

# Strong-stability-preserving Hermite–Birkhoff Time-discretization Methods Combining $k$ -step Methods and Explicit $s$ -stage RK4 Methods

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**Abstract** – New optimal strong-stability-preserving Hermite–Birkhoff (SSP HB) methods,  $\text{HB}(k, s, p)$ , of order  $p = 4, 5, \dots, 12$ , are constructed by combining  $k$ -step methods of order  $p = 1, 2, \dots, 9$  and  $s$ -stage explicit Runge–Kutta (RK) methods of order 4, where  $s = 4, 5, \dots, 10$ . These methods are well suited for solving discretized hyperbolic PDEs by the method of lines. The Shu–Osher form of RK methods is extended to our new methods. The  $\text{HB}(k, s, p)$  having the largest effective SSP coefficient have been numerically found among the HB methods of order  $p$  on hand. These SSP high-order methods are compared with other SSP methods and their main features are summarized.

**Keywords** – Strong stability preserving; Hermite–Birkhoff method; SSP coefficient; time discretization; method of lines; comparison with other SSP methods.

## I. INTRODUCTION

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

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

We assume that the function  $f$  is such that

$$\|y(t + \Delta t)\| \leq \|y(t)\|, \quad (2)$$

where  $\|\cdot\|$  is any norm or semi-norm. It is also assumed that  $f$  satisfies a discrete analog of inequality (2),

$$\|y_n + \Delta t f(t_n, y_n)\| \leq \|y_n\|, \quad (3)$$

for the forward Euler (FE) method with a step size  $\Delta t$  smaller than a maximal step size  $\Delta t_{\text{FE}} > 0$ . Here  $y_n$  is a numerical approximation of  $y(t_0 + n\Delta t)$ . We are interested in higher-order multistep Hermite–Birkhoff (HB) methods that preserve the strong stability property [4], also called monotonicity property [10],

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

for  $0 \leq \Delta t \leq \Delta t_{\text{max}}$  whenever condition (3) holds for the FE method. The positive integer  $k$  represents the number of previous steps used to compute the next solution value. The

SSP property(4) is desirable in that it mimics property (2) of the true solution and prevents error growth.

Strong-stability-preserving (SSP) methods have been developed to satisfy the SSP property (4) for system (1) whenever the FE condition (3) is fulfilled. The SSP property is guaranteed under the maximum time step  $\Delta t_{\text{max}} = c\Delta t_{\text{FE}}$ , where the SSP coefficient  $c$  depends only on the numerical integration method but not on  $f$ . Considerable research effort has been devoted to find numerical methods with largest  $c$  among various classes of methods (see [4], [8]).

The main application of such SSP results are found in the numerical solution of 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  $x_j$ ,  $j = 1, 2, \dots, N$ , (see, for example, [7], [21], [30], [1]). Such spatial semi-discretization will lead to system (1) of ODEs.

Recently, several new SSP methods have been constructed as combinations of multistep and explicit Runge–Kutta (RK) methods [13]–[18].

In this paper, to solve system (1), we construct new explicit, SSP,  $k$ -step,  $s$ -stage, general linear methods of order  $p$  with nonnegative coefficients as combinations of linear  $k$ -step methods of order  $p - 3$  and  $s$ -stage RK methods of order 4. We shall denote these new SSP methods by  $\text{HB}(k, s, p)$  since HB interpolation polynomials enter in their construction as it is briefly sketched in Section II (see [19] for fuller developments).

The objective of high-order SSP HB time discretizations is to maintain the SSP property (4) while achieving higher-order accuracy in time, perhaps with a modified CFL restriction, measured here with an SSP coefficient,  $c(\text{HB}(k, s, p))$ :

$$\Delta t \leq c(\text{HB}(k, s, p))\Delta t_{\text{FE}}, \quad (6)$$

The SSP coefficient, historically called CFL coefficient, describes the ratio of the SSP time step to the strongly stable FE time step (see [4]). Since our arguments are based on convex decompositions of high-order methods in terms the SSP FE method, such high-order methods are SSP in any norm once FE is shown to be strongly stable. We use this fact to extend the

Shu–Osher form of RK methods to methods which combine multistep and RK methods.

The new HB( $k, s, p$ ) have larger effective SSP coefficients than Huang’s [8] SSP hybrid methods (HM( $k, s, p$ )) with the same  $k$  and  $p$ , especially when  $k$  is small. In particular, no counterparts of HB( $k, s, p$ ) for  $p = 9, 10, 11, 12$  have been found in the literature among hybrid and general linear multistep methods.

Section II introduces  $k$ -step,  $s$ -stage HB( $k, s, p$ ) methods. Order conditions are listed in Section III. Section IV derives the Shu Osher form of HB( $k, s, p$ ) and formulates the optimization problem. Section V compares effective SSP coefficients which are the SSP coefficients divided by the number of functions evaluations by time step. Section VI compares SSP HB time discretization methods of orders 4 to 12 with known SSP RK methods of order 4 of same stage number.

### II. $K$ -STEP, $S$ -STAGE HB( $k, s, p$ ) OF ORDER $P$

We construct our  $k$ -step,  $s$ -stage HB methods as general linear methods by the following  $s$  formulae to perform integration from  $t_n$  to  $t_{n+1}$ . Let  $\Delta t$  be the time discretization step size. The abscissa vector  $[c_1, c_2, c_3, \dots, c_s]^T$  defines the  $s$  off-step points  $t_n + \Delta t c_j$ . In all cases,  $c_1 = 0$  and, by convention,  $c_1^0 = 1$ . Let  $F_1 = f_n$ .

With the initial stage value,  $Y_1 = y_n$ . HB polynomials of degree  $2k + i - 3$  are used as predictors  $P_i$  to obtain the stage values  $Y_i$ ,

$$Y_i = \sum_{j=0}^{k-1} A_{B,i,j} y_{n-j} + \Delta t \left[ \sum_{j=1}^{i-1} a_{ij} F_j + \sum_{j=1}^{k-1} B_{B,i,j} f_{n-j} \right], \quad (7)$$

for  $i = 2, 3, \dots, s$ , where  $F_j := f(t_n + c_j \Delta t, Y_j)$  denote the stage derivatives for  $j = 2, 3, \dots, s$ . An HB polynomial of degree  $2k + s - 2$  is used as integration formula to obtain  $y_{n+1}$  to order  $p$ ,

$$y_{n+1} = \sum_{j=0}^{k-1} A_{B,s+1,j} y_{n-j} + \Delta t \left[ \sum_{j=1}^s b_j F_j + \sum_{j=1}^{k-1} B_{B,s+1,j} f_{n-j} \right]. \quad (8)$$

Formulae (7)–(8) are the Butcher form of HB( $k, s, p$ ). The subscript B refers to Butcher, while, later, the subscript SO will refer to Shu–Osher.

*Notation 1:* We shall denote the  $k$ -step SSP methods of order  $p$  used in this paper as follows:

- HB( $k, s, p$ ):  $s$ -stage Hermite–Birkhoff method,
- HM( $k, p$ ): hybrid method,
- LM( $k, p$ ): linear multistep method,
- RK( $s, p$ ):  $s$ -stage Runge–Kutta method,
- TSRK( $s, p$ ): 2-step  $s$ -stage Runge–Kutta method.

All the methods considered in this work are SSP. Therefore the denomination SSP will often be omitted in what follows.

### III. ORDER CONDITIONS FOR HB( $k, s, p$ )

To derive the order conditions of  $s$ -stage HB( $k, s, p$ ) we shall use the following expressions coming from the backsteps of the methods:

$$B_i(j) = \sum_{\ell=0}^{k-1} A_{B,i,\ell} \frac{(-\ell)^j}{j!} + \sum_{\ell=1}^{k-1} B_{B,i,\ell} \frac{(-\ell)^{j-1}}{(j-1)!}, \quad (9)$$

for  $i = 2, 3, \dots, s$  and  $j = 1, 2, \dots, p$ . Forcing an expansion of the numerical solution produced by formulae (7)–(8) to agree with a Taylor expansion of the true solution, we obtain multistep- and several RK-type order conditions that must be satisfied by  $s$ -stage HB( $k, s, p$ ) methods.

First, we need to satisfy the following multistep-type consistency conditions:

$$\sum_{j=0}^{k-1} A_{B,i,j} = 1, \quad i = 2, 3, \dots, s + 1. \quad (10)$$

Second, to reduce the large number of RK-type order conditions (see [12]), we impose the following simplifying assumptions:

$$\sum_{j=1}^{i-1} a_{ij} c_j^k + k! B_i(k + 1) = \frac{1}{k + 1} c_i^{k+1}, \quad (11)$$

for  $i = 2, 3, \dots, s$  and  $k = 0, 1, \dots, p - 4$ . Thus, there remain only five sets of equations to be solved:

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

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

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

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

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

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

$$B(j) = \sum_{i=0}^{k-1} A_{\mathbf{B},s+1,i} \frac{(-i)^j}{j!} + \sum_{i=2}^{k-1} B_{\mathbf{B},s+1,i} \frac{(-i)^{j-1}}{(j-1)!}, \quad (17)$$

for  $j = 1, \dots, p+1$ . These order conditions are simply RK order conditions with backstep parts  $B_i(\cdot)$  and  $B(\cdot)$ .

