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CONTRACTIVITY-PRESERVING, 4-STEP EXPLICIT, HERMITE–OBRECHKOFF SERIES ODE SOLVERS OF ORDER 3 TO 20

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Abstract. New optimal, contractivity-preserving (CP), 4-step, explicit, d-derivative Hermite–Obrechkoff series methods up to order $p = 20$, denoted by HO(d, p), with nonnegative coefficients are constructed for solving nonstiff first-order initial value problems $y' = f(t, y)$, $y(t_0) = y_0$. The upper bound p_u of order p of HO(d, p) is approximately 1.8 times the number of derivatives d. It can be shown that HO(d, p)) are absolutely stable for $d = 1$ to infinity. Their stability regions have generally a good shape and grow with decreasing $p - d$. Two selected CP HO methods: 6-derivative HO of order 13, denoted by HO(6,13), which has maximum order 13 based on the CP conditions, and 7-derivative HO of order 14, denoted by HO(7,14), compare well with Adams–Bashforth–Moulton in Predict-Evaluate-Correct-Evaluate (PECE) mode, denoted by ABM(13), in solving several problems often used to test higher-order ODE solvers on the basis of the maximum global error as a function of the CPU time. These two selected CP HO methods also compare favorably with Adams–Cowell of order 13 in PECE mode, denoted by AC(13), in solving standard N-body problems over an interval of 1000 periods on the basis of the relative error of energy as a function of the CPU time.

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1. Introduction

In this paper, only $d = 2, 3, \dots, 10$, Taylor coefficients, with $d < p$, are required by a new contractivity-preserving (CP), explicit, d-derivative, 4-step Hermite–Obrechkoff method of order p up to 20, denoted by $\mathrm{HO}(d,p)$, for solving nonstiff ordinary differential equations (ODEs),

$$y' = f(t,y), \qquad y(t_0) = y_0, \qquad \text{where} \quad ' = \frac{d}{dt} \quad \text{and} \quad y \in \mathbb{R}^n. \tag{1}$$

$\mathrm{HO}(d,p)$ use y', y'',... $y^{(d)}$, as in Obrechkoff methods [23] and, when $d = p$, $\mathrm{HO}(d,p)$ reduce to Taylor series method of order p ($\mathrm{T}(p)$).

The Taylor series methods have been an excellent choice in astronomical calculations [3], numerical integration of ordinary differential equations (ODEs) and differential algebraic equations (DAEs) [1], sensitivity analysis of ODEs/DAEs [2], in solving general problems [7] and validating solutions of ODEs by means of interval analysis [21, 14].

More recently, the Taylor series and constant step Störmer's methods have been good choices in achieving Brouwers law [4, 11].

The main cost in solving ODEs by the Taylor method of order p ($\mathrm{T}(p)$) lies in the repeated evaluation of the p Taylor coefficients of the functions involved.

Following Steffensen and Rabe [26, 24], recursive computation of Taylor coefficients is used to compute sums, differences, products and powers of power series, etc. (see [3, 20], and [12, pp. 46–49]).

Deprit and Zahar [8] showed that such recursive computation is very effective in achieving high accuracy, even with little computing time and large step sizes.

In our construction of $\mathrm{HO}(d,p)$, we replace the forward Euler (FE) method,

$$y_{n+1} = y_n + \Delta t f(t_n, y_n), \tag{2}$$

used by Gottlieb et al. and Huang [9, 15] in establishing strong stability preserving (SSP) Runge–Kutta (RK) methods as convex combinations of FE methods, by rewriting $\mathrm{HO}(d,p)$ as a convex combination of the special d-derivative extension of FE, which we denote by $\mathrm{S}(d)$:

$$y_{n+1} = y_n + \Delta t f(t_n, y_n) + \sum_{m=2}^{d} \eta_m (\Delta t)^m f^{(m-1)}(t_n, y_n), \tag{3}$$

where the coefficients η_m satisfy the inequality $\eta_m \le \frac{1}{m!}$. If equality holds, then $\mathrm{S}(d)$ reduces to the Taylor method of order d, $\mathrm{T}(d)$. The error in $\mathrm{S}(d)$ is of order $\ell \ge 2$ if there exists a smallest $\ell \in \{2, 3, \dots, d\}$ such that $\eta_\ell < \frac{1}{\ell!}$. If $\mathrm{S}(d)$ is contractive in a given norm, then $\mathrm{HO}(d,p)$ will be contractive as a convex combination of $\mathrm{S}(d)$ with modified step sizes.

The region of absolute stability of $\mathrm{HO}(d,p)$ is derived under the assumption that two solutions, y and $\tilde{y}$, to problem (1) are *contractive*:

$$\|y(t+\Delta t) - \tilde{y}(t+\Delta t)\| \le \|y(t) - \tilde{y}(t)\|, \quad \forall\, \Delta t \ge 0. \tag{4}$$

We assume that there exists a maximum stepsize $\Delta t_{\mathrm{S}(d)}$ such that f satisfies a discrete analog of (4) when $\mathrm{S}(d)$ is employed with $\Delta t \le \Delta t_{\mathrm{S}(d)}$:

$$\|y_{n+1} - \tilde{y}_{n+1}\| \equiv \Bigg\| y_n + \Delta t f(t_n, y_n) + \sum_{m=2}^{d} \eta_m (\Delta t)^m f^{(m-1)}(t_n, y_n) - \Bigg(\tilde{y}_n + \Delta t f(t_n, \tilde{y}_n) + \sum_{m=2}^{d} \eta_m (\Delta t)^m f^{(m-1)}(t_n, \tilde{y}_n) \Bigg) \Bigg\| \le \|y_n - \tilde{y}_n\|. \quad (5)$$

Here y_n and $\tilde{y}_n$ are two numerical solutions generated by $\mathrm{S}(d)$ with different *neighbouring* starting values $y_0 = y(t_0)$ and $\tilde{y}_0 = \tilde{y}(t_0)$.

