ISSN 2286-4822
www.euacademic.org

EUROPEAN ACADEMIC RESEARCH
Vol. IV, Issue 3/ June 2016

Impact Factor: 3.4546 (UIF)
DRJI Value: 5.9 (B+)

Strong-stability-preserving Hermite – Birkhoff time discretization methods combining k-step methods and explicit s-stage Runge–Kutta methods of order 5

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Abstract:

New optimal strong-stability-preserving (SSP) Hermite–Birkhoff (HB) methods, $\mathrm{HB}(k,s,p)$ *of order* $p=5,6,\ldots,12$ *with nonnegative coefficients, are constructed by combining* k*-step methods of order* $(p-4)$ *and* s*-stage explicit Runge–Kutta methods of order 5 (RK5), where* $s=4,5,\ldots,10$. *These new methods preserve the monotonicity property of the solution, so they are suitable for solving ordinary differential equations (ODEs) coming from spatial discretization of hyperbolic partial differential equations (PDEs). The canonical Shu–*

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Osher form of the vector formulation of SSP RK methods is extended to SSP HB methods. The $\mathrm{HB}(k,s,p)$ *methods with largest effective SSP coefficient,* c_{eff}*, have been numerically found among the HB methods of order* p *on hand. These effective SSP coefficients are really good when compared to other well-known SSP methods such as Huang's hybrid methods (HM) and 2-step* s*-stage Runge–Kutta methods (TSRK). Their main features are summarized.*

Key words: Strong-stability-preserving, Hermite–Birkhoff method, SSP coefficient, Time discretization, Method of lines, Comparison with other SSP methods.

1. INTRODUCTION

In this paper, we shall concerned with the numerical solution of systems of N ordinary differential equations with initial conditions of the form:

$$\frac{dy}{dt} = f(t, y(t)), \qquad y(t_0) = y_0, \ (1)$$

where $y \in \mathbb{R}^N$ is the semi–discrete state and $f : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$ represents the discretization of the spatial variables forming a system of semi-discrete equations such that

$$\left\|y(t + \Delta t)\right\| \le \left\|y(t)\right\|, \ (2)$$

where $\|.\|$ is a norm, a semi-norm, or more generally, any convex functional.

It is also assumed that f satisfies a discrete analog of inequality (2),

$$\left\|y_n + \Delta t f(t_n, y_n)\right\| \le \left\|y_n\right\|, \ (3)$$

for a sufficiently small time step $0 < \Delta t \le \Delta t_{\mathrm{FE}}$ and all y_n where Δt_{FE} is a maximal step size for which (3) holds. Here y_n is a numerical approximation of $y(t_0 + n\Delta t)$. We are now interested in higher-order, explicit, multistep Hermite–Birkhoff methods that preserve the strong stability property [3], also called monotonicity property [8],

$$\|y_n\| \le \max_{1\le j\le k}\|y_{n-j}\|, \quad (4)$$

for $0 \le \Delta t \le \Delta t_{\max} = c\Delta t_{\mathrm{FE}}$ whenever the forward Euler (FE) condition (3) holds. The positive integer k represents the number of previous steps used to compute the numerical solution at the next step. The number c is called the strong-stability-preserving coefficient, which depends on the numerical integration method. Respectable efforts have been devoted to find numerical methods with highest c.

A multistage method is said to be SSP method if it satisfies SSP property. These methods have been developed to satisfy the SSP property (4) for system (1) whenever the FE condition (3) is fulfilled. The SSP property (4) is desirable in that it mimics property (2) of the true solution and prevents error growth and it is guaranteed under the maximum time step $\Delta t_{\max} = c\Delta t_{\mathrm{FE}}$.

Such SSP results are mainly applied for time integration of nonlinear hyperbolic PDEs, in particular, of conservation laws, an instance of which is the one-dimensional equation

$$y_t + g(y)_x = 0, \quad y(x,0) = y_0(x), \quad (5)$$

where the spatial derivative $g(y)_x$ is approximated by a conservative finite difference or finite element at x_j, $j = 1,2,\ldots,N$ (see, for example, [6,14,18,1]). This spatial semi–discretization will lead to system (1) of ODEs.

In our research, to solve system (1), we construct new explicit, SSP, k-step, s-stage, Hermite–Birkhoff methods of order p, $\mathrm{HB}(k,s,p)$ with nonnegative coefficients as combinations of linear k-step methods of order $p-4$ and s-stage RK methods of order 5.

These new methods involve HB interpolation polynomials. Furthermore, these methods are all SSP because they can be decomposed in terms of SSP FE methods by convexity and by using extension of the Shu–Osher representation RK methods to our methods. Therefore, the obtained high–order SSP HB time discretizations will maintain the SSP property (4), perhaps with an SSP coefficient, $c(\mathrm{HB}(k,s,p))$:

$$\Delta t \le c(\mathrm{HB}(k,s,p))\Delta t_{\mathrm{FE}}. \quad (6)$$

The new $\mathrm{HB}(k,s,p)$ have larger effective SSP coefficients than Huang's [7] SSP hybrid methods ($\mathrm{HM}(k,p)$) with the same k and p, especially when k is small. These new methods have far larger effective SSP coefficients than SSP TSRK methods when $k \ge 3$. In particular, no counterparts of $\mathrm{HB}(k,s,p)$ for $p = 9,10,11,12$ have been found in the literature among hybrid and general linear multistep methods.

Section 2 introduces the notation and general formulae of k-step, s-stage $\mathrm{HB}(k,s,p)$ methods of order p. Order conditions are listed in Section 3. Section 4 presents the canonical Shu-Osher form of $\mathrm{HB}(k,s,p)$ by means of the vector notation and formulates the optimization problem. Comparing effective SSP coefficients of $\mathrm{HB}(k,s,p)$ methods to $\mathrm{HM}(k,p)$ and $\mathrm{TSRK}(s,p)$ methods is displayed in Section 5.

2. k- STEP, s-STAGE $\mathrm{HB}(k,s,p)$ OF ORDER p

Throughout this paper, the following notation will be used:

Notation 1.

- k, s, p denote the number of steps, the number of stages and the order of a given method.