#### IV. HB( $k, s, p$ ) IN MODIFIED BUTCHER AND SHU–OSHER FORMS

By setting  $w_{\mathbf{B},i} = a_{i1}$ ,  $i = 2, 3, \dots, s$ , and  $w_{\mathbf{B},s+1} = b_1$  in (7)–(8) we have the modified Butcher form of HB( $k, s, p$ ):

$$Y_i = v_{\mathbf{B},i} y_n + \sum_{j=1}^{k-1} A_{\mathbf{B},i,j} y_{n-j} + \Delta t \left[ w_{\mathbf{B},i} f_n + \sum_{j=2}^{i-1} \alpha_{ij} F_j + \sum_{j=1}^{k-1} B_{\mathbf{B},i,j} f_{n-j} \right], \quad i = 2, 3, \dots, s, \quad (18)$$

$$y_{n+1} = v_{\mathbf{B},s+1} y_n + \sum_{j=1}^{k-1} A_{\mathbf{B},s+1,j} y_{n-j} + \Delta t \left[ w_{\mathbf{B},s+1} f_n + \sum_{j=2}^s b_j F_j + \sum_{j=1}^{k-1} B_{\mathbf{B},s+1,j} f_{n-j} \right], \quad (19)$$

where  $v_{\mathbf{B},i} = A_{\mathbf{B},i0}$ ,  $i = 2, 3, \dots, s+1$ .

As done in [16], (7)–(8) can be written as convex combinations of forward Euler methods as follows;

$$Y_i = \left[ \sum_{j=1}^{i-1} \alpha_{ij} Y_j + \Delta t \beta_{ij} F_j \right] + \left[ \sum_{j=1}^{k-1} A_{ij} y_{n-j} + \Delta t B_{ij} f_{n-j} \right], \quad i = 2, 3, \dots, s+1, \quad (20)$$

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

where consistency conditions are  $\sum_{j=1}^{i-1} \alpha_{ij} + \sum_{j=1}^{k-1} A_{ij} = 1$ ,  $i = 2, 3, \dots, s+1$ . The above form is called the Shu–Osher form of HB( $k, s, p$ ). This form is a generalization of the Shu–Osher form of RK first introduced by Shu and Osher in [27].

By setting  $v_i = \alpha_{i1}$  and  $w_i = \beta_{i1}$ ,  $i = 2, 3, \dots, s+1$ , in (20), we have the modified Shu–Osher form of HB( $k, s, p$ ) for  $i = 2, 3, \dots, s+1$ ,

$$Y_i = (v_i y_n + \Delta t w_i f_n) + \left[ \sum_{j=2}^{i-1} \alpha_{ij} Y_j + \Delta t \beta_{ij} F_j \right] + \left[ \sum_{j=1}^{k-1} A_{ij} y_{n-j} + \Delta t B_{ij} f_{n-j} \right], \quad (21)$$

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

The above form of HB( $k, s, p$ ) is a generalization of the modified Shu–Osher form for RK methods (see [5, p. 27]) since

it can be rearranged as three linear combinations of FE methods:

$$Y_i = \left[ v_i \left( y_n + \Delta t \frac{w_i}{v_i} f_n \right) \right] + \left[ \sum_{j=2}^{i-1} \alpha_{ij} \left( Y_j + \Delta t \frac{\beta_{ij}}{\alpha_{ij}} F_j \right) \right] + \left[ \sum_{j=0}^{k-1} A_{ij} \left( y_{n-j} + \Delta t \frac{B_{ij}}{A_{ij}} f_{n-j} \right) \right], \quad (22)$$

for  $i = 2, 3, \dots, s+1$ . As consistency requires that

$$v_i + \sum_{j=2}^{i-1} \alpha_{ij} + \sum_{j=1}^{k-1} A_{ij} = 1, \quad i = 2, 3, \dots, s+1, \quad (23)$$

then, if  $v_i, w_i, \alpha_{ij}, \beta_{ij}, A_{ij}, B_{ij}$  are nonnegative, each stage  $Y_i$  is a convex combination of forward Euler steps.

Hence, under these conditions, each representation  $v_i, w_i, \alpha_{ij}, \beta_{ij}, A_{ij}, B_{ij}$  of (22) will produce a *feasible* HB( $k, s, p$ ) in Shu Osher form (22) with *feasible* SSP coefficient.

The transformation of the HB( $k, s, p$ ) formulae (7)–(8) to the Shu–Osher form (21) and vice versa will be considered in subsection IV-B.

The next three subsections IV-A, IV-B and IV-C describe generalized results for the new HB( $k, s, p$ ), using the results for Runge–Kutta methods, following closely sections 3.1 to 3.4 of [5].

#### A. Vector notation

In the following three sections, it will be helpful to represent an HB method in a Shu–Osher form using a more compact notation. To this end, we define two real  $(s+1)$ -vectors

$$\mathbf{v} = [0, v_2, v_3, \dots, v_{s+1}]^T, \quad \mathbf{w} = [0, w_2, w_3, \dots, w_{s+1}]^T,$$

two strictly lower triangular  $(s+1) \times (s+1)$  real matrices

$$\boldsymbol{\alpha} = \{\alpha_{ij}\}, \quad \boldsymbol{\beta} = \{\beta_{ij}\},$$

two  $(s+1) \times (k-1)$  rectangular matrices with zero first row,

$$A_{\mathbf{SO}} = \{A_{ij}\}, \quad B_{\mathbf{SO}} = \{B_{ij}\},$$

where the components  $\alpha_{ij}, \beta_{ij}, A_{ij}, B_{ij}$  come from equations (20). Moreover, we have the four matrices,

$$\mathbf{Y} = [0, Y_2, \dots, Y_s, y_{n+1}]^T \in \mathbb{R}^{(s+1) \times N},$$

$$\mathbf{F} = [0, F_2, \dots, F_s, f_{n+1}]^T \in \mathbb{R}^{(s+1) \times N},$$

$$\mathbf{y}_{\text{back}} = [y_{n-1}, y_{n-2}, \dots, y_{n-(k-1)}]^T \in \mathbb{R}^{(k-1) \times N},$$

$$\mathbf{f}_{\text{back}} = [f_{n-1}, f_{n-2}, \dots, f_{n-(k-1)}]^T \in \mathbb{R}^{(k-1) \times N},$$

where the subscript “back” refers to backstep of an HB( $k, s, p$ ) method.

Thus, we can compactly write an HB method in the Shu–Osher form,

$$\begin{aligned}
 Y &= v y_n^T + \alpha Y + A_{SO} y_{back} \\
 &+ \Delta t (w f_n^T + \beta F + B_{SO} f_{back}), \quad (24) \\
 y_{n+1} &= Y_{s+1}.
 \end{aligned}$$

Here consistency requires that

$$v + \alpha e_{s+1} + A_{SO} e_{back} = e_{s+1},$$

where the  $(s + 1)$ -vector  $e_{s+1}$  and  $(k - 1)$ -vector  $e_{back}$  are, respectively,

$$\begin{aligned}
 e_{s+1} &= [0, 1, 1, \dots, 1]^T \in \mathbb{R}^{(s+1)}, \\
 e_{back} &= [1, 1, \dots, 1]^T \in \mathbb{R}^{(k-1)}. \quad (25)
 \end{aligned}$$

Provided all the coefficients of (22) are nonnegative, the following straightforward extension of a result presented in [6] and [8] holds.

*Theorem 1:* If  $f$  satisfies the forward Euler condition (3), then the  $k$ -step,  $s$ -stage HB( $k, s, p$ ) methods (22) of order  $p$  satisfy the SSP property

$$\|y_{n+1}\| \leq \max_{0 \leq j \leq k-1} \|y_{n-j}\|$$

provided

$$\Delta t \leq c(v, w, \alpha, \beta, A_{SO}, B_{SO}) \Delta t_{FE},$$

where the *feasible SSP coefficient*  $c(v, w, \alpha, \beta, A_{SO}, B_{SO})$  is

$$\min \left\{ \min_{i=2,3,\dots,s+1} \left\{ \frac{v_i}{w_i} \right\}, \min_{\substack{i=3,4,\dots,s+1 \\ j=2,3,\dots,i-1}} \left\{ \frac{\alpha_{ij}}{\beta_{ij}} \right\}, \min_{\substack{i=1,2,\dots,s+1 \\ j=1,2,\dots,k-1}} \left\{ \frac{A_{ij}}{B_{ij}} \right\} \right\}, \quad (26)$$

with the convention that  $a/0 = +\infty$ , under the assumption that all coefficients of (22) are nonnegative.

It is to be noted that each representation  $v_i, w_i, \alpha_{ij}, \beta_{ij}, A_{ij}, B_{ij}$  of (22) will produce a feasible SSP coefficient  $c(v, w, \alpha, \beta, A_{SO}, B_{SO})$  defined in Theorem 1.

What we really want is not a feasible HB( $k, s, p$ ) with feasible SSP coefficient  $c(v, w, \alpha, \beta, A_{SO}, B_{SO})$  but one with largest SSP coefficient. This question will be considered in subsection IV-C.