We are interested in a higher-order $\mathrm{HO}(d,p)$ that maintains the *contractivity-preserving property*

$$\|y_{n+1} - \tilde{y}_{n+1}\| \le \max_{0 \le \ell \le 3} \|y_{n-\ell} - \tilde{y}_{n-\ell}\|, \quad (6)$$

for $0 \le \Delta t \le \Delta t_{\max} = c \Delta t_{\mathrm{S}(d)}$ whenever inequality (5) holds. Here c, called a CP coefficient, depends only on the numerical integration method but not on f. This definition of a CP coefficient of $\mathrm{HO}(d,p)$ follows closely the definition of a SSP coefficient of RK (see [9]).

In [18], similar CP RK methods have been constructed and tested on DETEST problems [17].

The aim of $\mathrm{HO}(d,p)$ is to maintain the CP property (6) while achieving higher-order accuracy, perhaps with a modified time-step restriction, measured here with a CP coefficient $c(\mathrm{HO}(d,p))$:

$$\Delta t \le c(\mathrm{HO}(d,p)) \Delta t_{\mathrm{S}(d)}. \quad (7)$$

This coefficient describes the ratio of the maximal $\mathrm{HO}(d,p)$ time step to the time step $\Delta t_{\mathrm{S}(d)}$, for which condition (5) holds.

The upper bound p_u of order p of these methods is approximately 1.8 times the number of derivatives d. It can be shown that $\mathrm{HO}(d,p))$ are absolutely stable for $d = 1$ to infinity. Their stability regions have generally a good shape and grow with decreasing $p-d$. This result suggests that, for large d, $\mathrm{HO}(d,p)$ methods have order p large enough to take into account many problems where a very high precision of the solution is required, similar to Taylor methods.

The numerical performance of two selected CP HO methods: 6-derivative HO of order 13, denoted by HO(6,13), which has maximum order 13 based on the CP conditions, and 7-derivative HO of order 14, denoted by HO(7,14), and Adams–Bashforth–Moulton in PECE mode, denoted by ABM(13), is compared on several problems frequently used to test higher-order ODE solvers. It is seen that, generally, the two selected CP HO methods requires less CPU time than ABM(13).

Similar to Huang et al [16], we compare also the numerical performance of HO(6,13), HO(7,14) and Adams–Cowell of order 13 in PECE mode, denoted by AC(13), on Kepler orbit with eccentricity $e = 0.3$, $e = 0.5$ and $e = 0.7$ over an interval of 1000 periods on the basis of $\log_{10}$ of the absolute value of relative error in energy, denoted by $\log_{10}(\text{EE})$, as a function of CPU time. It is seen that HO(6,13) and HO(7,14) win. These two HO methods also compare well with AC(13) in solving eccentric Kepler orbit with eccentricity $e = 0.3$, $e = 0.5$ and $e = 0.7$ over an interval of 10000 periods on the basis of the growth of relative error of energy and long intervals of integration.

Section 2 introduces d-derivative HO(d, p) series methods and lists the necessary order conditions. In Section 3, the existence, stability properties and the principal error term of HO(d, p) methods are considered. Section 4 describes the region of absolute stability and the principal error term of two selected HO methods: HO(6,13) and HO(7,14). In Section 5, numerical results are used to compare HO(6,13), HO(7,14) with ABM(13) and AC(13). New selected HO(d, p) methods are listed in Appendix A.

2. d-derivative HO(d, p) series methods

To construct HO(d, p), we use a Hermite interpolation polynomial as a 4-step integration formula with d derivatives of y to obtain y_{n+1} to order p,

$$y_{n+1} = \sum_{\ell=0}^{3} \left[\gamma_{\ell,0}\, y_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \gamma_{\ell,m}\, y_{n-\ell}^{(m)} \right], \tag{8}$$

with step size Δt and consistency condition:

$$\sum_{\ell=0}^{3} \gamma_{\ell,0} = 1. \tag{9}$$

We also have to satisfy the following order conditions,

$$\sum_{m=0}^{j} \sum_{\ell=0}^{3} \gamma_{\ell,m} \frac{(-\ell)^{j-m}}{(j-m)!} = \frac{1}{j!}, \quad j = 1, 2, \ldots, d, \tag{10}$$

$$\sum_{m=0}^{d} \sum_{\ell=0}^{3} \gamma_{\ell,m} \frac{(-\ell)^{j-m}}{(j-m)!} = \frac{1}{j!}, \quad j = d+1, d+2, \ldots, p. \tag{11}$$

Upon factoring $\gamma_{\ell,0}$ in (8), the difference $y_{n+1} - \tilde{y}_{n+1}$ becomes

$$y_{n+1} - \tilde{y}_{n+1} = \sum_{\ell=0}^{3} \gamma_{\ell,0} \left[\left(y_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{\gamma_{\ell,m}}{\gamma_{\ell,0}} y_{n-\ell}^{(m)} \right) - \left(\tilde{y}_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{\gamma_{\ell,m}}{\gamma_{\ell,0}} \tilde{y}_{n-\ell}^{(m)} \right) \right]. \quad (12)$$

Provided all the coefficients $\gamma_{\ell,m}$ are nonnegative, the following straightforward extension of a result presented in [10, 15] holds.

Theorem. *If f satisfies condition* (5) *of the $S(d)$ method, then the* HO(d,p) *method* (8) *satisfies the CP property*

$$\|y_{n+1} - \tilde{y}_{n+1}\| \le \max_{0 \le \ell \le 3} \|y_{n-\ell} - \tilde{y}_{n-\ell}\|$$

provided

$$\Delta t \le c_{\text{feasible}}\, \Delta t_{S(d)},$$

where the feasible CP coefficient, $r = c_{\text{feasible}}$, satisfies the following conditions,

$$r \le r_\ell = \frac{\gamma_{\ell,0}}{\gamma_{\ell,1}}, \quad \textit{for} \quad \ell = 0, 1, 2, 3. \quad (13)$$

Here r_ℓ satisfy the conditions:

$$\frac{\gamma_{\ell,m}}{\gamma_{\ell,0}} \le \left[\frac{1}{r_\ell} \right]^m \frac{1}{m!}, \quad \textit{for} \quad \ell = 0, 1, 2, 3, \quad m = 2, 3, \dots, d, \quad (14)$$

with the convention that $a/0 = +\infty$, under the assumption that all coefficients of (8) *are nonnegative:*

$$\gamma_{\ell,m} \ge 0, \quad \ell = 0, 1, 2, 3, \quad m = 0, 1, \dots, d. \quad (15)$$