- HB(k,s,p): k-step, s-stage Hermite-Birkhoff method of order p.
- HM(k,p): k-step hybrid method of order p.
- RK(s,p): s-stage Runge-Kutta method of order p.
- TSRK(s,p): 2-step, s-stage Runge-Kutta method of order p.

All methods considered in this paper are SSP unless specified otherwise, so the denomination "SSP" will often be omitted in what follows.

Notation 2.

- The abscissa vector $s = [c_1, c_2, ..., c_s]^T$, $0 \le c_j \le 1$ defines the off-step points $t_n + c_j \Delta t, j = 1,2,...,s$. In all cases, $c_1 = 0$ and $c_1^0 = 1$ by convention.
- At each off-step point, let $F_j := f(t_n + c_j \Delta t, Y_j)$ be the jth-stage derivative where Y_j is the jth -stage value and set $Y_1 = y_n$.

To perform integration from t_n to t_{n+1}, an s-stage Hermite–Birkhoff method is defined by the following s formulae:

$(s-1)$ HB polynomials of degree $(2k+i-3)$ are used as predictors to obtain the stage values Y_i

$$Y_i = v_{B,i} y_n + \sum_{j=1}^{k-1} A_{B,ij} y_{n-j} + \Delta t \Big[\sum_{j=1}^{i-1} a_{ij} F_j + \sum_{j=1}^{k-1} B_{B,ij} f_{n-j} \Big], \qquad i = 2,3,\ldots,s, \quad (7)$$

and an HB polynomial of degree $(2k+s-2)$ is used as an integration formula to obtain y_{n+1} to order p,

$$y_{n+1} = v_{B,s+1} y_n + \sum_{j=1}^{k-1} A_{B,s+1,j} y_{n-j} + \Delta t \Big[\sum_{j=1}^{s} b_j F_j + \sum_{j=1}^{k-1} B_{B,s+1,j} f_{n-j} \Big]. \quad (8)$$

Here $v_{B,i}, A_{B,ij}, B_{B,ij}, a_{ij}$ and b_j for $i = 2,3,\ldots,s+1$ and $j = 1,2,\ldots,k-1$ are the constant coefficients that we can construct to obtain a good approximation, y_{n+1}, to the solution $y(t_{n+1}) = y(t_n + \Delta t)$.

The subscript B refers to the Butcher form, as opposed to the subscript SO and (SO,r), used later for Shu–Osher form and canonical Shu–Osher form, respectively.

3. ORDER CONDITIONS FOR $\mathrm{HB}(k,s,p)$

For the construction of the order conditions of s-stage $\mathrm{HB}(k,s,p)$, we have the conditions coming from the backsteps of the methods:

$$B_i(j) = \sum_{\ell=1}^{k-1} A_{B,i\ell} \frac{(-\ell)^j}{j!} + \sum_{\ell=1}^{k-1} B_{B,i\ell} \frac{(-\ell)^{j-1}}{(j-1)!}, \qquad \begin{cases} i = 2,3,\ldots,s, \\ j = 1,2,\ldots,p. \end{cases} \quad (9)$$

Matching expansion of the numerical solution from formulae (7)–(8) with Taylor expansion of the true solution, we obtain multistep and RK–type order conditions that must be satisfied by $\mathrm{HB}(k,s,p)$ methods.

First we have the consistency conditions of $\mathrm{HB}(k,s,p)$ methods:

$$v_{B,i} + \sum_{j=1}^{k-1} A_{B,ij} = 1, \qquad i = 2,3,\ldots,s+1. \quad (10)$$

Next we impose the following $(p-4)$ simplifying assumptions on the abscissa vector $s=[c_1,c_2,\ldots,c_s]^T$ (see [10]):

$$\sum_{j=1}^{i-1} a_{ij}c_j^m + m!B_i(m+1) = \frac{1}{m+1}c_i^{m+1}, \qquad \begin{cases} i=2,3,\ldots,s, \\ m=0,1,\ldots,p-4. \end{cases} \qquad (11)$$

Conditions (11) will help reduce the large number of RK–type order conditions to 12 conditions for the case $p>5$:

$$\sum_{i=1}^{s} b_i c_i^m + m!B(m+1) = \frac{1}{m+1}, \qquad m=0,1,\ldots,p-1, \quad (12)$$

$$\sum_{i=2}^{s} b_i\Big[\sum_{j=1}^{i-1} a_{ij}\frac{c_j^{p-4}}{(p-4)!} + B_i(p-3)\Big] + B(p-2) = \frac{1}{(p-2)!}, \quad (13)$$

$$\sum_{i=2}^{s} b_i \frac{c_i}{p-2}\Big[\sum_{j=1}^{i-1} a_{ij}\frac{c_j^{p-4}}{(p-4)!} + B_i(p-3)\Big] + B(p-1) = \frac{1}{(p-1)!}, \quad (14)$$

$$\sum_{i=2}^{s} b_i\Big[\sum_{j=1}^{i-1} a_{ij}\frac{c_j^{p-3}}{(p-3)!} + B_i(p-2)\Big] + B(p-1) = \frac{1}{(p-1)!}, \quad (15)$$

$$\sum_{i=2}^{s} b_i\Big[\sum_{j=1}^{i-1} a_{ij}\Big[\sum_{k=1}^{j-1} a_{jk}\frac{c_k^{p-4}}{(p-4)!} + B_j(p-3)\Big] + B_i(p-2)\Big] + B(p-1) = \frac{1}{(p-1)!}, \quad (16)$$

$$\sum_{i=2}^{s} b_i \frac{c_i^2}{(p-2)(p-1)}\Big[\sum_{j=1}^{i-1} a_{ij}\frac{c_j^{p-4}}{(p-4)!} + B_i(p-3)\Big] + B(p) = \frac{1}{p!}, \quad (17)$$

$$\sum_{i=2}^{s} b_i \frac{c_i}{p-1}\Big[\sum_{j=1}^{i-1} a_{ij}\frac{c_j^{p-3}}{(p-3)!} + B_i(p-2)\Big] + B(p) = \frac{1}{p!}, \quad (18)$$

