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Solving stiff systems using symbolic - numerical method

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Abstract In this paper, an efficient symbolic-numerical procedure based on the power series method is presented for solving a system of differential equations. The basic idea is to substitute power series into the differential equations and to find a polynomial system of coefficients, where a powerful symbolic computation technique (i.e., Gröbner basis) is used to solve the system. In fact, the proposed method is an excellent bridge between symbolic and numeric computation and specially, enables us to find the solution of linear and non-linear stiff systems. Numerical experiments were performed to justify our new approach.

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1. Introduction

Technically, problems with solutions changing quickly over a short period of time are called Stiff. The stiff problems have been studied in various fields of science such as physics, chemistry, and engineering. Solving such problems numerically is considerably hard because they are unstable. Curtiss and Hirschfelder [12] were the first who discussed stiff equations. These researchers used a numerical method for solving stiff initial value problems of the form

$$y' = f(x, y),\ y(x_0) = y_0,\ y \in R^S.$$

Since then, many studies have been conducted for the analysis of stiff problem. As a result, many numerical methods with acceptable accuracy have made afterward to solve this problem and continued so far. A few examples in this regard include homotopy perturbation method [13], variational iteration method [14], power series

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method [22], differential transformation method [23], and Taylor series method [3], which are based on the series solution.

The Taylor series is a high accuracy method for solving different types of differential equations. For instance, ordinary differential equations [4, 11], partial differential equations [8, 21], integral equations [24, 26], and other equations such as [3, 25, 28]. Rational Homotopy Perturbation Method (RHPM) [5] is a semi-analytic method that is expressed as the quotient of two power series.

Problems coming from applications typically have polynomial systems. Numerous standard techniques have been utilized to study solutions of polynomial systems. Among them, Gröbner bases have shown a great capability in recent decades. These bases were introduced by Bruno Buchberger [7] in 1965. He also produced the fundamental algorithms to compute them in his Ph.D. thesis. The Gröbner basis is one of the strongest tools for solving nonlinear system of equations in computer algebra. There are many applications of Gröbner bases such as graph coloring problems [15], robotics [10], coding theory [27], solving Diophantine equations (Pell) [9], solving fuzzy systems [1], and so on. A Görbner basis for an ideal generated by the equations is a finite set of polynomials that has a triangular structure that successively eliminates the variables in a proper way. With the advantages of computers and computing resources, Gröbner basis algorithms have been thoroughly improved; in particular, F_4 and F_5 algorithms by Jean-Charles Faugère [18, 19] have been sucessfully used to compute efficiently Gröbner bases for ideals in polynomial rings. These algorithms are used nowadays to solve systems of equations. These bases generalize Euclid's algorithm for computing polynomial greatest common divisors to multivariate, and Gaussian elimination for linear systems to non-linear. The solution can be deduced easily from a triangular form of Gröbner basis.

The present study was conducted to solve the linear and non-linear stiff systems via Gröbner basis techniques. For this purpose, we derive the solutions to form a power series in one variable with unknown coefficients and then substitute that variable by the appropriate step-size. By substituting this power series into a given problem, we obtain a system of polynomial equations. Next, Gröbner basis provides a system of the triangular form that is equivalent to the corresponding system of polynomial equations. From this form, it is easier to find the coefficients by the backward substitution.

We present an algorithm that gives the particular solution that will converge to the solution of the system of differential equations. Next, we compare the proposed approach with the RHPM and Taylor series methods. We will show that the proposed approach has the same accuracy of the Taylor series of Maple (TS Maple) with less computing time and more accuracy in larger intervals than RHPM.

The remainder of the paper is structured as follows: Section 2.1 introduces some basic definitions about the Gröbner basis. A new approach for solving a differential equation system using Gröbner basis is presented in section 2.2. The paper concludes in Section 3, with some numerical examples to compare the proposed method with the RHPM and Taylor series methods.

2. Symbolic - Numerical Method

2.1. **Basic definitions.** In this section, we present briefly the basic concepts of Gröbner basis. For a more detailed discussion, we refer the reader to [7, 10]. Using the method of Gröbner bases, we can solve systems of polynomial equations in a very nice fashion.

Let the ring of all polynomials in $x_1, x_2, \cdots, x_n$, with coefficients in field K is denoted by $R = K[x_1, x_2, \cdots, x_n]$. An expression of the form $x_1^{i_1} x_2^{i_2} \cdots x_n^{i_n} \in R$ with non-negative exponents is called a term. In order to define Gröbner basis, we need to define the term order.

