# Embedded Singly Diagonally Implicit RungeKutta -Nystrom Method Order 5(4) for the Integration of Special Second Order ODEs 

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#### Abstract

In this paper a new embedded Singly Diagonally Implicit Runge-Kutta Nystrom fourth order in fifth order method for solving special second order initial value problems is derived. A standard set of test problems are tested upon and comparisons on the numerical results are made when the same set of test problems are reduced to first order systems and solved using the existing embedded diagonally implicit Runge-Kutta method. The results suggests the superiority of the new method.


Keywords-Runge-Kutta Nystrom, Special second order problems.

## I. INTRODUCTION

SEVERAL methods have been proposed for the numerical solutions of the special second-order ordinary differential equations (ODEs) of the form:

$$
\begin{equation*}
y^{\prime \prime}=f(x, y), y\left(x_{0}\right)=y_{0}, y^{\prime}\left(x_{0}\right)=y_{0}^{\prime} \tag{1}
\end{equation*}
$$

In which $f$ does not depend on $y^{\prime}$. In general the second order equation (1) can be reduced to an equivalent first-order system of twice the dimension and solved using the standard Runge-Kutta ( RK) method. However, it is more efficient if the equation can be solved directly using Runge-Kutta Nystrom ( RKN) method, such work can be seen in Sharp and Fine [1], Dormand, El-Mikkawy and Prince [2] and ElMikkawy and El- Desouky [3]. Generally efficient RungeKutta and Runge-Kutta Nystrom codes involved the embedded pairs of orders $q(p)$ where the method of order $q=$ $p+1$ is used to obtain the numerical solutions of the problems and the method of order $p$ is used to obtain the local truncation error, hence, the next step of the integration can be calculated. In this paper we are going to derive embedded pairs which are diagonally implicit and all the diagonal element are equal, such method is very efficient in solving stiff differential equations, since the iteration matrix $\left(I-h^{2} \gamma J\right)$ (where $J$ is the Jacobian of the system of equations) of the Newton iteration can be used in all stages.

The Runge-Kutta Nystrom pair generates the approximations $y_{n+1}, \bar{y}_{n+1}, y_{n+1}^{\prime}, \bar{y}_{n+1}^{\prime}$ to $y\left(x_{n+1}\right)$ and $y^{\prime}\left(x_{n+1}\right)$, according to the following:

[^0]\[

$$
\begin{align*}
& y_{n+1}=y_{n}+h y_{n}^{\prime}+h^{2} \sum_{i=1}^{s} b_{i} k_{i}, y_{n+1}^{\prime}=y_{n}^{\prime}+h \sum_{i=1}^{s} b_{i}^{\prime} k_{i}  \tag{2a}\\
& \bar{y}_{n+1}=y_{n}+h y_{n}^{\prime}+h^{2} \sum_{i=1}^{s-1} \overline{b_{i}} k_{i}, \overline{y^{\prime}}{ }_{n+1}=y_{n}^{\prime}+h \sum_{i=}^{s-1} \overline{b_{i}^{\prime}} k_{i} \tag{2b}
\end{align*}
$$
\]

The first two formulae are order $q$ and the second two are order $p$ and

$$
\begin{align*}
& k_{i}=f\left(x_{n}+c_{i} h, y_{n}+c_{i} h y_{n}^{\prime}+h^{2} \sum_{j=1}^{i} a_{i j} k_{j}\right)  \tag{2c}\\
& i=1,2, \cdots, s
\end{align*}
$$

The method can also be written in Butcher Tableau

| $C$ | $A$ |
| :---: | :---: |
|  | $b$ |
|  | $b^{\prime}$ |
|  | $\bar{b}$ |
|  | $\overline{b^{\prime}}$ |