$$\sum_{i=2}^{s} b_i \frac{c_i}{p-1}\Big[\sum_{j=1}^{i-1} a_{ij}\Big[\sum_{k=1}^{j-1} a_{jk}\frac{c_k^{p-4}}{(p-4)!} + B_j(p-3)\Big] + B_i(p-2)\Big] + B(p) = \frac{1}{p!}, \quad (19)$$

$$\sum_{i=2}^{s} b_i\Big[\sum_{j=1}^{i-1} a_{ij}\frac{c_j^{p-2}}{(p-2)!} + B_i(p-1)\Big] + B(p) = \frac{1}{p!}, \quad (20)$$

$$\sum_{i=2}^{s} b_i\Big[\sum_{j=1}^{i-1} a_{ij}\frac{c_j}{p-2}\Big[\sum_{k=1}^{j-1} a_{jk}\frac{c_k^{p-4}}{(p-4)!} + B_j(p-3)\Big] + B_i(p-1)\Big] + B(p) = \frac{1}{p!}, \quad (21)$$

$$\sum_{i=2}^{s} b_i \Big[\sum_{j=1}^{i-1} a_{ij} \Big[\sum_{k=1}^{j-1} a_{jk} \frac{c_k^{p-3}}{(p-3)!} + B_j(p-2)\Big] + B_i(p-1)\Big] + B(p) = \frac{1}{p!}, \quad (22)$$

$$\sum_{i=2}^{s} b_i \Big\{\sum_{j=1}^{i-1} a_{ij} \Big[\sum_{k=1}^{j-1} a_{jk} \Big(\sum_{\ell=1}^{k-1} a_{k\ell} \frac{c_\ell^{p-4}}{(p-4)!} + B_k(p-3)\Big) + B_j(p-2)\Big] + B_i(p-1)\Big\} + B(p) = \frac{1}{p!}, \quad (23)$$

where the backstep parts, $B(j)$, are defined

$$B(j) = \sum_{i=1}^{k-1} A_{B,s+1,i} \frac{(-i)^j}{j!} + \sum_{i=1}^{k-1} B_{B,s+1,i} \frac{(-i)^{j-1}}{(j-1)!}, \qquad j = 1, \ldots, p+1. \quad (24)$$

In the case $p = 5$, $\mathrm{HB}(k,s,5)$ has to satisfy the following additional condition:

$$\sum_{i=2}^{s} \frac{b_i}{6} \Big[\sum_{j=1}^{i-1} a_{ij} c_j + B_i(2)\Big]^2 + B(5) = \frac{1}{5!}. \quad (25)$$

4. CANONICAL SHU – OSHER FORM AND OPTIMIZATION PROBLEM

As done in [13], (7)–(8) can be rewritten in modified Butcher form and Shu– Osher representation. Furthermore, Gottlieb, Ketcheson and Shu presented a more compact notation and the canonical Shu–Osher form for Runge–Kutta methods [5]. Following these results, we extended the canonical Shu–Osher form for our $\mathrm{HB}(k,s,p)$ methods.

The modified Shu–Osher form generalized from the Shu–Osher form of RK can be used to represent explicit HB methods (see more in [12]):

$$Y_i = \left(v_i y_n + \Delta t w_i f_n\right) + \sum_{j=1}^{k-1}\left[A_{ij} y_{n-j} + \Delta t B_{ij} f_{n-j}\right] + \sum_{j=2}^{i-1}\left[\alpha_{ij} Y_j + \Delta t \beta_{ij} F_j\right], \quad i = 2, 3, \ldots, s+1, \quad (26)$$

$$y_{n+1} = Y_{s+1}.$$

and the consistency condition now becomes

$$v_i + \sum_{j=1}^{k-1} A_{ij} + \sum_{j=2}^{i-1} \alpha_{ij} = 1, \qquad i = 2, 3, \ldots, s+1. \quad (27)$$

We can rearrange (28) as follows

$$Y_i = \left[v_i \left(y_n + \Delta t \frac{w_i}{v_i} f_n \right) \right] + \left[\sum_{j=0}^{k-1} A_{ij} \left(y_{n-j} + \Delta t \frac{B_{ij}}{A_{ij}} f_{n-j} \right) \right] + \left[\sum_{j=2}^{i-1} \alpha_{ij} \left(Y_j + \Delta t \frac{\beta_{ij}}{\alpha_{ij}} F_j \right) \right], \; i = 2,3,\ldots,s+1. \quad (28)$$

Clearly, (28) is the convex combination of forward Euler condition (3), with the step sizes $\frac{w_i}{v_i}\Delta t$, $\frac{B_{ij}}{A_{ij}}\Delta t$ and $\frac{\beta_{ij}}{\alpha_{ij}}\Delta t$ whenever $v_i, w_i, A_{ij}, B_{ij}, \alpha_{ij}, \beta_{ij} \geq 0$.

4.1 Vector notation

Now we define the vectors and matrices as follows [12]:

- $\mathbf{v}, \mathbf{w} \in \mathbb{R}^{s+1}$ have the form $\mathbf{v} = [0, v_2, v_3, \ldots, v_{s+1}]^T, \mathbf{w} = [0, w_2, w_3, \ldots, w_{s+1}]^T$.
- Two strictly lower triangular matrices $\alpha = (\alpha_{ij}),\ \beta = (\beta_{ij}) \in \mathbb{R}^{(s+1)\times(s+1)}$.
- Two $(s+1)\times(k-1)$ rectangular matrices $\mathbf{A}_{\mathrm{SO}} = (A_{ij})$ and $\mathbf{B}_{\mathrm{SO}} = (B_{ij})$ with zero first row.
- The matrices, $\mathbf{Y}, \mathbf{F} \in \mathbb{R}^{(s+1)\times N}$, $\mathbf{y}_{\mathrm{back}} \in \mathbb{R}^{(k-1)\times N}$ and $\mathbf{f}_{\mathrm{back}} \in \mathbb{R}^{(k-1)\times N}$ have the form: $\mathbf{Y} = [0, Y_2, \ldots, Y_{s+1}]^T$, $\mathbf{F} = [0, F_2, \ldots, F_{s+1}]^T$, $\mathbf{y}_{\mathrm{back}} = [y_{n-1}, y_{n-2}, \ldots, y_{n-(k-1)}]^T$, $\mathbf{f}_{\mathrm{back}} = [f_{n-1}, f_{n-2}, \ldots, f_{n-(k-1)}]^T$, with the following N-vectors: Y_j, F_j for $j = 1,2,\ldots,s+1$, y_j, f_j for $j = n-(k-1),\ldots,n$, $Y_1 = y_n$, $F_1 = f_n$, $Y_{s+1} = y_{n+1}$ and $F_{s+1} = f_{n+1}$.