One the most important of a term order will be *lexicographical order*(or *Lex order* for short). We now introduce that as follows:

Definition 2.1. [10] Let $\alpha = (\alpha_1, \ldots, \alpha_n)$ and $\beta = (\beta_1, \ldots, \beta_n) \in \mathbb{Z}^n_{\geqslant 0}$, We say $\alpha >_{lex} \beta$ if, in the vector difference $\alpha - \beta \in \mathbb{Z}^n$, the leftmost nonzero entry is positive. We will write $x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n} >_{lex} x_1^{\beta_1} x_2^{\beta_2} \cdots x_n^{\beta_n}$ if $\alpha >_{lex} \beta$.

Suppose $>$ be an arbitrary term order on R. For any non-zero polynomial f, the maximum term appearing in f with respect to $>$ is denoted by $LT(f)$, and is called the *leading term* of f. The coefficient of $LT(f)$ is the *leading coefficient* of f is denoted by $LC(f)$.

Now, we can define a Gröbner basis for an ideal in R as follows:

Definition 2.2. [10] Fix a monomial order $>$. A *Gröbner basis* of an ideal I in R with respect to $>$ is a finite set of polynomials $G = \{g_1, \ldots, g_m\} \subset I$ with the property that for every nonzero $f \in I$, $LT(f)$ is divisible by $LT(g_i)$ for some i. A Gröbner basis G is called a *reduced Gröbner basis* for I if for any $g_i \in G$, $LC(g_i) = 1$ and no term of g_i lies in the ideal generated by $\{LT(g_j) | 1 \leq j \neq i \leq m\}$.

The following theorem points out the essential properties of Gröbner basis.

Theorem 2.3. Let I be the ideal generated by $\{h_1, \cdots, h_m\}$ in $K[\mathbf{x}]$ and $K \subset \mathbb{C}$. For a given monomial order,

(1) I has a unique reduced Gröbner basis G.
(2) Every Gröbner basis G generates its ideal I.
(3) The equations $h_1 = 0, \cdots, h_m = 0$ have no solutions in any extending field of K if and only if $G = \{1\}$.
(4) The variety $V(I) \subset \mathbb{C}^n$ is a finite set if and only if for each variable x_i, there is a polynomial $g \in G$ such that $LT(g)$ is a power of x_i (the dimension of I is zero).
(5) $V(G) = V(h_1, \ldots, h_m)$

Proof. See [7, 10] □

In modern computer algebra packages, some versions of improvements of Gröbner basis have been applied. For example, package FGb by Jean-Charles Faugère [20] has been implemented in C.

2.2. **Solving a differential equation system using Gröbner basis.** In this subsection, we describe a new method for solving a differential equation system using

Gröbner basis. Let f_i be a polynomial in $K[y_1, y_2, \cdots, y_m]$ for $i = 1, 2, \cdots, m$, where our aim is to solve the following differential equation system:

$$\begin{cases} \frac{dy_1}{dt} & = & f_1(y_1, y_2, \cdots, y_m) \\ \frac{dy_2}{dt} & = & f_2(y_1, y_2, \cdots, y_m) \\ \vdots & & \\ \frac{dy_m}{dt} & = & f_m(y_1, y_2, \cdots, y_m) \end{cases} \tag{2.1}$$

with initial conditions $y_j(0) = c_j$ for $j = 1, \cdots, m$. We use the power series in a neighborhood of zero for each y_j, so:

$$y_j = c_j + \sum_{i=1}^{n} a_{i,j} t^i \quad for \;\; j = 1, \cdots, m. \tag{2.2}$$

Then, for a given n, t is substituted by $l * h$ for $l = 1, \cdots, n$, where h is a step-size, we obtain a polynomial system of mn equations

$$y_j(l) = c_j + \sum_{i=1}^{n} a_{i,j} l^i h^i \quad for \;\; j = 1, \cdots, m. \tag{2.3}$$

and mn unknowns $a_{i,j}$ for $i = 1, \cdots, n$ and $j = 1, \cdots, m$. Next, substitute (2.3) and its derivatives in ideal are generated by

$$\langle \frac{dy_1}{dt} - f_1(y_1, y_2, \cdots, y_m), \frac{dy_2}{dt} - f_2(y_1, y_2, \cdots, y_m), \ldots, \frac{dy_m}{dt} - f_m(y_1, y_2, \cdots, y_m)\rangle \tag{2.4}$$

