2 [A_2, A_1] \tag{20}$$

$$I_3(t) \approx h^3 [[A_2, A_1], (\frac{3}{80} + \frac{\sqrt{3}}{16}) A_1 - (\frac{3}{80} - \frac{\sqrt{3}}{16}) A_2] \tag{21}$$

$$I_4(t) \approx -h^3 [(\frac{3}{80} - \frac{\sqrt{3}}{48}) A_1 - (\frac{3}{80} + \frac{\sqrt{3}}{48}) A_2, [A_2, A_1]] \tag{22}$$

$$\vdots$$

The solution of Eq.(1) uses the truncated Magnus Series Expansion of fourth-order in the following way as given in [13]. For each-step of stepsize h from t_n to t_n+1 and with $y(t_n)=y_n$

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

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

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

$$y_{n+1} = exp(\Omega_4)y_n \tag{23}$$

This method is called as MG4 in literature [16].

In [16] Iserles et al. improved a sixth-order Magnus method based on Gauss-Legendre points.

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

$$A_2 = A(t_n + \frac{1}{2}h)$$

$$A_3 = A(t_n + (\frac{1}{2} + \frac{\sqrt{15}}{10})h)$$

where,

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

The method can be expressed as,

$$\begin{aligned}\Omega_6 = h(D_0 + \frac{1}{24}D_2) + h^2(\frac{1}{12}[D_1, D_0] - \frac{1}{480}[D_2, D_1]) \\ +h^3(\frac{1}{240}[D_1,[D_1,D_0]] - \frac{1}{720}[D_0,[D_2,D_0]]) \\ -h^4\frac{1}{720}[D_0,[D_0,[D_1,D_0]]]\end{aligned} \tag{24}$$

$$y_{n+1} = exp(\Omega_6)y_n \tag{25}$$

This method is called as MG6 in literature [16].

4 Stiff Systems of Ordinary Differential Equations

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 the equation contains some terms that can create a rapid change in related solution.

A linear differential system,

$$y'(t) = \lambda_i y(t) + \phi(t) \tag{26}$$

where $\lambda_i \in R^{n\times n}$ and y, $\phi \in R^n$ is stiff if and only if for all i, $Re(\lambda_i) < 0$ and stiffness ratio $S = \frac{max|Re(\lambda_i)|}{min|Re(\lambda_i)|} >> 1$, where $i = 1,2,...,n$ are eigenvalues of A.

Assuming that $Re(\lambda_i) < 0$ for all eigenvalues a commonly used stiffness index is

$$L = max|Re(\lambda_i)| \tag{27}$$

In addition, L is not invariant under a simple rescaling of the problem. Stiffness ratio is defined by

$$S = \frac{max|Re(\lambda_i)|}{min|Re(\lambda_i)|}. \tag{28}$$

5 Numerical Experiments

In this section, we applied Magnus Series Expansion Method to solve stiff systems of ordinary differential equations with constant and variable coefficient for various stiffness ratios. Then, we demonstrated approximate, exact solutions and absolute errors of each problems with figures in detail.

Example 1. Consider the following two-dimensional constant coefficient stiff ordinary differential equation [22].

$$\begin{cases} y_1'(t) = y_2(t), \\ y_2'(t) = -0.9999y_1(t) - 100y_2(t) \end{cases} \tag{29}$$

subject to initial conditions $y_1(0) = 1, y_2(0) = 0$. The exact solutions of the above system are

$$y_1(t) = -0.00010002000400080088e^{-99.99t} + 1.000100020004001e^{-0.009999999999990905t}$$

$$y_2(t) = 0.010001000200040078e^{-99.99t} - 0.010001000200040078e^{-0.009999999999990905t}$$

Case 1. Consider the stiff differential equation system (29), where $t \in [0,1]$ and $h = \frac{1}{100}$.

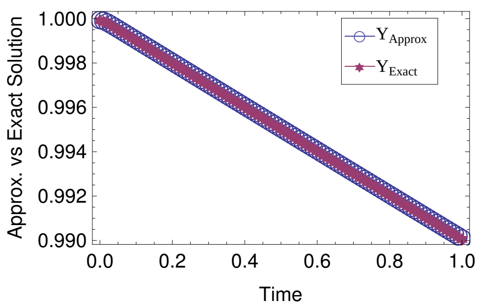

Fig. 1: Numerical results of Example 5.1 for $h = 0.01$

Case 2. Consider the stiff differential equation system (29), where $t \in [0,1]$ and $h = \frac{1}{1000}$.