Then, the modified Shu–Osher form of HB formulae can be rewritten compactly in vector notation:

$$\mathbf{Y} = \mathbf{v} y_n^T + \alpha \mathbf{Y} + \mathbf{A}_{\mathrm{SO}} \mathbf{y}_{\mathrm{back}} + \Delta t \left(\mathbf{w} f_n^T + \beta \mathbf{F} + \mathbf{B}_{\mathrm{SO}} \mathbf{f}_{\mathrm{back}} \right), \quad (29)$$
$$y_{n+1} = Y_{s+1}.$$

and the consistency condition (27) becomes

$$\mathbf{v} + \alpha \mathbf{e}_{s+1} + \mathbf{A}_{\mathrm{SO}} \mathbf{e}_{\mathrm{back}} = \mathbf{e}_{s+1}, \quad (30)$$

where $\mathbf{e}_{s+1} = [0,1,1,\ldots,1]^T \in \mathbb{R}^{(s+1)}$ and $\mathbf{e}_{\mathrm{back}} = [1,1,\ldots,1]^T \in \mathbb{R}^{(k-1)}$, respectively.

Also, the modified Butcher form of $\mathrm{HB}(k,s,p)$ is:

$$\mathbf{Y} = \mathbf{v}_{\mathrm{B}} y_n^T + \mathbf{A}_{\mathrm{B}} \mathbf{y}_{\mathrm{back}} + \Delta t \left(\mathbf{w}_{\mathrm{B}} f_n^T + \beta_{\mathrm{B}} \mathbf{F} + \mathbf{B}_{\mathrm{B}} \mathbf{f}_{\mathrm{back}} \right), \quad y_{n+1} = Y_{s+1}, \quad (31)$$

here the relations between Shu–Osher coefficients and Butcher coefficients are:

$$\mathbf{v}_{\mathrm{B}} = \left(\mathbf{I} - \alpha\right)^{-1} \mathbf{v}, \; \mathbf{w}_{\mathrm{B}} = \left(\mathbf{I} - \alpha\right)^{-1} \mathbf{w}, \; \mathbf{A}_{\mathrm{B}} = \left(\mathbf{I} - \alpha\right)^{-1} \mathbf{A}_{\mathrm{SO}},$$

$$\beta_{\mathrm{B}} = \left(\mathbf{I} - \alpha\right)^{-1} \beta, \quad \mathbf{B}_{\mathrm{B}} = \left(\mathbf{I} - \alpha\right)^{-1} \mathbf{B}_{\mathrm{SO}},$$

and the consistency condition: $\mathbf{v}_{\mathrm{B}} + \mathbf{A}_{\mathrm{B}} \mathbf{e}_{\mathrm{back}} = \mathbf{e}_{s+1}$.

4.2. Canonical Shu – Osher form in vector notation

It is useful to find the SSP coefficient of an HB method under a particular Shu–Osher form of the matrices α and β by assuming the ratio $r = \dfrac{\alpha_{ij}}{\beta_{ij}}$ for every i, j, $i = 2,3,\ldots,s+1$ and $j = 1,2,\ldots,i-1$ such that $\beta_{ij} \neq 0$. In vector notation, we can rewrite: $\alpha_r = r\beta_r$.

Then the canonical Shu – Osher form of $\mathrm{HB}(k,s,p)$ is defined as follows:

$$\mathbf{Y} = \left(\mathbf{v}_r y_n^T + \Delta t \mathbf{w}_r f_n^T \right) + \left(\alpha_r \mathbf{Y} + \Delta t \beta_r \mathbf{F} \right) + \left(\mathbf{A}_{\mathrm{SO},r} \mathbf{y}_{\mathrm{back}} + \Delta t \mathbf{B}_{\mathrm{SO},r} \mathbf{f}_{\mathrm{back}} \right), \quad (32)$$

where all the coefficients are determined by relations:

$$\mathbf{v}_r = \left(\mathbf{I} - \alpha_r\right) \mathbf{v}_{\mathrm{B}} = \left(\mathbf{I} + r\beta_{\mathrm{B}}\right)^{-1} \mathbf{v}_{\mathrm{B}}, \quad (33)$$

$$\mathbf{w}_r = \left(\mathbf{I} - \alpha_r\right) \mathbf{w}_{\mathrm{B}} = \left(\mathbf{I} + r\beta_{\mathrm{B}}\right)^{-1} \mathbf{w}_{\mathrm{B}}, \quad (34)$$

$$\beta_r = \beta_{\mathrm{B}}\left(\mathbf{I} - \alpha_r\right) = \left(\mathbf{I} + r\beta_{\mathrm{B}}\right)^{-1}\beta_{\mathrm{B}}, \quad (35)$$

$$\alpha_r = r\beta_{\mathrm{B}}\left(\mathbf{I} - \alpha_r\right) = r\left(\mathbf{I} + r\beta_{\mathrm{B}}\right)^{-1}\beta_{\mathrm{B}}, \quad (36)$$

$$\mathbf{A}_{\mathrm{SO},r} = \left(\mathbf{I} - \alpha_r\right)\mathbf{A}_{\mathrm{B}} = \left(\mathbf{I} + r\beta_{\mathrm{B}}\right)^{-1}\mathbf{A}_{\mathrm{B}}, \quad (37)$$

$$\mathbf{B}_{\mathrm{SO},r} = \left(\mathbf{I} - \alpha_r\right)\mathbf{B}_{\mathrm{B}} = \left(\mathbf{I} + r\beta_{\mathrm{B}}\right)^{-1}\mathbf{B}_{\mathrm{B}}, \quad (38)$$

with the consistency condition: $\mathbf{v}_r + \alpha_r \mathbf{e}_{s+1} + \mathbf{A}_{\mathrm{SO,r}}\mathbf{e}_{\mathrm{back}} = \mathbf{e}_{s+1}$. (39)

