Implementation of the Newton-Cotes and Mimetic Quadrature Coefficients for Numerical Integration

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1.0: INTRODUCTION

The numerical solution of partial differential equations (PDEs) obtained by preserving the properties of the original continuum differential operators is widely referred to as the Mimetic discretization methods. The spatial coordinates of the PDE can be discretized as divergence, gradient and curl that satisfy the underlying theorems of vector calculus (such as the Gauss Divergence theorem). These discretizations can then be used to solve higher order PDEs, Castillo et al [1]. Castillo [1] observed that the coefficient weights obtained for the 2nd order divergence Mimetic discretization method at the boundaries resemble those obtained from the Newton-Cotes formulation of numerical integration for ODE's. Navarro [2] compares the coefficients of higher order Newton-Cotes methods alongside with the equivalent Mimetic orders. Table 1 shows the

Method Source	Newton Cotes	Navarro				Castillo et al	
Method Name	**Newton**	**Mimetic**	**Mimetic**	**Newton**	**Newton**	**Mimetic**	**Mimetic**
Reference Name	**A**	**B**	**C**	**D**	**E**	**B1**	**C1**
Coefficients	3/8, 9/8, …	348/985, 473/384, 343/384, 612/599,…	1759/5586, 1224/877, 588/953, 2073/1657, 339/374, 746/735,…	1073/3527, 810/559, 343/640, 649/536,…	308/1123, 1499/880, -729/1783, 1899/596, -2716/2241, 1998/1021,…	407/1152, 473/384, 343/384, 1177/1152…	43531/138240, 192937/138240, 42647/69120, 86473/69120, 125303/138240, 140309/138240,…
# of function evaluations	4	8	12	8	12	8	12
Gradient order	2	4	6	4	6	4	6
Mimetic quadrature order	3	5	7	5	7	5	7

Table 1: Newton-Cotes and Mimetic coefficients

It is well known that the Newton-Cotes coefficients are symmetric about the median. Table 1 shows only the coefficients for the left of the symmetric median. In the case of the Newton-Cotes formulation, the numerical integration of a function

$$y'(x) = f(x) \text{ in the interval } [0,1]$$

can be represented as:

$$y_{x=1} = y_{x=0} + \frac{h}{3}\left(\frac{3}{8}f(0) + \frac{9}{8}f(\tfrac{1}{3}) + \frac{9}{8}f(\tfrac{2}{3}) + \frac{3}{8}f(1)\right) \qquad \dots \qquad \{1\}$$

The function f(x) is evaluated four times at each interval if a composite integration is to be performed. The equivalent Mimetic method is obtained by incorporating a divergence of order 2, which corresponds to the Mimetic quadrature order of 3.

Following this logic for higher orders, the numerical integration using a Mimetic quadrature method of order 5 (which has a gradient of order 4) is performed by incorporating 8 function evaluations at each time step. Likewise, integration using a Mimetic quadrature of order 7 (which has a gradient of 6) is performed using 12 function evaluations at each time step.

This report investigates the feasibility of using the coefficient weights obtained from Mimetic methods as a tool for numerical integration. The report also compares the Mimetic methods with the equivalent Newton-Cotes counterparts in order to study the performance of the numerical integration techniques.

To avoid confusion with the order numbers, the "Reference Names" A through E shown in Table 1 will be used in the remainder of this document to refer to a particular method. Coefficients with names "B1" and "C1" have only been shown for reference in Table 1. These coefficients as reported in Castillo at al [1] are identical to those of Navarro.

2.0: APPLICATION

This section describes the ODE problems that were numerically integrated using the coefficients from Table 1.

2.1: Baseline

To obtain a baseline, the test problem #1 of Navarro's thesis was incorporated. We call this problem BSLN.

$$F = \int_0^1 x^3 e^{-x} dx$$

The integration was performed for various constant step sizes. The solution at t=1 was compared with the exact value of F = 0.113928941256923 reported by Navarro, and the absolute of the error terms is shown in Table 2.