Proof. Taking the norm of (12), by the convexity of the norm and conditions (13) and (14), we obtain

$$\begin{aligned} &\|y_{n+1} - \tilde{y}_{n+1}\| \\ &\quad \le \sum_{\ell=0}^{3} \gamma_{\ell,0} \left\| \left(y_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{\gamma_{\ell,m}}{\gamma_{\ell,0}} y_{n-\ell}^{(m)} \right) - \left(\tilde{y}_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{\gamma_{\ell,m}}{\gamma_{\ell,0}} \tilde{y}_{n-\ell}^{(m)} \right) \right\| \\ &\quad \le \left[\sum_{\ell=0}^{3} \gamma_{\ell,0} \right] \max_{0 \le \ell \le 3} \|y_{n-\ell} - \tilde{y}_{n-\ell}\|, \quad \text{by (5)}, \\ &\quad \le \max_{0 \le \ell \le 3} \|y_{n-\ell} - \tilde{y}_{n-\ell}\|, \quad \text{by consistency condition (9)}, \end{aligned}$$

since, for $\ell = 0, 1, 2, 3$, $\quad \dfrac{1}{r_\ell}\Delta t \leq \dfrac{1}{r}\Delta t = \dfrac{\Delta t}{c_{\text{feasible}}} \leq \Delta t_{\text{S}(d)}$.

It is to be noted that each representation $\gamma_{\ell,m}$, for $\ell = 0, 1, 2, 3$ and $m = 0, 1, \ldots, d$, of $\text{HO}(d, p)$, given in (8), which satisfy (14), (15) and order conditions (9), (10), (11), will produce a feasible CP coefficient, c_{feasible}, defined in the Theorem and a *feasible* $\text{HO}(d, p)$.

What we really want is not merely a feasible $\text{HO}(d, p)$ but the $\text{HO}(d, p)$ with the largest c_{feasible}. This question will be considered in Subsection 2.1.

2.1. Obtaining $c(\mathbf{HO}(d, p))$

To obtain $c(\text{HO}(d, p))$, we maximize r,

$$\text{maximize } r, \tag{16}$$

subject to the inequalities (13)–(15) of the Theorem together with the order conditions (9)–(11). Let

$$c(\text{HO}(d, p)) = (\text{maximized})\ r. \tag{17}$$

It is to be noted that, using the above formulation of the optimization problem, when $d = p$, $c(\text{HO}(d, p))$ is equal to 1 and $\text{HO}(d, p)$ is the Taylor series method of order p, $\text{T}(p)$, and that a linear least square fit of $c(\text{T}(p))$ as a function of d will give a slope equal to 0.

Definition. A *effective CP coefficient* of a CP method, M, is denoted by

$$c_{\text{eff}}(M) = \frac{c(M)}{l}, \tag{18}$$

where l is the number of function evaluations of M per time step and $c(M)$ is a CP coefficient of M obtained in (17).

The effective coefficients c_{eff} provide a fair comparison between methods of the same order. Since $\text{HO}(d, p)$ contains many free parameters, the MATLAB Optimization Toolbox was used to search for the method with largest r under the tolerance 10^{-12} on the objective function r, provided all the constraints were satisfied to tolerance 8×10^{-14}.

The formulae of selected $\text{HO}(d, p)$ considered in this paper are listed in Appendix A with their $c(\text{HO}(d, p))$ and lower bounds $x_{\min}$ of the unscaled intervals of stability $(x_{\min}, 0)$.

Table 1: Given d, each cell of the table contains (1) $x_{\min}(p_\ell)$, (2) CP coefficient c_{p_ℓ} of HO(d, p_ℓ)) of order p_ℓ, (3) interval of order p, $[p_\ell, p_u]$, of HO(d, p) which exist, (4) $x_{\min}(p_u)$, and (5) CP coefficient c_{p_u} of HO(d, p_u)) of order p_u.

The set of HO(d,p) which exist as a function of d				
2	3	4	5	6
$x_{\min}(3) = -2.16$ $(c_3 = 0.785)$ $3 \le p \le 5$ $x_{\min}(5) = -1.11$ $(c_5 = 0.425)$	$x_{\min}(4) = -1.92$ $(c_4 = 0.905)$ $4 \le p \le 7$ $x_{\min}(7) = -1.06$ $(c_7 = 0.485)$	$x_{\min}(5) = -2.82$ $(c_5 = 0.976)$ $5 \le p \le 10$ $x_{\min}(10) = -0.92$ $(c_{10} = 0.423)$	$x_{\min}(6) = -3.00$ $(c_6 = 0.985)$ $6 \le p \le 11$ $x_{\min}(11) = -1.78$ $(c_{11} = 0.533)$	$x_{\min}(7) = -3.66$ $(c_7 = 0.993)$ $7 \le p \le 13$ $x_{\min}(13) = -0.85$ $(c_{13} = 0.330)$
The set of HO(d,p) which exist as a function of d				
7	8	9	10	11
$x_{\min}(8) = -3.84$ $(c_8 = 0.997)$ $8 \le p \le 15$ $x_{\min}(15) = -0.88$ $(c_{15} = 0.257)$	$x_{\min}(9) = -4.26$ $(c_9 = 0.998)$ $9 \le p \le 16$ $x_{\min}(16) = -1.54$ $(c_{16} = 0.502)$	$x_{\min}(10) = -4.56$ $(c_{10} = 0.999)$ $10 \le p \le 19$ $x_{\min}(19) = -1.38$ $(c_{19} = 0.431)$	$x_{\min}(11) = -5.10$ $(c_{11} = 0.999)$ $11 \le p \le 20$ $x_{\min}(20) = -1.38$ $(c_{20} = 0.547)$	$x_{\min}(12) = -5.46$ $(c_{12} = 0.999)$ $12 \le p$

3. Existence, stability properties and principal error term of HO(d, p) series methods

3.1. Existence of HO(d, p) methods as a function of d derivatives

Given a number d of derivatives, each cell of Table 1 contains:

1. Lower bound $x_{\min}(p_\ell)$ of the unscaled intervals of stability $(x_{\min}, 0)$ of HO(d, p_ℓ)) of order p_ℓ which is the lower bound of p,
2. CP coefficient $c_{p_\ell} = c(\text{HO}(d, p_\ell))$,
3. Interval of order p, $[p_\ell, p_u]$, of HO(d, p),
4. Lower bound $x_{\min}(p_u)$ of the unscaled intervals of stability $(x_{\min}, 0)$ of HO(d, p_u)) of order p_u which is the upper bound of p (if HO(d, p_u) exists),
5. CP coefficient $c_{p_u} = c(\text{HO}(d, p_u))$ of order p_u.