The ratio $r = \dfrac{\alpha_{ij}}{\beta_{ij}}$ for $i = 3,4,\ldots,s+1$ and $j = 2,3,\ldots,i-1$, becomes a feasible SSP coefficient of $\mathrm{HB}(k,s,p)$. Hence, this ratio r must satisfy two additional sets of conditions:

$$r \le \frac{v_i}{w_i}, \quad i = 2,3,\ldots,s+1,$$

and
$$r \leq \frac{A_{ij}}{B_{ij}}, \quad \begin{cases} j = 1,2,\ldots,k-1, \\ i = 2,3,\ldots,s+1. \end{cases}$$

Therefore, we have an extended result, which is slightly modification of the result presented in [11,12].

Theorem 1. ([10,11,12]) If f satisfies the forward Euler condition (3), then k -step, s-stage $\mathrm{HB}(k,s,p)$ (32) satisfies the strong–stability–preserving property

$$\left\|y_n\right\| \le \max_{1\le j\le k}\left\|y_{n-j}\right\|$$

provided $\Delta t \leq c(\mathbf{v}_r,\mathbf{w}_r,\alpha_r,\beta_r,\mathbf{A}_{\mathrm{SO,r}},\mathbf{B}_{\mathrm{SO,r}})\Delta t_{\mathrm{FE}}$,

where $c(\mathbf{v}_r,\mathbf{w}_r,\alpha_r,\beta_r,\mathbf{A}_{\mathrm{SO,r}},\mathbf{B}_{\mathrm{SO,r}})$ is equal to

$$r = \left\{\frac{\alpha_{ij}}{\beta_{ij}}\right\}, \quad \begin{cases} i = 3,4,\ldots,s+1, \\ j = 2,3,\ldots,i-1, \end{cases} \quad (40)$$

and less than or equal to

$$\min_{i=2,3,\ldots,s+1} \frac{v_i}{w_i}, \ (41)$$

$$\min_{j=1,2,\ldots,k-1} \left\{ \frac{A_{ij}}{B_{ij}} \right\}, \quad i = 2,3,\ldots,s+1, \ (42)$$

with the convention that $\alpha / 0 = +\infty$, under the assumption that all coefficients of (32) are nonnegative.

4.3. Optimization problem to obtain $c(\mathrm{HB}(k,s,p))$

To obtain optimal $\mathrm{HB}(k,s,p)$ and highest $c(\mathrm{HB}(k,s,p))$ canonical form, by above theorem, we maximize

$$\max_{\mathbf{v}_r,\mathbf{w}_r,\alpha_r,\beta_r,\mathbf{A}_{\mathrm{SO},\mathbf{r}},\mathbf{B}_{\mathrm{SO},\mathbf{r}}} = c(\mathbf{v}_r,\mathbf{w}_r,\alpha_r,\beta_r,\mathbf{A}_{\mathrm{SO},\mathbf{r}},\mathbf{B}_{\mathrm{SO},\mathbf{r}}) = c(\mathrm{HB}(k,s,p)).$$

In the optimization formulation with any feasible initial data, the ratio r becomes the variable r which satisfies the equation in three variables α_{ij}, r, β_{ij},

$$\alpha_{ij} - r\beta_{ij} = 0, \ i = 3,4,\ldots,s+1, \ j = 2,3,\ldots,i-1,$$

together with the two conditions (41) and (42).
So the problem of optimizing the canonical $\mathrm{HB}(k,s,p)$ can be formulated as

$$c(\mathrm{HB}(k,s,p)) = \max_{\mathbf{v}_\mathrm{B},\mathbf{w}_\mathrm{B},\beta_\mathrm{B},\mathbf{A}_\mathrm{B},\mathbf{B}_\mathrm{B}} = r, \ (43)$$

subject to the component – wise inequalities

$$\left(\mathbf{I} + r\beta_\mathrm{B}\right)^{-1} \mathbf{v}_\mathrm{B} \geq 0, \ (44)$$

$$\left(\mathbf{I} + r\beta_\mathrm{B}\right)^{-1} \mathbf{w}_\mathrm{B} \geq 0, \ (45)$$

$$\beta_\mathrm{B}\left(\mathbf{I} + r\beta_\mathrm{B}\right)^{-1} \geq 0, \ (46)$$

$$\left(\mathbf{I} + r\beta_\mathrm{B}\right)^{-1} \mathbf{A}_\mathrm{B} \geq 0, \ (47)$$

$$\left(\mathbf{I}+rb_{\mathrm{B}}\right)^{-1}\mathbf{B}_{\mathrm{B}} \geq 0, \quad (48)$$

$$\left(\mathbf{I}+rb_{\mathrm{B}}\right)^{-1}\left(-\mathbf{v}_{\mathrm{B}}+r\mathbf{w}_{\mathrm{B}}\right) \leq 0, \quad (49)$$

$$\left(\mathbf{I}+rb_{\mathrm{B}}\right)^{-1}\left(-\mathbf{A}_{\mathrm{B}}+r\mathbf{B}_{\mathrm{B}}\right) \leq 0, \quad (50)$$

$$rb_{\mathrm{B}}\left(\mathbf{I}+rb_{\mathrm{B}}\right)^{-1}\mathbf{e}_{s+1}+\left(\mathbf{I}+rb_{\mathrm{B}}\right)^{-1}\mathbf{A}_{\mathrm{B}}\mathbf{e}_{\mathrm{back}} \leq \mathbf{e}_{s+1}, \quad (51)$$

together with the set of order conditions (12)–(25).