$\left(C=\left[c_{1}, c_{2}, \cdots, c_{s}\right]^{T}, \quad A=\left[a_{i j}\right], \quad b=\left[b_{1}, b_{2}, \cdots, b_{s}\right]\right.$,
$b^{\prime}=\left[b_{1}^{\prime}, b_{2}^{\prime}, \cdots, b_{s}^{\prime}\right], \bar{b}=\left[\overline{b_{1}}, \overline{b_{2}}, \cdots, \overline{b_{s-1}}\right]$,
$\overline{b^{\prime}}=\left[\overline{b_{1}^{\prime}}, \overline{b_{2}^{\prime}}, \cdots, \overline{b_{s-1}^{\prime}}\right]$. We refer to (2) as the Runge-Kutta
Nystrom pair, where the approximations of order $p+1$ are being advanced from step to step and the approximations of order $p$ is used for the local truncation error so that the next stepsize can be obtained based on the local truncation error. Hence, the code developed here is the variable stepsize code.

## II. Derivation of the Method

According to Papageorgiou, Famwlis and Tsitouras [4] the coefficients of a fifth order Runge-Kutta-Nystrom method must satisfy the following order conditions after using two basic simplifying assumptions.

TABLE I
ORDER CONDITIONS FOR $y^{\prime}$

| Order <br> conditions: | 1 | $\sum_{i} b_{i}^{\prime}=1$ | (3) |
| :--- | ---: | :---: | :---: |
| Order <br> conditions: | 2 | $\sum_{i} b_{i}^{\prime} c_{i}=\frac{1}{2}$ | (4) |
| Order <br> conditions: | 3 | $\sum_{i} b_{i}^{\prime} c_{i}^{2}=\frac{1}{3}$ | (5) |
| Order <br> conditions: | 4 | $\sum_{i} b_{i}^{\prime} c_{i}^{3}=\frac{1}{4}$ | (6) |
| Order <br> conditions: | 5 | $\sum_{i} b_{i}^{\prime} c_{i}^{4}=\frac{1}{5}$ | (7) |

TABLE II
ORDER CONDITIONS FOR $\overline{y^{\prime}}$

| Order <br> conditions: | 1 | $\sum_{i} \overline{b_{i}^{\prime}}=1$ | $(3)^{*}$ |
| :--- | :--- | :--- | :--- |
| Order <br> conditions: | 2 | $\sum_{i} \overline{b_{i}^{\prime}} c_{i}=\frac{1}{2}$ | $(4)^{*}$ |
| Order <br> conditions: | 3 | $\sum_{i} \overline{b_{i}^{\prime}} c_{i}^{2}=\frac{1}{3}$ | $(5)^{*}$ |
| Order <br> conditions: | 4 | $\sum_{i} \overline{b_{i}^{\prime} c_{i}^{3}}=\frac{1}{4}$ | (6)* |
|  | $\sum_{i j} \overline{b_{i}^{\prime}} a_{i j} c_{j}=\frac{1}{24}$ | (7)* |  |

The simplifying assumptions are

$$
\begin{align*}
& \sum_{i j} a_{i j}=\frac{1}{2} c_{i}^{2}  \tag{11}\\
& b_{i}=b^{\prime}\left(1-c_{i}\right) \tag{12}
\end{align*}
$$

From which the values of $a_{i 1}$ and $b_{i}$ for $i=1,2, \cdots, s$ can be obtained respectively. The proof of using the simplifying assumptions can be found in Hairer and Wanner [5].

For the fifth order method all eight order equations for $y^{\prime}$
in Table I have to be satisfied and for the fourth order method
all the $\overline{b_{i}^{\prime}}$ have to satisfy all the equations in Table II and the values of $\overline{b_{i}}$ can be obtained from the following equation:

$$
\begin{equation*}
\overline{b_{i}}=\overline{b_{i}^{\prime}}\left(1-c_{i}\right) \tag{13}
\end{equation*}
$$

Here we are going to derive embedded singly diagonally implicit RKN method of order 4, 4-stage in order 5, 5 -stage or can be written as SDIRKN 5(4) method and $\gamma$ is the diagonal element.

