STRONG STABILITY PRESERVING HERMITE–BIRKHOFF TIME DISCRETIZATION METHODS

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Abstract

This thesis is concerned with strong-stability-preserving (SSP) high-order time discretizations, which have been specially developed for hyperbolic partial differential equations over the past 20 years. The main goal of the thesis is to construct explicit, s-stage, SSP Hermite–Birkhoff (HB) time discretization methods of order p with nonnegative coefficients for the integration of hyperbolic conservation laws.

The Shu–Osher form and the canonical Shu–Osher form by means of the vector formulation for SSP Runge–Kutta (RK) methods are extended to SSP HB methods. The SSP coefficients of k-step, s-stage methods of order p, HB(k, s, p), based on k-step methods of order $(p-3)$ with s-stage explicit RK methods of order 4, and based on k-step methods of order $(p-4)$ with s-stage explicit RK methods of order 5, respectively, for $s = 4, 5, \ldots, 10$ and $p = 4, 5, \ldots, 12$, are constructed and compared with other methods.

The fairly good efficiency gains of the new, numerically optimal, SSP HB methods over other SSP methods, such as Huang's hybrid methods and RK methods, are numerically shown by mean of their effective SSP coefficients and largest effective CFL numbers. The formulae of these new, optimal methods are presented in their Shu–Osher form.

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Dedication

In memory of my grandfather who was taken before I could complete this work. We always love you.

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List of Acronyms and Symbols

$\text{num}_{\text{eff}}(M)$	the largest effective CFL number of method M, see equation (4.1.5), page 71
$\text{HB}_{\text{RKq}}(k,s,p)$	Hermite–Birkhoff methods of order p combining k-step methods and s-stage RKq of order q, see equation (3.3.0), page 58
$\text{PEG}(\text{num}_{\text{eff}}(M_2), \text{num}_{\text{eff}}(M_1))$	the percentage efficiency gain of $\text{num}_{\text{eff}}(M2)$ over $\text{num}_{\text{eff}}(M1)$, see equation (4.1.8), page 71
$\text{PEG}(c_{\text{eff}}(\text{M2}), \text{c}_{\text{eff}}(\text{M1}))$	the percentage efficiency gain of c_{eff}(M2) over c_{eff}(M1), see equation (2.2.2), page 34
$c_{\text{eff}}(M)$	effective SSP coefficients of an SSP method M, see equation (2.2.1), page 34
$R_{\text{num/theor}}$	the ratio of the maximum numerical to theoretical stepsizes, see equation (4.1.7), page 71

Chapter 1

Introduction

In this thesis, we develop a class of high-order, time discretization, Hermite–Birkhoff (HB) methods for hyperbolic conservation laws. The main goal is to handle discontinuities even from smooth initial data, which result in spurious oscillations, overshoots and numerical instability in solving hyperbolic partial differential equations (PDEs). The thesis is concerned with strong stability preserving (SSP) HB methods to avoid these troubles. In this chapter, we provide background information and motivation for the SSP HB methods developed in this thesis.

1.1 Literature and motivation

1.1.1 The need for SSP methods

Numerical methods play an important role and made enormous progress for finding solutions of ordinary differential equations (ODEs). Such methods are valuable tools since finding analytic solutions is not often easy nor possible. There are many excellent books, for example [1], [13] and [26], which present many well-studied methods such as Runge–Kutta (RK), linear multistep (LMS) and general linear multistep (GLM) methods.

SSP methods are ODE solvers designed for solving ODEs obtained from the spatial discretization of time-dependent PDEs, specifically hyperbolic conservation laws.

In the one-dimensional scalar case, a hyperbolic conservation law has the form

$$y_t + g(y)_x = 0, \quad y(x,0) = y_0(x), \tag{1.1.1}$$

where y is a function of x and t.

There are some reasons to study hyperbolic conservation laws (see [30] for an introduction to hyperbolic conservation laws and their numerical solutions). For instance, this class of PDEs comes from many practical problems such as conservation of mass, energy and momentum problems. Moreover, solving these equations has some special difficulties like shock formation.

We consider a simple example of hyperbolic conservation laws, namely, a shock tube problem in one dimension ([31, p. 15–26], [30, p. 3–4], [27, p. 72]). In this physical example, a tube filled with gas is divided into two regions by a membrane. We suppose that the left region of the tube has gas with higher density and higher pressure than the right region. When the membrane is removed, the gas flows. Besides, the motion of the gas is from left to right. The initial velocity is always zero. The result gives shock and rarefaction waves. The shock wave propagates to the right region and the rarefaction moves in the opposite direction. The shock tube problem is a special case of the Riemann problem, which has the form (1.1.1) with

$$y_0(x) = \begin{cases} y_l & \text{if } x < 0, \\ y_r & \text{if } x > 0, \end{cases}$$

here y_l and y_r are constant states.

To find the numerical solution of (1.1.1), we use the method-of-lines. In particular, we first discretize the spatial derivative $g(y)_x$ by finite elements, finite difference, finite volumes or spectral methods (see [3, 14, 23, 44]). Thus, spatial discretization yields a set of time-dependent ODEs with initial condition of the form:

$$\frac{dy}{dt} = f(t, y(t)), \qquad y(t_0) = y_0, \tag{1.1.2}$$

where $y \in \mathbb{R}^N$ is a vector of approximations to the exact solution $y(x,t)$ of PDE (1.1.1) and $f : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$ represents a discretization of the spatial variables forming a system of semi-discrete equations. The size of system (1.1.2) is usually very large. It depends on Δx, the parameter in the spatial discretization. In other words, smaller Δx leads to larger ODE systems. Now these ODE systems can be integrated by using some standard time-stepping techniques such as general linear, linear multistep or RK methods. Here a relevant question concerns stability and convergence. For problems with smooth solutions, a linear stability analysis is enough. However, if the PDE is nonlinear and the solution is not smooth, for instance hyperbolic partial differential equations with discontinuous solutions, linear stability analysis is not adequate (see [10] for an example and detail explanation). One of the best known nonlinear stability conditions is total variation diminishing (TVD), which was suggested by Ami Harten in 1983 [14]. The TVD property is one important step to prove the convergence of the numerical solution.

The development of SSP methods is motivated by an observation about the solutions of PDEs. Indeed, the exact solutions of many important PDEs

$$y_t = f(t, y, y_x, y_{xx}, \ldots), \tag{1.1.3}$$

satisfy the monotonicity property

$$\|y(t + \Delta t)\| \leq \|y(t)\|, \tag{1.1.4}$$

where $\|\cdot\|$ is a norm, semi-norm, or, more generally, any convex functional. Therefore, when solving system (1.1.1) numerically, it is natural to require that the numerical solutions also reflect the qualitative property of the exact solution, that is,

$$\|y_{n+1}\| \leq \|y_n\|, \tag{1.1.5}$$

where y_n is a numerical approximation to $y(t_0 + n\Delta t)$.

In the context of scalar one-dimensional hyperbolic conservation laws, the total variation seminorm of the numerical solutions satisfies the monotonicity property (1.1.5) (see [14]).

Unlike linear stability, nonlinear stability is sometimes difficult to examine. Many attempts have been tried to find a convenient high-order spatial discretization so that when coupled with the forward Euler method (FE) time stepping method, one achieves the expected nonlinear stability when numerically solving hyperbolic conservation laws (see, for example, [14, 43, 58, 3, 32]). On the other hand, high-order time discretizations also have important effects, namely, suitable spatial discretizations may change the nonlinear stability property when coupled with linearly stable high-order time discretizations.

Therefore, it is necessary and useful to develop high-order time discretizations such that when coupled with spatial discretization, they will ensure (1.1.5) is satisfied by the same spatial discretization coupled with the FE method.

In our research, the semi-discretization is assumed to be designed such that the solution of the resulting ODE system (1.1.2) satisfies a monotonicity property analogous to (1.1.4) under the forward Euler method (FE), that is,

$$\|y_n + \Delta t f(t_n, y_n)\| \leq \|y_n\|, \tag{1.1.6}$$

for all $0 < \Delta t \leq \Delta t_{\mathrm{FE}}$ and all y_n where Δt_{FE} is a maximal step size for which (1.1.6) holds, and $\|\cdot\|$ is a given convex functional. Under this assumption, we are now interested in higher-order, explicit, HB methods, a class of multistep and multistage numerical methods which preserve the monotonicity property

$$\|y_{n+1}\| \leq \max_{0 \leq j \leq k-1} \|y_{n-j}\|, \quad 0 \leq \Delta t \leq c\Delta t_{\mathrm{FE}}, \tag{1.1.7}$$

when they are coupled with the spatial semi-discretization. Here k is a positive integer representing the number of previous steps used to compute the numerical solution at the next step.

