An Application of STWS Technique in Solving Stiff Non-linear System: 'High Irradiance Responses' (HIRES) of Photomorphogenesis

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Abstract

This paper illustrates an application of the Single Term Walsh Series (STWS) technique in solving stiff non-linear system: 'High Irradiance RESponses' (HIRES) of Photomorphogenesis from plant physiology. The chemical reaction scheme of HIRES problem has been modelled into system of stiff non-linear differential equations. This stiff system has been solved using the STWS technique. The STWS solutions are compared with the results obtained by the well-known solvers, namely, VODE and RADAU5. The applicability of the STWS technique has been tested.

Key Words: HIRES; STWS; WF; BPF; Stiff; Non-linear

Introduction

Many physical systems such as nuclear reactors and laser oscillators give rise to stiff non-linear ordinary differential equations (ODEs) in which the magnitudes of the eigenvalues vary greatly. Methods not designed for stiff problems are ineffective on intervals where the solution changes slowly because they use time steps small enough to resolve the fastest possible change. Stiff problems typically arise in chemical kinetics, nuclear reactor theory, control theory, biochemistry, climatology, electronics, fluid dynamics, etc. The numerical integration of a stiff system has attracted many researchers. This paper deals with the STWS technique to determine the numerical solution of stiff non-linear system.

The STWS technique was introduced by Rao et al. [1] using Walsh Functions (WFs). This is based on an approach called “single segment approximation” which avoids operational matrices of large size and maximizes the reduction in the computational effort. This method provides discrete solutions of problems, to any length of time, in an easy manner. Many researchers have made use of this STWS technique to solve different systems. Palanisamy [2] have used the STWS approach to the analysis and optimal control of linear time invariant and time varying systems. Subbayan et al. [3] have used the STWS method for the optimal control of singularly perturbed linear systems. Palanisamy and Arunachalam [4] have presented the STWS method for the analysis of bilinear systems. Balachandran and Murugesan [5] have applied STWS technique to the analysis of linear and non-linear singular systems. Murugesan et al. [6] have obtained the STWS solutions of the second order multi-variable linear system.

Sepehrian and Razzaghi [7] have proposed STWS method to find the solution of time-varying singular non-linear systems. Dhayabaran et al. [8] have obtained the numerical solution of Robot Arm Model using STWS method and extended Runge-Kutta method based on Heronian Mean (RKHeM). Emimal et al. [9] have proposed a generalised STWS technique to determine discrete solutions for the systems of IVPs of any higher order ‘n’ with ‘p’ variables. Dhayabaran et al. [10] have applied this generalised STWS technique to higher order time-varying singular systems.

This paper illustrates an application of the STWS technique in solving stiff non-linear system: 'High Irradiance RESponses' (HIRES) of Photomorphogenesis from the field of plant physiology. The chemical reaction scheme of HIRES problem has been modelled into system of eight stiff non-linear differential equations. This stiff system has been solved using the STWS technique. The STWS solutions are compared with the results obtained by the well-known solvers, namely, VODE and RADAU5.

STWS Technique

It is well known that a function, which is periodic, may be expanded into a Fourier series or Power series. In a similar manner, a function $f(t)$, which is integrable in $[0,1]$ may be approximated by using WFs as

$$f(t) = \sum_{i=0}^{\infty} f_i \psi_i(t)$$
where \( \psi_{0,i} \) is the \( i \)th WF and \( f_i \) is the corresponding coefficient. In practice, while approximating a function, only the first 'm' components are considered. If the coefficients of the WFs are concisely written as 'm' vectors, then

\[
F = (f_0, f_1, \ldots, f_{m-1})^T
\]

and

\[
\psi(t) = [\psi_{0,0}(t), \psi_{0,1}(t), \ldots, \psi_{0,m-1}(t)]^T
\]

where \( m = 2^k \), \( k \) is an integer and \( T \) denotes transpose.

