

# Computer Simulations of Second Order Initial Value Problems of Order Ordinary Differential Equations in Materials and Orbital Mechanics with Collocation Techniques Induced Hybrid Methods

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Abstract— This paper focuses on computer simulations intended for oscillatory problems formulated in special second order initial value problems (IVPs) of ordinary differential equations (ODEs) where first derivatives do not explicitly feature. These problems crop up in Mechanics of Materials (Macro-, Meso-, Micro-and Nano-Mechanics) as well as Celestial Mechanics and Orbital Mechanics. Computer simulation of the problems have always been of immense importance and attracted interests of scientist and researchers. We selected a sixorder Hybrid Method for current study. The method requires an extra back value after a change in step-size. Collocation technique inherits function evaluations at off-step points in an underlying interpolant that could be proficiently exploited to compute the extra back value. Accordingly, we embedded Collocation techniques into the selected *Hybrid Method.* We applied the method algorithm to the benchmark problems selected from linear Orbital Mechanics. At that point we programmed solution steps and procedures into commercially available MATLABTM 2020 code to obtain desired simulated results. We compared simulation generated results to the data results available in the literature and found to be within the acceptable range of  $(\pm 2\%)$  deviations. Additionally, the method is self-starting, requires fewer function evaluations, found to be quite proficient, and practically well suited for solving such problems. The selected results in terms of function value and point-wise absolute error evaluations are presented in graphical and tabular illustrations up to seven decimal places. Based on performance of the proposed Hybrid Method induced with Collocation techniques, we would like to recommend the proposed method for similar studies in the future.

*Keywords*— A. Second-order initial value problems; B. Direct Hybrid Methods; C. Mechanics of Materials; D. Celestial Mechanics; E. Orbital Mechanics.

# I. INTRODUCTION

The special second order initial value problems of ordinary differential equations with missing terms of time, function, or derivative of function formulate perturbed oscillatory problems in Mechanics of Materials (Macro-, Meso-, Micro-and Nano-Mechanics) as well as Celestial and Orbital Mechanics [1]. Computer simulations of the problems take up significant part at pre-design stage. As well as design parameters are identified, classified and evaluated for various design analyses. Nonetheless, the group of differential equations solvable for exact solutions is small. Either different techniques are required to solve system of equations or exact solutions cannot be found candidly. In so far as, the second order initial value problems are concerned the solutions could often be more challenging, complex, or almost impossible. Therefore, many researchers have resorted to numerical methods for solving the differential equations. A short appraisal of the relevant investigations is presented below.

The Spectral method applied to determine solutions on discretized set of Collocation points in series of bases functions: Legendre polynomials, Fourier series, and Chebyshev polynomials were reported in [2]. The single-step methods for illustration Euler and Runge-Kutta (RK) initiate more reliable starting values and predominantly suitable for computations were submitted in [3]. Bogie and Shampine developed method using two and three order RK methods with four stages for the same step to evaluate function for adaptive mesh size algorithms in [4]. Another four and five order RK process algorithm with stability analysis was proposed by Erwin Fehlberg in [4]. Conversely, the explicit RK methods of high order were instituted to boot complicated problems consisting of higher derivatives was mentioned in [5]. The family of high order single-step methods with truncation errors raised up to  $O(h^5)$  were presented in [6] The nonexistence of ten-stage eightorder explicit RK-method with rationalization, increasing stability limits, the dynamics of RK algorithms was proposed in [7]. Failures of the one-step method consisting of RK-Fehlberg solvers to higher order algorithms "embedded strong-stabilitypreserving pairs" was reported in [8]. The RK family of high order with Dormand and Prince algorithm was derived in [9]. The Implicit RK-methods with control of step size selection, increased stability limits, weaknesses of the single-step methods, and requirement for multistep methods were explained in [10]. Test sets for second ODE IVPs solvers, demonstration of lateral analyses, and multistep methods on manifold algorithms were presented in [11]. A collection on multistep algorithms/solvers for second order ODEs were



produced in [12]. Intuitively, the multistep methods are more efficient since function values at previous points were already computed and could be utilized in further simulations, and to achieve a higher order solution method were discussed in [13]. The multistep methods illustrated higher order of accuracy and suitability for the direct solutions of higher order differential equations without reduction to lower orders in [14]. Nonetheless, the major drawback in implementation of the methods still persists. Furthermore, the methods are not selfstarting and require lower order development of predictor was confirmed in [15] and [16]. The transformation from higher to lower order reduces the accuracy of the methods was established in [17]. To encounter requirements and difficulties in adopting multistep methods, the Predictor-Corrector method as well as a Block Multistep Methods were introduced and detailed in [18] and [19]. However, accuracy of these methods in terms of errors was found discouraging. Besides, the methods performed well, these methods also get affected by the Dahlquist barrier.

In overcoming the for-mentioned setbacks, researchers developed numerical methods for solution without reducing differential equations to a system of first order equations, to address limitations, circumvent the Dahlquist barrier, as well as persistent quest for versatile numerical methods with better accuracy led to introduction of the Hybrid Methods proposed in [11], [15] [20]. The Hybrid Methods combined features of single-step RK and linear multistep methods as well as function evaluations at off-step point(s) as described in [8] [19], [21]. As a consequence, to improve accuracy within the selected interval of integration, One-step and two-step Hybrid Method were proposed in [9], [20]. Some multi derivative Hybrid block for the problem was also presented in [21]. A five-step high order method with compact fourth-order-accurate embedded boundary method with a class of Hybrid Collocation methods were also conceded in [22]. The 2-Step two-point Hybrid Method for direct solution of second order IVPs for direct solutions of continuous ordinate-function Hybrid Methods were suggested in [23]. For analogous problems a class of implicit five step blocks methods and a class of six step block methods were also suggested in [24].