A multistage (and/or multistep) method is said to be SSP if it satisfies the monotonicity property (1.1.7) whenever the FE condition (1.1.6) is fulfilled (for one-step methods such as RK methods, see [10]). The number c in (1.1.7), referred to as the SSP coefficient, depends only on the numerical integration method. In the literature, c has been called the CFL coefficient. However, SSP coefficient is a more suitable term because the CFL condition is derived from the ratio between the time step and the spatial grid size, while the SSP coefficient comes from the ratio between the SSP time step and the strongly stable FE time step. Great effort has been devoted to search for numerical methods with largest SSP coefficients c among many different classes of methods (see [47], [9], [10] and [17]).

All the HB methods in our present work involve HB interpolation polynomials. Moreover, these methods are all SSP because they can be decomposed in terms of SSP FE methods by convexity and they use an extension of the Shu–Osher representation, thus they maintain the monotonicity property, while having high-order accuracy in time, perhaps under a modified restriction

$$\Delta t \leq c(\mathrm{HB}(k,s,p))\Delta t_{\mathrm{FE}}. \tag{1.1.8}$$

A typical numerical example given by Gottlieb and Shu [11], shows the necessity of using SSP methods. In this example, the test problem is inviscid Burgers' equation with Riemann initial data:

$$\frac{\partial}{\partial t}u(x,t) + \frac{\partial}{\partial x}\left[\frac{1}{2}\,u(x,t)^2\right] = 0, \quad u(x,0) = \begin{cases} 1, & x \leq 0, \\ -0.5, & x > 0. \end{cases} \tag{1.1.9}$$

This problem is discretized first by using the minmod limiter based on Monotone Upstream-centered Schemes for Conservation Law (MUSCL). After spatial discretization, two 2nd-order RK methods are applied, (a) the SSP 2nd-order RK,

$$\begin{aligned} u^{(1)} &= u^n + \Delta t\, L(u^n) \\ u^{(n+1)} &= \frac{1}{2}\,u^{(n)} + \frac{1}{2}\,\Delta t\, L(u^{(1)}) \end{aligned}$$

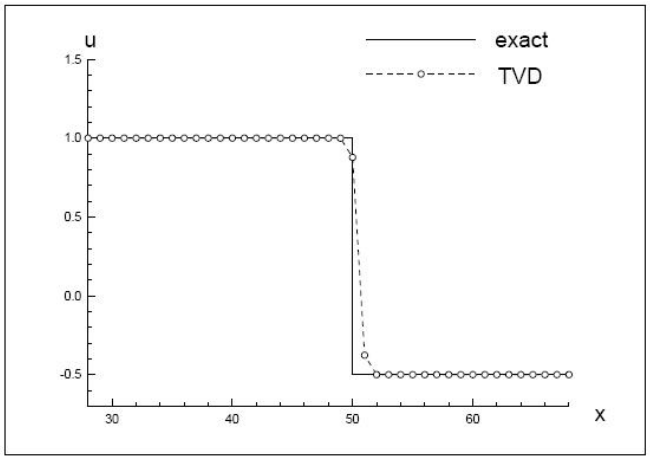


Figure 1.1: Solution after 400 time steps and 50 points in space with SSP RK method, taken from [11]

and (b) the non-SSP 2nd-order RK,

$$u^{(1)} = u^n - 20\Delta t\, L(u^n)$$
$$u^{(n+1)} = u^{(n)} + \frac{41}{40}\,\Delta t L(u^{(n)}) - \frac{1}{40}\,\Delta t L(u^{(1)})$$

where $L(.)$ approximates the spatial derivatives in (1.1.9).

From Figs. 1.1 and 1.2, we see clearly that the SSP result has no overshoot, but the non-SSP result has an overshoot. Therefore, in this case, it is safer to use SSP methods because they help to reduce the oscillatory and overshoot at discontinuous points. There are more examples ([20], [22], [9] for details) to compare the SSP methods and non-SSP methods and to demonstrate the safety of using SSP methods, especially for solving hyperbolic PDEs.

1.1.2 Some developments of SSP methods

We briefly review the development of SSP methods. After Ami Harten suggested TVD [14] in 1983, SSP methods were first developed by Shu [50] and then Shu and

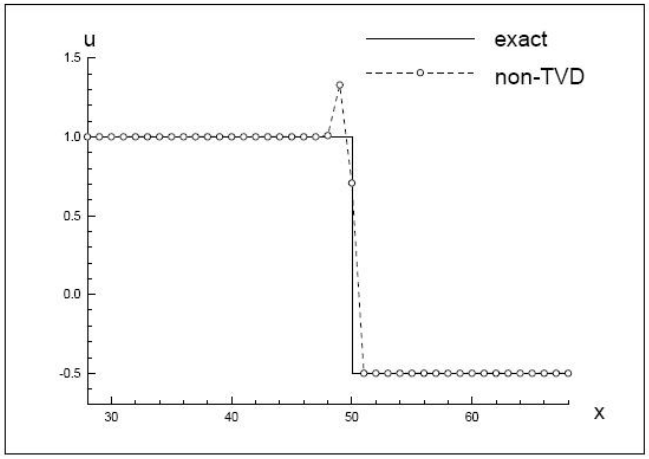


Figure 1.2: Solution after 528 time steps and 50 points in space with non-SSP RK method, taken from [11]

Osher [53]. In [50] and [53], the relevant norm was the total variation norm. The forward Euler time-discretization used in the method of lines was assumed to be TVD (total variation diminishing); therefore, the class was termed TVD time discretization methods. The term "strong stability preserving" was first used in [12] by Gottlieb, Shu and Tadmor and it is more suitable because these methods preserve *strong stability* in the same norm. Moreover, in [50], Shu and Osher constructed a series of second- to fifth-order SSP RK methods. Shu [50] found a class of first-order SSP RK methods with very large SSP coefficients, as well as a class of high-order SSP linear multistep methods. Later, Gottlieb and Shu [11] derived optimal s-stage SSP RK methods of order s for $s = 2, 3$, and proved that, for $s = 4$, there is no such SSP RK method of order 4 with nonnegative coefficients. In this paper, they also studied explicit SSP multistep methods and implicit SSP RK methods. Spiteri and Ruuth [56, 57] studied optimal s-stage SSP RK methods of order p with $s > p$ for $p \leq 4$. They proved the nonexistence of fifth-order SSP RK methods with nonnegative coefficients [46] and constructed some fifth-order methods of seven to nine stages with downwind-biased spatial discretization [47]. A 10-stage method of order 5 was given in [44]. Hundsdorfer, Ruuth and Spiteri [18] proved that the implicit Euler method can unconditionally preserve the strong stability of the FE method (see also [15]) and studied multistep methods with specific starting procedures.

Furthermore, some SSP methods for special purposes have also been investigated. For example, low storage RK methods were constructed in [11, 12, 44, 47, 56]. SSP methods for constant-coefficient linear systems were studied in [8, 12]. For a description of the state-of-the-art, we refer the reader to the review papers by Gottlieb, Shu and Tadmor [12], Shu [51], Gottlieb [7], and Gottlieb, Ketcheson and Shu [9].

Previous studies have investigated optimally contractive one-step, multistage methods [24, 59, 8] and one-stage, multistep methods [28, 29]. Several authors such as Spijker, Higueras and Ketcheson studied the equivalence between SSP coefficient and the radius of absolute monotonicity for general linear methods (see [55, 16, 21] for further details). Ferracina and Spijker [5, 6] and Higueras [15, 16] in their research established a connection between SSP and contractivity studies. These concepts have been developed independently (see, e.g., [25, 54, 28]). Therefore, some optimal SSP and optimal contractive methods agree. The SSP coefficient is also related to the radius of absolute monotonicity. This helps develop new optimal SSP methods [20, 22]. Ketcheson [21] surveyed the threshold factors for linear autonomous equations and also presented optimal explicit and implicit SSP linear multistep methods. Huang [17] explored hybrid methods (HM) based on linear multistep methods.

Spijker extended the theory of monotonicity to a larger class of general linear methods [55], which evaluate the next step by using input values at multiple steps and multiple stages.

1.2 Outline

This thesis includes six chapters in which Chapter 1 gives the general view of SSP methods in the literature and motivation to the study of this subject. The remainder of the thesis is organized as follows:

Chapter 2 can be divided into two parts. The first part deals with the general theory of SSP HB methods for hyperbolic conservation laws including the formulae and the order conditions of our methods. Moreover, it presents the transformation between the Butcher and Shu–Osher forms as well as canonical Shu–Osher form. All the SSP coefficients of HB methods obtained from combining k-step methods of order $(p-3)$ and RK4 are demonstrated in the second part, Section 2.2 of this chapter. Examples are found in chapter 4.