Then the above function \( f(t) \) becomes

\[
\Phi(t) \approx B_1 \tau \psi(t).
\]

The coefficients are given by

\[
f_i = \int_0^1 f(t) \psi_i(t) dt.
\]

It has been proved by Chen and Hsiao [13] that

\[
\int_0^1 f(t) dt \approx F^T E \psi(t).
\]

The constant square matrix \( E \) is called the operational matrix for integration in \( F \) and is given by

\[
E_{(m \times m)} = \begin{pmatrix}
E_{(m/2 \times m/2)} & -\frac{1}{2m} I_{(m/2 \times m/2)} \\
\frac{1}{2m} I_{(m/2 \times m/2)} & O_{(m/2 \times m/2)}
\end{pmatrix}
\]

with

\[
E_{(2 \times 2)} = \begin{pmatrix}
\frac{1}{2} & -1 \\
1 & 4
\end{pmatrix}
\]

and \( E_{(1 \times 1)} = \frac{1}{2} \).

A function \( x(t) \) may be expanded into a STWS in the normalised interval \( s \in [0,1) \) (which corresponds to \( t \in [0,1/m) \)) by defining \( s = mt \) as

\[
x(s) = B_1 \psi_{0,0}(s).
\]

Here \( B_1 \) is the block pulse function (BPF) value of \( x(t) \) in \( t \in [0,1/m) \). The operational matrix \( E \) for integration becomes a scalar, since

\[
E_{(1 \times 1)} = \frac{1}{2}.
\]

Consider the integral \( \int_0^1 \dot{x}(s) ds \).

Express \( \dot{x}(s) \) in STWS in the first normalized interval \( s \in [0,1) \) as

\[
\dot{x}(s) = C_1 \psi_{0,0}(s)
\]

where \( C_1 \) is the BPF value of the rate vector \( \dot{x}(t) \).

Integrating Eqn. (2.1) with the operational matrix \( E = \frac{1}{2} \)

\[
B_1 \psi_{0,0}(s) = \frac{1}{2} C_1 \psi_{0,0}(s) + x(0)
\]

According to the definition of Sannuti [14], the BPF value of \( \dot{x}(s) \) in the first interval is given by

\[
C_1 = m \int_0^{1/m} \dot{x}(s) ds, \quad t \in [0,1/m).
\]

When Eqn. (2.3) is normalized with \( t = s/m \)

\[
C_1 = \int_0^1 \dot{x}(s) ds = x(1) - x(0), \quad t \in [0,1),
\]

\[
x(1) = C_1 + x(0).
\]

For any interval \( k \),

\[
x(k) = C_1 + x(k-1).
\]

Eqn. (2.4) gives an important way to get discrete time values of \( x(t) \) and to continue the STWS solution to the next normalized interval.

**STWS Technique for Solving Non-linear Systems**

Consider a first order non-linear system of the following form:

\[
\dot{x}(t) = f(t, x(t), u(t)), \quad x(0) = x_0,
\]

where the non-linear function \( f \in R^n \), the state \( x(t) \in R^n \), and the control \( u(t) \in R^n \). With the STWS approach, the given function is expanded in the normalized interval \( t \in [0,1) \), which corresponds to \( s \in [0,1/m) \) by defining \( t = ms \), \( m \) being any integer. Normalizing Eqn. (3.1), we get

\[
m \dot{x}(s) = f(s, x(s), u(s)), \quad x(0) = x_0,
\]

Let \( \dot{x}(s) \) and \( x(s) \) be expanded by STWS series in the \( kth \) interval as

\[
\dot{x}(s) = \psi_{0,0}(s) \quad \text{and} \quad x(s) = \psi_{0,0}(s)
\]

Integrating Eqn. (3.3) with the operational matrix \( E = \frac{1}{2} \), we get

\[
x(k) = \frac{1}{2} V(k) + x(k-1).
\]

Therefore, \( x(s) = \left( \frac{1}{2} V^{(k)} + x(k-1) \right) \psi_{0,0}(s) \) (3.5)