Review of the previous literature on the topic revealed that a wide selection of methods and analyses are already available. The review provides valuable qualitative and quantitative information along evolution of problems and performance of methods. Nonetheless, none of those methods are effective for every type of applications. It also divulged the following pragmatic deficiencies: limitations in applications, complexity in implementation, computational burden, the accuracy in results, and time wastage. The lack of comprehensive studies on the topic is required to bridge the gap in the literature. It was desired to evaluate and choose method that could reliably and efficiently solve second-order initial value problem in-hand. Therefore, a relatively effective approach to utilize the direct Hybrid Method embedded with Collocation techniques was opted. Confidently, the current study would be another effort to complement manuscripts that offer a set of valuable computational tools. The study concludes that the solution approach is undemanding, dependable, and relatively efficient in performance. The proposed approach is thus recommended to solve real-world problems of perturbed and oscillatory nature in scientific and engineering dynamics.

### II. NUMERICAL METHODS FOR SPECIAL SECOND ORDER INITIAL VALUE PROBLEMS

#### 2.1 Single-step Methods

Many authors constructed a class of two-step methods for the second order periodic or oscillatory problem formulated in vector form in (1). The single-step methods require the high order IVPs may be replaced with an equivalent coupled first order system to obtain numerical solution as shown below:

$$\underbrace{y''(t) = \underline{f}(t, \underline{y}), \ a \le t \le b}_{\underline{y}'(a) = \underline{y}'_{0}(given), \qquad (1)}_{\underline{y}(a) = \underline{y}_{0}(given).}$$

where  $\underline{y}$ ,  $\underline{f}$ ,  $\underline{y}_0$  and  $\underline{y'}_0$  are vectors of dimension 'm' can be converted to a first order IVP. The equations may be solved by applying single-step (RK family) or linear multistep methods:

$$\begin{cases} Y^{[n]} = u_i, y_{n-1} + (1 - u_i)y_n + h^2 \sum_{j=1}^m a_{ij} f(x_n + c_j, Y_j^{[n]}), \\ y_{n+1} = \theta y_{n-1} + (1 - \theta)y_n + h^2. \end{cases}$$
(2)

The algorithms belong to the class of two-step methods.

The RK methods being too complicated, higher order nonexistent, involve large number of function evaluations, and exhibit increasing stability limits [2], [9]. In consequence, researchers started to develop and design advance solution methods.

#### 2.2 Second order Multistep Hybrid Methods

In general, the second order equations may be put in the following form:

$$y_{n+1} = \sum_{i=0}^{k} a_i y_{n-i+1} + h \sum_{i=0}^{k} b_i y'_{n-i+1}$$
(3)  
Symbolically, we may write (3) as

$$\rho(E)y_{n-k+1} - h\sigma(E)y'_{n-k+1} = 0$$
(4)

where  $\rho$  and  $\sigma$  are polynomials of degree k fined a:

$$\begin{cases}
\rho(\xi) = \xi^{\kappa} - a_1 \xi^{\kappa-1} - a_2 \xi^{\kappa-2} - \dots - a_k \\
\sigma(\xi) = b_0 \xi^k + b_1 \xi^{k-1} + \dots + b_k
\end{cases}$$
(5)

assuming the polynomials have no common factor. The difference equation (3) associated with the difference operator L may be defined by

$$\begin{cases} L[y(t),h] = y(t_{n+1}) - \sum_{i=0}^{k} a_i y(t_{n-i+1}) + h \sum_{i=0}^{k} b_i y'(t_{n-i+1}) \\ By \text{ expanding } \to y(t_{n-i+1}) \text{ and } y'(t_{n-i+1}) \text{ in Taylor series, we get} \\ L[y(t),h] = C_0 y(t_n) + C_1 h y'(t_n) + C_2 h^2 y'''(t_n) + \dots + C_p h^p y^{(p)}(t_n) + T_n \end{cases}$$
(6)
where

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(8)

$$\begin{cases} C_{0} = 1 - \sum_{i=0}^{k} a_{i} \\ \vdots \\ C_{q} = 1 - \frac{1}{q!} \left[ \sum_{i=0}^{k} a_{i} (1-i)^{q} \right] - \frac{1}{(q-1)!} \sum_{i=0}^{k} b_{i} (1-i)^{q-1}, q = 1, 2, \cdots, p. \\ and \\ T_{n} = \left[ \frac{1}{p!} \int_{t_{n}}^{t_{n-i+1}} (t_{n-i+1} - s) y^{(p)}(s) ds - \sum_{i=0}^{k} a_{i} \int_{t_{n}}^{t_{n-i+1}} (t_{n-i+1} - s) y^{(p+1)}(s) ds \\ -hp \int_{t_{n}}^{t_{n-i+1}} b_{0}(t_{n+1} - s)^{p-1} y^{(p+1)}(s) ds - hp \sum_{i=0}^{k} b_{i} \int_{t_{n}}^{t_{n-i+1}} (t_{n+1} - s)^{p-1} y^{(p+1)}_{*}(s) ds \right] \end{cases}$$
Definition 1: These methods associated with the difference operator are said to be of order p if  $C_{0} = C_{1} = C_{2} = \cdots + C_{p} = 0$  and  $C_{p} \neq 0$  in (9). Thus, for any function  $y(t) \in C_{p+2}$  with some nonzero  $C_{p+1}$  will yields

$$\begin{cases} L[y(t),h] = -C_{p+1}h^{p+1}y_{(t_n)}^{(p+1)} + o(h^{p+2}) \\ where \\ h^{p+1}\frac{C_{p+1}}{\sigma(1)} \text{ is an error constant} \end{cases}$$