Chapter 3 presents all the SSP coefficients of optimal HB methods obtained when combining k-step methods of order $(p-4)$ and RK5 and compares our methods with other methods and our methods themselves obtained from RK methods of different orders. An example is found in chapter 5.

Chapter 4 shows the numerical results of some typical SSP HB methods such as (a) 4-stage optimal, noncanonical SSP HB methods, (b) optimal, noncanonical SSP HB methods of order 4 and (c) 8-stage optimal, canonical SSP HB methods, when coupled with different spatial discretizations such as difference quotient and WENO5 applied to Burgers' equation and linear advection equation. These methods are considered as remarkable examples for chapter 3.

As an example for Chapter 3, in Chapter 5, 8-stage optimal, explicit, canonical SSP HB methods obtained from k-step methods and RK method of order 5 are applied to Burgers' equation to obtain the largest effective CFL numbers and are compared to other known methods.

The final chapter, Chapter 6, presents the conclusions and future work.

1.3 Contributions

The contribution of this thesis is presented in this section. We believe that these results are new and hope that they are remarkable contributions to the SSP theory. The principal contribution is the construction of new, explicit, optimal SSP Hermite–Birkhoff methods (here in our research HB(k, s, p) method with the largest SSP coefficients obtained by fmincon in the MATLAB Optimization Toolbox, and with nonnegative coefficients is regarded as the optimal method), as a class of general linear methods, with nonnegative coefficients and good SSP coefficients. Moreover, we show numerically the fairly good efficiency gain of the new methods over other well-known methods. In particular:

(1) Develop the SSP theory for new HB methods. Indeed, we extend the noncanonical and canonical Shu–Osher forms as well as the vector form of Runge–Kutta methods for HB methods (Section 2.1). Based on the optimization problems (Subsection 2.1.4 and 2.1.8), we achieve the formulae of some new optimal HB methods from RK4 or from RK5 of specific stage or specific order. These results are presented in [38, 35, 41] for noncanonical form and [40, 42] for canonical form.

(2) Find good SSP coefficients from constructing optimal s-stage SSP HB methods of order p, for $s = 4, 5, \ldots, 10$ and $p = 4, 5, \ldots, 12$, by combining k-step methods of order $(p-3)$ and RK4 (Section 2.2) or k-step methods of order $(p-4)$ and RK5 (Section 3.2). These SSP coefficients, which have not been investigated previously, are really good when compared to other methods. For example, HB(2,8,5), based on RK4, is 91% better than RK(8,5). Furthermore, they give extremely important results on the existence of SSP methods of order $p \geq 9$ with nonnegative coefficients and good SSP coefficients. The effective SSP coefficients obtained from these families show that HB methods from RK5 are better than HB methods from RK4.

(3) Show fairly good numerical efficiency of these newly obtained methods over other known methods and the suitable combinations of our new methods with some spatial discretizations methods through the largest effective CFL numbers

and their percentage efficiency gains. For instance, we combine (a) 4-stage, noncanonical HB methods (RK4) of order p with difference quotient [38], (b) s-stage, noncanonical HB methods (RK4) of order 4 with WENO5 [35], (c) 8-stage, canonical HB methods (RK4) of order p with WENO5, (d) 8-stage, canonical HB methods (RK5) of order p with WENO5.

Chapter 2

SSP s-Stage HB Methods Based on Combining k-Step with RK4 Methods

2.1 SSP Hermite–Birkhoff methods

2.1.1 General HB formulation and notation

Throughout this work, the following notation will be used:

Notation 2.1.1

- *k denotes the number of steps of a given method,*
- *s denotes the number of stages of a given method per time step,*
- *p denotes the order of a given method,*
- *HB(k, s, p) denotes k-step, s-stage SSP Hermite–Birkhoff methods of order p,*
- *LM(k, p)denotes linear multistep methods,*

- *GL(k,p) denotes k-step, 4-stage general linear methods of order p,*
- *HM(k,p) denotes k-step SSP hybrid methods of order p,*
- *RK(s,p) denotes s-stage SSP Runge–Kutta methods of order p,*
- *TSRK(s,p): 2-step, s-stage Runge–Kutta methods of order p.*

All the methods considered in this work are SSP, so the denominations “SSP” will generally be omitted in what follows.

Notation 2.1.2

- *The abscissa vector $\sigma = [c_1, c_2, c_3, \dots, c_s]^T$, $0 \le c_j \le 1$, defines the off-step points $t_n + c_j\Delta t$, $j = 1, 2, \dots, s$. 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 $Y_1 = y_n$.*

********CORRECTIONS FOLLOWED REPORTS********

Definition 2.1.3 *An HB(k,s,p) method to perform integration from t_n to t_{n+1} is defined by the following s formulae:*

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

$$Y_i = v_{B,i}y_n + \sum_{j=1}^{k-1} A_{B,ij}y_{n-j} + \Delta t\left[\sum_{j=1}^{i-1} a_{ij}F_j + \sum_{j=1}^{k-1} B_{B,ij}f_{n-j}\right], \qquad i = 2, 3, \dots, s. \tag{2.1.1}$$

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

$$y_{n+1} = v_{B,s+1}y_n + \sum_{j=1}^{k-1} A_{B,s+1,j}y_{n-j} + \Delta t\left[\sum_{j=1}^{s} b_jF_j + \sum_{j=1}^{k-1} B_{B,s+1,j}f_{n-j}\right]. \tag{2.1.2}$$

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 $y(t_{n+1}) = y(t_n + \Delta t)$.

**********END*********************

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.

2.1.2 Construction of the order conditions

For the construction of the order conditions of s-stage HB(k, s, p), we denote:

$$B_i(j) = \sum_{\ell=1}^{k-1} A_{B,i\ell} \frac{(-\ell)^j}{j!} + \sum_{\ell=1}^{k-1} B_{B,i\ell} \frac{(-\ell)^{j-1}}{(j-1)!}, \qquad \begin{cases} i = 2, 3, \ldots, s, \\ j = 1, 2, \ldots, p, \end{cases} \tag{2.1.3}$$

which comes from the backsteps of the methods.

Forcing an expansion of the numerical solution produced by formulae (2.1.1)–(2.1.2) to agree with a Taylor expansion of the true solution, we obtain multistep and RK type order conditions that must be satisfied by HB(k, s, p) methods.

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

$$v_{B,i} + \sum_{j=1}^{k-1} A_{B,ij} = 1, \qquad i = 2, 3, \ldots, s+1, \tag{2.1.4}$$

which are obtained when applying Taylor expansion (2.1.1)–(2.1.2) up to $O(\Delta t)$.

Second, to obtain HB methods of order p, we impose the following $(p-3)$ simplifying assumptions on the abscissa vector $\sigma = [c_1, c_2, c_3, \ldots, c_s]^T$:

$$\sum_{j=1}^{i-1} a_{ij} c_j^m + m! B_i(m+1) = \frac{1}{m+1} c_i^{m+1}, \qquad \begin{cases} i = 2, 3, \ldots, s, \\ m = 0, 1, \ldots, p-4. \end{cases} \tag{2.1.5}$$

The set of equations (2.1.5) is derived from the Taylor expansions of each stage Y_i up to order $(p-3)$. These assumptions help to reduce the large number of RK-type order conditions (see [36], [37]).