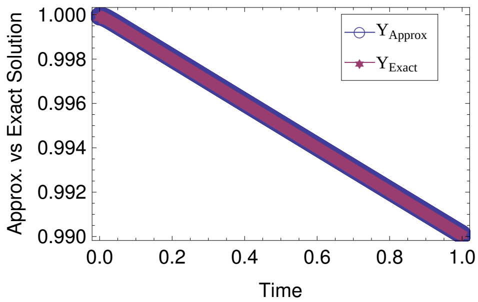

Fig. 2: Numerical results of Example 5.1 for $h = 0.001$

Case 3. Consider the stiff differential equation system (29), where $t \in [0,1]$ and $h = \frac{1}{10000}$.

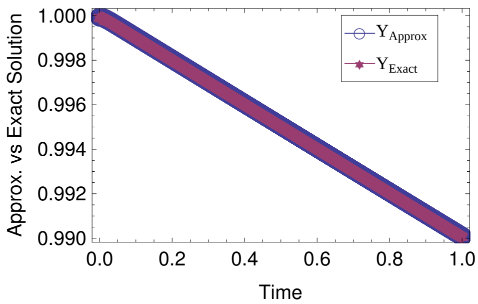

Fig. 3: Numerical results of Example 5.1 for $h = 0.0001$

Table 1: Numerical values of exact and approximate solutions obtained from second order Magnus Expansion Method (MG2) for Example 5.1.

t	*Exact*	$MG2(h=0.01)$	$MG2(h=0.001)$	$MG2(h=0.0001)$
0.1	0.99910041532	0.99910041532	0.99910041532	0.99910041532
0.2	0.99810181883	0.99810181883	0.99810181883	0.99810181883
0.3	0.99710421589	0.99710421589	0.99710421589	0.99710421589
0.4	0.99610761006	0.99610761006	0.99610761006	0.99610761006
0.5	0.99511200034	0.99511200034	0.99511200034	0.99511200034
0.6	0.99411738573	0.99411738573	0.99411738573	0.99411738573
0.7	0.99312376524	0.99312376524	0.99312376524	0.99312376524
0.8	0.99213113787	0.99213113787	0.99213113787	0.99213113787
0.9	0.99113950263	0.99113950263	0.99113950263	0.99113950263
1.0	0.99014885853	0.99014885853	0.99014885853	0.99014885853

Since $A(t)$ is constant in Eq.(1), we use only second order Magnus Expansion Method (MG2). In the following example $A(t)$ is not constant, so we can compare Magnus Expansion Method with different orders which are 4 and 6.

Example 2. Consider the following two-dimensional variable coefficient stiff ordinary differential equation [13].

$$\begin{cases} y_1'(t) = -1000ty_1(t) + y_2(t), \\ y_2'(t) = -ty_2(t) \end{cases} \tag{30}$$

subject to initial conditions $y_1(0) = -1, y_2(0) = 1$. The exact solutions of the above system are

$$y_1(t) = \frac{1}{666}e^{-500t^2}(-666 + \sqrt{222\pi}Erfi[3\sqrt{\frac{111}{2}}t])$$

$$y_2(t) = e^{\frac{-t^2}{2}}$$

Case 1. Consider the stiff differential equation system (30), where $t \in [0,1]$ and $h = \frac{1}{100}$.

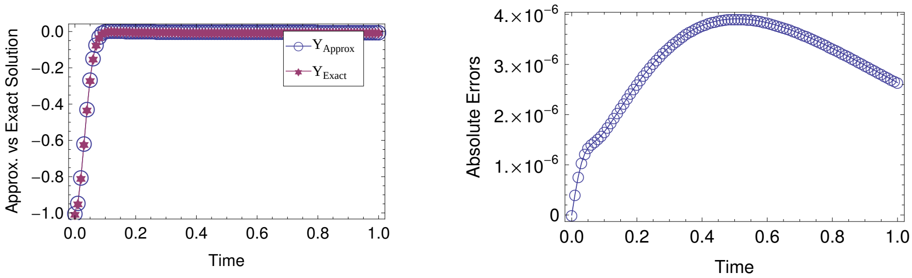

Fig. 4: Numerical results of Example 5.2 with MG4 for $h = 0.01$ (Left:approximation vs exact solution, Right:absolute errors)

Case 2. Consider the stiff differential equation system (30), where $t \in [0,1]$ and $h = \frac{1}{1000}$.