To solve Eqn. (3.2), we first substitute Eqn. (3.5) in \( f(s, x(s), u(s)) \). Then we express the resulting equation by STWS as

\[
f(s, \left( \frac{1}{2} V^{(k)} + x(k-1) \right) \psi_{0,0}(s), u(s)) = F^{(k)} \psi_{0,0}(s)
\]

(3.6)

Using the Eqns. (3.2), (3.3), (3.5), and (3.6), we get

\[
m V^{(k)} = F^{(k)}.
\]
By solving Eqn. (3.7), the components of $V^k$ can be obtained. Then, by substituting $V^k$ in Eqn. (3.4), we obtain discrete approximations of the state $x(t)$.

**Description of HIRES Problem**

The HIRES problem was proposed by Schäfer [15] in 1975. The parallel-IVP-algorithm group of Centre for Mathematics and Computer Science have contributed this problem to the test set [16]. This problem describes how light is involved in morphogenesis. It explains the ‘High Irradiance Responses’ of photomorphogenesis on the basis of phytochrome, by means of a chemical reaction involving eight reactants.

The reaction scheme for the HIRES problem is given in Fig. 4.1. $P_r$ and $P_{fr}$ refer to the red and far-red absorbing form of phytochrome, respectively. They can be bound by two receptors $X$ and $X'$, partially influenced by the enzyme $E$. The values of the parameters were taken as:

$$
k_1 = 1.71, \quad k_6 = 8.32 \quad k_2 = 0.43, \quad k_7 = 280 \quad k_3 = 8.32, \quad k_8 = 0.69 \quad k_4 = 0.69, \quad k_5 = 0.035, \quad o_{k_i} = 0.0007
$$

The chemical process is started at $t_0 = 0$ by mixing one mol of $P_r$ with 0.0057 mol of $E$. The integration process is continued during 321.8122 seconds. This value and the parameter values were chosen by Hairer and Wanner [17].

The reaction scheme for the HIRES problem can be described by a set of differential equations as follows:

$$
\begin{align*}
\frac{d[P_r]}{dt} &= -k_1[P_r] + k_2[P_{fr}] + k_3[P_rX] + o_{k_i} \\
\frac{d[P_{fr}]}{dt} &= k_1[P_r] - (k_2 + k_3)[P_{fr}] \\
\frac{d[P_rX]}{dt} &= -(k_3 + k_4)[P_rX] + k_2[P_rX] \quad + k_5[P_rX'] \\
\frac{d[P_{r}X']}{dt} &= -(k_3 + k_4)[P_{r}X'] \quad + k_5[P_{r}X'] \quad + k_6[P_{r}X] \\
\frac{d[P_{fr}]}{dt} &= k_1[P_{fr}] + k_4[P_{fr}] \\
\frac{d[P_{r}X']E}{dt} &= -(k_3 + k_4)[P_{r}X' E] + k_4[P_{fr}X'] \quad [E] \\
\frac{d[P_{fr}X'E]}{dt} &= -(k_3 + k_4)[P_{fr}X' E] + k_4[P_{fr}X'] \quad [E] \\
\frac{d[E]}{dt} &= (k_3 + k_4)[P_{fr} X' E] - k_4[P_{fr} X'] \quad [E].
\end{align*}
$$

The initial vector $y_0$ is given by $(1, 0, 0, 0, 0, 0, 0, 0.0057)^T$.

The square brackets ‘[ ]’ denote concentrations. Identifying the concentrations of $P_r$, $P_{fr}$, $P_rX$, $P_{fr}X$, $P_rX'$, $P_{fr}X'$, $P_rX'E$ and $E$ with $y_i, i \in \{1, 2, \ldots, 8\}$, respectively, the above reaction scheme for HIRES problem can be transformed into the system of stiff non-linear differential equations as follows:

$$
\frac{dy}{dt} = f(y), \quad y(0) = y_0, \text{ with } y \in R^8, 0 \leq t \leq 321.8122.
$$