5. COMPARING EFFECTIVE SSP COEFFICIENTS OF THE METHODS ON HAND

Since HB(k,s,p) methods contain many free parameters when k is sufficiently large, the optimization formulation, implemented by fmincon in the MATLAB Optimization Toolbox, was used to search for the methods with largest $c(\mathrm{HB}(k,s,p))$ for different values of k. In this work, the MATLAB Optimization Toolbox was used to tolerance 10^{-12} on the objective function $c(\mathrm{HB}(k,s,p))$ provided all the constraints were satisfied to tolerance 10^{-14}.

Gottlieb [2] showed that computational cost and orders also take into account when searching for high-order SSP methods with c as large as possible. Therefore, the effective coefficients c_{eff} provide a fair comparison between methods of the same order.

Definition 1. [15] The effective SSP coefficient of an SSP method M is denoted by

$$c_{\mathrm{eff}}(M)=\frac{c(M)}{\ell}, \quad (52)$$

where ℓ is the number of function evaluations of M per time step and $c(M)$ is the SSP coefficient of M.

For instance, $\ell = s$ for $\mathrm{HB}(k,s,p)$ or $\mathrm{RK}(s,p)$ methods and $\ell = 2$ for $\mathrm{HM}(k,p)$. By definition, $c_{\mathrm{eff}}(\mathrm{FE}) = 1$.

Definition 2. [17] The percentage efficiency gain (PEG) of the effective SSP coefficients $c_{\mathrm{eff}}(\mathrm{M2})$ of method 2 over $c_{\mathrm{eff}}(\mathrm{M1})$ of method 1 is evaluated by

$$\mathrm{PEG}(c_{\mathrm{eff}}(\mathrm{M2}),c_{\mathrm{eff}}(\mathrm{M1}))=\frac{c_{\mathrm{eff}}(\mathrm{M2}) - c_{\mathrm{eff}}(\mathrm{M1})}{c_{\mathrm{eff}}(\mathrm{M1})}. \quad (53)$$

In Tables 1–8, for each stage value s, the row–wise maxima, $\max_k c_{\mathrm{eff}}(\mathrm{HB}(k,s,p))$ are listed with an asterisk. The largest c_{eff} for each order p is in boldface. This data is summarized in Table 9 and Fig.2.

It is noted that, in Table 1–8, for a given k, $c_{\mathrm{eff}}(\mathrm{HB}(k,s,p))$ first increases with s and then decreases. On the other hand, for a given s, $c_{\mathrm{eff}}(\mathrm{HB}(k,s,p))$, first increases with k and then stabilizes. Therefore, empty entries in the tables correspond either to existing methods with a smaller c_{eff}.

5.1 Fifth – order method

Ruuth and Spiteri [16] showed that there are no fifth – order SSP RK methods with nonnegative coefficients. However, in [15], they found fifth – order $\mathrm{RK}(s,5)$, $s = 7,8,9,10$ methods with negative coefficients. Among them, $\mathrm{RK}(10,5)$ is the best method with $c_{\mathrm{eff}}(\mathrm{RK}(10,5)) = 0.339$.

In our work, optimal canonical $\mathrm{HB}(k,s,5)$ with stage number $s = 4,5,\ldots,10$ are found and their c_{eff} are listed in Table

1 with the largest $c_{\text{eff}}(\text{HB}(2,8,5)) = 0.447$. Comparing with RK(10,5), our method is much better with PEG(c_{eff}(HB(2,8,5),c_{eff}(RK(10,5)))=32% (by (53)) and it has the same c_{eff} with TSRK(8,5).

The best HM method is HM(7,5) with c_{eff}(HM(7,5))=0.373. Even with the lowest step number $k = 3$, our method is better than the best HM method, that is c_{eff}(HB(3,4,5))=0.341 > c_{eff}(HM(7,5))=0.373 (by (53)).

Except for c_{eff}(HB(2,4,5)), our methods are better than or equal to c_{eff}(TSRK(s,5)) of the same order.

			HM(4,5) 0.185	HM(5,5) 0.262	HM(6,5) 0.328	HM(7,5) 0.373	
$s \setminus k$	2	3	4	5	6	7	TSRK(s,5)
4	0.213	0.341	0.384	0.390	*0.392	0.392	0.214
5	0.328	0.364	0.400	*0.405	0.405		0.324
6	0.385	*0.404	0.404				0.385
7	0.418	*0.426	0.426				0.418
8	**0.447**	0.447	0.447				0.447
9	*0.438	0.438	0.438				0.438
10	*0.425	0.425	0.425				0.425

Table 1: c_{eff}(HB(k,s,5)) as function of k and s

5.2 Sixth – order method

Table 2 shows c_{eff} of HB as well as c_{eff} of HM [7] and TSRK [4] methods of order 6.

We see that two-step s-stage HB(2,s,6) have c_{eff} similar to c_{eff} of TSRK(2,s,6). But if we further increase the step number k, we can find HB(k,s,6) with considerably larger SSP coefficients.

Besides, it is not mentioned in [9] that 4-stage and 5-stage TSRK methods of order 6 exist. We found 3-step, 4-stage HB(3,4,6) with good c_{eff}(HB(3,4,6))=0.179.

				HM(5,6) 0.104	HM(6,6) 0.181	HM(7,6) 0.220	
$s\setminus k$	2	3	4	5	6	7	TSRK$(s,6)$
4		0.179	0.272	0.316	0.330	*0.339	
5		0.272	0.327	0.342	0.344	*0.345	
6		0.323	0.336	0.345	*0.349	0.349	0.099
7	0.182	0.341	0.349	*0.351	0.351	0.351	0.182
8	0.241	0.328	0.341	0.345	*0.347		0.242
9	0.287	0.334	0.343	*0.345			0.287
10	0.318	0.338	0.347	0.353	**0.355**		0.320

Table 2: $c_{\text{eff}}(\text{HB}(k,s,6))$ as function of k and s

Comparing with hybrid methods, we remark that HB$(k,4,6)$ with $k>4$ are competitive with Huang's best 7-step HM(7,6) of order 6. For instance, $c_{\text{eff}}(\text{HB}(4,4,6))=0.272 > c_{\text{eff}}(\text{HM}(7,6))=0.220$. Substantially, for the same step number $k=5$, HB(5,7,6) has really better c_{eff} than HM(5,6) with PEG$(c_{\text{eff}}(\text{HB}(5,7,6)),c_{\text{eff}}(\text{HM}(5,6)))=238\%$ (by (53)).