Reference Name	**A**	**B**	**C**	**D**	**E**
# of Steps	**Newton - A**	**Mimetic - B**	**Mimetic - C**	**Newton - D**	**Newton - E**
100	1.1529930E-11	7.5858849E-08	8.2761712E-09	3.0950673E-08	1.3278966E-08
200	7.2064577E-13	7.5858819E-08	8.2762242E-09	3.0951191E-08	1.3279085E-08
500	1.8415824E-14	7.5858760E-08	8.2762391E-09	3.0951336E-08	1.3279118E-08
1000	1.0685897E-15	7.5858750E-08	8.2762413E-09	3.0951357E-08	1.3279122E-08
2000	8.9234176E-15	7.5858739E-08	8.2762507E-09	3.0951371E-08	1.3279115E-08
5000	1.6042723E-14	7.5858730E-08	8.2762581E-09	3.0951380E-08	1.3279108E-08
10000	2.2287727E-14	7.5858724E-08	8.2762641E-09	3.0951386E-08	1.3279102E-08
20000	2.5424107E-14	7.5858722E-08	8.2762674E-09	3.0951389E-08	1.3279099E-08

Table 2: Comparison of error for the problem BSLN

The numerical integration performed with the Mimetic coefficients compares with those of the Newton-Cotes coefficients. A comparison of methods B and D shows that the average error of the Mimetic-B method is 2.45 times the error obtained from the Newton-D method. A comparison of methods C and E shows that the average error of the Mimetic-C method is 0.62 times the error obtained from the Newton-E method. That is, the error terms obtained from the 7th order Mimetic quadrature terms is lower than the error from the 12th order Newton-Cotes coefficients.

Nevertheless, this simple example illustrates the feasibility of utilizing the Mimetic coefficients as a viable alternative for numerical integration. We investigate this further in the following three example problems.

2.2: Application to Structural Mechanics

The structural mechanics problem from Piche [3] was solved using the coefficients from Table 1. The equations are shown below for reference, along with the boundary conditions. The problem will be referred to as PCHE in this report.

$$\boxed{\begin{aligned} &m_1\ddot{y}_1+(c_1+c_2)\dot{y}_1-c_2\dot{y}_2+(k_1+k_2)y_1-k_2y_2=0\\ &m_2\ddot{y}_1+c_2(\dot{y}_2-\dot{y}_1)+k_2(y_2-y_1)=0\\ &y_1(0)=y_2(0)=-1, \qquad \dot{y}_1(0)=\dot{y}_2(0)=0\end{aligned}}$$

This is a set of second order ODE's, which was converted into four first order ODE's and then solved numerically. The integration was performed for a time range of t=0 to 20 seconds. The reference numerical solution was obtained using a 4th order Runge-Kutta method with the embedded Cash-Karp coefficients as presented in Press et al [4]. A tolerance of 1E-8 was used for this reference solution. The plot of the variables y1 and y2 as a function of time is shown in Figure 1 below.

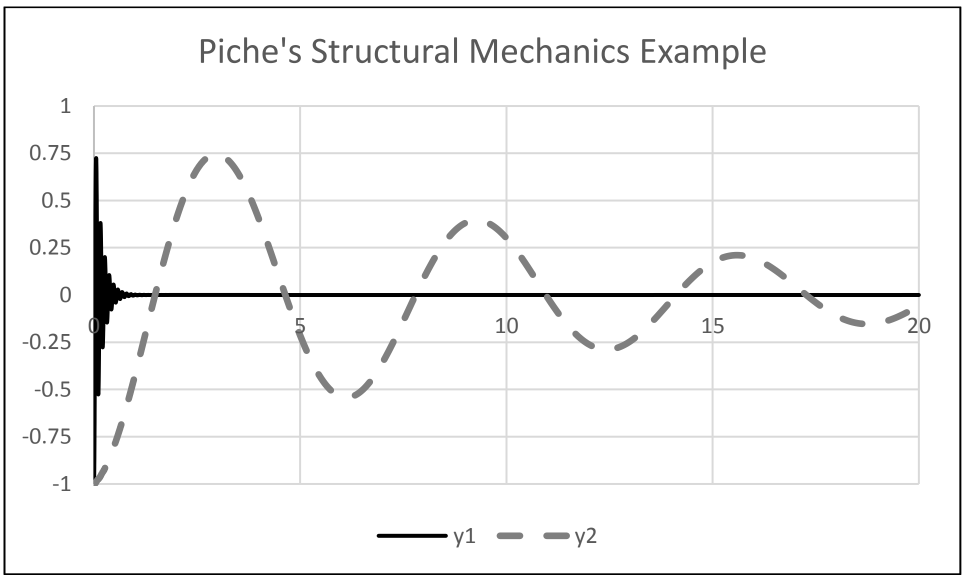

Figure 1: Solution to the structural mechanics problem PCHE obtained from a 4th order Runge Kutta method

Figure 1 clearly shows the largely varying settling rates of the solutions for y1 and y2. The solution for y1 settles down to zero within ~1 second, while the solution for y2 continues to exhibit oscillatory behavior over the 20 second time period. This set of equations was solved using the Newton-Cotes and Mimetic coefficients. In order to compare the solutions from the various methods, the error comparison was performed at times t=0.05 and t=20 seconds.