The function $f$ is defined by

$$
f(y) = 
\begin{pmatrix}
-1.71y_1 + 0.43y_2 + 8.32y_5 + 0.0007 \\
1.71y_1 - 8.75y_2 \\
-10.03y_3 + 0.43y_4 + 0.085y_5 \\
8.32y_3 + 1.71y_4 - 1.12y_6 \\
-1.74y_5 + 0.43y_6 + 0.43y_7 \\
-280y_3 + 0.69y_4 + 1.71y_5 - 0.43y_6 + 0.69y_7 \\
280y_5 - 1.81y_7 \\
-280y_3 + 1.81y_7
\end{pmatrix}
$$

Fig. 4.1
Applicability of STWS Technique in Solving HIRES Problem

The discrete solutions of HIRES problem can be determined using the STWS technique discussed in Section 3. The STWS solutions at the end of the integration interval are compared with the results obtained by the well-known solvers VODE and RADAU5. These results have been shown in Table 5.1. The solution graphs by the solver RADAU5 are given in Fig. 5.2(a) – Fig. 5.2(h) and the solution graphs by the STWS technique are given in Fig. 5.3(a)–Fig. 5.3(h).

<table>
<thead>
<tr>
<th>Variables</th>
<th>STWS</th>
<th>VODE</th>
<th>RADAU5</th>
</tr>
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<tr>
<td>y1</td>
<td>0.0007382</td>
<td>0.0007405</td>
<td>0.0007371</td>
</tr>
<tr>
<td>y2</td>
<td>0.0001445</td>
<td>0.0001449</td>
<td>0.0001442</td>
</tr>
<tr>
<td>y3</td>
<td>0.0000591</td>
<td>0.0000595</td>
<td>0.0000599</td>
</tr>
<tr>
<td>y4</td>
<td>0.0011776</td>
<td>0.0011821</td>
<td>0.0011757</td>
</tr>
<tr>
<td>y5</td>
<td>0.0024179</td>
<td>0.0024836</td>
<td>0.0023863</td>
</tr>
<tr>
<td>y6</td>
<td>0.0063381</td>
<td>0.0064948</td>
<td>0.0062390</td>
</tr>
<tr>
<td>y7</td>
<td>0.0028720</td>
<td>0.0029543</td>
<td>0.0028500</td>
</tr>
<tr>
<td>y8</td>
<td>0.0027926</td>
<td>0.0027457</td>
<td>0.0028500</td>
</tr>
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</table>
To demonstrate the applicability of the STWS technique, the discrete solutions of this problem have been determined in the interval \([0, 5]\) by varying the values of ‘m’ (involved in the STWS technique), for example, \(m = 100, 200, 300, 400, 500, 600\). The absolute errors between the STWS solutions of \(y_1, y_2, \ldots, y_8\) in \([0, 5]\) at two consecutive values of ‘m’, say \(m_1\) and \(m_2\), have been determined which may be denoted as \(Err_m\).

But in this paper, as an illustration, the error results for the variables \(y_1\) and \(y_4\) have been given in Tables 5.2 - 5.5. Further, the maximum errors for the variables \(y_1, y_2, \ldots, y_8\) in \([0, 5]\) have been determined and shown in Table 5.6.

### Table 5.2

<table>
<thead>
<tr>
<th>Time t</th>
<th>STWS Solution of (y_1)</th>
<th>(m = 100)</th>
<th>(m = 200)</th>
<th>(m = 300)</th>
<th>(m = 400)</th>
<th>(m = 500)</th>
<th>(m = 600)</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
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<td>1</td>
</tr>
<tr>
<td>1</td>
<td>0.255485</td>
<td>0.255491</td>
<td>0.255492</td>
<td>0.255492</td>
<td>0.255492</td>
<td>0.255492</td>
<td>0.255493</td>
</tr>
<tr>
<td>2</td>
<td>0.123519</td>
<td>0.123520</td>
<td>0.123520</td>
<td>0.123520</td>
<td>0.123520</td>
<td>0.123520</td>
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</tr>
<tr>
<td>3</td>
<td>0.07470</td>
<td>0.074697</td>
<td>0.074697</td>
<td>0.074697</td>
<td>0.074697</td>
<td>0.074697</td>
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</tr>
<tr>
<td>4</td>
<td>0.047824</td>
<td>0.047823</td>
<td>0.047823</td>
<td>0.047823</td>
<td>0.047823</td>
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<tr>
<td>5</td>
<td>0.031652</td>
<td>0.031652</td>
<td>0.031652</td>
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### Table 5.3