In 1989, Deuflhard [16] presented uniqueness theorems for stiff ODE initial value problems, which indicate the existence and uniqueness of the solution of the ODE. Therefore, the ideal generated by (2.4) is zero- dimensional. Then, a Gröbner basis for the ideal generated by (2.4) in $K[a_{i,j} \mid i = 1 \cdots n, \; j = 1 \cdots m]$ with respect to lex order can be computed. The Gröbner basis w.r.t Lex order has the upper triangular structure; i.e., it has the following form:

$$\begin{cases} g_{1,1}(t_1) \in K[t_1] \\ g_{2,1}(t_1, t_2), g_{2,p_2}(t_1, t_2) \in K[t_1, t_2] \\ \vdots \\ g_{n,1}(t_1, \ldots, t_n), \ldots, g_{n,p_n}(t_1, \ldots, t_n) \in K[t_1, \ldots, t_n] \end{cases} \tag{2.5}$$

So, we can find the solutions of equation (2.5) by the backward substitution. The main algorithm for solving a differential equation system is presented here. We now illustrate the algorithm with an example as follows:

Example 2.4. ([13, 14]) Consider the following non-linear stiff system:

$$\begin{cases} y_1'(t) & = & -1002 y_1(t) + 1000 y_2^2(t) \\ y_2'(t) & = & y_1(t) - y_2(t)(1 + y_2(t)) \end{cases} \tag{2.6}$$

with initial condition $y_1(0) = 1$ and $y_2(0) = 1$. The exact solution is $y_1(t) = e^{-2t}$ and $y_2(t) = e^{-t}$.

Algorithm 1 (Main Algorithm)

Input: IVP systems of ODEs and n.
Output: a solution for problem.

- 1. Compute power series expansion (2.2) to order n in one variable.
- 2. Substitute the variable by the appropriate step-size (2.3).
- 3. Substitute the solution obtained from the step 2 and its derivatives in the ideal generated by (2.4).
- 4. Compute the Gröbner basis for the ideal generated by (2.4) in $K[a_{i,j} \mid i = 1\cdots n,\ j = 1\cdots m]$ with respect to the lexicographical order.
- 5. Find the solutions of the system in Step 4 with the forward substitution.

We put $n = 7$ and $c_1 = 1$, $c_2 = 1$. Power series expansion y_j's (2.2) to order $n = 7$ in one variable is as follows:

$$y_j(l) = c_j + \sum_{i=1}^{7} a_{i,j} l^i (h)^i \quad \textit{for} \;\; j = 1, 2, \tag{2.7}$$

where we concider a step-size of $h = 10^{-7}$ in Step 2. Now, we substitute solution (2.7) and its derivatives in ideal generated by $\langle y_1'(t) + 1002y_1(t) - 1000y_2^2(t), y_2'(t) - y_1(t) + y_2(t)(1 + y_2(t))\rangle$. We obtain a polynomial system of 14 equations with 14 unknowns $a_{i,j}$ for $i = 1, \cdots, 7$ and $j = 1, 2$. Then, Gröbner basis for the mentioned ideal with respect to the lex order is computed, which gives the following solutions for (2.7):

$$y_1 = 1 - 2t + 2t^2 - \frac{4}{3}t^3 + \frac{2}{3}t^4 - \frac{4}{15}t^5 + \frac{4}{45}t^6 - \frac{8}{315}t^7 + \dots,$$

$$y_2 = 1 - t + \frac{1}{2}t^2 - \frac{1}{6}t^3 + \frac{1}{24}t^4 - \frac{1}{120}t^5 + \frac{1}{720}t^6 - \frac{1}{5040}t^7 + \dots.$$

The power series solution of Example 2.4 coincides with the exact solution. Figure 1 presents a comparison between SNM with the exact solution.