Tables 3 & 4 show that both the Newton-Cotes and the Mimetic methods yield error terms are identical for y1 and y2 at t=0.05 s. The percentage error for y1 and y2 at t=20 s between methods B&D and C&E is shown in Table 5. A positive error percentage indicates the Mimetic method generates an error more than the corresponding Newton-Cotes method, while a negative error indicates the Mimetic method generates a smaller error. Table 5 shows that the Mimetic method B performs better than Newton-Cotes method D. It is instructional to note here that the error terms for y1 and y2 at t=20 s are well below 3E-8.

Reference Name	A	B	C	D	E
No of Steps	Newton - A	Newton - D	Newton - E	Mimetic - B	Mimetic - C
	Error of y1 @ t=0.05				
10000	1.4558E-01	1.4558E-01	1.4558E-01	1.4558E-01	1.4558E-01
50000	2.7139E-02	2.7138E-02	2.7139E-02	2.7139E-02	2.7139E-02
100000	1.3449E-02	1.3449E-02	1.3449E-02	1.3449E-02	1.3449E-02
	Error of y2 @ t=0.05				
10000	1.9349E-04	1.9350E-04	1.9349E-04	1.9348E-04	1.9349E-04
50000	3.1692E-05	3.1697E-05	3.1690E-05	3.1679E-05	3.1693E-05
100000	1.5468E-05	1.5473E-05	1.5466E-05	1.5455E-05	1.5469E-05

Table 3: Comparison of error for PCHE at t=0.05 s

Reference Name	A	B	C	D	E
No of Steps	Newton - A	Newton - D	Newton - E	Mimetic - B	Mimetic - C
	Error of y1 @ t=20				
10000	2.1723E-08	2.1931E-08	2.1634E-08	2.1213E-08	2.1778E-08
50000	4.3895E-09	4.5943E-09	4.3017E-09	3.8876E-09	4.4443E-09
100000	2.1976E-09	2.4020E-09	2.1099E-09	1.6967E-09	2.2523E-09
	Error of y2 @ t=20				
10000	6.1496E-04	6.1567E-04	6.1465E-04	6.1320E-04	6.1515E-04
50000	1.2229E-04	1.2300E-04	1.2199E-04	1.2057E-04	1.2248E-04
100000	6.1104E-05	6.1807E-05	6.0803E-05	5.9382E-05	6.1292E-05

Table 4: Comparison of error PCHE at t=20 s

% Error between methods B & D	% Error between methods C & E
y1 @ t=20	
-3.39	0.67
-18.18	3.21
-41.57	6.32
y2 @ t=20	
-0.40	0.08
-2.02	0.40
-4.08	0.80

Table 5: Percentage Error for y1 & y2 at t=20 s for PCHE

2.3: Application to an induction motor transient start-up analysis [MOTR]

The second example is adapted from Krause et al [5]. This problem describes the transient start-up analysis for an induction motor as it accelerates from rest to full rotor speed when voltage is applied at the motor terminals. The set of ODEs is as shown below.

$$\psi_{qs} = \frac{\omega_b}{p}\left[v_{qs} - \frac{\omega}{\omega_b}\psi_{ds} + \frac{r_s}{X_{ls}}(\psi_{mq} - \psi_{qs})\right]$$

$$\psi_{ds} = \frac{\omega_b}{p}\left[v_{ds} + \frac{\omega}{\omega_b}\psi_{qs} + \frac{r_s}{X_{ls}}(\psi_{md} - \psi_{ds})\right]$$

$$\psi_{0s} = \frac{\omega_b}{p}\left[v_{0s} - \frac{r_s}{X_{ls}}\psi_{0s}\right]$$

$$\psi'_{qr} = \frac{\omega_b}{p}\left[v'_{qr} - \left(\frac{\omega - \omega_r}{\omega_b}\right)\psi'_{dr} + \frac{r'_r}{X'_{lr}}(\psi_{mq} - \psi'_{qr})\right]$$