<table>
<thead>
<tr>
<th>Time t</th>
<th>Absolute Error in (y_1)</th>
<th>(Err_{100}^{m=200})</th>
<th>(Err_{200}^{m=300})</th>
<th>(Err_{300}^{m=400})</th>
<th>(Err_{400}^{m=500})</th>
<th>(Err_{500}^{m=600})</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>5.0E-06</td>
<td>1.0E-06</td>
<td>4.0E-07</td>
<td>2.0E-07</td>
<td>1.0E-07</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>8.0E-07</td>
<td>2.0E-07</td>
<td>1.0E-07</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>3.0E-07</td>
<td>0</td>
<td>0</td>
<td>1.0E-07</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>6.0E-07</td>
<td>0</td>
<td>1.0E-07</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>7.0E-07</td>
<td>1.0E-07</td>
<td>0</td>
<td>0</td>
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Table 5.4

<table>
<thead>
<tr>
<th>Time t</th>
<th>STWS Solution of y4</th>
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<tbody>
<tr>
<td></td>
<td>m = 100</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0.458531</td>
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<tr>
<td>2</td>
<td>0.344056</td>
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<tr>
<td>3</td>
<td>0.220462</td>
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<tr>
<td>4</td>
<td>0.139693</td>
</tr>
<tr>
<td>5</td>
<td>0.089744</td>
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Table 5.5

<table>
<thead>
<tr>
<th>Time t</th>
<th>Absolute Error in y4</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>Error Err^200_100</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>8.8E-06</td>
</tr>
<tr>
<td>2</td>
<td>1.8E-06</td>
</tr>
<tr>
<td>3</td>
<td>7E-07</td>
</tr>
<tr>
<td>4</td>
<td>7E-07</td>
</tr>
<tr>
<td>5</td>
<td>1E-06</td>
</tr>
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Table 5.6

<table>
<thead>
<tr>
<th>Variables</th>
<th>Maximum Error in [0, 5]</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>Error Err^200_100</td>
</tr>
<tr>
<td>y1</td>
<td>5.50E-06</td>
</tr>
<tr>
<td>y2</td>
<td>1.20E-06</td>
</tr>
<tr>
<td>y3</td>
<td>6.00E-07</td>
</tr>
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<td>y4</td>
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<td>y7</td>
<td>1.00E-07</td>
</tr>
<tr>
<td>y8</td>
<td>1.00E-07</td>
</tr>
</tbody>
</table>

Conclusion

In this paper, the chemical reaction scheme of HIRES problem has been transformed into a system of eight stiff non-linear differential equations. The STWS technique has been applied to solve this problem. From the graphs given in Fig. 5.3(a) – (h), it is observed that after about 320 seconds, the concentrations of the species are very small, which indicates that almost all phytochrome has been transformed to Pfr'. The amount of Pfr' can be derived from the conservation of the total amount of phytochrome.

From Table 5.1, it is observed that the STWS solutions agree well with that of the solvers VODE and RADAU5. In order to ascertain the applicability of the STWS technique, a thorough study has been undertaken by determining the STWS solutions for the decision variables involved in HIRES problem in [0, 5] by varying the values of m = 100, 200, 300, 400, 500, 600. From Table 5.6, it is observed that the error decreases as the value of 'm' increases.

Hence, it is concluded that the proposed STWS technique is stable and very much applicable in solving the real-world problems like HIRES problem and similar realistic problems existing in various fields of science and engineering.

References