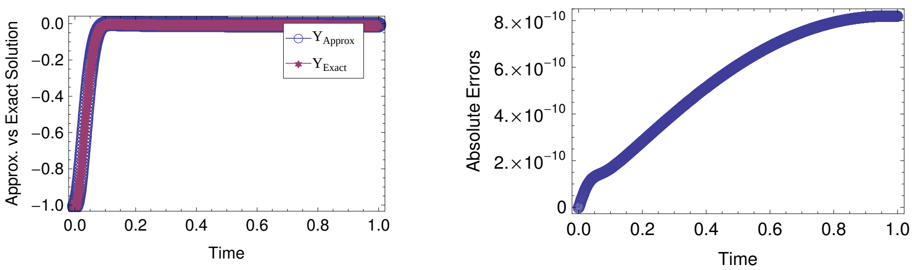

Fig. 5: Numerical results of Example 5.2 with MG4 for $h = 0.001$ (Left:approximation vs exact solution, Right:absolute errors)

Case 3. Consider the stiff differential equation system (30), where $t \in [0,1]$ and $h = \frac{1}{10000}$.

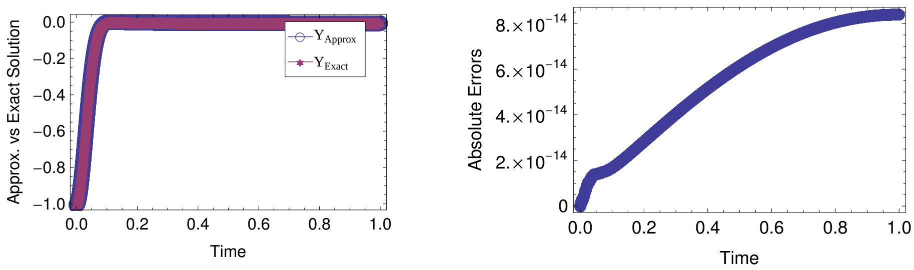

Fig. 6: Numerical results of Example 5.2 with MG4 for $h = 0.0001$ (Left:approximation vs exact solution, Right:absolute errors)

Table 2: Numerical values of exact and approximate solutions obtained from fourth-order Magnus Expansion Method (MG4) for Example 5.2.

t	*Exact*	$MG4(h=0.01)$	$MG4(h=0.001)$	$MG4(h=0.0001)$
0.1	0.004788438856654205	0.004786780414370417	0.004788438686822496	0.004788438856637138
0.2	0.005039304792290868	0.005036698696919041	0.005039304506867239	0.005039304792262303
0.3	0.003226581691867235	0.0032232292695685526	0.003226581286266913	0.0032265816918266017
0.4	0.002324833687128679	0.0023210594126784148	0.0023248331708462643	0.002324833687076848
0.5	0.0017739214071528352	0.001770011684693963	0.0017739207942755724	0.0017739214070911957
0.6	0.001397418047002593	0.0013935848714085597	0.0013974173544071232	0.0013974180469327792
0.7	0.0011215692753747594	0.0011179517261896757	0.0011215685216204355	0.0011215692752985864
0.8	0.0009100227126543259	0.0009067018069023954	0.0009100219170289942	0.0009100227125735789
0.9	0.0007427473453034181	0.0007397623404288402	0.0007427465269526064	0.00074274734522001
1.0	0.0006077473773139123	0.0006051092160958073	0.0006077465544652914	0.0006077473772296983

The numerical results for Example 5.2 by using sixth-order Magnus series expansion method are presented with figure (7-9) and Table 3.

Case 4. Consider the stiff differential equation system (30), where $t \in [0,1]$ and $h = \frac{1}{100}$.

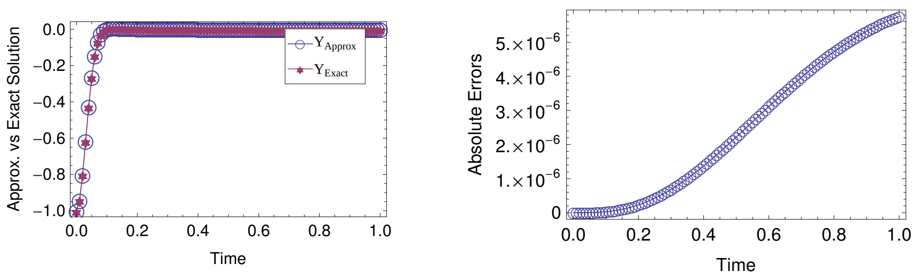

Fig. 7: Numerical results of Example 5.2 with MG6 for $h = 0.01$ (Left:approximation vs exact solution, Right:absolute errors)

Case 5. Consider the stiff differential equation system (30), where $t \in [0,1]$ and $h = \frac{1}{1000}$.