Table 2 also gives a new phenomenon, that is c_{eff} increases again when $s>8$ after it has decreased for $k=3,4,5,6$

5.3 Seventh – order methods

Table 3 lists c_{eff} of HB methods of order 7 together with HM(7,7) and TSRK of the same order.

$s\setminus k$	2	3	4	5	6	7	TSRK$(s,7)$	HM(7,7)
4			0.141	0.219	0.256	*0.287		0.117
5		0.173	0.239	0.282	0.293	*0.296		"
6		0.232	0.290	0.301	**0.305**	0.305		"
7		0.231	0.286	0.292	*0.293	0.293		"
8	0.040	0.248	0.284	0.285	0.286	*0.287	0.071	"
9	0.113	0.250	0.280	*0.290	0.290		0.124	"
10	0.161	0.277	*0.283	0.283	0.283		0.179	"

Table 3: $c_{\text{eff}}(\text{HB}(k,s,7))$ as function of k and s

The SSP coefficients of HB$(2,s,7)$ are slightly lower than those of TSRK$(s,7)$ as seen in the second and eighth columns.

Nevertheless, increasing the step number to $k = 3,4,...,7$, we found $\text{HB}(k,s,7)$, $s = 4,5,...,10$, with larger effective SSP coefficients. For example, the best optimal method of order 7 is the 6-step, 6-stage HB(6,6,7) with $c_{\text{eff}}(\text{HB}(6,6,7)) = 0.305$. Ketcheson, Gotlieb and Macdonald [4] found a two-step, 8-stage RK method of order 7 with c_{eff}(TSRK(8,7))=0.071 with the best c_{eff}(TSRK(12,7))=0.231. However, they did not mention that with lower stage number $s < 8$, two-step, s-stage TSRK methods of order 7 exist. Our investigation for HB methods shows that HB methods of order 7 with only 4 stages exist. Despite their low stage number, HB methods of order 7 are competitive with the best two-step RK of order 7. For example, HB(7,4,7) has $c_{\text{eff}}(\text{HB}(7,4,7)) = 0.287$, larger than c_{eff}(TSRK(12,7))=0.231 of the best 12-stage method TSRK(12,7).

Compared with hybrid methods, despite the lower step number, $k = 4$ our optimal $\text{HB}(4,s,7)$ are competitive with the 7-step HM(7,7), the best hybrid method at present. Additionally, the PEG between our best method with HM(7,8) is nonnegligible with PEG(c_{eff}(HB(6,6,7),c_{eff}(HM(7,7)))=161% (by (53)).

Except for HB(2,8,7) and HB(2,9,7), all our HB methods have better c_{eff} than HM(7,7).

5.3 Eighth-order methods

The c_{eff} of optimal $\text{HB}(k,s,8)$ with stage number $s = 4,5,...,10$ and 3,4,...8 are presented in Table 4 with largest $c_{\text{eff}}(\text{HB}(8,6,8)) = 0.261$. Ketcheson, Gottlieb, Macdonald and Shu found c_{eff} of 11- and 12-stage TSRK ([9,4]) of order 8. The best of these has $c_{\text{eff}}(\text{TSRK}(12,8)) = 0.078$. It is not mentioned in

Ketcheson, Gottlieb and Macdonald [9] that two-step, 4- to 10-stage RK methods of order 8 exist. Our study of HB methods shows that these new methods of order 8 with only 4 stages exist. We found $\text{HB}(8,s,8)$ with good $c_{\text{eff}}(\text{HB}(8,s,8)) \geq 0.237$ with stage number $s=4,5,...,10$.

Though general linear multistep, multistage SSP methods of order 9 to 12 with nonnegative coefficients have not been found in the literature, we discovered $\text{HB}(k,s,p)$ of these high orders with good effective SSP coefficients described in the following subsection.

$s \setminus k$	3	4	5	6	7	8
4			0.123	0.180	0.213	*0.239
5		0.121	0.200	0.230	0.253	*0.259
6		0.169	0.239	0.256	0.258	**0.261**
7		0.169	0.236	0.240	0.243	*0.244
8	0.160	0.198	0.235	0.241	0.243	*0.244
9	0.174	0.202	0.224	0.236	0.239	*0.240
10	0.186	0.217	0.231	0.234	*0.237	0.237

Table 4: $c_{\text{eff}}(\text{HB}(k,s,8))$ as function of k and s

5.4 High order methods

We numerically found optimal $\text{HB}(k,s,9)$ with stage number $s=4,5,...,10$. Their c_{eff} are listed in Table 5 with the largest $c_{\text{eff}}(\text{HB}(8,6,9))=0.228$.

In addition to the above results, the optimal $\text{HB}(k,s,10)$ with stage number $s=4,5,...10$ are found numerically and Table 6 lists all the c_{eff} of our optimal methods with the largest $c_{\text{eff}}(\text{HB}(8,8,10))=0.186$.

The optimal $\text{HB}(k,s,11)$ as well as $\text{HB}(k,s,12)$ with stage number $s=4,5,...10$ and their c_{eff} are listed in Table 7 and 8, respectively.

We see in Tables 7 and 8 that $c_{\text{eff}}(\text{HB}(8,8,11))=0.156$ and $c_{\text{eff}}(\text{HB}(8,8,12))=0.116$ are largest for the values of k and s on hand, corresponding to order 11 and 12.