$$\psi'_{dr} = \frac{\omega_b}{p}\left[v'_{dr} + \left(\frac{\omega - \omega_r}{\omega_b}\right)\psi'_{qr} + \frac{r'_r}{X'_{lr}}(\psi_{md} - \psi'_{dr})\right]$$

$$\psi'_{0r} = \frac{\omega_b}{p}\left[v'_{0r} - \frac{r'_r}{X'_{lr}}\psi'_{0r}\right]$$

$$\psi_{mq} = X_{aq}\left(\frac{\psi_{qs}}{X_{ls}} + \frac{\psi'_{qr}}{X'_{lr}}\right)$$

$$\psi_{md} = X_{ad}\left(\frac{\psi_{ds}}{X_{ls}} + \frac{\psi'_{dr}}{X'_{lr}}\right)$$

$$X_{aq} = X_{ad} = \left(\frac{1}{X_M} + \frac{1}{X_{ls}} + \frac{1}{X'_{lr}}\right)^{-1}$$

$$T_e = \psi_{ds} i_{qs} - \psi_{qs} i_{ds}$$

$$\omega_r = \frac{\omega_b}{2Hp}(T_e - T_L)$$

The original set of equations is 8 ODEs as shown in. The problem was modified to solve only for the direct and quadrature flux terms, along with the rotor angular velocity. The total number of ODE's is thus 6.

The reference solution was obtained using the Runge-Kutta 4th order Cash-Karp coefficients as mentioned earlier for PCHE. A tolerance of 1E-7 was used for the MOTR reference solution. The plot of Torque and angular velocity (omega) versus time is shown in Figure 2.

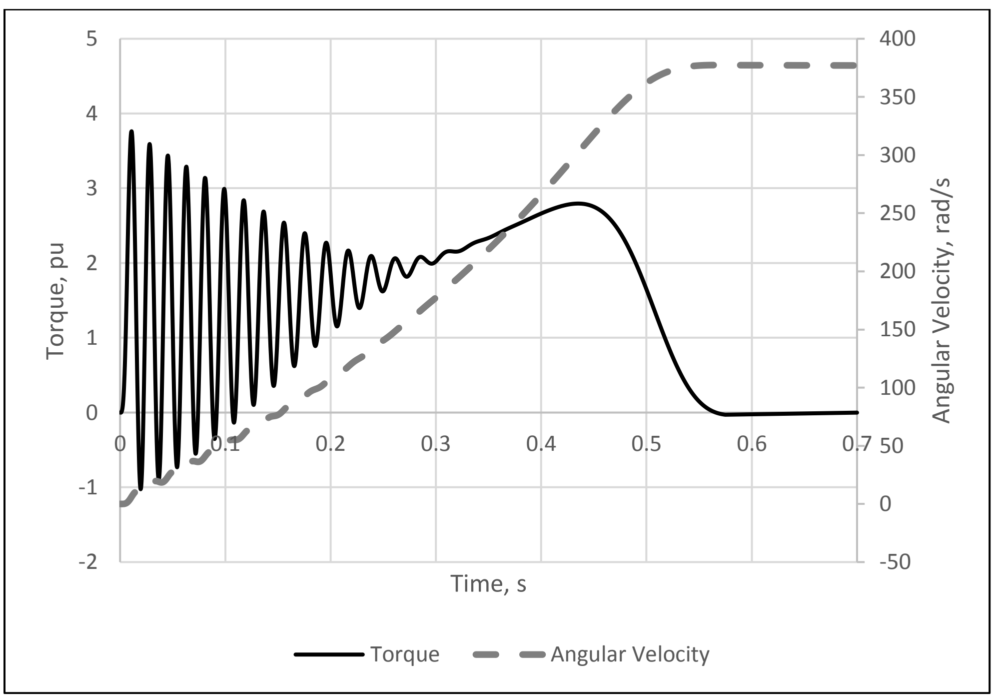

Figure 2: Solution to the induction motor problem MOTR obtained from a 4th order Runge Kutta method

Tables 6 & 7 show the error comparisons for Torque and Angular Velocity for the various methods at t=0.01 s and t=0.45 s. These two time slices were chosen to capture the responses at the transient (i.e., oscillatory) and the peak pull-out Torque locations as shown in Figure 2.