*Example 1:* We consider a simple 3-step 3-stage HB method of order 3 denoted by HB(3, 3, 3). With  $A_{SO} = 0, B_{SO} = 0$ , this method becomes the well known Shu–Osher RK(3, 3) given in [27] with abscissae vector  $\sigma = [0, 1, \frac{1}{2}]^T$ :

$$\begin{aligned}
 Y_2 &= y_n + \Delta t f_n, \\
 Y_3 &= \frac{1}{4} Y_2 + \frac{1}{4} \Delta t F_2 + \frac{3}{4} y_n, \\
 y_{n+1} &= \frac{2}{3} Y_3 + \frac{2}{3} \Delta t F_3 + \frac{1}{3} y_n. \quad (27)
 \end{aligned}$$

Note that this is in the Shu–Osher form (20) and produces the well known SSP coefficient  $c(RK(3, 3)) = 1$  of RK(3, 3). This coefficient is a feasible SSP coefficient  $c(v, w, \alpha, \beta, A_{SO}, B_{SO}) = 1$  of HB(3, 3, 3). However, we

can rewrite the method with the new abscissa vector  $\sigma = [0, \frac{2}{3}, \frac{153901}{283168}]^T$  and by dropping conditions  $A_{SO} = 0$  and  $B_{SO} = 0$  we obtain a better result:

$$\begin{aligned}
 Y_2 &= y_n + \frac{2}{3} \Delta t f_n, \\
 Y_3 &= \frac{1420255}{2340227} Y_2 + \frac{1045855}{2584967} \Delta t F_2 + \frac{458404}{1374219} y_{n-1} + \frac{217149}{1422944} \Delta t f_{n-1} \\
 &+ \frac{147561}{2478430} y_{n-2} + \frac{30158}{877731} \Delta t f_{n-2}, \quad (28) \\
 y_{n+1} &= \frac{1038099}{1617767} Y_3 + \frac{412233}{963632} \Delta t F_3 + \frac{120175}{804846} Y_2 + \frac{138081}{1387153} \Delta t F_2 \\
 &+ \frac{67868}{679793} y_n + \frac{69677}{1046869} \Delta t f_n + \frac{140082}{1355255} y_{n-1} + \frac{93388}{1355255} \Delta t f_{n-1} \\
 &+ \frac{6335}{1092053} y_{n-2} + \frac{6381}{1649974} \Delta t f_{n-2},
 \end{aligned}$$

which produces  $c(v, w, \alpha, \beta, A_{SO}, B_{SO}) = 1.5$ . This is still not optimal. Rewriting the method with the abscissa vector  $\sigma = [0, \frac{646123}{1613385}, \frac{543161}{833453}]^T$ , we have

$$\begin{aligned}
 Y_2 &= \frac{428284}{469581} y_n + \frac{649438}{1235431} \Delta t f_n + \frac{41297}{469581} y_{n-2} + \frac{411103}{8110447} \Delta t f_{n-2}, \\
 Y_3 &= \frac{61125}{79607} Y_2 + \frac{343435}{776031} \Delta t F_2 + \frac{18482}{79607} y_{n-1} + \frac{109753}{820202} \Delta t f_{n-1}, \quad (29) \\
 y_{n+1} &= \frac{1105643}{1282766} Y_3 + \frac{758390}{1526607} \Delta t F_3 + \frac{177123}{1282766} y_{n-1} + \frac{38171}{479632} \Delta t f_{n-1}.
 \end{aligned}$$

Thus, one easily verifies that  $c(v, w, \alpha, \beta, A_{SO}, B_{SO}) = 1.735$ . This value turns out numerically to be the largest possible value of  $c(v, w, \alpha, \beta, A_{SO}, B_{SO})$  for this method. We denote this value,  $c(HB(3, 3, 3)) = 1.735$  which is the SSP coefficient of HB(3, 3, 3).

*B. Butcher form*

If  $\alpha = 0$ , then the Shu–Osher form (24) becomes

$$\begin{aligned}
 Y &= v y_n^T + A_{SO} y_{back} \\
 &+ \Delta t (w f_n^T + \beta F + B_{SO} f_{back}), \quad (30) \\
 y_{n+1} &= Y_{s+1}.
 \end{aligned}$$

which is the Butcher form. If  $v, w, \beta, A_{SO}, B_{SO}$  of (30) are denoted as  $v_0, w_0, \beta_0, A_B, B_B$ , respectively, then the Butcher form (30) can be rewritten as

$$\begin{aligned}
 Y &= v_0 y_n^T + A_B y_{back} \\
 &+ \Delta t (w_0 f_n^T + \beta_0 F + B_B f_{back}), \quad (31) \\
 y_{n+1} &= Y_{s+1}.
 \end{aligned}$$

Here consistency conditions (10) are written in vector form:

$$v_0 + A_B e_{back} = e_{s+1} \quad (32)$$

where  $e_{s+1}$  and  $e_{back}$  are defined in (25).

To find the relation between the Shu–Osher coefficients and the Butcher coefficients, we simply solve (24) for  $Y$ , since  $I - \alpha$  is invertible because  $\alpha$  is strictly lower triangular. From  $Y = v y_n^T + \alpha Y + A_{SO} y_{back} + \Delta t (w f_n^T + \beta F + B_{SO} f_{back})$  we have

$$(I - \alpha) Y = v y_n^T + A_{SO} y_{back} + \Delta t (w f_n^T + \beta F + B_{SO} f_{back}).$$

Thus,

$$\begin{aligned}
 Y &= (I - \alpha)^{-1} v y_n^T + (I - \alpha)^{-1} A_{SO} y_{\text{back}} \\
 &+ \Delta t \left[ (I - \alpha)^{-1} w f_n^T \right. \\
 &\left. + (I - \alpha)^{-1} \beta F + (I - \alpha)^{-1} B_{SO} f_{\text{back}} \right]. \tag{33}
 \end{aligned}$$

Comparing (33) with (31), we have the following relations between the Shu–Osher coefficients and the Butcher coefficients for our HB methods,

$$v_0 = (I - \alpha)^{-1} v, \tag{34}$$

$$w_0 = (I - \alpha)^{-1} w, \tag{35}$$

$$\beta_0 = (I - \alpha)^{-1} \beta, \tag{36}$$

$$A_B = (I - \alpha)^{-1} A_{SO}, \tag{37}$$

$$B_B = (I - \alpha)^{-1} B_{SO}. \tag{38}$$

These relations allow a simple transformation of the vectors and matrices  $v, w, \beta, A_{SO}, B_{SO}$  of a Shu–Osher form into  $v_0, w_0, \beta_0, A_B, B_B$  of a Butcher form and vice versa. In fact, form (31) is the Butcher form (7) and (8) with

$$v_0 = [0, A_{B,2,0}, A_{B,3,0}, \dots, A_{B,s+1,0}]^T, \tag{39}$$

$$w_0 = [0, a_{21}, a_{31}, \dots, a_{s1}, b_1]^T, \tag{40}$$

$$\beta_0 = \begin{bmatrix} 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ a_{21} & 0 & 0 & 0 & \dots & 0 & 0 \\ a_{31} & a_{32} & 0 & 0 & \dots & 0 & 0 \\ a_{41} & a_{42} & a_{43} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{s1} & a_{s2} & a_{s3} & \dots & a_{s,s-1} & 0 & 0 \\ b_1 & b_2 & b_3 & \dots & b_{s-1} & b_s & 0 \end{bmatrix}, \tag{41}$$

$$A_B = \begin{bmatrix} 0 & 0 & \dots & 0 \\ A_{B,2,1} & A_{B,2,2} & \dots & A_{B,2,k-1} \\ A_{B,3,1} & A_{B,3,2} & \dots & A_{B,3,k-1} \\ \vdots & \vdots & \dots & \vdots \\ A_{B,s+1,1} & A_{B,s+1,2} & \dots & A_{B,s+1,k-1} \end{bmatrix}, \tag{42}$$

$$B_B = \begin{bmatrix} 0 & 0 & \dots & 0 \\ B_{B,2,1} & B_{B,2,2} & \dots & B_{B,2,k-1} \\ B_{B,3,1} & B_{B,3,2} & \dots & B_{B,3,k-1} \\ \vdots & \vdots & \dots & \vdots \\ B_{B,s+1,1} & B_{B,s+1,2} & \dots & B_{B,s+1,k-1} \end{bmatrix}. \tag{43}$$

### C. Canonical Shu–Osher form and formulation of the optimization problem

To find the SSP coefficient of a Hermite–Birkhoff method, it is useful to consider a particular Shu–Osher form of the matrices  $\alpha, \beta$ , in which the ratio  $r = \frac{\alpha_{ij}}{\beta_{ij}}$  is the same for every  $i, j$  such that  $\beta_{ij} \neq 0$ , that is, in a convex combination of forward Euler steps, the step length,

$$\Delta t \frac{\beta_{ij}}{\alpha_{ij}} = \frac{1}{r} \Delta t \leq \Delta t_{FE},$$

is the same for every step in the second member of the righthand side of (22).