Algorithm to find the coefficients of SDIRKN 5(4) method.
Step 1: Let $\gamma=0.25$
Step 2: $c_{1}=\sqrt{2 \gamma} \quad$ (from equation 11 for $i=1$ ).
Step 3: Give the values of $c_{2}, c_{3}, c_{4}, c_{5}$, with all the values of $c$ 's obtain $b_{1}^{\prime}, b_{2}^{\prime}, b_{3}^{\prime}, b_{4}^{\prime}$ and $b_{5}^{\prime}$ from equations (3),(4),(5),(6) and (8).

Step 4: Use (12) to get the values of $b_{1}, b_{2}, b_{3}, b_{4}$ and $b_{5}$.
Step 5: Use (3)*, (4)*,(5)* and (6)* and solve for $\overline{b_{1}^{\prime}}, \overline{b_{2}^{\prime}}, \overline{b_{3}^{\prime}}$ and $\overline{b_{4}^{\prime}}$.

Step 6: Use (13) to get the values of $\overline{b_{1}}, \overline{b_{2}}, \overline{b_{3}}$ and $\overline{b_{4}}$.
Step 7: Give the values of $a_{52}$ and $a_{54}$ and use (7), $(7)^{*},(9)$ and (10) to obtain the values of $a_{i j}$ where $i \neq 1$.
Step 8: Use (11) to get the values of $a_{i 1}$.
By using MAPLE, the following are the parameters of the SDIRKN 5(4) method with free parameters are chosen to be $\gamma=0.25, \quad c_{2}=0.2, c_{3}=0.4, c_{4}=0.6, c_{5}=0.9, \quad a_{52}=-0.1$ and $a_{53}=0.15$
$c_{1}=0.7071067811865475$
$c_{2}=0.2$
$c_{3}=0.4$
$C_{4}=0.6$
$c_{5}=0.9$
$a_{11}=a_{22}=a_{33}=a_{44}=a_{55}=0.25$
$a_{21}=-0.23$
$a_{31}=-0.3925002502501825$
$a_{32}=0.2225002502501825$
$a_{41}=-0.008891426702213870$
$a_{42}=0.2120976370788504$
$a_{43}=-0.2732062103766366$
$a_{51}=-1.672156796751771$
$a_{52}=-0.1$
$a_{53}=0.15$
$a_{54}=1.777156796751771$
$b_{1}^{\prime}=-0.8909522811353591$
$b_{2}^{\prime}=0.6247556718194198$
$b_{3}^{\prime}=-0.7000548195198433$
$b_{4}^{\prime}=1.615190309345717$
$b_{5}^{\prime}=0.3510611194900651$
$b_{1}=-0.2609538814309234$
$b_{2}=0.4998045374555358$
$b_{3}=-0.4200328917119060$
$b_{4}=0.6460761237382868$
$b_{5}=0.03510611194900651$
$\overline{b_{1}^{\prime}}=1.318915246389200$
$\overline{b_{2}^{\prime}}=0.3743745692181844$
$\overline{b_{3}^{\prime}}=0.4575746950566785$
$\overline{b_{4}^{\prime}}=-1.150864510664063$
$\overline{b_{1}}=0.3863013318570706$
$\overline{b_{2}}=0.2994996553745475$
$\overline{b_{3}}=0.2745448170340071$
$\overline{b_{4}}=-0.4603458042656252$

The above coefficients are substituted into the error equations of the sixth order method both for $y$ and $y^{\prime}$ see Dormand [6] and we obtained the error norm of the method which is:

$$
\left\|\tau^{(6)}\right\|_{2}=8.29696 \times 10^{-3} \text { and }\left\|\tau^{\prime(6)}\right\|_{2}=9.94999 \times 10^{-3} .
$$

Where $\left\|\tau^{(6)}\right\|_{2}=\sqrt{\sum_{j=1}^{n_{6}}\left(\tau_{j}^{(6)}\right)^{2}}$ and
$\left\|\tau^{\prime(6)}\right\|_{2}=\sqrt{\sum_{j=1}^{n_{6}}\left(\tau_{j}^{\prime(6)}\right)^{2}}, \tau$ and $\tau^{\prime}$ are error equations associated with the method. The error norms are smaller compared to other methods such as method in [4] which has error norms $10^{-2}$.