Finally, matching Taylor expansions of the exact solution and numerical solution (2.1.2) up to order p and using the set of simplifying assumptions (2.1.5) to reduce the order conditions, we obtain five sets of equations to be solved for order p, and these order conditions are analogous to the set of order conditions of RK of order 4:

$$\sum_{i=1}^{s} b_i c_i^m + m!B(m+1) = \frac{1}{m+1}, \qquad m = 0, 1, \ldots, p-1, \tag{2.1.6}$$

$$\sum_{i=2}^{s} b_i \left[\sum_{j=1}^{i-1} a_{ij} \, \frac{c_j^{p-3}}{(p-3)!} + B_i(p-2) \right] + B(p-1) = \frac{1}{(p-1)!}, \tag{2.1.7}$$

$$\sum_{i=2}^{s} b_i \frac{c_i}{p-1} \left[\sum_{j=1}^{i-1} a_{ij} \, \frac{c_j^{p-3}}{(p-3)!} + B_i(p-2) \right] + B(p) = \frac{1}{p!}, \tag{2.1.8}$$

$$\sum_{i=2}^{s} b_i \left[\sum_{j=1}^{i-1} a_{ij} \, \frac{c_j^{p-2}}{(p-2)!} + B_i(p-1) \right] + B(p) = \frac{1}{p!}, \tag{2.1.9}$$

$$\sum_{i=2}^{s} b_i \left[\sum_{j=1}^{i-1} a_{ij} \left[\sum_{k=1}^{j-1} a_{jk} \, \frac{c_k^{p-3}}{(p-3)!} + B_j(p-2) \right] + B_i(p-1) \right] + B(p) = \frac{1}{p!}, \tag{2.1.10}$$

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

$$B(j) = \sum_{i=1}^{k-1} A_{B,s+1,i} \, \frac{(-i)^j}{j!} + \sum_{i=1}^{k-1} B_{B,s+1,i} \, \frac{(-i)^{j-1}}{(j-1)!}, \qquad j = 1, \ldots, p. \tag{2.1.11}$$

These order conditions are simply RK order conditions with backstep parts $B_i(\cdot)$ and $B(\cdot)$. The HB(k, s, p) methods with order conditions (2.1.4)–(2.1.10) are what we call HB(k, s, p) based on s-stage RK4 or HB(k, s, p) obtained from combining k-step methods of order $(p-3)$ with s-stage RK4.

HB(k, s, p) based on s-stage RK5 or HB(k, s, p) obtained from combining k-step methods of order $(p-4)$ with s-stage RK5 will be considered in the next chapter, Chapter 3.

2.1.3 A Shu–Osher form of s-stage HB methods for deriving the SSP property

Now we extend the Shu–Osher representation to our methods so that we can rewrite our s-stage HB(k,s,p) methods in formulae (2.1.1)–(2.1.2) as convex combinations of FE method [53] to show that they will preserve the monotonicity property (1.1.7). The following procedure presents how we can transform HB(k,s,p) formulae into Shu–Osher form (see also in [41]).

Firstly, let

$$\lambda_{i\ell}, \lambda_{s+1,\ell} \geq 0, \qquad \sum_{\ell=1}^{i-1} \lambda_{i\ell} = 1, \quad i = 3, 4, \ldots, s, \quad \text{and} \quad \sum_{\ell=1}^{s} \lambda_{s+1,\ell} = 1. \tag{2.1.12}$$

Then, formulae (2.1.1) and (2.1.2) become

$$Y_i = \left[\sum_{\ell=1}^{i-1} \lambda_{i\ell}\right] v_{B,i} y_n + \sum_{j=1}^{k-1} A_{B,ij} y_{n-j} + \Delta t \left[\sum_{j=1}^{i-1} a_{ij} F_j + \sum_{j=1}^{k-1} B_{B,ij} f_{n-j}\right], \quad i = 3, 4, \ldots, s, \tag{2.1.13}$$

$$y_{n+1} = \left[\sum_{\ell=1}^{s} \lambda_{s+1,\ell}\right] v_{B,s+1} y_n + \sum_{j=1}^{k-1} A_{B,s+1,j} y_{n-j} + \Delta t \left[\sum_{j=1}^{s} b_j F_j + \sum_{j=1}^{k-1} B_{B,s+1,j} f_{n-j}\right]. \tag{2.1.14}$$

Secondly, we express the term y_n in formulae (2.1.1) as a function of Y_i,

$$y_n = \frac{1}{v_{B,i}} \left\{ Y_i - \sum_{j=1}^{k-1} A_{B,ij} y_{n-j} - \Delta t \left[\sum_{j=1}^{i-1} a_{ij} F_j + \sum_{j=1}^{k-1} B_{B,ij} f_{n-j}\right] \right\}, \qquad i = 2, 3, \ldots, s. \tag{2.1.15}$$

To avoid confusion, we replace the index i by m in formulae (2.1.15) to obtain

$$y_n = \frac{1}{v_{B,m}} \left\{ Y_m - \sum_{j=1}^{k-1} A_{B,mj} y_{n-j} - \Delta t \left[\sum_{j=1}^{m-1} a_{mj} F_j + \sum_{j=1}^{k-1} B_{B,mj} f_{n-j}\right] \right\}, \qquad m = 2, 3, \ldots, s. \tag{2.1.16}$$

Thirdly, for $i = 3, 4, \ldots, s$ and $\ell = 1, 2, \ldots, i-1$, we substitute (2.1.16) into the terms $\lambda_{i\ell} v_{B,i} y_n$ in (2.1.13) with $m = \ell$. Similarly, we replace y_n in the terms $\lambda_{s+1,\ell} v_{B,s+1} y_n$ in (2.1.14) by (2.1.16) with $m = \ell$. If we set

$$\alpha_{ij} = \lambda_{ij} v_{B,i}/v_{B,j}, \qquad j = 2, 3, \ldots, i-1, \quad i = 3, 4, \ldots, s, s+1, \tag{2.1.17}$$

$$A_{B,i0} = v_{B,i}, \qquad i = 3, 4, \ldots, s, s+1, \tag{2.1.18}$$

$$B_{B,i0} = a_{i1}, \qquad i = 2, 3, \ldots, s, \tag{2.1.19}$$

$$B_{B,s+1,0} = b_1, \tag{2.1.20}$$

after some calculations, formulae (2.1.1) with $i = 2$, (2.1.13) and (2.1.14) become:

$$\begin{aligned} Y_i &= \sum_{j=1}^{k-1} \Big[A_{ij} y_{n-j} + \Delta t B_{ij} f_{n-j} \Big] + \sum_{j=1}^{i-1} \Big[\alpha_{ij} Y_j + \Delta t \, \beta_{ij} F_j \Big], \; i = 2, 3, \ldots, s+1, \\ y_{n+1} &= Y_{s+1}, \end{aligned} \tag{2.1.21}$$

where the coefficients are

$$A_{ij} = A_{B,ij} - \sum_{\ell=2}^{i-1} \alpha_{i\ell} A_{B,\ell j}, \quad j = 0, 1, \ldots, k-1, \quad i = 3, \ldots, s, s+1, \tag{2.1.22}$$

$$A_{2j} = A_{B,2j} \qquad j = 1, \ldots, k-1, \tag{2.1.23}$$

$$\alpha_{i1} = A_{i0}, \qquad i = 3, \ldots, s, s+1, \tag{2.1.24}$$

$$\alpha_{21} = v_{B,2}, \tag{2.1.25}$$

$$B_{ij} = B_{B,ij} - \sum_{\ell=2}^{i-1} \alpha_{i\ell} B_{B,\ell j}, \quad j = 0, 1, \ldots, k-1, \quad i = 3, \ldots, s, s+1, \tag{2.1.26}$$

$$B_{2j} = B_{B,2j} \qquad j = 1, \ldots, k-1, \tag{2.1.27}$$

$$\beta_{ij} = a_{ij} - \sum_{\ell=j+1}^{i-1} \alpha_{i\ell} a_{\ell j}, \qquad j = 2, 3, \ldots, i-1, \quad i = 3, 4, \ldots, s, \tag{2.1.28}$$

$$\beta_{i1} = B_{i0}, \qquad i = 3, \ldots, s, s+1, \tag{2.1.29}$$

$$\beta_{21} = a_{21}, \tag{2.1.30}$$

$$\beta_{s+1,j} = b_j - \sum_{\ell=j+1}^{s} \alpha_{s+1,\ell} a_{\ell j}, \qquad j = 2, 3, \ldots, s. \tag{2.1.31}$$

Thus, the form (2.1.21) can be rewritten as:

$$\begin{aligned} Y_i &= \left[\sum_{j=1}^{k-1} A_{ij} \left(y_{n-j} + \Delta t \frac{B_{ij}}{A_{ij}} f_{n-j} \right)\right] + \left[\sum_{j=1}^{i-1} \alpha_{ij} \left(Y_j + \Delta t \, \frac{\beta_{ij}}{\alpha_{ij}} F_j \right)\right], \\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad i = 2, 3, \ldots, s+1, \\ y_{n+1} &= Y_{s+1}. \end{aligned} \tag{2.1.32}$$

Since methods with negative coefficients will require additional spatial discretization (see [12]), we assume that all the coefficients in the Shu–Osher form are nonnegative.

From the condition (2.1.4), we have:

$$\sum_{j=1}^{k-1} A_{ij} + \sum_{j=1}^{i-1} \alpha_{ij} = 1, \qquad i = 2, 3, \ldots, s+1, \tag{2.1.33}$$

which is a so-called consistency condition.