Each cell of Table 1 shows the set of HO(d, p) of order p, $p_\ell \le p \le p_u$, which exist and associated $x_{\min}(p_\ell), x_{\min}(p_u)$, CP coefficients c_{p_ℓ}, c_{p_u}.

Table 1 lists the upper bounds p_u of CP HO(d, p) methods as an increasing function of d, number of derivatives and shows that the upper bound p_u of order p seems to be linear with the number of derivatives d and a linear least square fit is

$$p_u = 1.8667d + 1.6887, \tag{19}$$

where the slope $\eta = 1.8667$ is expected, since an increase of order p by one requires one additional order condition while an increase of d by one yields 4 additional variables. Here, for any positive d, lower bounds $x_{\min}$ of the unscaled intervals of stability $(x_{\min}, 0)$ of HO(d, p_u)) satisfy generally the relation $|x_{\min}| \geq 2 \times c(\text{HO}(d, p_u))$ from condition (7) and, hence, CP HO(d, p)) are absolutely stable for $d = 1$ to infinity. This analysis suggests that, for large d, HO(d, p) methods have order p large enough to take into account many problems which require a very high precision of the solution, similar to Taylor methods which have the slope $\eta = 1$.

Since p_u follows the equation (19), when we slow down the growth of order p as d increases as follows: p being the integer part of $\eta\, d$, denoted by $p = \lfloor \eta\, d \rfloor$ where

$$1 \leq \eta \leq \eta_{\max}, \tag{20}$$

HO(d, p) method has desirable stability properties considered in Subsection 3.2. Here, $\eta_{\max} > 1$ should not be much larger than 1. From Table 3, $\eta_{\max}$ seems to be about 1.4 or less.

The existence of CP HO(d, p) would suggest the existence of series of contractivity-preserving Hermite–Birkhoff-Obrechkoff methods, HBO$_{\text{RK2}}(p+1)$, HBO$_{\text{RK3}}(p+2)$, HBO$_{\text{RK4}}(p+3)$, etc., based on combining HO(d, p) with RK2, RK3, RK4, etc., respectively.

3.2. Stability properties and principal error term of HO(d, p) methods with $p = \lfloor \eta\, d \rfloor$

In this section, we analyze some stability properties and list the principal error term of CP HO(d, p) methods with $p = \lfloor \eta\, d \rfloor$ and η satisfying (20). Similar to the case of Taylor series methods, the use of high number d gives HO series methods of high order.

We are now interested in the size of the stability regions of CP HO(d, p) methods.

As an example, Table 2 lists bounds $|x_{\min}|$ of unscaled intervals of stability $(x_{\min}, 0)$ of CP HO(d, p) method with $p = \lfloor 1.3\, d \rfloor$, $d = 4, 5, \dots, 13$ as a generally increasing function of d and $c(\text{HO}(d, p = \lfloor 1.3\, d \rfloor))$ as an almost constant function of d.

Similar to Barrio et al. [3], we use a linear least square fit of $|x_{\min}|$ as a function of d, the number of derivatives of the method. We also use a linear least square fit of $c(\text{HO}(d, p))$ as a function of d. These linear least square fits give different positive slopes ρ and σ of $|x_{\min}| = \rho\, d + \sigma$ and slopes μ and ν of $c(\text{HO}(d, p)) = \mu\, d + \nu$ depending on the values of η. The values of ρ, σ, μ and ν are presented in Table 3. It is seen that HO$(d, p = \lfloor \eta\, d \rfloor)$ series methods have slopes ρ positive and non negligible up to $\eta = 1.4$ and slopes μ near 0 and positive similar to Taylor series methods.

Table 2: Unscaled $|x_{\min}|$ and $c(\mathrm{HO}(d, p = \lfloor 1.3\, d \rfloor))$ of $\mathrm{HO}(d, p = \lfloor 1.3\, d \rfloor)$ series method as a function of p.

p	d	$\lvert x_{\min}\rvert$	$c(\mathrm{HO}(d, \lfloor 1.3\, d \rfloor))$
5	4	2.82	0.9759
6	5	3.00	0.9847
7	6	3.66	0.9928
9	7	3.72	0.9866
10	8	4.80	0.9901
11	9	4.08	0.9951
13	10	4.20	0.9908
14	11	3.50	0.9876
15	12	5.80	0.9932
16	13	6.30	0.9981

Table 3: Slope ρ and σ of a linear least square fit of $|x_{\min}| = \rho\, d + \sigma$ and slope μ and ν of a linear least square fit of $c(\mathrm{HO}(d, p)) = \mu\, d + \nu$ for the listed methods.

method	Order p as a function of d $p = \lfloor \eta\, d \rfloor$	ρ	σ	μ	ν
$\mathrm{HO}(d, p_u)$		0.0392	0.9741		
$\mathrm{HO}(d, p)$	$p = \lfloor 1.6\, d \rfloor$	0.0352	2.4432	0.005298	0.8702
”	$p = \lfloor 1.5\, d \rfloor$	0.0990	2.2836	0.006602	0.8894
”	$p = \lfloor 1.4\, d \rfloor$	0.1575	2.2366	0.003544	0.9462
”	$p = \lfloor 1.3\, d \rfloor$	0.2476	1.9720	0.001382	0.9775
$\mathrm{T}(p)$	$p = d$	0.3725	1.3614	0	1