## III. Test Problems

Below are some of the problems tested:
Problem 1: A nonlinear problem.

$$
\begin{aligned}
& y^{\prime \prime}+100 y=\sin (y) \\
& y(0)=0, \quad y^{\prime}(0)=1, \quad 0 \leq x \leq 20 \pi
\end{aligned}
$$

There is no true solution but the value at $20 \pi$ is 0.000392823991 .

Source: Chawla and Rao [7]
The first order system: The new variables are $y_{1}=y$
and $y_{2}=y^{\prime}$

$$
\begin{aligned}
& y_{1}^{\prime}=y_{2} \\
& y_{2}^{\prime}+100 y_{1}=\sin \left(y_{1}\right)
\end{aligned}
$$

$$
y_{1}(0)=0, \quad y_{2}(0)=1 \quad 0 \leq x \leq 20 \pi
$$

Problem 2:

$$
\begin{aligned}
& y^{\prime \prime}=-y+x \\
& y(0)=1, \quad y^{\prime}(0)=2, \quad 0 \leq x \leq 16 \pi
\end{aligned}
$$

$$
\text { Solution: } y(x)=\sin (x)+\cos (x)+x
$$

Source: Allen and Wing [8]
The first order system :

$$
\begin{aligned}
& y_{1}^{\prime}=y_{2} \\
& y_{2}^{\prime}=-y_{1}+x \quad, \quad y_{1}(0)=1, \quad y_{2}(0)=2, \\
& 0 \leq x \leq 20 \pi \\
& \text { Solutions: } \\
& y_{1}(x)=\sin (x)+\cos (x)+x, \\
& y_{2}(x)=\cos (x)-\sin (x)+1 .
\end{aligned}
$$

Problem 3:

$$
\begin{aligned}
& y_{1}^{\prime \prime}=-4 x^{2} y_{1}-\frac{2 y_{2}}{\sqrt{y_{1}^{2}+y_{2}^{2}}}, \\
& y_{1}\left(x_{0}\right)=0, \quad y_{1}^{\prime}\left(x_{0}\right)=-\sqrt{2 \pi} \\
& y_{2}^{\prime \prime}=-4 x^{2} y_{2}+\frac{2 y_{1}}{\sqrt{y_{1}^{2}+y_{2}^{2}}}, \\
& y_{2}\left(x_{0}\right)=1, \quad y_{2}^{\prime}\left(x_{0}\right)=0 \\
& \sqrt{\frac{\pi}{2}} \leq x \leq 5 \pi
\end{aligned}
$$

Solution: $y_{1}(x)=\cos \left(x^{2}\right), \quad y_{2}(x)=\sin \left(x^{2}\right)$
Source: Sharp and Fine [1]
The first order system:

$$
\begin{aligned}
& y_{1}^{\prime}=y_{3}, y_{2}^{\prime}=y_{4}, y_{3}^{\prime}=-4 x^{2} y_{1}-\frac{2 y_{2}}{\sqrt{y_{1}^{2}+y_{2}^{2}}}, \\
& y_{4}^{\prime}=-4 x^{2} y_{2}+\frac{2 y_{1}}{\sqrt{y_{1}^{2}+y_{2}^{2}}} \\
& y_{1}\left(x_{0}\right)=0, \quad y_{2}\left(x_{0}\right)=1, \quad y_{3}\left(x_{0}\right)=-\sqrt{2 \pi}, \\
& y_{4}\left(x_{0}\right)=0 \\
& \text { Solution: } \quad y_{1}(x)=\cos \left(x^{2}\right), \quad y_{2}(x)=\sin \left(x^{2}\right), \\
& y_{3}(x)=-2 x \sin \left(x^{2}\right), \quad y_{4}(x)=2 x \cos \left(x^{2}\right) .
\end{aligned}
$$