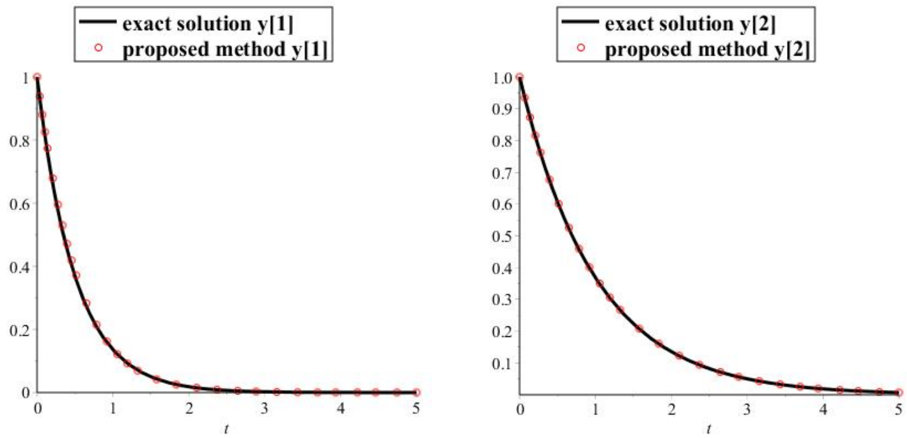
Proposition 2.5. [10] Let $I \subset \mathbb{C}[x_1, \dots, x_n]$ be an ideal such that for each i, some power $x_i^{m_i} \in < LT(I) >$. Then the number of points of $V(I)$ is at most $m_1 \cdot m_2 \cdots m_n$.

Proof. This follows by the Theorem 2.3. □

According to the above, several classes of the power series coefficient are calculated by the Gröbner basis. After substituting these roots in the system, we choose the minimum error as a special class coefficient. Let $y_{j,n}$ be the n^{th} degree power series for the corresponding component of y_j. We estimate the error $\|y_{j,n+1} - y_{j,n}\|$,

$$\begin{aligned}
\|y_{j,n+1} - y_{j,n}\| = \|\sum_{i=1}^{n+1} a_{i,j} t^i - \sum_{i=1}^{n} \alpha_{i,j} t^i\| &= \|a_{n+1,j} t^{n+1} + \sum_{i=1}^{n} (a_{i,j} - \alpha_{i,j}) t^i\| \\
&\leq \|a_{n+1,j} t^{n+1}\| + \|\sum_{i=1}^{n} (a_{i,j} - \alpha_{i,j}) t^i\| \leq \|a_{n+1,j} t^{n+1}\| \\
&\leq \frac{f^{(n)}(y(t), 0) t^{n+1}}{(n+1)!}.
\end{aligned}$$

FIGURE 1. Comparison of SNM with exact solution.



Where the limit of the second sum goes to zero, because Gröbner basis finds the special class coefficient in $y_{j,n}$ and $y_{j,n+1}$, which is a minimum error with the original solution of the system.
Now, let y_j be the exact solution of the differential equation system (2.1),

$$\|y_j - y_{j,n}\| \leq \frac{K|t^{n+1}|}{(n+1)!}$$

where K is a constant such that:

$$\|f^{(n)}(y(t), 0)\| \leq K.$$

Theorem 2.6. The main algorithm finds the particular solution that will converge to the solution of the differential equation.

Proof. We are looking for the coefficients of the power series that is the same variety ideal (2.4). Thus, ideal (2.4), according to the Theorem 2.3, has a unique reduced Gröbner basis G, where G generates its ideal (2.4) and variety of the mentioned ideal equal $V(G)$. In the above Proposition, we show that the number of points of $V(G)$ is at most $m_1 \cdot m_2 \cdots m_n$. Thus, by solving the upper triangular system from (2.5), we can find all the series solutions to the differential equations. The particular solution can be selected among the series solutions by substituting in the differential equation that has the minimum error.

□

3. Numerical examples

In this section, three numerical examples are given to illustrate the performance and accuracy of solving stiff systems by the proposed method.

Remark. We received the Maple implementation of RHPM algorithm from the authors to compare an approximation of stiff systems.

Remark. Execution time of the proposed method is compared with RHPM and Taylor series methods in Table 4.

Example 3.1. [17, 2] Consider the following differential equation system: $y^{'} = Ay$, where

$$A=\begin{bmatrix} -10^4 & 100 & -10 & 1 \\ 0 & -1000 & 10 & -10 \\ 0 & 0 & -1 & 10 \\ 0 & 0 & 0 & -0.1 \end{bmatrix} \text{y, } y(0) = (1,1,1,1)^T,\ 0 \leq t \leq 20.$$