In fact, for $i = 2, 3, \ldots, s+1$, we have:

$$
\begin{aligned}
\sum_{j=1}^{k-1} A_{ij} + \sum_{j=1}^{i-1} \alpha_{ij} &= \sum_{j=1}^{k-1} A_{ij} + \alpha_{i1} + \sum_{j=2}^{i-1} \alpha_{ij} \\
&= \sum_{j=1}^{k-1} A_{ij} + A_{i0} + \sum_{j=2}^{i-1} \alpha_{ij} \qquad \text{(by (2.1.24))} \\
&= \sum_{j=0}^{k-1} A_{ij} + \sum_{j=2}^{i-1} \alpha_{ij} \\
&= \sum_{j=0}^{k-1} \left[A_{B,ij} - \sum_{\ell=2}^{i-1} \alpha_{i\ell} A_{B,\ell j} \right] + \sum_{j=2}^{i-1} \alpha_{ij} \qquad \text{(by (2.1.22))} \\
&= \sum_{j=0}^{k-1} A_{B,ij} - \sum_{\ell=2}^{i-1} \alpha_{i\ell} \left[\sum_{j=0}^{k-1} A_{B,\ell j} \right] + \sum_{j=2}^{i-1} \alpha_{ij} \\
&= \sum_{j=1}^{k-1} A_{B,ij} + v_{B,i} - \sum_{\ell=2}^{i-1} \alpha_{i\ell} \left[\sum_{j=1}^{k-1} A_{B,\ell j} + v_{B,l} \right] + \sum_{j=2}^{i-1} \alpha_{ij} \quad \text{(by (2.1.18))} \\
&= 1 - \sum_{\ell=2}^{i-1} \alpha_{i\ell} + \sum_{j=2}^{i-1} \alpha_{ij} = 1. \qquad \text{(by (2.1.4))}
\end{aligned}
$$

The form (2.1.21) is the generalization to HB(k, s, p) methods of the Shu–Osher form introduced by Shu and Osher in [53].

Clearly, the HB(k, s, p) methods can be decomposed into a combination of FE methods with new step sizes. Indeed, in (2.1.32) for $i = 2, 3, \ldots, s, s+1$, the step sizes are $\frac{B_{ij}}{A_{ij}} \Delta t$, $j = 1, \ldots, k-1$, and $\frac{\beta_{ij}}{\alpha_{ij}} \Delta t$, $j = 1, 2, \ldots, i-1$, for the first and second bracketed terms, respectively.

Thus, we can conclude:

Theorem 2.1.4 *If f satisfies the forward Euler condition* (1.1.6)*, then the k-step, s-stage* HB*(k, s, p) methods* (2.1.32) *preserve the monotonicity property* (1.1.7)*, that is, the method is SSP under the restriction*

$$\Delta t \leq c(A_{ij}, B_{ij}, \alpha_{ij}, \beta_{ij}) \Delta t_{\mathrm{FE}},$$

where the feasible SSP coefficient $c(A_{ij}, B_{ij}, \alpha_{ij}, \beta_{ij})$ *is the minimum of the following quotients:*

$$
\begin{aligned}
&\min_{j=1,2,\dots,k-1} \left\{\frac{A_{ij}}{B_{ij}}\right\}, \quad i = 2,3,\dots,s+1, \\
&\min_{j=1,2,\dots,i-1} \left\{\frac{\alpha_{ij}}{\beta_{ij}}\right\}, \quad i = 2,3,\dots,s+1,
\end{aligned}
\tag{2.1.34}
$$

with the convention that $a/0 = +\infty$ *and under the assumption that all coefficients of* (2.1.32) *are nonnegative.*

This result is a straightforward extension of the result presented in [12, 17] and the idea for the proof is in [50].

2.1.4 Formulation of the optimization problem to obtain a non-canonical optimal HB(k,s,p)

We now turn to the task of finding optimal HB(k, s, p) schemes. To start, we search for an optimal s-stage SSP HB(k, s, p) scheme by maximizing its feasible SSP coefficients according to Theorem 2.1.4. This means we look for the global maximum of the nonlinear programming problem:

$$
\max_{A_{ij}, B_{ij}, \alpha_{ij}, \beta_{ij}} c(A_{ij}, B_{ij}, \alpha_{ij}, \beta_{ij}), \tag{2.1.35}
$$

where all the numbers in all pairs

$$
\begin{aligned}
&\{A_{ij}, B_{ij}\}, \quad i = 2,3,\dots,s+1, \quad j = 1,\dots,k-1, \\
&\{\alpha_{ij}, \beta_{ij}\}, \quad i = 2,3,\dots,s+1, \quad j = 1,2,\dots,i-1,
\end{aligned}
$$

are nonnegative. Note that if the coefficients in a pair are zero, it is not included in the minimization process. Here the obtained value $\max_{A_{ij}, B_{ij}, \alpha_{ij}, \beta_{ij}} c(A_{ij}, B_{ij}, \alpha_{ij}, \beta_{ij}) = c(\text{HB}(k,s,p))$ is the *SSP coefficient* of HB(k,s,p).

However, as in [56], Spiteri and Ruuth mentioned that there are two factors contributing to the poor performance of optimization problems. Firstly, the objective function (2.1.35) is nonsmooth and hence it is difficult to obtain numerically reliable derivative estimations with an optimization method using gradient information. Another trouble is that the $\min\{\cdot\}$ function is not sensitive to its arguments. Fortunately, using a dummy variable z to reformulate the nonlinear programming problem may improve the performance of the optimization routine

$$\max_{A_{ij},B_{ij},\alpha_{ij},\beta_{ij}} z, \tag{2.1.36}$$

such that z satisfies the inequalities

$$\begin{aligned} A_{ij} - zB_{ij} \geq 0, &\quad i = 2,3,\dots,s+1 \quad j = 1,2,\dots,k-1, \\ \alpha_{ij} - z\beta_{ij} \geq 0, &\quad i = 2,3,\dots,s+1 \quad j = 1,2,\dots,k-1, \end{aligned} \tag{2.1.37}$$

together with the conditions

- all the coefficients of (2.1.32) are nonnegative;
- the convex combinations constraints (2.1.12);
- the simplifying assumptions (2.1.4) and (2.1.5) for HB(k,s,p);
- the order conditions (2.1.6)–(2.1.10) for HB(k,s,p);
- the conditions on the abscissae c_i: $c_1 = 0$, $0 \leq c_i \leq 1$, $i = 2,3,\dots,s$.

Some HB methods under noncanonical Shu–Osher forms, presented in Chapter 4, are remarkable illustrations for this optimization problem.

2.1.5 HB(k,s,p) in Butcher and Shu–Osher modified forms

By setting $w_{B,i} = a_{i1}$, $i = 2,3,\dots,s$, and $w_{B,s+1} = b_1$ in (2.1.1)–(2.1.2), we have the HB(k,s,p) modified Butcher form:

$$Y_i = v_{B,i}y_n + \sum_{j=1}^{k-1} A_{B,ij}y_{n-j} + \Delta t\left[w_{B,i}f_n + \sum_{j=2}^{i-1} a_{ij}F_j + \sum_{j=1}^{k-1} B_{B,ij}f_{n-j}\right],$$

$$i = 2,3,\dots,s, \tag{2.1.38}$$

$$y_{n+1} = v_{B,s+1}y_n + \sum_{j=1}^{k-1} A_{B,s+1,j}y_{n-j} + \Delta t\Big[w_{B,s+1}f_n + \sum_{j=2}^{s} b_j F_j + \sum_{j=1}^{k-1} B_{B,s+1,j}f_{n-j}\Big], \tag{2.1.39}$$

As done in Subsection 2.1.3, the Butcher form (2.1.1)–(2.1.2) or the modified Butcher form (2.1.38)–(2.1.39) can be written in the Shu–Osher form (2.1.32).