We shall denote the coefficient matrices of this special form by  $\alpha_r, \beta_r$ , and require that  $\alpha_r = r\beta_r$ . Substituting this relation into (36), we can solve for  $\beta_r$  in terms of  $\beta_0$  and  $r$ . Thus, we find

$$\begin{aligned}
 (I - r\beta_r)^{-1} \beta_r &= \beta_0, \\
 \beta_r &= \beta_0 - r\beta_r\beta_0, \\
 \beta_r (I + r\beta_0) &= \beta_0.
 \end{aligned}$$

Since  $I + r\beta_0$  is invertible, the coefficients for this form are given by

$$v_r = (I + r\beta_0)^{-1} v_0 = (I - \alpha_r) v_0, \tag{44}$$

$$w_r = (I + r\beta_0)^{-1} w_0 = (I - \alpha_r) w_0, \tag{45}$$

$$\alpha_r = r\beta_r = r\beta_0 (I + r\beta_0)^{-1} = r\beta_0 (I - \alpha_r), \tag{46}$$

$$\beta_r = \beta_0 (I + r\beta_0)^{-1} = \beta_0 (I - \alpha_r), \tag{47}$$

$$A_{SO,r} = (I - \alpha_r) A_B = (I + r\beta_0)^{-1} A_B, \tag{48}$$

$$B_{SO,r} = (I - \alpha_r) B_B = (I + r\beta_0)^{-1} B_B, \tag{49}$$

where the identity  $(I - \alpha_r) = (I + r\beta_0)^{-1}$  follows from

$$\begin{aligned}
 (I - \alpha_r) (I + r\beta_0) &= (I - r\beta_r) (I + r\beta_0) \\
 &= I + r\beta_0 - r\beta_r - r^2\beta_r\beta_0 = I,
 \end{aligned}$$

since  $r\beta_r = r\beta_0 - r^2\beta_r\beta_0$ .

It is to be noted that using (36) and (46),  $\beta_r$  can be written as

$$\begin{aligned}
 \beta_r &= \beta_0 (I + r\beta_0)^{-1} = \beta_0 (I - \alpha_r) \\
 &= (I - \alpha_r) \beta_0 = (I + r\beta_0)^{-1} \beta_0.
 \end{aligned} \tag{50}$$

As in [5, p. 34], we shall refer to the form given by (44)–(49) as a *canonical Shu–Osher form* of an HB method,

$$\begin{aligned}
 Y &= (v_r y_n^T + \Delta t w_r f_n^T) + (\alpha_r Y + \Delta t \beta_r F) \\
 &+ (A_{SO,r} y_{\text{back}} + \Delta t B_{SO,r} f_{\text{back}}), \tag{51}
 \end{aligned}$$

which can be written only in terms of the vectors  $v_0, w_0$  and matrices  $\beta_0, A_B, B_B$  of the Butcher form:

$$\begin{aligned}
 Y &= \left[ (I + r\beta_0)^{-1} v_0 y_n^T + \Delta t (I + r\beta_0)^{-1} w_0 f_n^T \right] \\
 &+ \left[ r\beta_0 (I + r\beta_0)^{-1} Y \right] + \left[ \Delta t \beta_0 (I + r\beta_0)^{-1} F \right] \\
 &+ \left[ (I + r\beta_0)^{-1} A_B y_{\text{back}} + \Delta t (I + r\beta_0)^{-1} B_B f_{\text{back}} \right]. \tag{52}
 \end{aligned}$$

Using the relation  $\beta_0 (I + r\beta_0)^{-1} = (I + r\beta_0)^{-1} \beta_0$  obtained in (50), result (52) can be written as,

$$\begin{aligned}
 Y &= (I + r\beta_0)^{-1} \left[ v_0 y_n^T + \Delta t w_0 f_n^T + \beta_0 (rY + \Delta t F) \right. \\
 &\left. + (A_B y_{\text{back}} + \Delta t B_B f_{\text{back}}) \right]. \tag{53}
 \end{aligned}$$

The zeroth-order term of the Taylor expansion of (53) about  $t_n$  leads to the consistency condition:

$$(I + r\beta_0)^{-1} v_0 + r(I + r\beta_0)^{-1} \beta_0 e_{s+1} + (I + r\beta_0)^{-1} A_B e_{\text{back}} = e_{s+1}, \quad (54)$$

which is equivalent to (32).

Note also that the Butcher form (31), with the coefficient vectors  $v_0, w_0$  and the coefficient matrices  $\beta_0, A_B, B_B$ , corresponds to the canonical Shu–Osher form (51) or (53) with  $r = 0$ .

To simplify notation, in the following theorem the ratio  $r = \frac{\alpha_{ij}}{\beta_{ij}}$ , which is the same for every  $i, j, i = 3, 4, \dots, s + 1$  and  $j = 2, 3, \dots, i - 1$ , becomes a feasible SSP coefficient of  $\text{HB}(k, s, p)$ . Hence, this ratio  $r$  must satisfy two additional conditions:

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

which is (56) and (63) and

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

which is (57) and (64). Therefore, the following slight modification of Theorem 1 holds.

*Theorem 2:* If  $f$  satisfies the forward Euler condition (3), then the  $k$ -step,  $s$ -stage  $\text{HB}(k, s, p)$  methods (22) satisfy the monotonicity property

$$\|y_{n+1}\| \leq \max_{0 \leq j \leq k-1} \|y_{n-j}\|$$

provided

$$\Delta t \leq c(v_r, w_r, \alpha_r, \beta_r, A_{SO,r}, B_{SO,r}) \Delta t_{FE},$$

where the coefficient  $c(v_r, w_r, \alpha_r, \beta_r, A_{SO,r}, B_{SO,r})$  is equal to

$$r = \left\{ \frac{\alpha_{ij}}{\beta_{ij}} \right\}, \quad \begin{cases} i = 3, 4, \dots, s + 1, \\ j = 2, 3, \dots, i - 1, \end{cases} \quad (55)$$

and less than or equal to:

$$\min_{i=2,3,\dots,s+1} \frac{v_i}{w_i}, \quad (56)$$

$$\min_{j=1,2,\dots,k-1} \left\{ \frac{A_{ij}}{B_{ij}} \right\}, \quad i = 2, 3, \dots, s + 1, \quad (57)$$

with the convention that  $a/0 = +\infty$ , under the assumption that all coefficients of (22) are nonnegative.

With the newly defined  $r$ , to optimize  $\text{HB}(k, s, p)$  and obtain  $c(\text{HB}(k, s, p))$ , by Theorem 2, we maximize

$$r = c(v_r, w_r, \alpha_r, \beta_r, A_{SO,r}, B_{SO,r}).$$

Hence, the problem of optimizing  $\text{HB}(k, s, p)$  can be formulated as

$$c(\text{HB}(k, s, p)) = \max_{v_r, w_r, \alpha_r, \beta_r, A_{SO,r}, B_{SO,r}} r, \quad (58)$$

subject to the component-wise inequalities

$$(I + r\beta_0)^{-1} v_0 \geq 0, \quad (59)$$

$$\beta_0 (I + r\beta_0)^{-1} \geq 0, \quad (60)$$

$$(I + r\beta_0)^{-1} A_B \geq 0, \quad (61)$$

$$(I + r\beta_0)^{-1} B_B \geq 0, \quad (62)$$

$$(I + r\beta_0)^{-1} (-v_0 + r w_0) \leq 0, \quad (63)$$

$$(I + r\beta_0)^{-1} (-A_B + r B_B) \leq 0, \quad (64)$$

together with the order conditions (10)–(16) for order  $p$ .

Since the consistency condition (54) is satisfied, inequality (59) implies the following inequality,

$$r\beta_0 (I + r\beta_0)^{-1} e_{s+1} + (I + r\beta_0)^{-1} A_B e_{\text{back}} \leq e_{s+1}, \quad (65)$$

and inequality (65) implies inequality (59).

It is to be noted here that each representation  $(v_r, w_r, \alpha_r, \beta_r, A_{SO,r}, B_{SO,r})$  which satisfies conditions (59)–(64) together with the order conditions (10)–(16) for order  $p$ , will produce a feasible SSP coefficient  $c(v_r, w_r, \alpha_r, \beta_r, A_{SO,r}, B_{SO,r})$  and a feasible SSP  $\text{HB}(k, s, p)$  in Shu–Osher form (22). For example, it is easy to verify that the coefficients of each of methods (27), (28) and (29) verifies condition (59)–(64) together with the order conditions (10)–(16) for order 3.

## V. COMPARING EFFECTIVE SSP COEFFICIENTS OF THE METHODS ON HAND

*Definition 1:* (See [25]) The *effective SSP coefficient* of an SSP method  $M$  is denoted by

$$c_{\text{eff}}(M) = \frac{c(M)}{\ell}, \quad (66)$$

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

The effective SSP coefficients,  $c_{\text{eff}}(\text{HM})$ , of hybrid methods are found in [8]. In this paper,  $\ell = 4, 5, \dots, 10$  for HB methods,  $\ell = 2$  for hybrid methods and  $\ell = 1$  for linear multistep methods.

The coefficients  $c_{\text{eff}}$  provide a fair comparison between methods of the same order, although, in practice, starting methods and storage issues are also important. Gottlieb [3] pointed out that one looks for high-order SSP methods  $M$  with  $c(M)$  as large as possible, taking their computational costs and orders into account.

In Tables I–IX, for each stage value  $s$ , the row-wise maximum,  $\max_k c_{\text{eff}}(\text{HB}(k, s, p))$ , is listed with an asterisk and the global maximum is in boldface for each order  $p$ . This data is summarized in Table X and Fig. 9. It will be seen that, for a

given  $k$ ,  $c_{\text{eff}}(\text{HB}(k, s, p))$  first increases with  $s$  and then decreases. On the other hand, for a given  $s$ ,  $c_{\text{eff}}(\text{HB}(k, s, p))$  first increases with  $k$  and then stabilizes. For these two reasons, further columns to the right and rows to the bottom are not added to the tables, or because the omitted methods are numerically worse than the included ones.