Problem 4: (The two-body gravitational problem)

$$
\begin{aligned}
& y_{1}^{\prime \prime}=\frac{-y_{1}}{\left(\sqrt{y_{1}^{2}+y_{2}^{2}}\right)^{3}}, \quad y_{1}(0)=1, y_{1}^{\prime}(0)=0 \\
& y_{2}^{\prime \prime}=\frac{-y_{2}}{\left(\sqrt{y_{1}^{2}+y_{2}^{2}}\right)^{3}}, \quad y_{2}(0)=0, \quad y_{2}^{\prime}(0)=1 \\
& 0 \leq x \leq 16 \pi, \\
& \text { Solution: } y_{1}(x)=\cos (x), \quad y_{2}(x)=\sin (x) . \\
& \text { Source: Dorman et. al. }[2]
\end{aligned}
$$

The first order system:

$$
\begin{gathered}
y_{1}^{\prime}=y_{3}, y_{2}^{\prime}=y_{4}, y_{3}^{\prime}=\frac{-y_{1}}{\left(\sqrt{y_{1}^{2}+y_{2}^{2}}\right)^{3}}, y_{4}^{\prime}=\frac{-y_{2}}{\left(\sqrt{\left.y_{1}^{2}+y_{2}^{2}\right)^{3}}\right.} \\
y_{1}(0)=1, \quad y_{2}(0)=0, \quad y_{3}(0)=0, \quad y_{4}(0)=1
\end{gathered}
$$

$$
\text { Solutions: } \quad y_{1}(x)=\cos (x), \quad y_{2}(x)=\sin (x),
$$

$$
y_{3}(x)=-\sin (x), \quad y_{4}(x)=\cos (x) .
$$

## IV. Implementation and Numerical Results

The set of tested problems in section III is solved using the new method and the results are compared with the numerical results when the same set of test problems are reduced to first order system twice the dimension and solve using method by Butcher and Chen [9].

For all the problems, they are considered as nonstiff and solve using simple iterations where every $k$ 's are iterated three times once stiffness is detected through $h_{\text {acc }}>h_{\text {iter }}$, the whole system is considered stiff and solve using Newton iterations. $h_{a c c}$ is the stepsize which is expected to meet the specified accuracy .
$h_{i t e r}$ is the stepsize which will make the iteration converge. Coefficient matrix for the Newton iteration is $\left(I-h^{2} \gamma J\right)$. Local truncation error : LTE $=y_{n}-\overline{y_{n}}=h^{2} \sum_{i}^{s}\left(b_{i} k_{i}-\bar{b}_{i} k_{i}\right)$. In this paper we just control the stepsize for $y$ because we feel that the formula for $y$ contained the value of $y^{\prime}$, thus controlling $y$ means we are also indirectly controlling the value of $y^{\prime}$.

For the new method (F1) the next stepsize is

$$
h_{\text {new }}=0.5\left[\frac{t o l}{2\left|y_{n}-\overline{y_{n}}\right|}\right]^{\frac{1}{p+1}} h_{\text {old }}
$$

and for the second method (B1)

$$
h_{\text {new }}=0.2\left[\frac{t o l}{2\left|y_{n}-\overline{y_{n}}\right|}\right]^{\frac{1}{p+1}} h_{\text {old }}
$$

and for the second method

Where tol is the chosen tolerance, $h_{\text {old }}$ is the current stepsize, $p$ is the order of the method and $\left|y_{n}-\overline{y_{n}}\right|$ is the local truncation error. The reason why we used safety factor 0.2 here is that to keep the global error small enough so that it is comparable with method F1.

Some of the notations used:
$2.345789\left(10^{-2}\right)$ means $2.345789 \times 10^{-2}$
TOL ~ The tolerance chosen
MTD ~ The method used.
F1 - SDIRKN 5(4) which has been derived in this paper.
B1 - SDIRK $3^{\text {rd }}$ order 4 -stage embedded in $4^{\text {th }}$ order
5-stage method by Butcher and Chen [9].
FCN ~ Number of functions evaluated.
STEP ~ Number of steps.
JAC ~ The number of Jacobian evaluation.
FS ~ The number of failed steps.
GE $\sim$ Maximum global error (max $\left\|y_{n}-y\left(x_{n}\right)\right\|$ ), that is the computed solution minus the true solution.