No of steps	Newton - A	Newton - D	Newton - E	Mimetic - B	Mimetic - C
	Error of Angular Velocity @ t=0.01				
10000	2.3773E-03	2.3730E-03	2.3791E-03	2.3878E-03	2.3762E-03
50000	3.7400E-04	3.6973E-04	3.7583E-04	3.8447E-04	3.7286E-04
100000	9.3866E-05	8.9597E-05	9.5698E-05	1.0433E-04	9.2725E-05
	Error of Angular Velocity @ t=0.45				
10000	9.1876E+00	9.1872E+00	9.1878E+00	9.1887E+00	9.1875E+00
50000	1.8053E+00	1.8049E+00	1.8055E+00	1.8064E+00	1.8052E+00
100000	9.0061E-01	9.0017E-01	9.0080E-01	9.0170E-01	9.0049E-01

Table 6: Comparison of error in Angular Velocity for MTOR

No of steps	Newton - A	Newton - D	Newton - E	Mimetic - B	Mimetic - C
	Error of Torque @ t=0.01				
10000	1.7183E-02	1.7181E-02	1.7184E-02	1.7188E-02	1.7183E-02
50000	4.1052E-03	4.1031E-03	4.1061E-03	4.1102E-03	4.1046E-03
100000	2.4202E-03	2.4182E-03	2.4211E-03	2.4252E-03	2.4197E-03
	Error of Torque @ t=0.45				
10000	8.7476E-02	8.7481E-02	8.7475E-02	8.7466E-02	8.7477E-02
50000	1.8933E-02	1.8936E-02	1.8932E-02	1.8927E-02	1.8934E-02
100000	9.5425E-03	9.5447E-03	9.5415E-03	9.5370E-03	9.5431E-03

Table 7: Comparison of error in Torque for MTOR

2.4: Application to a Stiff ODE Problem

The sample problem D4 from Enright & Pryce [6] was solved using the Newton Cotes & Mimetic coefficients. We call this problem as EPD4. The reference solution was once again obtained using the procedure of Press et al [4] with a tolerance of 1E-8.

D4:
$$\begin{aligned} y_1' &= -.013y_1 - 1000y_1y_3 & y_1(0) &= 1 \\ y_2' &= -2500y_2y_3 & y_2(0) &= 1 \\ y_3' &= -.013y_1 - 1000y_1y_3 - 2500y_2y_3 & y_3(0) &= 0 \end{aligned}$$

$$x_f = 50 \qquad h_0 = 2.9 \times 10^{-4}$$

(chemistry: Gear (1969),
eigenvalues: 0, $-9.3\times10^{-3} \rightarrow -4.0\times10^{-3} \rightarrow -6.3\times10^{-3}$,
$-3.5\times10^{3} \rightarrow -3.8\times10^{3}$)

Since this is a stiff set of ODEs, an adaptive step-size calculation was implemented. At each step, the numerical integration was performed three times – once for a full step h, followed by two half-h steps. The two solutions were then compared to determine the subsequent step size to advance the integration process. The process was repeated for various tolerance values, and the results are compared in Table 8.

Tolerance	Newton - A	Newton - D	Newton - E	Mimetic - B	Mimetic - C
	Error of y1 at t=50				
1.00E-03	5.9184E-07	5.0160E-07	6.3060E-07	8.1275E-07	5.6797E-07
1.00E-04	5.9201E-07	5.0188E-07	6.3074E-07	8.1296E-07	5.6789E-07
1.00E-05	5.9191E-07	5.0177E-07	6.3069E-07	8.1286E-07	5.6781E-07
	Error of y2 at t=50				
1.00E-03	5.9225E-07	5.0159E-07	6.3004E-07	8.1335E-07	5.6690E-07
1.00E-04	5.9195E-07	5.0191E-07	6.3078E-07	8.1310E-07	5.6788E-07
1.00E-05	5.9191E-07	5.0177E-07	6.3068E-07	8.1287E-07	5.6782E-07
	Error of y3 at t=50				
1.00E-03	4.0749E-10	5.8528E-12	5.5470E-10	5.9300E-10	1.0739E-09
1.00E-04	5.3176E-11	3.4980E-11	4.7147E-11	1.3561E-10	7.5780E-12
1.00E-05	2.2356E-12	4.3841E-12	5.1854E-12	8.8255E-12	1.2170E-11
	Evaluation steps				
1.00E-03	94486	94497	94492	94490	94490
1.00E-04	94602	94608	94610	94611	94612
1.00E-05	95013	95037	95039	95040	95043

Table 8: Comparison of error for EPD4

3.0: OBSERVATIONS

The Mimetic quadrature coefficients were compared with the equivalent Newton-Cotes coefficients for three examples (PCHE, MTOR and EPD4). The numerical error at specific temporal locations for the series of ODEs were evaluated and compared. The Mimetic quadrature coefficients provide error estimates that are comparable with those from the Newton-Cotes of equivalent order. Simply stated, the Mimetic quadrature coefficients serve as a viable alternative for numerical integration.