Using eigenvalue-eigenvector method from [6], exact solution would be as follows:

$$y_1(t) = \frac{818090}{89901009}e^{-t} + \frac{9989911}{899010090}e^{-1000t} + \frac{89071119179}{89990100090}e^{-10000t} - \frac{89990090}{8999010009}e^{-0.1t}$$
$$y_2(t) = -\frac{910}{8991}e^{-t} + \frac{9989911}{9989001}e^{-1000t} + \frac{9100}{89991}e^{-0.1t}$$
$$y_3(t) = -\frac{91}{9}e^{-t} + \frac{100}{9}e^{-0.1t}$$
$$y_4(t) = e^{-0.1t}.$$

In the power series of y_j's (2.2), we put $n = 20$ and $c_1 = 1$, $c_2 = 1$, $c_3 = 1$ and $c_4 = 1$ and substitute x by $\ell \times h$ for $l = 1, \cdots, 20$. Then, we obtain a polynomial system of 80 equations and 80 unknowns as follows:

$$y_j(l) = 1 + \sum_{i=1}^{20} a_{i,j} l^i (h)^i \quad \textit{for} \quad j = 1, \cdots, 4. \tag{3.1}$$

where $a_{i,j}$ for $i = 1, \cdots, 20$ and $j = 1, \cdots, 4$. Now, we substitute solution (3.1) and its derivatives in ideal generated by

$$\langle y_1^{'} + 10^4 y_1 - 100y_2 + 10y_3 - y_4, y_2^{'} + 1000y_2 - 10y_3 + 10y_4, y_3^{'} + y_3 - 10y_4, y_4^{'} + 0.1y_4\rangle.$$

Then, we compute a Gröbner basis for the ideal generated with respect to lex order and we obtain the $a_{i,j}$ for $i = 1, \cdots, 20$ and $j = 1, \cdots, 4$. Figure 2 shows the comparison between absolute error for the SNM and RHPM and exact solutions. As can be seen, at the beginning of the interval, the error is high but error tends to zero in the larger intervals. The numerical results and execution time of the proposed method, RHPM, and Taylor series method are displayed in Tables 1 and 4.

Figure 2. Comparison between absolute error for the SNM and RHPM.