Now, if we let $v_i = \alpha_{i1}$ and $w_i = \beta_{i1}$, $i = 2, 3, \ldots, s+1$, formulae (2.1.21) become the HB(k, s, p) modified Shu–Osher form, which is a generalization of the modified Shu–Osher form for RK methods (see [53, 10]):

$$\begin{aligned} Y_i = (v_i y_n + \Delta t\, w_i f_n) &+ \sum_{j=1}^{k-1}\Big[A_{ij}y_{n-j} + \Delta t B_{ij} f_{n-j}\Big] \\ &+ \sum_{j=2}^{i-1}\Big[\alpha_{ij}Y_j + \Delta t\,\beta_{ij}F_j\Big], \quad i = 2, 3, \ldots, s+1, \end{aligned} \tag{2.1.40}$$

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

We can rearrange (2.1.40) as follows:

$$\begin{aligned} Y_i = \left[v_i\left(y_n + \Delta t\,\frac{w_i}{v_i}f_n\right)\right] &+ \left[\sum_{j=1}^{k-1} A_{ij}\left(y_{n-j} + \Delta t\frac{B_{ij}}{A_{ij}}f_{n-j}\right)\right] \\ &+ \left[\sum_{j=2}^{i-1}\alpha_{ij}\left(Y_j + \Delta t\,\frac{\beta_{ij}}{\alpha_{ij}}F_j\right)\right], \qquad i = 2, 3, \ldots, s+1. \end{aligned} \tag{2.1.41}$$

Now the consistency condition (2.1.33) becomes

$$v_i + \sum_{j=1}^{k-1} A_{ij} + \sum_{j=2}^{i-1}\alpha_{ij} = 1, \qquad i = 2, 3, \ldots, s+1. \tag{2.1.42}$$

Clearly, (2.1.41) is the convex combination of forward Euler steps 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 $v_i, w_i, A_{ij}, B_{ij}, \alpha_{ij}, \beta_{ij} \geq 0$.

This immediately gives the following result:

Theorem 2.1.5 *If f satisfies the forward Euler condition* (1.1.6)*, then the k-step, s-stage* HB*(k, s, p) methods* (2.1.41) *satisfy the monotonicity property*

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

provided

$$\Delta t \leq c(A_{ij}, B_{ij}, \alpha_{ij}, \beta_{ij}, v_i, w_i)\Delta t_{\mathrm{FE}},$$

where the feasible SSP coefficient $c(A_{ij}, B_{ij}, \alpha_{ij}, \beta_{ij}, v_i, w_i)$ *is the minimum of the following numbers:*

$$\begin{aligned} \min_{j=1,2,\dots,k-1}\left\{\frac{A_{ij}}{B_{ij}}\right\}, &\quad i = 2,3,\dots,s+1, \\ \min_{j=2,3,\dots,i-1}\left\{\frac{\alpha_{ij}}{\beta_{ij}}\right\}, &\quad i = 3,4,\dots,s+1, \\ \frac{v_i}{w_i}, &\quad i = 2,3,\dots,s+1, \end{aligned} \tag{2.1.43}$$

with the convention that $a/0 = +\infty$ *and under the assumption that all coefficients of* (2.1.41) *are nonnegative.*

Gottlieb, Ketcheson and Shu presented a more compact notation as well as the canonical Shu–Osher form for RK methods (See more in Sections 3.1-3.4 in [10] for details). Following these results, in our work, we extended the canonical Shu–Osher form for our HB(k, s, p) methods. This generalization will be described in the next three subsections. Like optimal explicit SSP Runge–Kutta methods [20], the new sparse canonical Shu–Osher forms of HB methods might allow for reduced-storage implementation.

2.1.6 Butcher form in compact vector notation

A. Vector notation

In this part, we define the following vectors and matrices, which are very helpful to represent an HB method in Shu–Osher form. In particular, we set $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^{s+1}$:

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

and strictly lower triangular matrices $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{R}^{(s+1)\times(s+1)}$, and rectangular matrices $\boldsymbol{A}_{\mathrm{SO}} \in \mathbb{R}^{(s+1)\times(k-1)}$, $\boldsymbol{B}_{\mathrm{SO}} \in \mathbb{R}^{(s+1)\times(k-1)}$, $\boldsymbol{Y}, \boldsymbol{F} \in \mathbb{R}^{(s+1)\times N}$, $\boldsymbol{y}_{\mathrm{back}} \in \mathbb{R}^{(k-1)\times N}$ and

$\boldsymbol{f}_{\text{back}} \in \mathbb{R}^{(k-1)\times N}$:

$$(\boldsymbol{\alpha})_{ij} = \begin{cases} \alpha_{ij} & i = 2,3,\dots,s+1, \quad j = 1,2,\dots,i-1, \\ 0 & \text{otherwise}, \end{cases}$$

$$(\boldsymbol{\beta})_{ij} = \begin{cases} \beta_{ij} & i = 2,3,\dots,s+1, \quad j = 1,2,\dots,i-1, \\ 0 & \text{otherwise}, \end{cases}$$

$$(\boldsymbol{A}_{\text{SO}})_{ij} = \begin{cases} A_{ij} & i = 2,3,\dots,s+1, \quad j = 1,2,\dots,k-1, \\ 0 & \text{otherwise}, \end{cases}$$

$$(\boldsymbol{B}_{\text{SO}})_{ij} = \begin{cases} B_{ij} & i = 2,3,\dots,s+1, \quad j = 1,2,\dots,k-1, \\ 0 & \text{otherwise}, \end{cases}$$

where the numbers $\alpha_{ij}, \beta_{ij}, A_{ij}, B_{ij}$ come from equation (2.1.21). Moreover,

$$\begin{aligned} \boldsymbol{Y} &= [0, Y_2, \dots, Y_{s+1}]^T, & \boldsymbol{F} &= [0, F_2, \dots, F_{s+1}]^T, \\ \boldsymbol{y}_{\text{back}} &= [y_{n-1}, y_{n-2}, \dots, y_{n-(k-1)}]^T, & \boldsymbol{f}_{\text{back}} &= [f_{n-1}, f_{n-2}, \dots, f_{n-(k-1)}]^T, \end{aligned}$$

with the following N-vectors: Y_j, F_j for $j = 1,2,\dots,s+1$, y_j, f_j for $j = n-(k-1),\dots,n$, $Y_1 = y_n$, $F_1 = f_n$, $Y_{s+1} = y_{n+1}$ and $F_{s+1} = f_{n+1}$.

Therefore, the modified Shu–Osher form of HB formulae can be rewritten compactly:

$$\begin{aligned} \boldsymbol{Y} &= \boldsymbol{v} y_n^T + \boldsymbol{\alpha}\boldsymbol{Y} + \boldsymbol{A}_{\text{SO}}\boldsymbol{y}_{\text{back}} + \Delta t \left(\boldsymbol{w} f_n^T + \boldsymbol{\beta}\boldsymbol{F} + \boldsymbol{B}_{\text{SO}}\boldsymbol{f}_{\text{back}} \right), \\ y_{n+1} &= Y_{s+1}. \end{aligned} \tag{2.1.44}$$

Here, consistency (2.1.42) can be rewritten as

$$\boldsymbol{v} + \boldsymbol{\alpha}\boldsymbol{e}_{s+1} + \boldsymbol{A}_{\text{SO}}\boldsymbol{e}_{\text{back}} = \boldsymbol{e}_{s+1}, \tag{2.1.45}$$

where the $(s+1)$- and $(k-1)$-vectors $\boldsymbol{e}_{s+1}$ and $\boldsymbol{e}_{\text{back}}$ are

$$\boldsymbol{e}_{s+1} = [0, 1, 1, \dots, 1]^T \in \mathbb{R}^{(s+1)}, \quad \boldsymbol{e}_{\text{back}} = [1, 1, \dots, 1]^T \in \mathbb{R}^{(k-1)}, \tag{2.1.46}$$

respectively. Note that, by setting the first row of matrix $\boldsymbol{Y}$ and the first row of matrix $\boldsymbol{F}$ equal zero, respectively, α_{i1} and β_{i1}, $i = 2, 3, \ldots, s+1$, are not used in formulae (2.1.44) and the coefficients of $Y_1 = y_n$ and $F_1 = f_n$ are then replaced by v_i and w_i, $i = 2, 3, \ldots, s+1$.