Table 4: Ordered pair (scaled bound $\hat{x}_{\min}(\cdot)$, scaled norm SPLTC$(\cdot)$) of HO(d, p) series method and ABM(p) method as a function of p.

p	HO$(d, p = \lfloor 1.3\, d \rfloor)$	HO$(d, p = \lfloor 1.6\, d \rfloor)$	HO(d, p_u)	ABM(p)
5	(0.70, 3.66e-02)		(0.55, 1.75e-01)	(0.70, 2.44e-01)
6	(0.60, 8.04e-03)	(0.61, 2.28e-02)		(0.52, 2.18e-01)
7	(0.61, 1.31e-03)		(0.35, 1.36e-02)	(0.39, 2.00e-01)
8		(0.40, 1.39e-03)		(0.30, 1.86e-01)
9	(0.53, 1.18e-04)	(0.36, 2.78e-04)		(0.22, 1.75e-01)
10	(0.60, 1.39e-05)		(0.23, 3.51e-04)	(0.17, 1.65e-01)
11	(0.45, 1.53e-06)	(0.59, 1.00e-05)	(0.35, 5.64e-05)	(0.13, 1.57e-01)
12		(0.39, 1.16e-06)		(0.11, 1.51e-01)
13	(0.42, 5.65e-08)		(0.14, 2.41e-06)	(0.03, 1.45e-01)
14	(0.31, 5.80e-09)	(0.32, 2.94e-08)		
15	(0.48, 2.98e-10)		(0.12, 7.40e-08)	
16	(0.48, 3.94e-11)	(0.22, 5.84e-10)	(0.19, 4.03e-09)	
17		(0.23, 5.69e-11)		
18				
19			(0.15, 1.50e-11)	
20			(0.13, 8.34e-13)	

The principal error term of HO(d, p) series methods is of the form

$$[\delta\, \{f^p\}]\, h^{p+1}, \tag{21}$$

where $\{f^p\}$ is an elementary differential defined in [6], [19] and [12] and δ is the principal local truncation error coefficient (PLTC) of the principal error term.

The PLTC of ABM(p) are $[\beta_k C_p*, C_{p+1}]$ [19, p. 107].

The scaled bound $\hat{x}_{\min}(\text{HO}(d,p)) = |x_{\min}/d|$, scaled norm SPLTC(HO$(d,p)$) $= d \times \|\text{PLTC}\|_2$ of HO(d, p) and the scaled bound $\hat{x}_{\min}(\text{ABM}(p)) = |x_{\min}/2|$, scaled norm SPLTC(ABM$(p)$) $= 2 \times \|\text{PLTC}\|_2$ of ABM(p) for a given order p are listed in Table 4. It is seen that, generally, $\hat{x}_{\min}(\text{HO}(d,p)) > \hat{x}_{\min}(\text{ABM}(p))$, SPLTC(HO$(d,p)$) $<$ SPLTC(ABM(p)) for the same order p and SPLTC(HO(d,p)) decrease much more rapidly than SPLTC(ABM(p)) with increasing p.

4. Region of absolute stability and principal error term of two selected methods: HO(6,13) and HO(7,14)

To obtain the region of absolute stability, $\mathcal{R}$, of HO(d,p), we apply the integration formula (8) with constant step $h = \Delta t$ to the linear test equation

$$y' = \lambda y, \qquad y_0 = 1.$$

Thus, we obtain

$$y_{n+1} = \sum_{\ell=0}^{3}\left[\gamma_{\ell,0}y_{n-\ell} + \sum_{m=1}^{d}(\lambda h)^m \gamma_{\ell,m}y_{n-\ell}\right]. \tag{22}$$

If we let $\hat{h} = \lambda h$ and replace y_{n+1}, y_n, y_{n-1}, y_{n-2}, y_{n-3} with y_{n+4}, y_{n+3}, y_{n+2}, y_{n+1}, y_n, respectively, then (22) can be written as a function of y_{n+4}, y_{n+3}, y_{n+2}, y_{n+1}, y_n only, then follow the following fourth-order difference equation and associated linear characteristic equation:

$$\sum_{j=0}^{4} C_j y_{n+j} = 0, \qquad \sum_{j=0}^{4} C_j r^j = 0. \tag{23}$$

A complex number $\hat{h} = \lambda h$ is in $\mathcal{R}$ if the 4 roots of the characteristic equation satisfy the root condition $|r_s| \leq 1$, $s = 1,2,3,4$, provided the multiple roots satisfy $|r_s| < 1$. The scanning method used to find $\mathcal{R}$ is similar to the one used for Runge–Kutta methods (see [19, pp. 70 and 204]).

The unscaled intervals of stability of HO(6,13) and HO(7,14) are (-0.85, 0) and (-1.22, 0) respectively.

The principal error term of HO(6,13) and HO(7,14) is of the form $[\delta\,\{f^p\}]\,h^{p+1}$ where $\{f^p\}$ is an elementary differential defined in [6], [19] and [12] and the principal local truncation error coefficients δ of HO(6,13) and HO(7,14) are respectively 1/2489338 and 1/29274190.

5. Numerical results

Since HO(d,p) is not a one-step method, we must provide not only an initial value, i.e., y_0 but also $k-1$ additional starting value, i.e., $y_1, y_2, \ldots, y_{k-1}$. The starting values for HO(d,p) are calculated by the one-step, 4-stage, Hermite–Birkhoff–Taylor method of order $d+3$ using y' to $y^{(d)}$ with appropriate small step sizes [22]. The d derivatives, y' to $y^{(d)}$, of the Taylor series are calculated at each integration step by known recurrence formulae (see, for example, [12, pp. 46–49], [20]).

The numerical performances of HO(6,13), HO(7,14), Adams–Bashforth–Moulton in PECE mode, denoted by ABM(13) and Adams–Cowell of order 13 in PECE mode, denoted by AC(13), were compared on the problems mentioned in Subsections 5.1, 5.2 and 5.3.