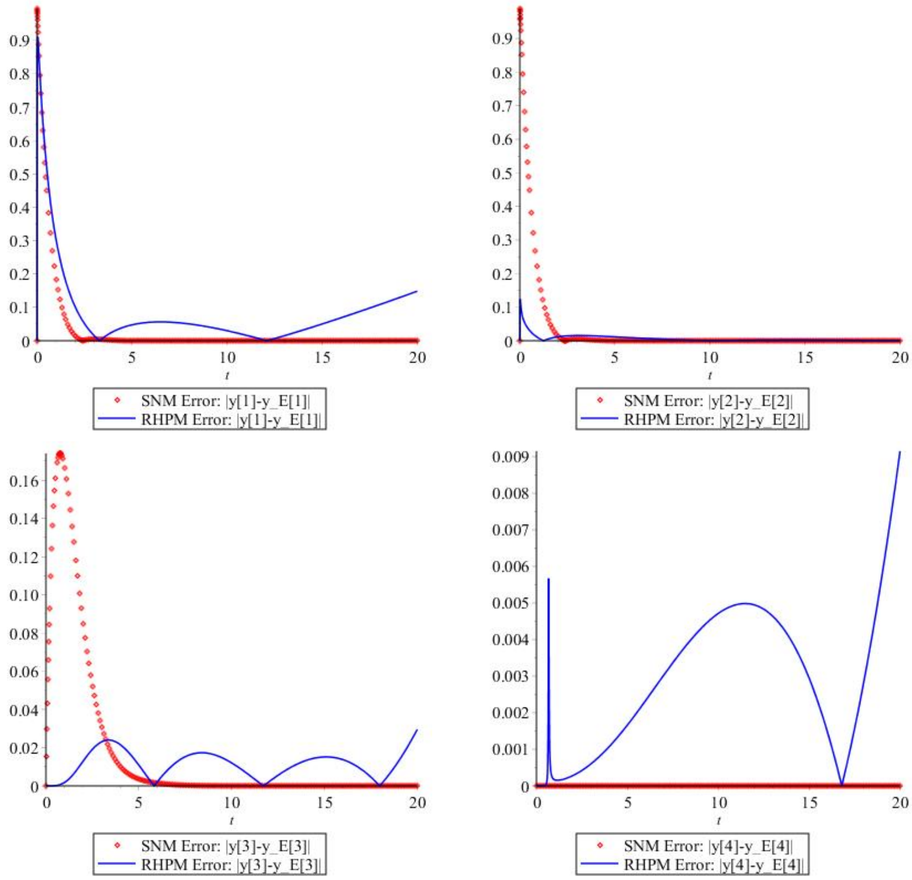


Table 1. Absolute error on [0,20] for Example 3.1

t	Method	y_1	y_2	y_3	y_4
	SNM	1.8694e-01	1.8503e-01	1.6696e-01	0.0000e+00
1	RHPM	3.0273e-01	7.2098e-03	1.7752e-03	1.6396e-04
	SNM	1.7983e-04	1.3953e-04	3.6011e-03	0.0000e+00
5	RHPM	4.7867e-02	1.1578e-02	1.0876e-02	1.6638e-03
	SNM	7.6890e-06	6.1252e-06	2.2164e-05	1.0000e-010
10	RHPM	2.9990e-02	3.4665e-04	1.2035e-02	4.7161e-03
	SNM	1.0412e-05	1.1339e-05	2.6333e-05	0.0000e+00
15	RHPM	5.0370e-02	2.3100e-03	1.5157e-02	2.9430e-03
	SNM	4.0963e-05	9.8658e-06	2.7533e-05	9.0000e-10
20	RHPM	1.4874e-01	7.2612e-04	2.9615e-02	9.1540e-03

Example 3.2. [17, 2] Consider the following non-linear stiff problem:

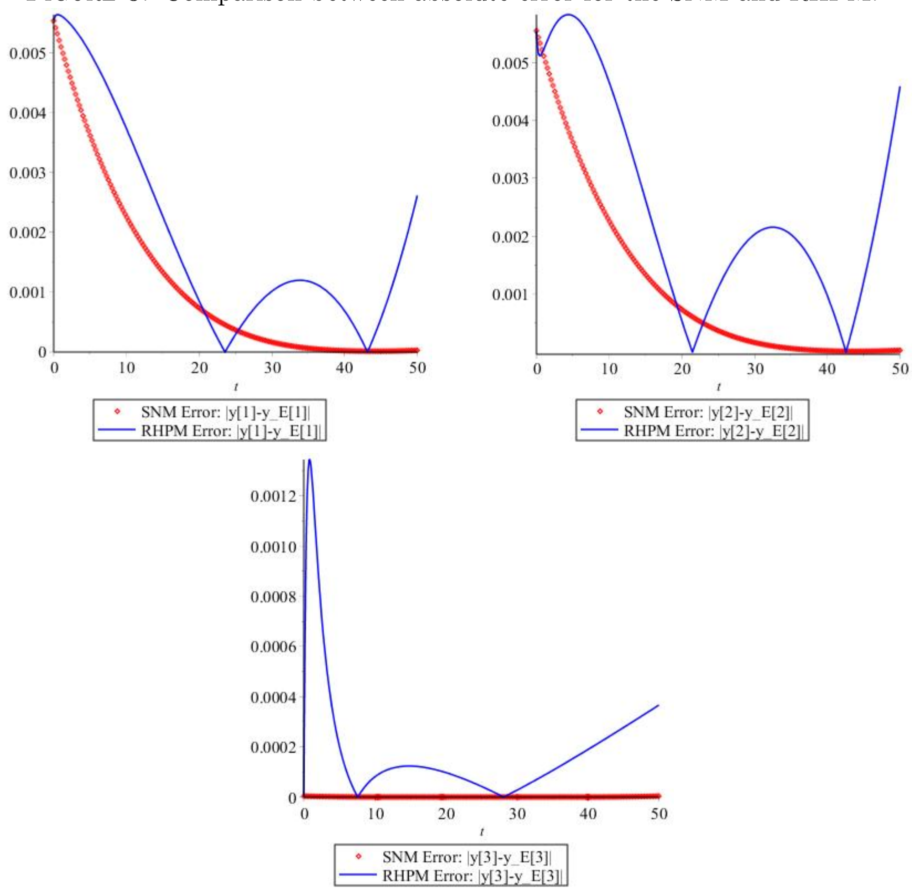
$$\begin{cases} y_1^{'} = -0.013y_1 - 1000y_1y_3 & y_1(0) = 1 \\ y_2^{'} = -2500y_2y_3 & y_2(0) = 1 \\ y_3^{'} = -0.013y_1 - 1000y_1y_3 - 2500y_2y_3 & y_3(0) = 0. \end{cases}$$