B. Butcher form

At first glance, we can see that if $\boldsymbol{\alpha} = \mathbf{0}$, then the Shu–Osher form (2.1.44) becomes,

$$\begin{aligned} \boldsymbol{Y} &= \boldsymbol{v} y_n^T + \boldsymbol{A}_{\mathrm{SO}} \boldsymbol{y}_{\mathrm{back}} + \Delta t \left(\boldsymbol{w} f_n^T + \boldsymbol{\beta} \boldsymbol{F} + \boldsymbol{B}_{\mathrm{SO}} \boldsymbol{f}_{\mathrm{back}} \right), \\ y_{n+1} &= Y_{s+1}, \end{aligned} \tag{2.1.47}$$

which is the Butcher form. So, to distinguish the Butcher form from the Shu–Osher form, the elements $\boldsymbol{v}$, $\boldsymbol{w}$, $\boldsymbol{A}_{\mathrm{SO}}$, $\boldsymbol{B}_{\mathrm{SO}}$, $\boldsymbol{\beta}$ in (2.1.47) are replaced by $\boldsymbol{v}_{\mathrm{B}}$, $\boldsymbol{w}_{\mathrm{B}}$, $\boldsymbol{A}_{\mathrm{B}}$, $\boldsymbol{B}_{\mathrm{B}}$, $\boldsymbol{\beta}_{\mathrm{B}}$, respectively, and hence the Butcher form (2.1.47) can be rewritten as

$$\begin{aligned} \boldsymbol{Y} &= \boldsymbol{v}_{\mathrm{B}} y_n^T + \boldsymbol{A}_{\mathrm{B}} \boldsymbol{y}_{\mathrm{back}} + \Delta t \left(\boldsymbol{w}_{\mathrm{B}} f_n^T + \boldsymbol{\beta}_{\mathrm{B}} \boldsymbol{F} + \boldsymbol{B}_{\mathrm{B}} \boldsymbol{f}_{\mathrm{back}} \right), \\ y_{n+1} &= Y_{s+1}, \end{aligned} \tag{2.1.48}$$

where the consistency condition (2.1.45) reduces to

$$\boldsymbol{v}_{\mathrm{B}} + \boldsymbol{A}_{\mathrm{B}} \boldsymbol{e}_{\mathrm{back}} = \boldsymbol{e}_{s+1}, \tag{2.1.49}$$

and $\boldsymbol{e}_{s+1}$ and $\boldsymbol{e}_{\mathrm{back}}$ are defined in (2.1.46).

In fact, the form (2.1.48) is the Butcher form (2.1.1) and (2.1.2) with

$$\boldsymbol{v}_{\mathrm{B}} = [0, v_{B,2}, v_{B,3}, \ldots, v_{B,s+1}]^T, \tag{2.1.50}$$

$$\boldsymbol{A}_{\mathrm{B}} = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ A_{B,2,1} & A_{B,2,2} & \cdots & A_{B,2,k-1} \\ A_{B,3,1} & A_{B,3,2} & \cdots & A_{B,3,k-1} \\ \vdots & & \cdots & \vdots \\ A_{B,s+1,1} & A_{B,s+1,2} & \cdots & A_{B,s+1,k-1} \end{bmatrix}, \tag{2.1.51}$$

$$\boldsymbol{w}_{\mathrm{B}} = [0, a_{21}, a_{31}, \ldots, a_{s1}, b_1]^T, \tag{2.1.52}$$

$$\boldsymbol{\beta}_{\mathrm{B}} = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ a_{21} & 0 & 0 & 0 & \cdots & 0 & 0 \\ a_{31} & a_{32} & 0 & 0 & \cdots & 0 & 0 \\ a_{41} & a_{42} & a_{43} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & & \ddots & \ddots & & \vdots \\ a_{s1} & a_{s2} & a_{s3} & \cdots & a_{s,s-1} & 0 & 0 \\ b_1 & b_2 & b_3 & \cdots & b_{s-1} & b_s & 0 \end{bmatrix}, \tag{2.1.53}$$

$$\boldsymbol{B}_{\mathrm{B}} = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ B_{B,2,1} & B_{B,2,2} & \cdots & B_{B,2,k-1} \\ B_{B,3,1} & B_{B,3,2} & \cdots & B_{B,3,k-1} \\ \vdots & & \cdots & \vdots \\ B_{B,s+1,1} & B_{B,s+1,2} & \cdots & B_{B,s+1,k-1} \end{bmatrix}. \tag{2.1.54}$$

Our task now is to find the relationship between the Shu–Osher coefficients and the Butcher coefficients.

Firstly, solving (2.1.44) for $\boldsymbol{Y}$, we have

$$\begin{aligned} \boldsymbol{Y} = {} & (\boldsymbol{I} - \boldsymbol{\alpha})^{-1} \boldsymbol{v} y_n^T + (\boldsymbol{I} - \boldsymbol{\alpha})^{-1} \boldsymbol{A}_{\mathrm{SO}} \boldsymbol{y}_{\mathrm{back}} \\ & + \Delta t \left[(\boldsymbol{I} - \boldsymbol{\alpha})^{-1} \boldsymbol{w} f_n^T + (\boldsymbol{I} - \boldsymbol{\alpha})^{-1} \boldsymbol{\beta} \boldsymbol{F} + (\boldsymbol{I} - \boldsymbol{\alpha})^{-1} \boldsymbol{B}_{\mathrm{SO}} \boldsymbol{f}_{\mathrm{back}} \right]. \end{aligned} \tag{2.1.55}$$

Secondly, comparing (2.1.48) with (2.1.55), we obtain the following relations between the generalized Shu–Osher coefficients and the Butcher coefficients,

$$\boldsymbol{v}_{\mathrm{B}} = (\boldsymbol{I} - \boldsymbol{\alpha})^{-1}\boldsymbol{v}, \quad \boldsymbol{w}_{\mathrm{B}} = (\boldsymbol{I} - \boldsymbol{\alpha})^{-1}\boldsymbol{w}, \quad \boldsymbol{A}_{\mathrm{B}} = (\boldsymbol{I} - \boldsymbol{\alpha})^{-1}\boldsymbol{A}_{\mathrm{SO}}, \tag{2.1.56}$$

$$\boldsymbol{\beta}_{\mathrm{B}} = (\boldsymbol{I} - \boldsymbol{\alpha})^{-1}\boldsymbol{\beta}, \quad \boldsymbol{B}_{\mathrm{B}} = (\boldsymbol{I} - \boldsymbol{\alpha})^{-1}\boldsymbol{B}_{\mathrm{SO}}. \tag{2.1.57}$$

Remark 2.1.6

- *If the stepnumber $k = 1$, then* (2.1.48) *becomes*

$$\begin{aligned} \boldsymbol{Y} &= \boldsymbol{v}_B y_n^T + \Delta t\left(\boldsymbol{w}_B f_n^T + \boldsymbol{\beta}_B \boldsymbol{F}\right), \\ y_{n+1} &= Y_{s+1}, \end{aligned} \tag{2.1.58}$$

  that is the Butcher form of RK methods.

- *The process of obtaining* (2.1.55) *is always valid since* $(\boldsymbol{I} - \boldsymbol{\alpha})$ *is non-singular. Indeed, this matrix is always invertible because, by definition,* $\boldsymbol{\alpha}$ *is strictly lower triangular.*

2.1.7 Canonical Shu–Osher form of s-stage HB methods for deriving the SSP property

It is useful to find the SSP coefficient of an HB method under a particular Shu–Osher form of the matrices $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ by assuming the ratio $r = \frac{\alpha_{ij}}{\beta_{ij}}$ for every i, j, $i = 2, 3, 4, \ldots, s+1$ and $j = 1, 2, 3, \ldots, i-1$ such that $\beta_{ij} \neq 0$.

First of all, denote the coefficient matrices of this special form by $\boldsymbol{\alpha}_r$, $\boldsymbol{\beta}_r$. Thus,

$$\boldsymbol{\alpha}_r = r\boldsymbol{\beta}_r. \tag{2.1.59}$$

Then substituting (2.1.59) into (2.1.57), we can solve for $\boldsymbol{\beta}_r$ in terms of $\boldsymbol{\beta}_{\mathrm{B}}$ and r. In fact,

$$\begin{aligned}
(\boldsymbol{I} - r\boldsymbol{\beta}_r)^{-1}\boldsymbol{\beta}_r &= \boldsymbol{\beta}_{\mathrm{B}}, \\
\boldsymbol{\beta}_r &= \boldsymbol{\beta}_{\mathrm{B}} - r\boldsymbol{\beta}_r\boldsymbol{\beta}_{\mathrm{B}}, \\
\boldsymbol{\beta}_r(\boldsymbol{I} + r\boldsymbol{\beta}_{\mathrm{B}}) &= \boldsymbol{\beta}_{\mathrm{B}}.
\end{aligned}$$

Since $\boldsymbol{I} + r\boldsymbol{\beta}_{\mathrm{B}}$ is invertible, we obtain

$$\boldsymbol{\beta}_r = \boldsymbol{\beta}_{\mathrm{B}}(\boldsymbol{I} + r\boldsymbol{\beta}_{\mathrm{B}})^{-1} \tag{2.1.60}$$

Next by (2.1.59) and (2.1.60), we have

$$\boldsymbol{\alpha}_r = r\boldsymbol{\beta}_r = r\boldsymbol{\beta}_{\mathrm{B}}(\boldsymbol{I} + r\boldsymbol{\beta}_{\mathrm{B}})^{-1}. \tag{2.1.61}$$