The maximum global error (MGE) is taken in the uniform norm,

$$\text{MGE} = \max_n \{\|y_n - z_n\|_\infty\},$$

where y_n is the numerical value obtained by HO(d, p) and z_n is the "exact solution" obtained by DP(8,7)13M, with stringent tolerance 5×10^{-14}. Computations were performed in C++ on a PC with the following characteristics: Memory: 5.8 GB, Processor 0,1,...,7: Intel(R) Core(TM) i7 CPU 920 @ 2.67GHz, Operating system: Ubuntu Release 11.04, Kernel Linux 2.6.38-12-generic, GNOME 2.32.1.

5.1. CPU time of HO(6,13), HO(7,14) and ABM(13)

In Table 5, the performance of HO(6,13), HO(7,14) and ABM(13) is compared on the seven problems on hand: the equatorial main problem in artificial satellite theory [5, 3, 27], Hénon–Heiles' problem [13], and the following nonstiff DETEST problems: growth problem B1 of two conflicting populations, two-body problems D2, D3, D4 and Van der Pol's equation E2 with $\epsilon = 1$ [17], on the basis of Maximum Global Errors (MGE) as a function of CPU time in seconds (CPU).

It is seen that HO(6,13) and HO(7,14) compare favorably with ABM(13) at almost all tolerances.

The *CPU percentage efficiency gain* (CPU PEG) is defined by the formula (cf. Sharp [25]),

$$(\text{CPU PEG})_i = 100 \left[\frac{\sum_j \text{CPU}_{2,ij}}{\sum_j \text{CPU}_{1,ij}} - 1 \right], \tag{24}$$

where $\text{CPU}_{1,ij}$ and $\text{CPU}_{2,ij}$ are the estimates of CPU time of methods 1 and 2, respectively, associated with problem i, and estimate of MGE $= 10^{-j}$. To compute $\text{CPU}_{2,j}$ and $\text{CPU}_{1,j}$ appearing in (24), we approximate the data $(\log_{10}(\text{MGE}), \log_{10}(\text{CPU}))$ in a least-squares sense by MATLAB's `polyfit`. Then, for chosen integer values of the summation index j, we take $-\log_{10}(\text{MGE estimate}) = j$ and obtain $\log_{10}(\text{CPU estimate})$ from the approximating curve, and finally the estimate of CPU time.

Table 6 lists the CPU PEG of HO(6,13) and HO(7,14) over ABM(13) for the seven problems on hand. It is seen that HO(6,13) and HO(7,14) win.

Table 5: Maximum Global Errors (MGE) as a function of CPU time in seconds of HO(6,13), HO(7,14) and ABM(13) for the problems on hand.

Problem: equatorial main problem

MGE	CPU in HO(6,13)	CPU in HO(7,14)	CPU in ABM(13)
6.89e-02	1.13e-03	1.45e-03	3.52e-03
2.46e-04	1.40e-03	1.96e-03	3.98e-03
1.44e-05	1.65e-03	2.28e-03	4.23e-03
2.14e-06	1.97e-03	2.52e-03	4.41e-03
1.14e-07	2.43e-03	2.94e-03	4.70e-03
2.45e-08	2.68e-03	3.20e-03	4.86e-03
1.93e-09	3.25e-03	3.66e-03	5.13e-03
1.99e-10	3.72e-03	4.13e-03	5.39e-03

Problem: Hénon–Heiles' problem

MGE	CPU in HO(6,13)	CPU in HO(7,14)	CPU in ABM(13)
1.11e-07	2.67e-04	2.93e-04	8.20e-04
1.37e-08	3.00e-04	3.33e-04	8.24e-04
2.60e-09	3.33e-04	3.69e-04	8.28e-04
1.60e-10	4.00e-04	4.37e-04	8.33e-04
1.44e-11	4.67e-04	5.06e-04	8.38e-04
2.22e-12	5.50e-04	5.67e-04	8.42e-04

Problem: DETEST B1

MGE	CPU in HO(6,13)	CPU in HO(7,14)	CPU in ABM(13)
2.76e-04	1.08e-04	1.14e-04	1.82e-04
1.10e-05	1.25e-04	1.35e-04	2.02e-04
1.23e-06	1.33e-04	1.51e-04	2.17e-04
1.73e-07	1.50e-04	1.67e-04	2.32e-04
2.87e-08	1.67e-04	1.83e-04	2.46e-04
1.39e-09	2.00e-04	2.14e-04	2.71e-04
3.39e-10	2.25e-04	2.31e-04	2.84e-04
9.27e-11	2.42e-04	2.47e-04	2.97e-04
2.81e-11	2.58e-04	2.62e-04	3.08e-04

Problem: DETEST D2

MGE	CPU in HO(6,13)	CPU in HO(7,14)	CPU in ABM(13)
6.68e-04	3.33e-04	3.85e-04	1.04e-03
7.32e-06	4.00e-04	5.15e-04	1.16e-03
5.66e-07	5.50e-04	6.07e-04	1.24e-03
1.37e-08	6.50e-04	7.71e-04	1.35e-03
5.19e-10	7.00e-04	9.51e-04	1.46e-03
1.43e-10	9.50e-04	1.03e-03	1.51e-03
3.20e-11	1.08e-03	1.14e-03	1.56e-03

Problem: DETEST D3

MGE	CPU in HO(6,13)	CPU in HO(7,14)	CPU in ABM(13)
5.63e-04	6.00e-04	6.83e-04	1.06e-03
2.09e-05	7.17e-04	8.97e-04	1.33e-03
1.89e-06	9.17e-04	1.09e-03	1.57e-03
1.30e-07	1.13e-03	1.36e-03	1.90e-03
2.84e-08	1.23e-03	1.55e-03	2.12e-03
4.58e-09	1.57e-03	1.80e-03	2.41e-03
2.67e-10	1.62e-03	2.28e-03	2.94e-03