First, we assume the power series expansion y_j's (2.2) to order $n = 4$ in one variable as follows:

$$y_j(l) = c_j + \sum_{i=1}^{4} a_{i,j} l^i (h)^i \quad for \;\; j = 1, \ldots, 3, \tag{3.2}$$

where c_j is as $c_1 = 1$, $c_2 = 1$ and $c_3 = 0$. We obtain a polynomial system of 12 equations and 12 unknowns $a_{i,j}$ for $i = 1, \cdots, 4$ and $j = 1, \ldots, 3$. Next, we substitute

FIGURE 3. Comparison between absolute error for the SNM and RHPM.



the solution (3.2) and its derivatives in ideal generated by

$$\langle y_1^{'} + 0.013y_1 + 1000y_1y_3, y_2^{'} + 2500y_2y_3, y_3^{'} + 0.013y_1 + 1000y_1y_3 + 2500y_2y_3 \rangle.$$

Then, a Gröbner basis for the above ideal with respect to lex order is computed to obtain these unknown coefficients. Figure 3 shows the comparison between absolute error for the SNM and RHPM and exact solutions is given by the Taylor series. We describe the numerical results on [0, 50] in Table 2 and present the execution time of these methods in Table 4.

TABLE 2. Results for Example 3.2 on [0,50]

t	y_i	TS(Maple)	SNM	RHPM
	y_1	0.9907319	0.9907284	0.9902109
1	y_2	1.0092644	1.0092708	1.00938416
	y_3	-0.000003665	-0.000000672	-0.001322989
	y_1	0.9091683	.9091519	0.9076808
10	y_2	1.0908284	1.0908448	1.0932356
	y_3	-0.000003250	-0.000003250	0.00007710
	y_1	0.8229907	0.8229766	0.8228569
20	y_2	1.1770063	1.177020549	1.1768228
	y_3	-0.000002841	-0.000002841	0.00009464
	y_1	0.7421287	0.7421148	0.7432978
30	y_2	1.2578687	1.2578827	1.2556842
	y_3	-0.000002482	-0.000002482	-0.00002960
	y_1	0.6669652	0.6669536	0.6676638
40	y_2	1.3330326	1.3330442	1.3320474
	y_3	-0.000002167	-0.000002167	-0.0001913
	y_1	0.5976546	0.5976263	0.59503493
50	y_2	1.4023434	1.4023754	1.40693084
	y_3	-0.000001893	-0.000001821	-0.0003683

Example 3.3. [17] Consider the initial value problem

$$\begin{cases} y_1^{'} = -y_1 + 10^8 y_3(1-y_1) & y_1(0) = 1 \\ y_2^{'} = -10y_2 + 3.10^7 y_3(1-y_2) & y_2(0) = 1 \;\; 0 \leq t \leq 1. \\ y_3^{'} = -y_1^{'} - y_2^{'} & y_3(0) = 0 \end{cases}$$

Like the previous examples, we consider the solutions as a power series expansion to order $n = 4$ in one variable. We substitute these solutions and its derivatives in ideal generated by

$$\langle y_1^{'} + y_1 - 10^8.y_3(1-y_1), y_2^{'} + 10y_2 - 3.10^7 y_3(1-y_2), y_3^{'} + y_1^{'} + y_2^{'} \rangle.$$

Then, a Gröbner basis for the mentioned ideal with respect to lex order is computed. The numerical results and execution time of these methods are presented in Tables 3 and 4.

Table 3. Results for Example 3.3

Method	y_1	y_2	y_3
TS (Maple)	0.9999829	0.9994312	0.0005857
SNM	0.99998332	0.9994446	0.00057205
RHPM	1.3253315	0.70307088	0.00058218531

Table 4. Execution time at final state of examples

Method	Example 3.1	Example 3.2	Example 3.3
SNM	1.096	8.492	9.325
RHPM	90.262	56.909	24.648
TS(Maple)	68.500	118.560	22.480

4. Conclusion

The symbolic-numerical method is an excellent method that allows finding approximate solutions for stiff problems using Maple software. We implemented our algorithm in Maple 13 on Linux. Combining a Gröbner basis technique with power series method, we obtained a conceptually simple method to solve stiff systems of linear and non-linear differential equations. The simulation results showed the effectiveness of the proposed method. The results obtained using SNM and RHPM show that SNM can solve stiff systems more accurately and in the larger intervals than RHPM. Also, we see that the series solution obtained by Gröbner basis requires less execution time than the Taylor series method with an accuracy close to the same results.

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