In particular, the term L[y(t), h] vanishes identically when y(t) is a polynomial of degree  $\leq p$ . The method is said to be consistent if it has order  $p \geq 1$  and satisfies the root condition if the roots satisfy the equation  $\rho(\xi) = 0$ . In the same way all roots lie inside the unit circle in the complex plane and are simple if they lie on the circle. We use definitions of order,

consistency, and root condition to determine the parameters  $a_i$  and  $b_i$  in linear multistep method. Since (4) holds good for any  $(t) \in C_{p+2}$ . The constants  $C_i$  and p are independent of y(t). Thus, the constants can be determined by a particular case  $y(t) = e^t$  on substituting in (4):

$$\begin{cases} L[e^{t},h] = e^{t_{n+1}} - a_{1} e^{t_{n}} \cdots - a_{k} e^{t_{n-k+1}} - h(b_{0} e^{t_{n+1}} + b_{1} e^{t_{n}} + \dots + b_{k} e^{t_{n-k+1}}) \\ = -C_{p+1} h^{p+1} e^{t_{n}} + o(h^{p}) \\ after simplifying \\ = \left[ \left( e^{kh} - a_{1} e^{(k-1)h} \cdots - a_{k} \right) - h\left( b_{0} e^{kh} + b_{1} e^{(k-1)h} + \dots + b_{k} \right) \right] e^{t_{n-k+1}} \\ = -C_{p+1} h^{p+1} e^{t_{n}} + o(h^{p}) \\ or \\ \rho(e^{h}) - h\sigma(e^{h}) \approx -C_{p+1} h^{p+1} e^{t_{n}} + o(h^{p+2}) \\ Putting e^{h} = \xi, as h \rightarrow 0, \xi \rightarrow 1, the (9) becomes \\ \left\{ \begin{array}{c} \rho(\xi) - (\log\xi)\sigma(\xi) &= -C_{p+1}(\xi - 1)^{p+1} + o((\xi - 1)^{p+2}) \\ or \\ \frac{\rho(\xi)}{\log\xi} - \sigma(\xi) &= -C_{p+1}(\xi - 1)^{p} + o((\xi - 1)^{p+1}) \end{array} \right\}$$
(10)

The equations (7) and (8) provide methods for determining  $\rho(\xi)$  or  $\sigma(\xi)$  for maximum order. If  $\sigma(\xi)$  is specified, then (10) can be used to determine  $\rho(\xi)$  of degree k such that the order is at least k. The term  $(\log \xi)\sigma(\xi)$  in (10) may be expanded in a power series  $(\xi - 1)$  up to  $(\xi - 1)^k$  terms to find  $\rho(\xi)$ . On the other hand, if  $\rho(\xi)$  is given one can determine  $\sigma(\xi)$  of degree  $\leq k$  such that the order is at least k+1. The ratio  $\frac{\rho(\xi)}{\log \xi}$  may be expanded as a power in  $(\xi - 1)$  series, ..., and terms up to  $(\xi - 1)^k$  are used to get  $\sigma(\xi)$ . A choice of polynomial  $\rho(\xi)$  and the resulting polynomials  $\sigma(\xi)$  pave a way to produce other various well-known methods.

The linear k-step Hybrid Method contains 2k+1 arbitrary parameters that satisfy 2k+1 relations that gives 2k order of the method. Nonetheless, the stability requirements restrict the order up to k+1 if k is odd and to k+2 if k is even. Thus, the order of the k-step Hybrid Methods remains fixed. Nonetheless, no linear multistep method can be of order greater than two was confirmed in [12] and [15]. Thus, we to increase stability order of the k-step Hybrid Methods we modified the (3) to include a linear combination of the slopes at several points between  $t_n$ 

and  $t_{n+1}$ . Since stability of higher order methods requires implementation of collocation algorithm to evaluate function values at off-step points in a variable step code. Thus, we would introduce the Collocation algorithm and then imbed the same within Hybrid Method.

# 2.3 The Collocation algorithm to evaluate function values at off-step points

We derive parameters of the methods by using a Collocation technique based on algebraic polynomials. Thus, it takes various possibilities into account: construction of off-step, in the step-point solutions, different derivative of the solution, stages associated to the previous points, and order of the resulting method.

**Definition 2:** The Collocation polynomial  $y(t) \in P$  of s-stage Collocation method with pair-wise different points  $c_0, c_1, \dots, c_s$  is defined through the s + 1 conditions:

$$\begin{cases} y(t_0) = y_0 \\ y'(t_0 + c_i h) = f(t_0 + c_i h, y(t_0 + c_i h)), & i = 1, \dots s. \\ the next step becomes \\ y_1 = y(t_0 + h) \end{cases}$$
(11)



Definition 3: In an s-stage Gauss-Collocation method is the Collocation points are the set of a Gauss points in an interval [0, 1] namely the roots of the Legendre polynomial of degree s. Thus, a general single-step m-stage RK method is used to define off-step points:

$$\begin{cases} \underline{y}_{n+1} = \underline{y}_n + h \sum_{j=1}^m b_j \underline{f}_{nj}, & 0 \le n \le N-1 \\ \underline{f}_{nj} = \underline{f} \left( t_{nj}, \underline{y}_n + h \sum_{l=1}^m \underline{a}_{jl} \underline{f}_{nl} \right) & 1 \le j \le m, \\ t_{nj} = t_n + hc_j, & 1 \le j \le m, 0 \le n \le N-1. \end{cases}$$
(12)

The off-step point may be assumed as  $0 \le c_1 \le c_2 \le \ldots \le$  $c_m \leq 1$ . The points  $t_{nj}$  are known as Collocation points,  $c_n =$  $\sum_{i=1}^{m} a_{ni}$  are coefficients. The constants  $a_{ii}$ ,  $i = 1, 2, \ldots, m$ , and  $b_i, c_i, j = 1, 2, \ldots, m$  are coefficients of the formula. We observed that the sum in (3) is a quadrature rule for with weights  $a_{j1}, a_{j2}, \ldots, a_{jm}$  while the sum is a quadrature rule for with weights  $b_1, b_2, \ldots, b_m$ . We also assume that the quadrature rule has the same order for all  $j, 1 \le j \le m$ , and  $1 \le m$  $s \leq m$ , uniform step size, and limits  $0 \rightarrow c_i$ ,  $P_s$  denote the set of polynomials of degree order < s.