Problem: DETEST D4

MGE	CPU in HO(6,13)	CPU in HO(7,14)	CPU in ABM(13)
1.62e-02	1.23e-03	1.31e-03	1.54e-03
2.26e-04	1.58e-03	1.86e-03	2.22e-03
1.36e-05	1.95e-03	2.34e-03	2.82e-03
4.46e-06	2.28e-03	2.56e-03	3.10e-03
1.15e-07	3.00e-03	3.44e-03	4.24e-03
1.12e-08	3.33e-03	4.16e-03	5.18e-03
1.62e-09	3.72e-03	4.87e-03	6.11e-03
4.68e-10	4.77e-03	5.39e-03	6.80e-03

Problem: DETEST E2

MGE	CPU in HO(6,13)	CPU in HO(7,14)	CPU in ABM(13)
1.60e-03	9.17e-05	9.39e-05	1.80e-04
6.04e-05	1.08e-04	1.13e-04	1.98e-04
4.12e-06	1.25e-04	1.32e-04	2.14e-04
4.12e-07	1.42e-04	1.50e-04	2.29e-04
9.63e-09	1.75e-04	1.85e-04	2.55e-04
2.07e-09	1.92e-04	2.02e-04	2.66e-04
1.09e-10	2.25e-04	2.39e-04	2.90e-04
1.24e-11	2.50e-04	2.70e-04	3.09e-04
4.07e-12	2.67e-04	2.88e-04	3.19e-04

Table 6: CPU PEG of HO(6,13) and HO(7,14) over ABM(13) for the listed problems.

Problem	CPU PEG of HO(6,13) over ABM(13)	CPU PEG of HO(7,14) over ABM(13)
Equat. main prob.	104 %	67 %
Hénon–Heiles	183 %	160 %
B1	46 %	37 %
D2	121 %	90 %
D3	67 %	40 %
D4	43 %	23 %
E2	49 %	41 %

5.2. CPU time of HO(6,13), HO(7,14) and AC(13) after a 1000 periods integration of Kepler's two-body problem

The relative energy error (EE(t)) at time t is defined as

$$\mathrm{EE}(t) = \left| \frac{\mathrm{E}(t) - \mathrm{E}(0)}{\mathrm{E}(0)} \right|,$$

where E(t) is the energy at time t.

Our second result is a comparison of the relative energy error (EE(t)) as a function of CPU time of HO(6,13), HO(7,14) and AC(13) after a 1000 periods integration of a Hamiltonian system as in [16]. For this comparison, we used Kepler's two-body problem with eccentricities of 0.3, 0.5 and 0.7 and an interval of integration of $[0, 2000\pi]$.

Table 7 lists the relative energy error (EE) as a function of CPU time in seconds of HO(6,13), HO(7,14) and AC(13) after a 1000 periods integration of Kepler's two-body problem. It is seen, from Table 7, that HO(6,13) and HO(7,14) compare favorably with AC(13) at stringent tolerances.

Table 8 lists the CPU PEGs of HO(6,13) and HO(7,14) over AC(13) after a 1000 periods integration of Kepler's two-body problem with $e = 0.3$, $e = 0.5$ and $e = 0.7$ respectively. It is seen that HO(6,13) and HO(7,14) win on the basis of $\log_{10}$(EE) as a function of CPU time.

5.3. Error growth of HO(6,13), HO(7,14) and AC(13) on a 10000 periods integration of Kepler's two-body problem

In our last test, we compared the growth of relative energy error (EE(t)) on a 10000 periods integration of Kepler's two-body problem for different eccentricities.

Table 7: Relative energy error (EE) as a function of CPU time in seconds of HO(6,13), HO(7,14) and AC(13) after a 1000 periods integration of Kepler's two-body problems.

Kepler's two-body problem with $e = 0.3$				Kepler's two-body problem with $e = 0.5$			
	CPU in		CPU in		CPU in		CPU in
EE	HO(6,13)	HO(7,14)	AC(13)	EE	HO(6,13)	HO(7,14)	AC(13)
1.29e-04	3.62e-02	3.76e-02	3.82e-02	8.55e-03	5.30e-02	4.27e-02	4.80e-02
2.96e-06	4.40e-02	4.84e-02	5.30e-02	3.58e-04	6.64e-02	5.55e-02	6.36e-02
1.39e-08	5.14e-02	6.91e-02	8.44e-02	2.38e-05	7.96e-02	6.94e-02	8.09e-02
1.46e-09	6.66e-02	8.03e-02	1.03e-01	9.23e-07	9.26e-02	9.07e-02	1.08e-01
1.35e-10	7.46e-02	9.41e-02	1.26e-01	1.27e-08	1.06e-01	1.29e-01	1.58e-01
1.82e-11	8.24e-02	1.07e-01	1.50e-01	4.22e-09	1.19e-01	1.41e-01	1.74e-01
5.79e-12	1.06e-01	1.16e-01	1.66e-01	4.72e-10	1.34e-01	1.69e-01	2.12e-01
				6.65e-11	1.61e-01	1.99e-01	2.52e-01
				2.05e-12	2.05e-01	2.65e-01	3.44e-01

Problem: Kepler's two-body problem with $e = 0.7$			
	CPU in		CPU in
EE	HO(6,13)	HO(7,14)	AC(13)
2.97e-03	1.40e-01	1.20e-01	1.23e-01
1.60e-04	1.74e-01	1.49e-01	1.62e-01
1.28e-05	2.06e-01	1.80e-01	2.05e-01
4.03e-07	2.39e-01	2.32e-01	2.83e-01
4.87e-09	2.72e-01	3.23e-01	4.28e-01
1.09e-10	4.05e-01	3.85e-01	6.10e-01
2.78e-11	4.38e-01	4.74e-01	6.93e-01
1.89e-12	4.71e-01	5.79e-01	8.92e-01

Table 8: CPU PEG of HO(6,13) and HO(7,14) over AC(13) after a 1000 periods integration of Kepler's two-body problem with $e = 0.3$, $e = 0.5$ and $e = 0.7$ respectively.

	CPU PEG for two-body problem with:		
HO method	$e = 0.3$	$e = 0.5$	$e = 0.7$
HO(6,13)	44 %	37 %	37 %
HO(7,14)	24 %	23 %	32 %

Table 9: Values of C_1 and C_2 of power law $C_1 t^{C_2}$ fitted to the graphs of log(EE(t)) as a function of log(t) for a 10000 periods integration of Kepler's two-body problem with $e = 0.3$, $e = 0.5$ and $e = 0.7$ respectively.