A. Fourth-order methods

Spiteri and Ruuth [28] found a 5-stage SSP RK method of order 4, called RK(5,4), with  $c(\text{RK}(5,4)) = 1.508$  and  $c_{\text{eff}}(\text{RK}(5,4)) = 0.302$ . Other fourth-order SSP RK methods with more stages can be found in [29] and [9]. Gottlieb, Shu and Tadmor [6] proved that there are no HM(2, 4) with nonnegative coefficients. Huang [8] found  $k$ -step HM( $k$ , 4) of

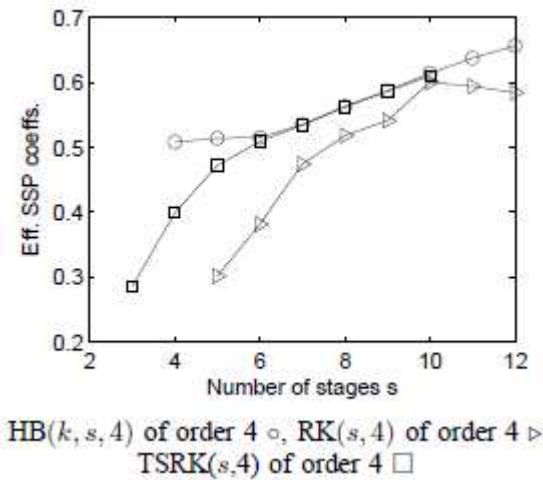


Fig. 1.  $\max_k c_{\text{eff}}(\text{HB}(k, s, 4))$ ,  $c_{\text{eff}}(\text{RK}(s, 4))$ , and  $c_{\text{eff}}(\text{TSRK}(s, 4))$  as functions of  $s$ .

order 4 for  $k = 3, 4, \dots, 7$ ,

$$\begin{aligned} c(\text{HM}(3,4)) &= 0.494, & c_{\text{eff}}(\text{HM}(3,4)) &= 0.247, \\ c(\text{HM}(4,4)) &= 0.682, & c_{\text{eff}}(\text{HM}(4,4)) &= 0.341, \\ c(\text{HM}(5,4)) &= 0.793, & c_{\text{eff}}(\text{HM}(5,4)) &= 0.396, \\ c(\text{HM}(6,4)) &= 0.879, & c_{\text{eff}}(\text{HM}(6,4)) &= 0.439, \\ c(\text{HM}(7,4)) &= 0.938, & c_{\text{eff}}(\text{HM}(7,4)) &= 0.469. \end{aligned}$$

Recently, Constantinescu and Sandu [2] obtained optimal 2-step general linear SSP methods of order 4, with certificates of global optimality for some of them. Ketcheson, Gottlieb and Macdonald [11] found 2-step RK(TSRK) methods of order 4 with nonnegative coefficients. Among these, the 10-stage method has the best effective SSP coefficient,  $c_{\text{eff}}(\text{TSRK}(10,4)) = 0.610$ .

We numerically found optimal HB( $k$ ,  $s$ , 4) with stage number  $s = 4, 5, \dots, 12$  [20]. Their  $c_{\text{eff}}$  are listed in Table I with largest  $c_{\text{eff}}(\text{HB}(3,12,4)) = 0.656$ . It is seen that  $c_{\text{eff}}(\text{HB}(2, s, 4)) > c_{\text{eff}}(\text{RK}(s, 4))$  especially when  $s$  is small.

All our new methods (except HB (2,4,4) and HB (3,4,4)) have greater  $c_{\text{eff}}$  than those of the hybrid methods listed above.

Even with only 4 steps, HB (4, 4, 4) has larger  $c_{\text{eff}}$  than Huang's best 7-step, HM(7,4), that is,  $c_{\text{eff}}(\text{HB}(4,4,4)) = 0.483 > c_{\text{eff}}(\text{HM}(7,4)) = 0.469$ . Moreover,  $c_{\text{eff}}(\text{HB}(k, s, 4)) \geq c_{\text{eff}}(\text{TSRK}(s, 4))$ ,  $k \geq 3$ , and  $c_{\text{eff}}(\text{HB}(k, s, 4)) = c_{\text{eff}}(\text{TSRK}(s, 4))$ ,  $s = 9, 10$ . HB and RK methods of order 4, including Ketcheson RK(10, 4), are compared in Fig. 1 on the basis of  $\max_k c_{\text{eff}}(\text{HB}(k, s, 4))$  as a function of the number of stages  $s$ . It is seen that  $\max_k c_{\text{eff}}(\text{HB}(k, s, 4))$  increases with  $s \leq 12$  while  $c_{\text{eff}}(\text{RK}(s, 4))$  decreases with  $s \geq 11$ . At stages  $s = 7, 8, 9$ , Fig. 1 shows that  $c_{\text{eff}}$  of HB methods and TSRK methods are almost equal.

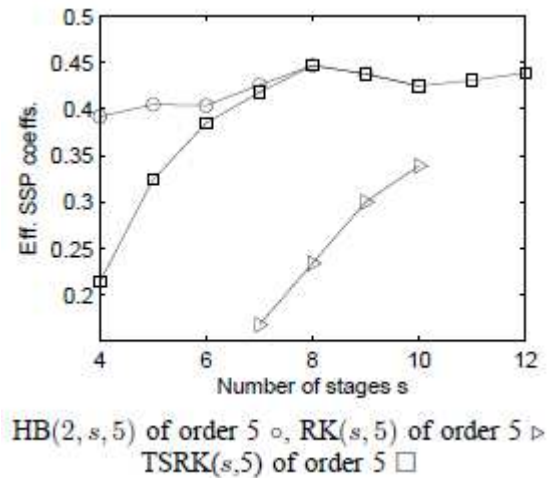


Fig. 2.  $c_{\text{eff}}(\text{HB}(2, s, 5))$ ,  $c_{\text{eff}}(\text{RK}(s, 5))$ , and  $c_{\text{eff}}(\text{TSRK}(s, 5))$  as functions of  $s$ .

B. Fifth-order methods

Ruuth and Spiteri [24] proved that there are no fifth-order SSP RK methods with nonnegative coefficients. In [22] and [25], they recently considered fifth-order methods with negative coefficients with:

$$\begin{aligned} c(\text{RK}(7,5)) &= 1.178, & c_{\text{eff}}(\text{RK}(7,5)) &= 0.168, \\ c(\text{RK}(8,5)) &= 1.875, & c_{\text{eff}}(\text{RK}(8,5)) &= 0.234, \\ c(\text{RK}(9,5)) &= 2.696, & c_{\text{eff}}(\text{RK}(9,5)) &= 0.300, \\ c(\text{RK}(10,5)) &= 3.395, & c_{\text{eff}}(\text{RK}(10,5)) &= 0.339. \end{aligned}$$

Ruuth and Hundsdorfer [23] pointed out that fifth-order linear multistep methods with nonnegative coefficients require at least  $k = 7$  steps with  $c_{\text{eff}}(\text{LM}(7,5)) = 0.038$ . In [8], one finds HMs with nonnegative coefficients and the following SSP coefficients,

$$\begin{aligned} c(\text{HM}(4,5)) &= 0.371, & c_{\text{eff}}(\text{HM}(4,5)) &= 0.185, \\ c(\text{HM}(5,5)) &= 0.525, & c_{\text{eff}}(\text{HM}(5,5)) &= 0.262, \\ c(\text{HM}(6,5)) &= 0.657, & c_{\text{eff}}(\text{HM}(6,5)) &= 0.328, \\ c(\text{HM}(7,5)) &= 0.746, & c_{\text{eff}}(\text{HM}(7,5)) &= 0.373. \end{aligned}$$

Gottlieb, Shu and Tadmor [6] proved that there are no 2-step HMs of order 4 with nonnegative coefficients. Two-step RK methods of order 5 with nonnegative coefficients are found in [11]. Among these, the 8-stage method has the best  $c_{\text{eff}}(\text{TSRK}(8, 5)) = 0.447$ .

We numerically found optimal HB( $k, s, 5$ ) with stage number  $s = 4, 5, \dots, 10$ . Their  $c_{\text{eff}}$  are listed in Table II with largest  $c_{\text{eff}}(\text{HB}(2, 8, 5)) = 0.447$ .

The effective SSP coefficients of HB ( $2, s, 5$ ), for  $s = 4, 5, \dots, 10$ , and RK( $s, 5$ ), for  $s = 7, 8, 9, 10$ , are plotted in Fig. 2. It is seen that the new methods have larger effective SSP coefficients when  $s > 6$ .

We remark that, even with a low step number, some of the new methods are competitive with the best general linear and

Table I  
 $c_{\text{eff}}(\text{HB}(k, s, 4))$  AS FUNCTION OF  $k$  AND  $s$ , AND  $c_{\text{eff}}(\text{RK}(s, 4))$  AND  $c_{\text{eff}}(\text{TSRK}(s, 4))$  AS FUNCTIONS OF  $s$ .