 $\begin{cases} t = t_n + xh \\ \int_0^{c_j} \psi(x) dx = \sum_{l=1}^m a_{jl} \psi(c_l) & \forall \psi \in P_s, \ 1 \le j \le m \end{cases}$ (13) We assume quadrature rule order is  $p \ge s$ , it gives:

$$\begin{cases} \int_0^1 \psi(x) dx = \sum_{l=1}^m b_l \psi(c_l), & \forall \psi \in P_p \\ & \text{the schemes satisfy } p \ge s \ge 1 \\ \sum_{l=1}^m b_l = 1, & \sum_{l=1}^m a_{jl} = c_j, & 1 \le j \le m. \end{cases}$$

The weights  $b_i$  and  $a_{ii}$  may be constructed by Lagrangian interpolation when the values of  $c_m$  are given. With these values, we define the Collocation points  $t_{ij}$  in each subinterval  $[t_i, t_{i+1}]$ . Thus write the function y'(t) on the interval in terms of its Lagrangian interpolant of order m with an error term  $\underline{\Delta}(t)$ :

Integrating (16) with respect to t when  $t = t_n \rightarrow t_{nj}$  and ignoring the error term, we obtain

$$\begin{array}{rcl}
\underbrace{y_{nj} - y_n}{t} &= & h \sum_{l=1}^m \int_0^{C_j} (L_l(t)dt) \underbrace{f_{nl}}_{nl}, and \\
t &= & t_n \operatorname{to} t_{n+1} \\
\underbrace{y_{n+1} - y_n}_{n} &= & h \sum_{j=1}^m (\int_0^1 L_j(t)dt) \underbrace{f_{nj}}_{nj} \quad (16)
\end{array}$$

Thus, we obtain  $b_j = \int_0^1 L_j(t) dt$ , and  $a_{ji} = \int_0^{C_j} L_1(t) dt$ .

The process is identical with an m-stage implicit RK method shown in [4]. The RK methods furnish a discrete solution with values  $y_n$  approximating the truncation error at mesh points  $t_n$ and values  $y_{nj}$  defined by (13), approximating the true solution at Collocation points  $t_{nj}$ . Let  $y_{\pi}(t)$  be a polynomial of order m + 1 defines on  $[t_n, t_{n+1}]$  by the interpolation conditions.  $\underline{y}_{\pi}(t_n)$  $f(t_{ni}, y_{ni}) = 1, 2, \dots, m$  $y'_{\pi}(t_{ni})$ 

$$\underline{y}_{\pi}(t) \text{ in terms of its first derivative:}$$

$$\underline{y}_{\pi}(t) = \underline{y}_{n} + \int_{t_{n}}^{t} \underline{y}'_{\pi}(\eta) d\eta$$
(17)

and replacing  $y'_{\pi}(t)$  by its Lagrangian interpolant form (17). Using the results in (15) and (16) and noting that the error term  $\underline{\Delta}(t) = \underline{0}$  since  $y_{\pi}(t)$  is a polynomial of degree m or less, we obtain

$$\begin{pmatrix}
\underbrace{y_{\pi}(t_{nj}) = \underbrace{y_{n}}_{l} + \int_{t_{n}}^{t_{nj}} \sum_{l=1}^{m} \underbrace{f(t_{nl}, \underbrace{y_{nl}}_{l}) L_{l}\left(\frac{\eta - t_{n}}{h}\right) d\eta}_{l} \\
= \underbrace{y_{n}}_{l} + h \sum_{l=1}^{m} a_{jl} \underbrace{f_{nl}}_{l} = \underbrace{y_{nj}}_{l} \\
\underbrace{y_{\pi}(t_{n+1}) = \underbrace{y_{n}}_{l} + \int_{t_{n}}^{t_{n+1}} \sum_{l=1}^{m} \underbrace{f(t_{nl}, \underbrace{y_{nl}}_{l}) L_{l}\left(\frac{\eta - t_{n}}{h}\right) d\eta}_{l} \\
= \underbrace{y_{n}}_{l} + h \sum_{l=1}^{m} b_{l} \underbrace{f_{nl}}_{l} = \underbrace{y_{n+1}}_{l}$$
(18)

We extended the polynomial to the next subinterval  $[t_{n+1}, t_{n+2}]$ . By using the same conditions, replacing n by n + 11, we observed that the polynomial continuously marched to  $t_{n+1}$  values. We observed that by expanding the subintervals for all n  $1 \le n \le N$ , over[a, b] in (14)-(19) the piecewise polynomial function  $y_{\pi}(t)$  satisfies the Collocation points:

$$\frac{y'_{\pi}(t) = f(t_{nj}), y_{\pi}(t_{nj}), n = 0, 1, 2, \dots, N, j = 1, 2, \dots, m.$$
(19)

The process steps are useful to overcome the difficulty of obtaining the extra back value after a change of step-size using the Collocation method as stated in [17]. We apply the same algorithm based on  $\underline{P}_{3,n}(t)$  a polynomial of degree three defined on  $[t_{n-1}, t_{n+1}]$  with the following interpolation conditions:

$$\begin{cases} (i) & \underline{P}_{3,n}(t_n) = \underline{y}_n \\ (ii) & \underline{P}_{3,n}(t_{n-1}) = \underline{y}_{n-1} \\ (iii) & \underline{P}_{3,n}'(t_{n+\alpha_1}) = \underline{y}_{n+\alpha_1}' \\ (iv) & \underline{P}_{3,n}''(t_{n-\alpha_1}) = \underline{y}_{n-\alpha_1}'' \end{cases}$$
(20)

where  $y_{n-\alpha_1}$  denotes the numerical solution at  $t_{n\pm\alpha_1} \equiv t_n \pm$  $\alpha_1 h$ , and  $\alpha_1$  is a parameter to be determined.