$s \setminus k$	4	5	6	7	8
4			0.091	0.135	*0.171
5		0.121	0.177	0.204	*0.220
6		0.168	0.194	0.215	**0.228**
7		0.162	0.196	0.207	*0.215
8	0.138	0.178	0.203	0.216	*0.218
9	0.154	0.195	0.206	0.208	*0.208
10	0.164	0.189	0.191	0.191	*0.191

Table 5: $c_{\text{eff}}(\text{HB}(k,s,9))$ as function of k and s

$s \setminus k$	6	7	8
4		0.073	*0.117
5	0.088	0.143	*0.172
6	0.126	0.168	*0.185
7	0.131	0.171	*0.182
8	0.156	0.182	**0.186**
9	0.169	0.179	*0.180
10	0.155	0.167	*0.172

Table 6: $c_{\text{eff}}(\text{HB}(k,s,10))$ as function of k and s

$s \setminus k$	6	7	8
4			*0.053
5		0.080	*0.126
6	0.029	0.092	*0.142
7	0.086	0.123	*0.143
8	0.106	0.135	**0.156**
9	0.114	0.146	*0.155
10	0.115	0.139	*0.143

Table 7: $c_{\text{eff}}(\text{HB}(k,s,11))$ as function of k and s

$s \setminus k$	7	8
5	0.010	*0.057
6	0.035	*0.091
7	0.062	*0.097
8	0.100	**0.116**
9	0.097	*0.112
10	0.089	*0.103

Table 8: $c_{\text{eff}}(\text{HB}(k,s,12))$ as function of k and s

Table 9 lists $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$, which are the numbers with an asterisk and the boldface numbers in Table 1–8.

In Table 9, as expected, for a given s, $c_{\text{eff}}(\text{HB}(k,s,p))$ decreases with increasing p. It is also seen that $c_{\text{eff}}(\text{HB}(k,s,p))$ of orders $p=5,6,...,12$ are among the highest when the number of stages is about 6 to 10.

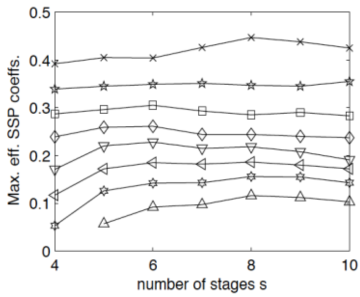
Hence, based on the c_{eff}, it seems that there are very few HB families which can have methods up to order 12 with good c_{eff}, namely, the 7-, 8-, 9- and 10-stage HB methods of order 5 to 12. Especially, the 8-stage HB methods are among the most efficient methods on hand at least in term of stability constraints.

$p \setminus s$	4	5	6	7	8	9	10
5	HB(6,4,5) 0.392	HB(5,5,5) 0.405	HB(3,6,5) 0.404	HB(3,7,5) 0.426	HB(2,8,5) 0.447	HB(2,9,5) 0.438	HB(2,10,5) 0.425
6	HB(7,4,6) 0.339	HB(7,5,6) 0.345	HB(6,6,6) 0.349	HB(5,7,6) 0.351	HB(6,8,6) 0.347	HB(5,9,6) 0.345	HB(5,10,6) 0.355
7	HB(7,4,7) 0.287	HB(7,5,7) 0.296	HB(6,6,7) 0.305	HB(6,7,7) 0.293	HB(7,8,7) 0.287	HB(5,9,7) 0.290	HB(4,10,7) 0.283
8	HB(8,4,8) 0.239	HB(8,5,8) 0.259	HB(8,6,8) 0.261	HB(8,7,8) 0.244	HB(7,8,8) 0.244	HB(7,9,8) 0.240	HB(6,10,8) 0.237
9	HB(8,4,9) 0.171	HB(8,5,9) 0.220	HB(8,6,9) 0.228	HB(8,7,9) 0.215	HB(8,8,9) 0.218	HB(8,9,9) 0.208	HB(6,10,9) 0.191
10	HB(8,4,10) 0.171	HB(8,5,10) 0.172	HB(8,6,10) 0.185	HB(8,7,10) 0.182	HB(8,8,10) 0.186	HB(8,9,10) 0.180	HB(8,10,10) 0.172
11	HB(8,4,11) 0.053	HB(8,5,11) 0.126	HB(8,6,11) 0.142	HB(8,7,11) 0.143	HB(8,8,11) 0.158	HB(8,9,11) 0.155	HB(8,10,11) 0.143
12		HB(8,5,12) 0.057	HB(8,6,12) 0.091	HB(8,7,12) 0.097	HB(8,8,12) 0.116	HB(8,9,12) 0.112	HB(8,10,12) 0.103

Table 9: $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$ of $\text{HB}(k,s,p)$ for k-step methods combined with RK5 as function of s and p.

In Fig.1, $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$, $p = 5,6,\dots,12$, is plotted as a function of the stage number s. We note that, for a given $p \geq 5$, generally, $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$ first increases with s and then decreases.

Figure 2 plots $\max_{k,s} c_{\text{eff}}(\text{HB}(k,s,p))$ as a function of the order p. We note that, as expected, $\max_{k,s} c_{\text{eff}}(\text{HB}(k,s,p))$ decreases with increasing p.



HB order 5 ´ , HB order 6 ★, HB order 7□, HB order 8 à, HB order 9 ∇, HB order 10 □ , HB order 11 *, HB order 12 ⌴ .

Figure 1: $\max_{k} c_{\text{eff}}(\text{HB}(k,s,p))$ as function of s for orders $p=5,6,...,12$.

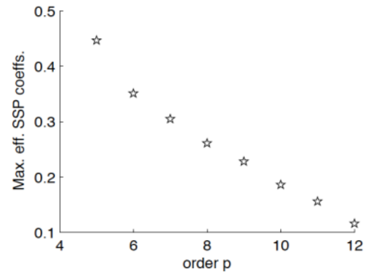


Figure 2: $\max_{k,s} c_{\text{eff}}(\text{HB}(k,s,p))$ versus order p.

6. CONCLUSION

In our work, a collection of new optimal SSP explicit, k-step, 4- to 10-stage Hermite–Birkhoff methods, $\text{HB}(k,s,p)$, of orders $p=5,6,...,12$ with nonnegative coefficients are constructed by combining k-step methods with s-stage RK methods of order 5. The canonical Shu–Osher by means of vector is also introduced. Moreover, the largest effective SSP coefficients of HB methods of order p have also been found on hand. Compared to some well–known methods of the same orders such as $\text{HM}(k,p)$ and $\text{TSRK}(s,p)$, our new methods have larger effective SSP coefficients.

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