TABLE III

| NUMERICAL RESULTS FOR PROBLEM 1 |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| TOL | MTD | FCN | STEP | JAC | FS | GE |
| $10^{-2}$ | F1 | 976 | 882 | 1 | 0 | 0.115425 |
|  | B1 | 10366 | 797 | 1 | 0 | $5.808069(-4)$ |
| $10^{-4}$ | F1 | 26707 | 2413 | 1 | 16 | $4.023551(-4)$ |
|  | B1 | 26880 | 2067 | 1 | 1 | $2.448647(-2)$ |
| $10^{-6}$ | F1 | 85927 | 7807 | 0 | 5 | $9.651620(-7)$ |
|  | B1 | 67691 | 5206 | 1 | 2 | $2.502111(-2)$ |
| $10^{-8}$ | F1 | 216716 | 19700 | 0 | 2 | $1.265587(-8)$ |
|  | B1 | 170070 | 13081 | 1 | 3 | $2.503427(-2)$ |

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TABLE IV
Numerical Results for Problem 2

| TOL | MTD | FCN | STEP | JAC | FSTEP | GE |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $10^{-2}$ | F1 | 1740 | 158 | 0 | 0 | $1.434827(-2)$ |
|  | B1 | 2537 | 195 | 0 | 0 | $3.715717(-2)$ |
| $10^{-4}$ | F1 | 4655 | 423 | 0 | 0 | $6.379218(-6)$ |
|  | B1 | 6385 | 491 | 0 | 0 | $2.361495(-3)$ |
| $10^{-6}$ | F1 | 11783 | 1071 | 0 | 0 | $3.575833(-8)$ |
|  | B1 | 16044 | 1234 | 0 | 0 | $1.487438(-4)$ |
| $10^{-8}$ | F1 | 29614 | 2692 | 0 | 0 | $3.005017(-10)$ |
|  | B1 | 40289 | 3099 | 0 | 0 | $9.376044(-6)$ |

TABLE V

| TOL | MTD | FCN | STEP | JAC | FS | GE |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $10^{-2}$ | F1 | 1916 | 174 | 0 | 0 | 0.183162 |
|  | B1 | 2386 | 183 | 1 | 0 | $2.470289(-2)$ |
| $10^{-4}$ | F1 | 4853 | 441 | 0 | 0 | $1.589209(-3)$ |
|  | B1 | 5917 | 455 | 0 | 0 | $1.582103(-1)$ |
| $10^{-6}$ | F1 | 12201 | 1109 | 0 | 0 | $1.542600(-5)$ |
| $10^{-8}$ | F1 | 30648 | 2786 | 0 | 0 | $1.533881(-7)$ |
|  | B1 | 37585 | 2891 | 0 | 0 | $6.256793(-4)$ |

TABLE VI

| TOL | MTD | FCN | STEP | JAC | FS | GE |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $10^{-2}$ | F1 | 9018 | 819 | 1 | 1 | $6.219093(-3)$ |
|  | B1 | 20928 | 3201 | 1 | 1 | $6.784609(-1)$ |
| $10^{-4}$ | F1 | 23590 | 2144 | 0 | 1 | $4.094247(-5)$ |
| $10^{-6}$ | F1 | 59505 | 5409 | 0 | 1 | $3.777785(-7)$ |
| $10^{-8}$ | B1 | 132736 | 20420 | 0 | 1 | $2.663875(-3)$ |
|  | F1 | 149631 | 13601 | 0 | 2 | $3.654645(-9)$ |
|  | 333534 | 51312 | 0 | 1 | $1.675455(-4)$ |  |

## V. Conclusion

From the tables we observed that the new embedded SDIRKN 5(4) method produced better results in terms of function evaluations, number of steps and maximal global error. Problem 1 is considered stiff for all the tolerances whereas problem 4 is only stiff for lower tolerance. The numerical results suggest that, the new method is more efficient than the existing technique whereby the problem is reduce to first order system of ODEs.

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