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 $f_{n\pm\alpha_1} = f\left(t_{n\pm\alpha_1}, y_{n\pm\alpha_1}\right) = y_{n+\alpha_1}''$ Function  $\underline{f}_{n\pm\alpha_1}$ may be written  $\rightarrow$ Polynomial as:  $a_0 + a_1(t - t_n) + a_2(t - t_n)^2 + a_3(t - t_n)^3$ (21) $P_{3,n}(t)$ = Differentiating twice gives:  $P_{3,n}''(t)$  $2\underline{a}_2 + 6\underline{a}_3(t - t_n)$ where the parameters  $a_i$ , i = 0, 1, 2, and 3 are to be chosen to satisfy the interpolating conditions. The conditions (iii) and (iv) becomes: *Choose parameters*  $\underline{a}_i$ , i = 0, 1, 2, and 3 that satisfy conditions (iii) and (iv) and gives: (22) $2a_2 + 6a_1ha_3$ =  $\underline{y}_{n+a_1}^{\prime\prime}$  $y_{n-a}^{\prime\prime}$  $2a_2 - 6a_1ha_3$ \_ Solving for  $\underline{a}_2$  and  $\underline{a}_3$  gives  $\frac{\underline{y}_{n+a_1}'-\underline{y}_{n-a_1}'}{12a_1h},$  $\frac{1}{4}\left(\underline{y}_{n+a_1}''+\underline{y}_{n-a_1}''\right).$  $\underline{a}_0 = \underline{y}_n$  $\underline{a}_3$  $a_2$ (23)Using condition (i)  $\rightarrow$  $\underline{a_0} = \underline{y_n}$  $\underline{\underline{y_n}}_{\underline{y_{n-1}}} + \frac{h}{4} \left( \underline{y_{n+a_1}''} + \underline{y_{n-a_1}''} \right) - \frac{h}{12a_1} \left( \underline{y_{n+a_1}''} + \underline{y_{n-a_1}''} \right)$  $\underline{a}_1$ We arrived at values of  $y_{n\pm a_1}$  from the equation We arrive atfunction values  $\underline{P}_{3,n}(\underline{t}_{n+a_1})$ \_  $y_{n\pm a_1}$ of f - step function values are  $\underbrace{\underline{y}_{n+a_1}}_{\text{To obtain}\underline{y}_{n+1}} = (1+a_1)\underline{y}_n - a_1\underline{y}_{n-1} + \frac{h^2}{12} \qquad \{4a_1^2 + 3a_1 - 1\}\underline{y}_{n+a_1}'' + \frac{h^2}{12}\{2a_1^2 + 3a_1 + 1\}\underline{y}_{n-a_1}'' \\ = (1-a_1)\underline{y}_n + a_1\underline{y}_{n-1} + \frac{h^2}{12} \qquad \{2a_1^2 - 3a_1 + 1\}\underline{y}_{n+a_1}'' + \frac{h^2}{12}\{4a_1^2 - 3a_1 - 1\}\underline{y}_{n-a_1}'' \\ = (1-a_1)\underline{y}_n + a_1\underline{y}_{n-1} + \frac{h^2}{12} \qquad \{2a_1^2 - 3a_1 + 1\}\underline{y}_{n+a_1}'' + \frac{h^2}{12}\{4a_1^2 - 3a_1 - 1\}\underline{y}_{n-a_1}'' \\ = (1-a_1)\underline{y}_n + a_1\underline{y}_{n-1} + \frac{h^2}{12} \qquad \{2a_1^2 - 3a_1 + 1\}\underline{y}_{n+a_1}'' + \frac{h^2}{12}\{4a_1^2 - 3a_1 - 1\}\underline{y}_{n-a_1}'' \\ = (1-a_1)\underline{y}_n + a_1\underline{y}_{n-1} + \frac{h^2}{12} \qquad \{2a_1^2 - 3a_1 + 1\}\underline{y}_{n+a_1}'' + \frac{h^2}{12}\{4a_1^2 - 3a_1 - 1]\underline{y}_{n-a_1}'' \\ = (1-a_1)\underline{y}_n + a_1\underline{y}_{n-1} + \frac{h^2}{12} \qquad \{2a_1^2 - 3a_1 + 1\}\underline{y}_{n+a_1}'' + \frac{h^2}{12}\{4a_1^2 - 3a_1 - 1]\underline{y}_{n-a_1}'' \\ = (1-a_1)\underline{y}_n + a_1\underline{y}_{n-1} + \frac{h^2}{12} \qquad \{2a_1^2 - 3a_1 + 1\}\underline{y}_{n+a_1}'' + \frac{h^2}{12}\{4a_1^2 - 3a_1 - 1]\underline{y}_{n-a_1}'' \\ = (1-a_1)\underline{y}_n + a_1\underline{y}_{n-1} + \frac{h^2}{12} \qquad (1-a_1)\underline{y}_n + \frac{h^2}{12} + \frac{h^2}{12$ (24)that gives  $y_{n+1} \equiv \underline{P}_{3,n}(t_{n+1}) = 2\underline{y}_n - \underline{y}_{n-1} + \frac{h^2}{2} \left( \underline{y}_{n+a_1}'' + \underline{y}_{n-a_1}'' \right)$ (25)Comparing (24) and (25) with the direct Hybrid formulae in equivalent. The method incorporates the features of single-steps as well as linear multistep methods. It can also make use of

[17], the method this is a new one. The off-step values  $\underline{y}_{n\pm a_1}$  are defined in terms of  $\underline{y}_{n\pm a_1}''$  which do not appear to relate with the multistep Hybrid Method.

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Therefore, we require to solve the equations simultaneously for  $\underline{y}_{n\pm a_1}$  to find  $\underline{y}_{n+1}$  and accept  $\underline{y}_n$  a new step-size,  $\overline{h}$ , predicted for the next step to advance to the next step. Thus, approximations of back value  $\underline{y}(t_n - \overline{h})$  is required that can be calculated by evaluating from the polynomial  $\underline{P}_{3,n}(t)$  at t = $t_n - \overline{h}$  using the conditions (iii) and (iv) as:  $\left( P_{1,n}^{\prime\prime}(t_{n+1}) \right) = \int_{0}^{t} \left( t_{n+1} - y_{n+1} \right)$ 

$$\begin{cases} \underline{P}_{3,n}^{"}(t_{n\pm a_{1}}) = \underline{f}\left(t_{n\pm a_{1}}, \underline{y}_{n\pm a_{1}}\right) \\ \text{and we have} \\ \underline{P}_{3,n}^{"}(t_{n\pm a_{1}}) = \underline{f}\left(t_{n\pm a_{1}}, \underline{P}_{3,n}(t_{n\pm a_{1}})\right) \end{cases}$$
Accordingly, it follows that the interpolating polynomial

Accordingly, it follows that the interpolating polynomial  $\underline{P}_{3,n}(t)$  satisfied the equation at the Collocation points  $t_{n\pm a_1}$ .