$s \backslash k$	2	3	4	5	6	7	RK( $s, 4$ )	TSRK( $s, 4$ )
3								0.286
4	0.398	0.461	0.483	0.495	0.503	*0.508		0.399
5	0.472	0.504	0.508	0.511	0.513	*0.514	0.302	0.472
6	0.502	0.511	0.514	*0.515			0.382	0.509
7	0.532	0.534	*0.535				0.474	0.534
8	0.561	0.562	*0.563				0.518	0.562
9	0.586	*0.587					0.541	0.586
10	0.610	*0.614					0.600	0.610
11	0.634	*0.637					0.594	
12	0.653	0.656					0.584	

Table II  
 $c_{\text{eff}}(\text{HB}(k, s, 5))$  AS FUNCTION OF  $k$  AND  $s$ , AND  $c_{\text{eff}}(\text{TSRK}(s, 5))$  AS FUNCTIONS OF  $s$ .

$s \backslash k$	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
11							0.431
12							0.439

RK methods on hand:

- All Huang's HM ( $k, 5$ ). For example, the 4-step HB(4, 4, 5) has  $c_{\text{eff}}(\text{HB}(4, 4, 5)) = 0.384 > c_{\text{eff}}(\text{HM}(7, 5)) = 0.373$  compared to Huang's best 7-step HM(7, 5).
- Ruuth's 10-stage RK(10, 5). The 4-stage HB(3, 4, 5) has  $c_{\text{eff}}(\text{HB}(3, 4, 5)) = 0.341 > c_{\text{eff}}(\text{RK}(10, 5)) = 0.339$ .
- With  $k = 2$ , although  $c_{\text{eff}}(\text{HB}(2, s, 5))$  are slightly smaller than  $c_{\text{eff}}(\text{TSRK}(s, 5))$ , they are equal when  $s \geq 6$ . However, as  $k > 2$ ,  $c_{\text{eff}}(\text{HB}(k, s, 5)) > c_{\text{eff}}(\text{TSRK}(s, 5))$ . Unlike the fourth order methods, the fifth order methods present an unusual behavior: for all step numbers, as the number of stages is greater than eight, it is not possible to obtain larger  $c_{\text{eff}}$  than with 8-stage methods. This phenomenon, which will happen differently at different order, will be seen clearly in the next subsections.

$$\begin{aligned}
 c(\text{HM}(5, 6)) &= 0.209, & c_{\text{eff}}(\text{HM}(5, 6)) &= 0.104, \\
 c(\text{HM}(6, 6)) &= 0.362, & c_{\text{eff}}(\text{HM}(6, 6)) &= 0.181, \\
 c(\text{HM}(7, 6)) &= 0.440, & c_{\text{eff}}(\text{HM}(7, 6)) &= 0.220.
 \end{aligned}$$

Two-step RK methods of order 6 with nonnegative coefficients are found in [11]. Among these, the 12-stage method has the best  $c_{\text{eff}}(\text{TSRK}(12, 6)) = 0.365$ .

We numerically found optimal HB( $k, s, 6$ ) with stage number  $s = 4, 5, \dots, 10$ . Their  $c_{\text{eff}}$  are listed in Table III with largest  $c_{\text{eff}}(\text{HB}(5, 7, 6)) = 0.351$ . 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,  $c_{\text{eff}}(\text{HB}(4, 4, 6)) = 0.272 > c_{\text{eff}}(\text{HM}(7, 6)) = 0.220$ . Note the existence of the 2-step method HB(2, 7, 6) with only 7 stages.

With  $s = 6, 7$ , HB methods have significantly better  $c_{\text{eff}}$  than TSRK methods.

In Fig. 3,  $c_{\text{eff}}(\text{HB}(5, s, 6))$  and  $c_{\text{eff}}(\text{RK}(s, 5))$  are plotted as functions of the number of stages  $s$ . It is seen that the new methods generally have larger effective SSP coefficients, especially when the number of stages of both methods are

C. Sixth-order methods

Ketcheson [10] pointed out that LM methods of order 6 with nonnegative coefficients require at least  $k = 10$  steps with  $c_{\text{eff}}(\text{LM}(10, 6)) = 0.052$ .

In [8], one finds  $k$ -step HM( $k, 6$ ) with  $k = 5, 6, 7$  and

small. It is also observed that HB(5, s, 6), for s = 5, 6, 7, have larger  $c_{\text{eff}}$  than the 10-stage RK(10, 5).

D. Seventh-order methods

In [10], LM methods of order 7 with nonnegative coefficients require at least  $k = 12$  steps with  $c_{\text{eff}}(\text{LM}(12, 7)) = 0.018$ .

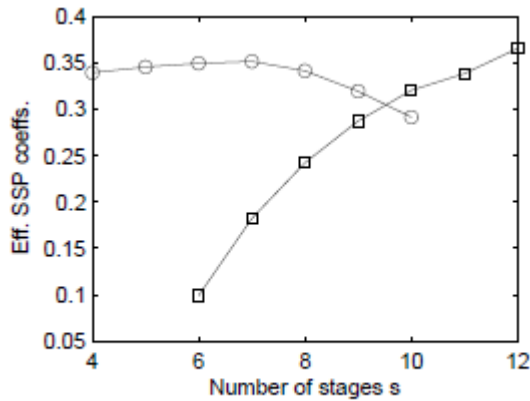
The 7-step HM(7, 7) of order 7 with  $c(\text{HM}(7, 7)) = 0.234$  and  $c_{\text{eff}}(\text{HM}(7, 7)) = 0.117$  was introduced by Huang in [8].

Two-step RK methods of order 7 with nonnegative coefficients are found in [11]. Among these, the 12-stage method has the best  $c_{\text{eff}}(\text{TSRK}(12, 7)) = 0.231$ .

We numerically found optimal HB(k, s, 7) with stage number s = 4, 5, . . . , 10 [14]. Their  $c_{\text{eff}}$  are listed in Table IV with largest  $c_{\text{eff}}(\text{HB}(6, 6, 7)) = 0.305$ .

Table III  
 $c_{\text{EFF}}(\text{HB}(k, s, 6))$  AS FUNCTION OF k AND s, AND  $c_{\text{EFF}}(\text{TSRK}(s, 6))$  AS FUNCTIONS OF s.

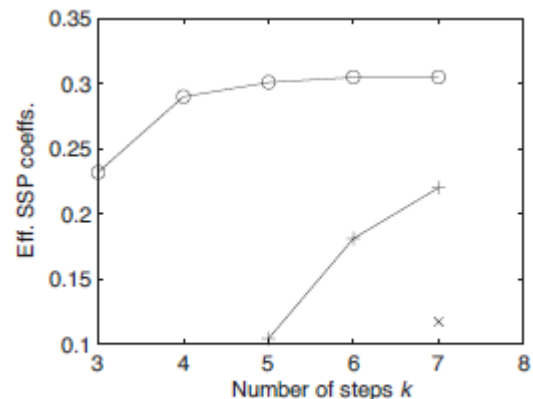
s \ k	2	3	4	5	6	7	TSRK(s, 6)
4		0.179	0.272	0.316	0.330	*0.339	
5		0.272	0.327	0.342	0.344	*0.345	
6		0.323	0.336	0.345	*0.349	0.349	0.099
7	0.182	0.341	0.349	0.351	0.351	0.351	0.182
8	0.240	0.328	0.336	0.339	*0.341	0.341	0.242
9	0.285	0.316	0.317	0.318	*0.319	0.319	0.287
10	0.284	0.288	0.290	*0.291	0.291		0.320
11							0.338
12							0.365



HB(k, s, 6) of order 6 ○, TSRK(s, 6) of order 6 □

Fig. 3.  $\max_k c_{\text{eff}}(\text{HB}(k, s, 6))$  and  $c_{\text{eff}}(\text{TSRK}(s, 6))$  versus stage number s.

In Fig. 4, the  $c_{\text{eff}}$  of HB(k, 6, 7) and HM(7,7), both of order 7, and HM(k, 6) of order 6 are plotted as functions of the number of steps, k. It is seen that HB(k, 6, 7) have larger  $c_{\text{eff}}$  than HM(7, 7) and HM(k, 6), for k = 5, 6, 7. Even with smaller step number k = 3, HB(3, 6, 7) has larger  $c_{\text{eff}}$  than HM(7,7) and HM(k, 6) which require more steps, namely,



HB(k, 6, 7) ○, HM(7, 7) ×, HM(k, 6) +

Fig. 4. Effective SSP coefficients versus number of steps k of 6-stage HB(k, 6, 7) of order 7, HM(7, 7) of order 7, and HM(k, 6) of order 6.

Table IV  
 $c_{\text{EFF}}(\text{HB}(k, s, 7))$  AS FUNCTION OF k AND s, AND  $c_{\text{EFF}}(\text{TSRK}(s, 7))$  AS FUNCTIONS OF s.

s \ k	3	4	5	6	7	TSRK(s, 7)
4		0.141	0.219	0.256	*0.287	
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	0.228	0.280	*0.285	0.285	0.285	0.071
9	0.209	0.262	*0.277	0.277	0.277	0.124
10	0.191	0.240	0.255	*0.260	0.260	0.179
11						0.218
12						0.231

Our optimal HB(k, 4, 7) are competitive with the 7-step HM(7,7), since  $c_{\text{eff}}(\text{HB}(k, 4, 7))$  increases with  $k \geq 4$ , and  $c_{\text{eff}}(\text{HB}(4, 4, 7)) = 0.141 > c_{\text{eff}}(\text{HM}(7, 7)) = 0.117$ .