	(C_1, C_2) of $C_1 t^{C_2}$ for two-body problem with:		
Method	$e = 0.3$	$e = 0.5$	$e = 0.7$
HO(6,13)	(4.48e-15, 1.047)	(3.48e-15, 1.043)	(1.53e-14, 0.990)
HO(7,14)	(1.25e-13, 0.926)	(1.25e-13, 0.887)	(4.89e-13, 0.862)
AC(13)	(4.25e-13, 0.980)	(2.81e-13, 0.982)	(4.22e-13, 1.011)

We compute the smoothed graphs of EE(t) for $e = 0.3$, $e = 0.5$ and $e = 0.7$ over an interval of 10000 periods. The smoothing removed the small amplitude high frequency oscillations in the original data and was done by using the MATLAB's `filter` command with the window size of 20. The initial stepsize was chosen so that HO(6,13), HO(7,14) and AC(13) used the same CPU time.

For $e = 0.3$, $e = 0.5$ and $e = 0.7$, the relative energy errors of HO(6,13) and HO(7,14) are less than the relative energy error of AC(13) across the interval of integration. These results are consistent with the CPU PEGs listed in Table 8 for two-body problem with $e = 0.3$, $e = 0.5$ and $e = 0.7$.

We use linear least-squares to fit the power law $C_1 t^{C_2}$ to the graphs of log(EE(t)) as a function of log(t):

$$\log(\mathrm{EE}(t)) = \log(C_1) + C_2 \log(t), \tag{25}$$

to obtain C_1 and C_2 shown in Table 9. It is seen, from Table 9, that HO(6,13) and HO(7,14) compare favorably with AC(13) on the basis of the growth of relative error of energy as a function of 10000 periods of integration. The values of C_2 of HO(7,14) and AC(13), listed in Table 9, are in good agreement with the expected asymptotic value of one for non-symplectic methods.

6. Conclusion

A family of optimal, contractivity-preserving (CP), explicit, d-derivative, 4-step Hermite–Obrechkoff series methods up to order $p = 20$, denoted by CP HO(d, p), with nonnegative coefficients were constructed for solving nonstiff first-order initial value problems $y' = f(t, y)$, $y(t_0) = y_0$. Given a number of derivatives d, HO(d, p) of highest order p uses less than 56% of the number of Taylor coefficients of Taylor methods of the same order. This result suggests that, for large d, these methods have order p large enough to take into account many problems where a very high precision of the solution is required, similar to Taylor series methods. The stability regions of HO(d, p) have generally a good shape and grow with decreasing $p - d$. The scaled stability intervals are often larger than those of multistep methods of the same order. Two selected CP HO methods: 6-derivative HO of order 13, denoted by HO(6,13), and 7-derivative HO of order 14, denoted by HO(7,14), use less CPU time than Adams–Bashforth–Moulton in PECE mode, denoted by ABM(13), in solving several problems often used to test higher-order ODE solvers. These two selected CP HO methods use less CPU time than Adams–Cowell of order 13 in PECE mode, denoted by AC(13), in solving Kepler orbit over an interval of 1000 periods. They also compare well with AC(13) in solving standard N-body problems over an interval of 10000 periods on the basis of the growth of relative error of energy and long intervals of integration.

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A. Coefficients of two selected methods: HO(6,13) and HO(7,14)

Table 10 of the appendix lists the two selected CP HO(d, p) methods: HO(6,13) and HO(7,14) with their $c(\text{HO}(d, p))$ and $x_{\min}$ (of the unscaled stability intervals $(x_{\min}, 0)$).

Table 10: $c(\mathrm{HO}(d,p))$, $x_{\min}$ and coefficients of the integration formulae of HO(6,13), HO(7,14).

d	6	7
coeffs\\p	13	14
$c(\mathrm{HO}(d,p))$	3.3025394065636432e-01	4.7268433700409124e-01
$x_{\min}$	-0.855	-1.22
γ_{00}	1.6052468542707576e-01	4.9432740404963976e-01
γ_{10}	4.1759122711146152e-02	1.0527345602885479e-01
γ_{20}	4.0693474508191280e-01	1.9089411194696357e-01
γ_{30}	3.9078144677986532e-01	2.0950502797454187e-01
γ_{01}	4.8606440579646210e-01	1.0457875697399324e+00
γ_{11}	1.2644549411931874e-01	2.2271407742445171e-01
γ_{21}	1.2321874018312966e+00	4.0385114759009105e-01
γ_{31}	1.1832756514674903e+00	4.4322396909193235e-01
γ_{02}	4.1638457012384050e-01	5.7741196630557468e-01
γ_{12}	5.4986045182230367e-02	2.3558436359032986e-01
γ_{22}	1.7845477404290651e+00	4.2718905194715134e-01
γ_{32}	1.7914633344204538e+00	2.4270532024358202e-01
γ_{03}	3.7865294247369558e-01	1.2139104439649467e-02
γ_{13}	1.9322178537733983e-01	0.0
γ_{23}	1.2408140024282908e+00	0.0
γ_{33}	1.8081675077669057e+00	2.7388248012249139e-01
γ_{04}	0.0	1.0827718623571250e-01
γ_{14}	0.0	8.7866391747489392e-02
γ_{24}	1.4253499250222528e+00	1.5932959223855614e-01
γ_{34}	4.5430958685346723e-01	1.7486317591809836e-01
γ_{05}	0.0	0.0
γ_{15}	0.0	3.4868906851863285e-03
γ_{25}	0.0	6.7414796626602450e-02
γ_{35}	3.7029795031462455e-02	3.8734303403132678e-02
γ_{06}	4.8539162580120768e-03	0.0
γ_{16}	0.0	0.0
γ_{26}	9.1603142928411638e-02	0.0
γ_{36}	0.0	3.0033072855333107e-03
γ_{07}		6.7870368979688195e-04
γ_{17}		0.0
γ_{27}		5.4332960764999893e-03
γ_{37}		0.0

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