# 2.4 Six-order Hybrid Method embedded with off-step Collocation points

The Direct Hybrid Methods can be applied directly to a second order problem without first converting it to first order

equivalent. The method incorporates the features of single-steps as well as linear multistep methods. It can also make use of function values at the points  $l_n = a + nh, n = 0, 1, \ldots$  as well as at the off-step points  $t_n \pm \alpha_i h$ , where  $\alpha_i \in (0, 1)$ . To increase order of the k-step Hybrid Methods, we require to modify (3), and include a linear combination of the slopes at several points between  $t_n$  and  $t_{n+1}$ . We may let function  $\underline{y}_{n+1}$ be an approximation to the theoretical solution at  $(t_{n+k}, \underline{f}(t_{n+k}))$  where function is  $\underline{f}_{n+k} \equiv \underline{f}(t_{n+k}, \underline{y}_{n+k})$  and change (3) by adding v slopes up to k-steps as

$$y_{n+1} = \sum_{j=1}^{\kappa} a_j y_{n-j+1} + h \sum_{j=0}^{\kappa} b_j y_{n-j+1} + h \sum_{j=1}^{\nu} c_j y_{n-\alpha_j+1}$$
(27)

whereas  $a_j$ 's,  $b_j$ 's,  $c_j$ 's,  $\alpha_j$ 's coefficients and 2k + 2v + 1 arbitrary parameters that obey relations:  $0 < \alpha_j < 1, j = 1, 2, \dots, v$ . If we choose  $b_0 = 0$ , the formula (27) is called an explicit Hybrid Method, otherwise it is an implicit Hybrid Method. We select two non-step points, so k-step method can be written in the form:



y<sub>n+</sub>

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(28)

$$-$$
 Using  $k = 2$  into give

$$\sum_{j=1}^{k} a_{j} y_{n-j+1} + h \sum_{j=0}^{k} b_{j} f_{n-j+1} + h c_{1} f_{n-\alpha_{1}+1}$$

 $\begin{pmatrix} y_{n+1} &= a_1y_n + a_2y_{n-1} + h(b_0f_{n+1} + b_1f_n + b_2f_{n-1}) + hc_1f_{n-\alpha_1+1} \\ \text{where } a_j\text{'s, } b_j\text{'s, } c_1, \text{ and } \alpha_1 \text{ are arbitrary and } 0 < \alpha_1 < 1, \text{ and letting } a_1, a_2, b_0, b_1, b_2, c_1, \text{ and } \alpha_1, \text{ the seven arbitrary parameters, } \end{pmatrix}$  $0 < \alpha_1 < 1$ . We proceed to achieve Hybrid Method of order six by expanding (28) in Taylor series and correlating coefficients produce the following relations:

$$\begin{pmatrix}
a_1 + a_2 &= 1 \\
-a_2 + b_0 + b_1 + b_2 + c_1 &= 1 \\
a_2 + 2b_0 - 2b_2 + 2(1 - \alpha_1)c_1 &= 1 \\
-a_2 + 3b_0 + 3b_2 + 3(1 - \alpha_1)^2c_1 &= 1 \\
a_2 + 4b_0 - 4b_2 + 4(1 - \alpha_1)^3c_1 &= 1 \\
-a_2 + 5b_0 + 5b_2 + 5(1 - \alpha_1)^4c_1 &= 1 \\
a_2 + 6b_0 - 6b_2 + 6(1 - \alpha_1)^5c_1 &= 1
\end{cases}$$
(29)

By comparing the coefficients, we find the principal truncation error term  $(1 + a_2 - 7b_0 - 7b_2 74(1 - b_2 74))$  $\alpha_1)^6 c_1) \frac{h^7}{7!} y_{(t_n)}^{(7)} + o(h^8)$ . Putting  $b_1 = b_2 = 0$ , and solving the first five equations in (29) and choosing the value of  $\alpha_1$  in (0, 1) we find  $a_1, a_2, b_0, c_1$ . The  $\alpha_1$  vale satisfies polynomial of order 5, thus we obtained fourth order method. In order to get the method of order 5, we solve the first six equations in (29) in terms of one arbitrary parameter say  $\alpha_1 \neq 0, 1 \text{ or } 2$  and get methods of order 5 with principal truncation error as:  $\frac{h^{6} (16 - 48\alpha_{1} + 24\alpha_{1}^{2})}{6! (23 - 15\alpha_{1})} y_{(t_{n})}^{(6)} + o(h^{7}). \text{ If we take } b_{0} = 0, \text{ i.e. } \alpha_{1} = \frac{(9 - \sqrt{41})}{10}, \text{ we have an explicit Hybrid Method of order 5 as:}$  $v_{r+1} = \frac{1}{2}(32v_r - v_{r-1}) + \frac{h}{2}(15f_{r+1} + 12f_r - f_{r-1}) + \frac{h}{2}(15f_{r+1}$ 

$$64f_{n+1/2}$$
(30)

The value  $\alpha_1 = \frac{1}{2}$  gives an implicit Hybrid Method of order 5. The principal term of the truncation error vanishes for  $\alpha_1 =$  $1 - \frac{1}{\sqrt{3}}$  value, so we get a six-order method with following values of the parameters:

$$\begin{cases} a_1 = \frac{16}{(8+5\sqrt{3})} & a_2 = \frac{-(8-5\sqrt{3})}{(8+5\sqrt{3})} \\ b_0 = \frac{(\sqrt{3}+1)}{[(8+5\sqrt{3})(3-\sqrt{3})]} & b_1 = \frac{8\sqrt{3}}{[3(8+5\sqrt{3})]} \\ b_2 = \frac{(\sqrt{3}-1)}{[(8+5\sqrt{3})(3+\sqrt{3})]} & c_1 = \frac{6\sqrt{3}}{(8+5\sqrt{3})} & \alpha_1 = 1 - \frac{1}{\sqrt{3}} \end{cases}$$
(31)