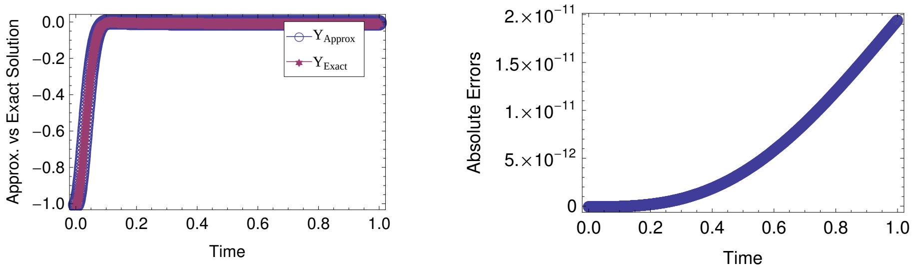

Fig. 8: Numerical results of Example 5.2 with MG6 for $h = 0.001$ (Left:approximation vs exact solution, Right:absolute errors)

Case 6. Consider the stiff differential equation system (30), where $t \in [0,1]$ and $h = \frac{1}{10000}$.

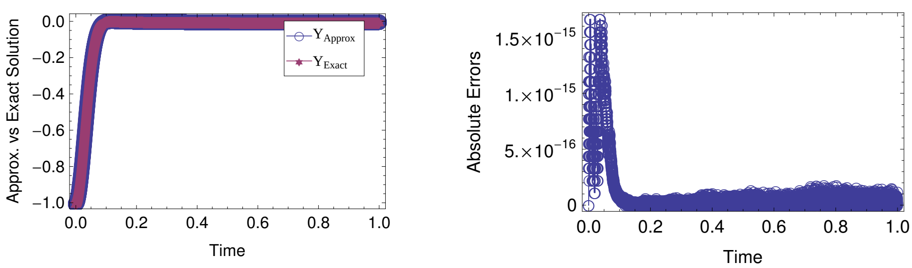

Fig. 9: Numerical results of Example 5.2 with MG6 for $h = 0.0001$ (Left:approximation vs exact solution, Right:absolute errors)

Table 3: Numerical values of exact and approximate solutions obtained from sixth-order Magnus Expansion Method (MG6) for Example 5.2.

t	*Exact*	$MG6(h = 0.01)$	$MG6(h = 0.001)$	$MG6(h = 0.0001)$
0.1	0.004788438856654205	0.00478847186232619	0.004788438856688662	0.00478843885665412
0.2	0.005039304792290868	0.005039536215136678	0.005039304792549599	0.005039304792290874
0.3	0.003226581691867235	0.0032272661441778506	0.003226581692715816	0.0032265816918672498
0.4	0.002324833687128679	0.00232620840809544	0.002324833689066781	0.0023248336871286774
0.5	0.0017739214071528352	0.0017761400659024726	0.0017739214107631868	0.00177392140715285
0.6	0.001397418047002593	0.0014005317854346511	0.0013974180528911677	0.001397418047002634
0.7	0.0011215692753747594	0.0011255386698003145	0.001121569284108935	0.0011215692753748425
0.8	0.0009100227126543259	0.0009147416591928036	0.0009100227247051727	0.0009100227126543534
0.9	0.0007427473453034181	0.0007480676671897068	0.00074274736099798	0.0007427473453034218
1.0	0.0006077473773139123	0.0006134997470667265	0.0006077473968011909	0.0006077473773139392

6 Conclusion

When the results are examined, Magnus Series Expansion Method gives smaller errors for stiff ordinary differential equations. In the case of Example 5.1, all orders of Magnus series expansion method are giving same errors since A(t) is constant. For Example 5.2, MG6 gives better results than MG4 for smaller step sizes at the same interval. To sum up, MG4 and MG6 is very effective for stiff ordinary differential equations with different stiffness ratios. An important advantage of Magnus Series Expansion is that the Magnus Series is truncated but it maintaining geometric properties of the exact solution. Also, MG4 and MG6 have similar stability to the implicit methods. Therefore, these methods are suitable and reliable for stiff systems of ordinary differential equations.

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