For the same number of stages, the HB methods have better  $c_{\text{eff}}$  than the TSRK methods in a row-wise comparison.

Table V  
 $c_{\text{EFF}}(\text{HB}(k, s, 8))$  AS FUNCTION OF k AND s.

s \ k	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	0.192	0.231	*0.233	0.233	0.233
9	0.202	0.210	0.211	*0.212	0.212
10	0.189	0.191	*0.193	0.193	0.193

k = 5, 6, 7.

**E. Eighth-order methods**

In [10], LM methods of order 8 with nonnegative coefficients require at least  $k = 15$  steps with  $c_{\text{eff}}(\text{LM}(15, 8)) = 0.012$ .

Two-step RK methods of order 8 with nonnegative coefficients are found in [11]. Among these, the 12-stage method has the best  $c_{\text{eff}}(\text{TSRK}(12, 8)) = 0.078$ .

We numerically found optimal HB( $k, s, 8$ ) with stage number  $s = 4, 5, \dots, 10$ . Their  $c_{\text{eff}}$  are listed in Table V with largest  $c_{\text{eff}}(\text{HB}(8, 6, 8)) = 0.261$ .

Even with only 5 steps, these new methods are competitive with HM(7,7). For instance,  $c_{\text{eff}}(\text{HB}(5, 4, 8)) = 0.123 >$

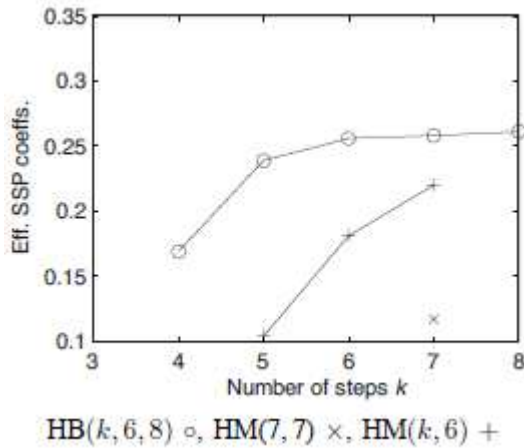


Fig. 5. Effective SSP coefficients versus number of steps  $k$  of 6-stage HB( $k, 6, 8$ ) of order 8, HM(7, 7) of order 7, and HM( $k, 6$ ) of order 6.

Table VI  
 $c_{\text{eff}}(\text{HB}(k, s, 9))$  AS FUNCTION OF  $k$  AND  $s$ .

$s \setminus k$	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	<b>0.228</b>
7	0.162	0.196	0.207	*0.215
8	0.153	0.191	0.206	*0.210
9	0.138	0.172	0.185	*0.191
10	0.126	0.157	0.168	*0.174

$c_{\text{eff}}(\text{HM}(7, 7)) = 0.117$ .

In Fig. 5, the  $c_{\text{eff}}$  of HB( $k, 6, 8$ ), HM(7, 7) of order 7 and HM( $k, 6$ ) of order 6 are compared as functions of  $k$ . It is seen that HB( $k, 6, 8$ ) have larger  $c_{\text{eff}}$  than HM(7,7) and HM( $k, 6$ ) for  $k = 5, 6, 7$ .

**F. Ninth-order methods**

In [10], LM methods of order 9 with nonnegative coefficients require at least  $k = 18$  steps with  $c_{\text{eff}}(\text{LM}(18, 9)) = 0.003$ .

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

Even with only 5 steps, these new methods are competitive with HM(7,7) of order 7. For instance,  $c_{\text{eff}}(\text{HB}(5, 6, 9)) = 0.168 > c_{\text{eff}}(\text{HM}(7, 7)) = 0.117$ .

In Fig. 6, it is seen that, for all  $k$ , HB( $k, 6, 9$ ) have larger  $c_{\text{eff}}$  than HM(7,7).

**G. Tenth-order methods**

In [10], LM methods of order 10 with nonnegative coefficients require at least  $k = 22$  steps with  $c_{\text{eff}}(\text{LM}(22, 10)) = 0.010$ .

We numerically found optimal HB( $k, s, 10$ ) with stage number  $s = 4, 5, \dots, 10$ . Their  $c_{\text{eff}}$  are listed in Table VII with largest  $c_{\text{eff}}(\text{HB}(8, 6, 10)) = 0.185$ .

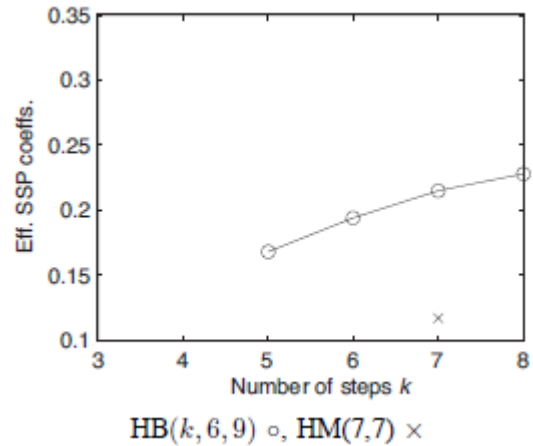


Fig. 6.  $c_{\text{eff}}(\text{HB}(k, 6, 9))$  of order 9 as function of  $k$  and HM(7,7) of order 7.

Table VII  
 $c_{\text{eff}}(\text{HB}(k, s, 10))$  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	<b>0.185</b>
7	0.131	0.171	*0.182
8	0.141	0.170	*0.176
9	0.128	0.154	*0.159
10	0.117	0.140	*0.144

Even with only 6 steps, we have  $c_{\text{eff}}(\text{HB}(6, 6, 10)) = 0.126 > 0.117 = c_{\text{eff}}(\text{HM}(7, 7))$ .

In Fig. 7, the  $c_{\text{eff}}$  of HB( $k, 6, 10$ ) of order 10 and HM(7, 7) of order 7 are compared as functions of  $k$ . It is seen that all HB( $k, 6, 10$ ) have larger  $c_{\text{eff}}$  than HM(7, 7).

**H. Eleventh-order methods**

In [10], LM methods of order 11 with nonnegative coefficients require at least  $k = 26$  steps with  $c_{\text{eff}}(\text{LM}(26, 11)) = 0.012$ .

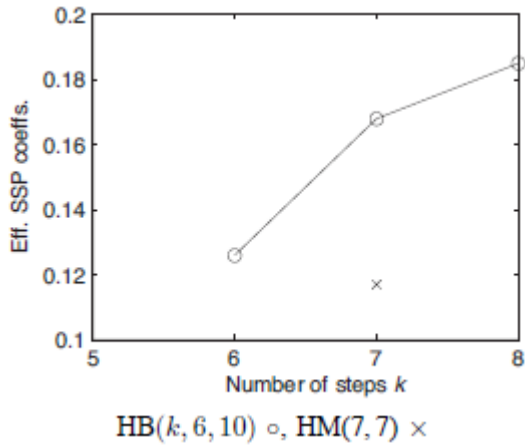


Fig. 7.  $c_{\text{eff}}(\text{HB}(k, 6, 10))$  of order 10 as function of  $k$  and  $\text{HM}(7, 7)$  of order 7.

Table VIII  
 $c_{\text{eff}}(\text{HB}(k, 7, 11))$  AS FUNCTION OF  $k$  AND  $s$ .

$s \backslash k$	6	7	8
4			*0.053
5		0.080	*0.126
6	0.029	0.092	0.142
7	0.029	0.121	0.142
8	0.028	0.110	*0.127
9	0.027	0.099	*0.114
10	0.025	0.091	*0.104

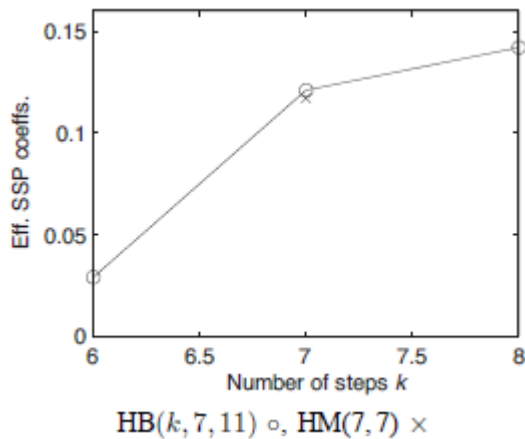


Fig. 8. Effective SSP coefficients versus number of steps  $k$  of 7-stage  $\text{HB}(k, 7, 11)$  of order 11 and  $\text{HM}(7, 7)$  of order 7.

We numerically found optimal  $\text{HB}(k, s, 11)$  with stage number  $s = 4, 5, \dots, 10$  [15]. Their  $c_{\text{eff}}$  are listed in Table VIII.

We remark that  $\text{HB}(8, 5, 11)$  is competitive with  $\text{HM}(7, 7)$  since  $c_{\text{eff}}(\text{HB}(8, 5, 11)) = 0.126 > c_{\text{eff}}(\text{HM}(7, 7)) = 0.117$ . We see that  $c_{\text{eff}}(\text{HB}(8, 6, 11)) = c_{\text{eff}}(\text{HB}(8, 7, 11)) = 0.142$  are largest for the values of  $k$  and  $s$  on hand.