Substituting these values of the parameters from (31) into (30), we obtain the principal term of the truncation error  $\frac{-8\sqrt{3}}{[9(8+5\sqrt{3})]}\frac{h^{7}}{7!}y_{(t_{n})}^{(7)} + o(h^{8}).$  Thus, the maximum order attained with two off-step points is 6, a principal truncation error attained is:  $T_n = \frac{42r^2 - 13}{302400}h^8 y^{(8)}_{(\xi)}$ . To embed the six-order Hybrid Method with off-step points, we may write it as follows:

$$y_{n+1} - 2y_n - y_{n-1} = h^2 \left[ \frac{25r^2 - 3}{30r^2} y_n'' + \frac{2 - 5r^2}{60(1 - 3r^2)} (y_{n+1}'' + y_{n-1}'') + \frac{1}{20r^2(1 - r^2)} (y_{n+1}'' + y_{n-1}'') \right]$$
(32)

Use of parameter r fixes the positions of the off-step points at arbitrary position to minimize function evaluation. A twostep six-order Hybrid Method embedded with off-step points is given in (32):

$$\begin{cases} y_{n+1} - 2y_n - y_{n-1} = h^2 \left[ \frac{7}{12} y_n'' + \frac{5}{24} (y_{n+r}'' + y_{n-r}'') \right], & r^2 = \frac{2}{5} \\ and \\ y_{n+1} - 2y_n - y_{n-1} = h^2 \left[ \frac{7}{264} (y_{n+1}'' + y_{n-1}'') + \frac{125}{264} (y_{n+r}'' + y_{n-r}'') \right], & r^2 = \frac{3}{25} \\ (33)$$

# **III. NUMERICAL EXPERIMENTS**

We perform some numerical experiments to complement the theoretical discussion presented in Section 2. We discretized the domain occupied by the problems using different step sizes, apply solution algorithms, and implement solution steps and procedures into MATLAB<sup>TM</sup>2020 to obtain simulated results. Since simulation generated results by using single-step methods to solve Example 1 below were available in [17], we went ahead to simulate the test the same (Example 1) to verify the proposed solution method and program. As expected, the simulated result obtained by applying Hybrid Methods with and without embedded Collocation off-step points matched well, as can be seen in Section 4 (Results and discussions).

1:

$$\begin{cases} \overline{y''} + 7 = t, & y(0) = -1, y'(0) = 1, \text{ in the interval } 0 \le t \le 1. \\ Analytical solution, & given & as \\ y = \frac{1}{6}t^3 - \frac{7}{2}t^2 + t - 1 & for step size & h = 0,025. \end{cases}$$

$$(1)$$

After verification of the code, we considered benchmark second order IVPs oscillatory in nature presented below in Example 2. Succeeding with the same algorithms (solver of Example 1), we introduced additional subroutines based on three choices of parameter  $(\alpha_1)$  for two-, four-, and six-order Hybrid Methods as well as provision of Collocation techniques in the program to simulate Example 2. We utilized time step at t = 0 and the analytical solution at t = h as starting values. Instead of running program for a certain number of iterations, we introduced stopping criteria based on the following relative error tolerance:

Relative error = absolute error/measured value.

The iteration process of program execution terminates when simulation produced error is deemed to be below the tolerance (relative error) for every step-sizes:

$$h = \frac{\pi}{4}, \frac{\pi}{8}, \frac{\pi}{16}, \frac{\pi}{32}, \frac{\pi}{64}, \frac{\pi}{128}$$

Example 2: Simulated results are required for the motion on a perturbed circular orbit formulated in the second order initial value problems of ordinary differential equations (35) with initial conditions: distance|z(t)| from origin is given at  $|z(40\pi)| = 1.001972$  given in [17]:



(Z	$z'' + z = 0.001e^{it}$	z(0) = 1,	z'(0) = 0.9995i	
	and	z(t) =	$0.001e^{it}(1 - 0.0005it)$	
Į	We compute	z(t)  =	$\sqrt{x(t)^2 + y(t)^2}$ (2)	)
	in polar	coordinates	as:	<i>'</i>
	x(t)	=	$\cos(t) + 0.0005(t)\sin(t)$ ,	
l	y(t)	=	sint – 0.0005(t)cos (t).	
	1 1 11	1		

The scalar problem can be rewritten in the (equivalent) form of two real, uncoupled initial value problems

 $\begin{cases} x'' + x = 0.001 \text{cost}, \quad x(0) = 1, \qquad x'(0) = 0.0\\ and\\ y'' + y = 0.001 \text{sint}, \quad y(0) = 0, \quad y'(0) = 0.9995. \end{cases}$ (3)

The simulation generated results of the examples are being presented with brief discussions in the next Section 4.

#### IV. RESULTS AND DISCUSSIONS

In this Section, we make intra and inter comparisons of simulated results to understand convergence properties, accuracy of solutions, quantify errors in results, and discover bugs in code. Furthermore, to verify results and validate applied solution methods, suitability of the method for a specific problem, future usages, performance, as well as explain associated advantages.