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APPENDIX

The coefficients generated for the 4^{th} order Mimetic differential operator, with 5 weights. The P-coefficients are:

P = 227/641 941/766 811/903 659/647 1349/1348 1349/1348 659/647 811/903 941/766 227/641

This method is denoted by “Mimetic F”. The table below shows the comparison of error for the sample problem NVRO. The error obtained from the Mimetic-F method is quantitatively smaller compared to the equivalent Mimetic-C method.

	Error					
Reference Name	**A**	**B**	**C**	**D**	**E**	**F**
NoSteps	**Newton - A**	**Mimetic - B**	**Mimetic - C**	**Newton - D**	**Newton - E**	**Mimetic - F**
100	1.1529930E-11	7.5858849E-08	8.2761712E-09	3.0950673E-08	1.3278966E-08	**1.5766273E-09**
200	7.2064577E-13	7.5858819E-08	8.2762242E-09	3.0951191E-08	1.3279085E-08	**1.5770204E-09**
500	1.8415824E-14	7.5858760E-08	8.2762391E-09	3.0951336E-08	1.3279118E-08	**1.5771133E-09**
1000	1.0685897E-15	7.5858750E-08	8.2762413E-09	3.0951357E-08	1.3279122E-08	**1.5771260E-09**
2000	8.9234176E-15	7.5858739E-08	8.2762507E-09	3.0951371E-08	1.3279115E-08	**1.5771201E-09**
5000	1.6042723E-14	7.5858730E-08	8.2762581E-09	3.0951380E-08	1.3279108E-08	**1.5771136E-09**
10000	2.2287727E-14	7.5858724E-08	8.2762641E-09	3.0951386E-08	1.3279102E-08	**1.5771079E-09**
20000	2.5424107E-14	7.5858722E-08	8.2762674E-09	3.0951389E-08	1.3279099E-08	**1.5771046E-09**

The table below shows the comparison of error terms for problem PCHE.

Reference Name	**A**	**B**	**C**	**D**	**E**	**F**
No of Steps	**Newton - A**	**Newton - D**	**Newton - E**	**Mimetic - B**	**Mimetic - C**	**Mimetic F**
	Error of y1 @ t=20					
10000	2.1723E-08	2.1931E-08	2.1634E-08	2.1213E-08	2.1778E-08	2.1723E-08
50000	4.3895E-09	4.5943E-09	4.3017E-09	3.8876E-09	4.4443E-09	4.3813E-09
100000	2.1976E-09	2.4020E-09	2.1099E-09	1.6967E-09	2.2523E-09	2.1883E-09
	Error of y2 @ t=20					
10000	6.1496E-04	6.1567E-04	6.1465E-04	6.1320E-04	6.1515E-04	6.1523E-04
50000	1.2229E-04	1.2300E-04	1.2199E-04	1.2057E-04	1.2248E-04	1.2232E-04
100000	6.1104E-05	6.1807E-05	6.0803E-05	5.9382E-05	6.1292E-05	6.1099E-05

Reference Name	**A**	**B**	**C**	**D**	**E**	**F**
No of Steps	**Newton - A**	**Newton - D**	**Newton - E**	**Mimetic - B**	**Mimetic - C**	**Mimetic - F**
	Error of y1 @ t=0.05					
10000	1.4558E-01	1.4558E-01	1.4558E-01	1.4558E-01	1.4558E-01	1.4558E-01
50000	2.7139E-02	2.7138E-02	2.7139E-02	2.7139E-02	2.7139E-02	2.7139E-02
100000	1.3449E-02	1.3449E-02	1.3449E-02	1.3449E-02	1.3449E-02	1.3450E-02
	Error of y2 @ t=0.05					
10000	1.9349E-04	1.9350E-04	1.9349E-04	1.9348E-04	1.9349E-04	1.9349E-04
50000	3.1692E-05	3.1697E-05	3.1690E-05	3.1679E-05	3.1693E-05	3.1693E-05
100000	1.5468E-05	1.5473E-05	1.5466E-05	1.5455E-05	1.5469E-05	1.5469E-05

The error for the PCHE problem with the Mimetic- F method is comparable to those obtained from the Mimetic-C method.