It is seen in Figure 8 that  $c_{\text{eff}}(\text{HB}(8, 7, 11)) > c_{\text{eff}}(\text{HB}(7, 7, 11)) > c_{\text{eff}}(\text{HM}(7, 7)) = 0.117$ .

I. Twelfth-order methods

In [10], LM methods of order 12 with nonnegative coefficients require at least  $k = 30$  steps with  $c_{\text{eff}}(\text{LM}(30, 12)) = 0.002$ .

We numerically found optimal  $\text{HB}(k, s, 12)$  with stage number  $s = 5, 6, \dots, 10$  [17]. Their  $c_{\text{eff}}$  are listed in Table IX with largest  $c_{\text{eff}}(\text{HB}(8, 7, 12)) = 0.096$ .

VI. COMPARING  $\text{HB}(k, s, p)$  AND  $\text{RK}(s, 4)$

Table X lists  $\max_k c_{\text{eff}}(\text{HB}(k, s, p))$  which are the numbers with an asterisk and the boldface numbers in Tables I–IX, and also  $c_{\text{eff}}(\text{RK}(s, 4))$  from Table I.

In Table X, as expected, for a given  $s$ ,  $c_{\text{eff}}(\text{HB}(k, s, p))$  decreases as  $p$  increases. It is also seen that  $c_{\text{eff}}(\text{HB}(k, s, p))$  for  $p = 6, 7, \dots, 12$  are among the largest when the number of stages are about 6 to 8.

Table IX  
 $c_{\text{eff}}(\text{HB}(k, s, 12))$  AS FUNCTION OF  $k$  AND  $s$ .

$s \backslash k$	7	8
5	0.010	*0.057
6	0.035	*0.091
7	0.060	0.096
8	0.055	*0.091
9	0.051	*0.083
10	0.047	*0.076

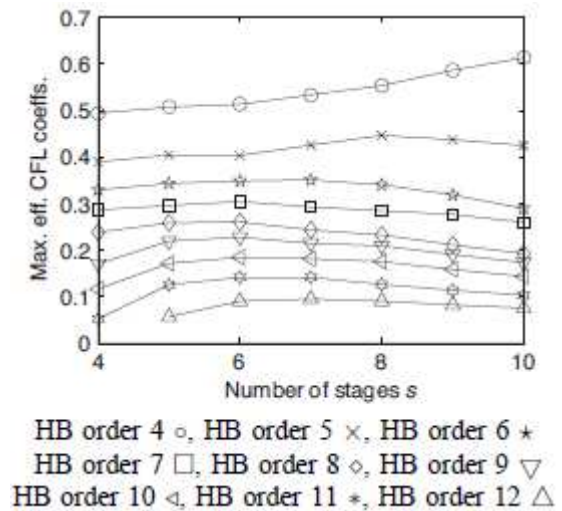


Fig. 9.  $\max_k c_{\text{eff}}(\text{HB}(k, s, p))$  as function of  $s$  for orders  $p = 4, 5, \dots, 12$ .

Hence, based on the  $c_{\text{eff}}$ , it seems that there are only 3 HB families which can have methods up to order 12 with good  $c_{\text{eff}}$ , namely, the 6-, 7- and 8-stage HB methods of order 4 to 12, are among the most efficient methods on hand.

In Fig. 9,  $\max_k c_{\text{eff}}(\text{HB}(k, s, p))$ ,  $p = 4, 5, \dots, 12$ , is plotted as a function of the stage number  $s$ . We note that, for

each  $p \geq 5$ ,  $\max_k c_{\text{eff}}(\text{HB}(k, s, p))$  first increases with  $s$  and then decreases.

Figure 10 plots  $\max_{k,s} c_{\text{eff}}(\text{HB}(k, s, p))$  as a function of the order  $p$ . We note that  $\max_{k,s} c_{\text{eff}}(\text{HB}(k, s, p))$  decreases with  $p$ .

VIII. CONCLUSION

In recent years, a collection of new optimal SSP explicit four- to ten-stage and  $k$  - step Hermite–Birkhoff methods,  $\text{HB}(k, s, p)$ , of orders  $p = 4, 5, \dots, 12$  with nonnegative

coefficients have been constructed by combining  $k$ -step methods of order one to nine and four- to ten-stage Runge–Kutta methods of order 4. Moreover, the  $\text{HB}(k, s, p)$  having the largest effective SSP coefficient have also been found among the HB methods of order  $p$  on hand. No counterparts of most of these new methods have been numerically found in the literature among hybrid and general linear multistep methods. The SSP HB methods mentioned in this paper can be obtained from the corresponding author.

Table X

$c_{\text{EFF}}(\text{RK}(s, 4))$  OF THE  $s$ -STAGE  $\text{RK}(s, 4)$  OF ORDER 4 AND  $\max_k c_{\text{EFF}}(\text{HB}(k, s, p))$  AS FUNCTION OF STAGE NUMBER  $s$  AND ORDER  $p$ .

$p \setminus s$	4	5	6	7	8	9	10
$\text{RK}(s, 4)$		0.302	0.382	0.474	0.518	0.541	0.600
4	$\text{HB}(7,4,4)$ 0.508	$\text{HB}(7,5,4)$ 0.514	$\text{HB}(5,6,4)$ 0.515	$\text{HB}(4,7,4)$ 0.535	$\text{HB}(3,8,4)$ 0.554	$\text{HB}(3,9,4)$ 0.587	$\text{HB}(3,10,4)$ 0.614
5	$\text{HB}(6,4,5)$ 0.392	$\text{HB}(5,5,5)$ 0.405	$\text{HB}(3,6,5)$ 0.404	$\text{HB}(3,7,5)$ 0.426	$\text{HB}(2,8,5)$ 0.447	$\text{HB}(2,9,5)$ 0.438	$\text{HB}(2,10,5)$ 0.425
6	$\text{HB}(7,4,6)$ 0.339	$\text{HB}(7,5,6)$ 0.345	$\text{HB}(6,6,6)$ 0.349	$\text{HB}(5,7,6)$ 0.351	$\text{HB}(6,8,6)$ 0.341	$\text{HB}(6,9,6)$ 0.319	$\text{HB}(4,10,6)$ 0.290
7	$\text{HB}(7,4,7)$ 0.287	$\text{HB}(7,5,7)$ 0.296	$\text{HB}(6,6,7)$ 0.305	$\text{HB}(6,7,7)$ 0.293	$\text{HB}(5,8,7)$ 0.285	$\text{HB}(5,9,7)$ 0.277	$\text{HB}(6,10,7)$ 0.260
8	$\text{HB}(8,4,8)$ 0.239	$\text{HB}(8,5,8)$ 0.259	$\text{HB}(8,6,8)$ 0.261	$\text{HB}(8,7,8)$ 0.244	$\text{HB}(6,8,8)$ 0.233	$\text{HB}(7,9,8)$ 0.212	$\text{HB}(6,10,8)$ 0.193
9	$\text{HB}(8,4,9)$ 0.171	$\text{HB}(8,5,9)$ 0.220	$\text{HB}(8,6,9)$ 0.228	$\text{HB}(8,7,9)$ 0.215	$\text{HB}(8,8,9)$ 0.210	$\text{HB}(8,9,9)$ 0.191	$\text{HB}(8,10,9)$ 0.174
10	$\text{HB}(8,4,10)$ 0.117	$\text{HB}(8,5,10)$ 0.172	$\text{HB}(8,6,10)$ 0.185	$\text{HB}(8,7,10)$ 0.182	$\text{HB}(8,8,10)$ 0.176	$\text{HB}(8,9,10)$ 0.159	$\text{HB}(8,10,10)$ 0.144
11	$\text{HB}(8,4,11)$ 0.053	$\text{HB}(8,5,11)$ 0.126	$\text{HB}(8,6,11)$ 0.142	$\text{HB}(8,7,11)$ 0.142	$\text{HB}(8,8,11)$ 0.127	$\text{HB}(8,9,11)$ 0.114	$\text{HB}(8,10,11)$ 0.104
12		$\text{HB}(8,5,12)$ 0.057	$\text{HB}(8,6,12)$ 0.091	$\text{HB}(8,7,12)$ 0.096	$\text{HB}(8,8,12)$ 0.091	$\text{HB}(8,9,12)$ 0.083	$\text{HB}(8,10,12)$ 0.076

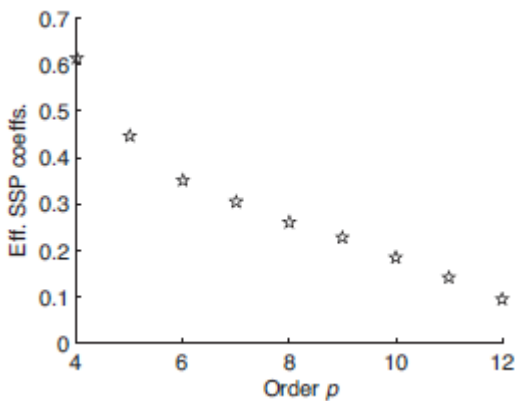


Fig. 10.  $\max_{k,s} c_{\text{eff}}(\text{HB}(k, s, p))$  versus order  $p$ .

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