We present simulated results from Example 1 in Figure 1 to illustrate mesh-wise comparison of solution errors with the results available in literature [17]. It is evident from plotted curves that simulated results satisfactorily commute with the exact solutions. The curves demonstrate that simulated error quantities decrease rapidly within the intervals relatively closer to boundary-end of the mesh. The errors decrease in turn depict the better simulated values. The comparison justifies and

verifies applicability, accuracy, and performance of the method applied. In the same way, we illustrated comparison of pointwise absolute errors values in Figure 2. Both the error curves demonstrate proportionated increase within a certain range of time interval during simulation progression. Nonetheless, the curve representing single-step method demonstrates steady increase while the Hybrid Method curve turns smoothly into straight line within the last portion of interval. The smooth straight-line portion of curve represents simulated results in turn illustrates that the solution has converged. Therefore, the comparison confirms that the Hybrid Method provides the better approximate values. As expected, based on the acquired results presented in Figures: (1-2), we conclude that the Collocation technique induced six-order Hybrid Method produced more accurate results than the results produced by using single-step Classical RK methods [17].

Therefore, the comparison confirms that the Hybrid Method provides the better approximate values. As expected, based on the acquired results presented in Figures: (1-2), we conclude that the Collocation technique induced six-order Hybrid Method produced more accurate results than the single-step Classical RK methods

We selected simulated results from Example 2 for display in tabular forms. The simulated results obtained with the sixth order Hybrid Methods embedded with off-step Collocation points are shown in TABLE 1. Correspondingly, the simulated results obtained with the fourth order Hybrid Methods embedded with off-step Collocation points are shown in TABLE 2. Additionally, the simulated results obtained with the second order Hybrid Methods embedded with off-step Collocation points are shown in TABLE 3.



Figure 1: Plot of point-wise errors in solution values (Example 1).







TABLE 1: Six-order Hybrid Method with vs without collocation points

Ston	Computed solution		Error	
size	M Malik	Current study	M Malik	Current study
π/4	.10141184E+01	.10029005E+01	21461E- 02	.714835E-04
π/8	.10131084E+01	.10109712E+01	136384E- 03	.771366E-06
π/16	.10029806E+01	.10019720E+01	860559E- 05	354450E- 07
π/32	.10039725E+01	.10019820E+01	566253E- 06	306178E- 07
π/64	.10119720E+01	.10010720E+01	628977E- 06	294203E- 07
π/128	.10018720E+01	.10009720E+01	314147E- 07	293220E- 07

TABLE 2: Fourth-order Hybrid Method with vs without collocation points

<i>a</i> .	Computed solution		Error	
Step size	M Malik	Current study	M Malik	Current study
π/4	.9988215E+00	1047683E+01	.315051E	- .457110E+01
π/8	.1001760E+01	.1014874E+01	.195822E	129023E-01
π/16	.1001960E+01	.1005120E+01	.121861E	314796E-02
π/32	.1001971E+01	.1002759E+01	.760755E	787316E-03
π/64	.1001972E+01	.1002169E+01	.475334E	197011E-03
π/128	.1001972E+01	.1002021E+01	.297053E	492683E-04

We can see from column titles of the Tables (1-3) that stepsize are consistently presented in columns 1 for step sizes used in the simulation. Furthermore, the referred results in column 2 for comparison with simulated solution quantities illustrated in column 3 of all tabular figures. Simulated results matched well at every step size with respective quantities. The simulated were also compared with the given distance values  $|z(40\pi)| =$ 1.001972 to six decimal places at every step-size in [17]. We observed no major difference among compared quantities. Likewise, reference error values are presented for comparison in column 4 while simulated error quantities are given in column 5 in all tabular figures. The absolute errors in  $\gamma(40\pi)$  are compared against defined tolerance in every iteration. Simulated absolute error quantities matched well at every step size with respective quantities. We observed no major difference among error comparisons. On forming the ratio of the errors obtained by these methods with steps h and h/2 we find that, as expected, the ratio approaches 16 for the fourth order methods. As expected, the 4<sup>th</sup> order methods produce more accurate results than the 2<sup>nd</sup> order methods. The second order method with  $\alpha_1 = 0.5$  has the smallest principal error constants of all the second order methods.

The simulated results vis-a-vis the reference seen in tabular comparison together with the total number of function evaluations, the sixth order methods is more efficient than the second and four order formula for this type of problem.

Ston	Compute	d Solution	Error	
size	M Malik	Current study	M Malik	Current study
π/4	.1041506E+01	1091456E+01	395339E- 01	89491E- 01
π/8	.1049986E+01	.1037340E+01	480137E- 01	353679E- 01
π/16	.1020613E+01	.1027770E+01	186409E- 01	257977E- 01
π/32	.1006452E+01	.1008071E+01	447957E- 02	609917E- 02
π/64	.1003090E+01	.1003492E+01	111841E- 02	151976E- 02
π/128	.1002252E+01	.1002352E+01	279782E- 03	380226E- 03

TABLE 3: Second Order Hybrid Method with vs without collocation points

As expected, we observed from the problems tested with this proposed method the results converged within acceptable range to exact solutions as well as compared favourably with

existing similar methods. The six-order methods produced more accurate results with the smallest principal error constant of all the second order methods and it has produced relatively accurate results than the lower order methods. Based on the comparison of the results of the simulated examples, the proposed method is effective for the direct solution of secondorder ordinary differential equations.

# V. CONCLUSIONS

In this work, we applied Hybrid Methods for numerical solution of second order initial value problems of ordinary differential equations where first derivative does not feature explicitly. The Direct Hybrid Method of order six embedded with off-step points was successfully applied for the direct solution of tested benchmark problems. Two illustrative examples were solved to test performance of the algorithms in terms of the absolute relative errors computed with the use of MATLAB<sup>TM</sup> 2020 code. It proved to be efficient in solving, the simulated results compared favourably with existing methods. In terms of accuracy, the comparisons are evident in Figures 1-2 and Tables 1-3. The proposed method has been tested and found to be reliable, efficient and less tedious compared to single-step and linear multi-step methods that require reduction of higher-order equations to first-order equations.

It is worth taking note of that the methods used in comparison also methods with second order, fourth order or equal order (order 6). Nonetheless, the other method approximate function quantities at step-points only not at the off-step points. Hence, the basis of the comparison is fair, as Hybrid Method embedded with off-step points was applied in current study.

Therefore, the proposed six-order Hybrid Method is recommended for adoption as a solver of second order IVPs of ODEs in scientific and engineering mechanics.

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