Remark 2.1.7

- *The matrix* $(\boldsymbol{I} + r\boldsymbol{\beta}_B)$ *is invertible because the matrix* $\boldsymbol{\beta}_B$ *is strictly lower triangular by* (2.1.53)*, which implies that the determinant of* $(\boldsymbol{I} + r\boldsymbol{\beta}_B)$ *is always equal to one.*

- *We always have* $(\boldsymbol{I} + r\boldsymbol{\beta}_B)^{-1} = \boldsymbol{I} - \boldsymbol{\alpha}_r$*. Actually,*

$$\begin{aligned}
(\boldsymbol{I} + r\boldsymbol{\beta}_B)^{-1} &= [(\boldsymbol{I} + r\boldsymbol{\beta}_B) - r\boldsymbol{\beta}_B](\boldsymbol{I} + r\boldsymbol{\beta}_B)^{-1} \\
&= \boldsymbol{I} - r\boldsymbol{\beta}_B(\boldsymbol{I} + r\boldsymbol{\beta}_B)^{-1} \\
&= \boldsymbol{I} - \boldsymbol{\alpha}_r \qquad (\textit{by } (2.1.61)).
\end{aligned}$$

Therefore, from (2.1.56) *and* (2.1.57)*, we have:*

$$\boldsymbol{v}_r = (\boldsymbol{I} - \boldsymbol{\alpha}_r)\boldsymbol{v}_B = (\boldsymbol{I} + r\boldsymbol{\beta}_B)^{-1}\boldsymbol{v}_B, \tag{2.1.62}$$

$$\boldsymbol{w}_r = (\boldsymbol{I} - \boldsymbol{\alpha}_r)\boldsymbol{w}_B = (\boldsymbol{I} + r\boldsymbol{\beta}_B)^{-1}\boldsymbol{w}_B, \tag{2.1.63}$$

$$\boldsymbol{A}_{SO,r} = (\boldsymbol{I} - \boldsymbol{\alpha}_r)\boldsymbol{A}_B = (\boldsymbol{I} + r\boldsymbol{\beta}_B)^{-1}\boldsymbol{A}_B, \tag{2.1.64}$$

$$\boldsymbol{B}_{SO,r} = (\boldsymbol{I} - \boldsymbol{\alpha}_r)\boldsymbol{B}_B = (\boldsymbol{I} + r\boldsymbol{\beta}_B)^{-1}\boldsymbol{B}_B, \tag{2.1.65}$$

and from (2.1.57), (2.1.60) *and* (2.1.61), $\boldsymbol{\beta}_r$ *and* $\boldsymbol{\alpha}_r$ *are also given by:*

$$\boldsymbol{\beta}_r = \boldsymbol{\beta}_B \left(\boldsymbol{I} - \boldsymbol{\alpha}_r\right) = \left(\boldsymbol{I} + r\boldsymbol{\beta}_B\right)^{-1} \boldsymbol{\beta}_B, \tag{2.1.66}$$

$$\boldsymbol{\alpha}_r = r\boldsymbol{\beta}_B \left(\boldsymbol{I} - \boldsymbol{\alpha}_r\right) = r\left(\boldsymbol{I} + r\boldsymbol{\beta}_B\right)^{-1} \boldsymbol{\beta}_B, \tag{2.1.67}$$

*********CORRECTION FOLLOWED REPORTS********

Definition 2.1.8 *The canonical Shu–Osher form of the HB method is defined as follow:*

$$\boldsymbol{Y} = \left(\boldsymbol{v}_r y_n^T + \Delta t \boldsymbol{w}_r f_n^T\right) + \left(\boldsymbol{\alpha}_r \boldsymbol{Y} + \Delta t \boldsymbol{\beta}_r \boldsymbol{F}\right) + \left(\boldsymbol{A}_{SO,r} \boldsymbol{y}_{back} + \Delta t \boldsymbol{B}_{SO,r} \boldsymbol{f}_{back}\right) \tag{2.1.68}$$

where all the coefficients are determined by the relations (2.1.60)–(2.1.65) *with the consistency condition*

$$\boldsymbol{v}_r + \boldsymbol{\alpha}_r \boldsymbol{e}_{s+1} + \boldsymbol{A}_{SO,r} \boldsymbol{e}_{back} = \boldsymbol{e}_{s+1}. \tag{2.1.69}$$

**************END******************

It is noted that the form (2.1.68) can be also presented in terms of the Butcher coefficients by using (2.1.62)–(2.1.67),

$$\boldsymbol{Y} = \left(\boldsymbol{I} + r\boldsymbol{\beta}_{\mathrm{B}}\right)^{-1} \left[\boldsymbol{v}_{\mathrm{B}} y_n^T + \Delta t \boldsymbol{w}_{\mathrm{B}} f_n^T + \boldsymbol{\beta}_{\mathrm{B}} \left(r\boldsymbol{Y} + \Delta t \boldsymbol{F}\right) + \left(\boldsymbol{A}_{\mathrm{B}} \boldsymbol{y}_{\mathrm{back}} + \Delta t \boldsymbol{B}_{\mathrm{B}} \boldsymbol{f}_{\mathrm{back}}\right)\right]. \tag{2.1.70}$$

with the consistency condition

$$\left(\boldsymbol{I} + r\boldsymbol{\beta}_{\mathrm{B}}\right)^{-1} \boldsymbol{v}_{\mathrm{B}} + r\left(\boldsymbol{I} + r\boldsymbol{\beta}_{\mathrm{B}}\right)^{-1} \boldsymbol{\beta}_{\mathrm{B}} \boldsymbol{e}_{s+1} + \left(\boldsymbol{I} + r\boldsymbol{\beta}_{\mathrm{B}}\right)^{-1} \boldsymbol{A}_{\mathrm{B}} \boldsymbol{e}_{\mathrm{back}} = \boldsymbol{e}_{s+1}. \tag{2.1.71}$$

*******CORRECTION FOLLOWED REPORTS**********

Definition 2.1.9 *The canonical Shu–Osher form of the HB method* (2.1.68) *is called sparse form if matrices* $\boldsymbol{\alpha}_r$ *and* $\boldsymbol{\beta}_r$ *have few non-zero entries.*

The sparsity gives significant advantages such as memory management and computational efficiency.

*************END******************

Remark 2.1.10

- *If $r = 0$, then the Butcher form* (2.1.48) *and the form* (2.1.71) *are identical.*
- *The relations* (2.1.60)–(2.1.67) *will enable us to transform simply a Butcher form into a canonical Shu–Osher form and vice versa.*

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

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

which is (2.1.73) and (2.1.82) and

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

which is (2.1.73) and (2.1.83). Therefore, the following slight modification of the result presented in Theorem 2.1.5 holds.

Theorem 2.1.11 *If f satisfies the forward Euler condition* (1.1.6)*, then the k-step, s-stage* HB*(k, s, p)* (2.1.68) *satisfy the monotonicity property*

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

provided

$$\Delta t \leq c(\boldsymbol{v}_r, \boldsymbol{w}_r, \boldsymbol{\alpha}_r, \boldsymbol{\beta}_r, \boldsymbol{A}_{SO,r}, \boldsymbol{B}_{SO,r})\Delta t_{\mathrm{FE}},$$

where the coefficient $c(\boldsymbol{v}_r, \boldsymbol{w}_r, \boldsymbol{\alpha}_r, \boldsymbol{\beta}_r, \boldsymbol{A}_{\mathrm{SO,r}}, \boldsymbol{B}_{\mathrm{SO,r}})$ is equal to

$$r = \left\{ \frac{\alpha_{ij}}{\beta_{ij}} \right\}, \quad \begin{cases} i = 3, 4, \ldots, s+1, \\ j = 2, 3, \ldots, i-1, \end{cases} \tag{2.1.72}$$

and less than or equal to:

$$\min_{i=2,3,\dots,s+1} \frac{v_i}{w_i}, \tag{2.1.73}$$

$$\min_{j=1,2,\dots,k-1} \left\{ \frac{A_{ij}}{B_{ij}} \right\}, \quad i = 2, 3, \dots, s+1, \tag{2.1.74}$$

with the convention that $a/0 = +\infty$*, under the assumption that all coefficients of* (2.1.68) *are nonnegative.*

2.1.8 Formulation of the optimization problem to obtain the canonical optimal HB(k,s,p)

Similar to Subsection 2.1.4, we would like to optimize HB(k,s,p) and obtain $c(\text{HB}(k,s,p))$ in canonical form, so by Theorem 2.1.11, we maximize

$$\max_{\boldsymbol{v}_r,\boldsymbol{w}_r,\boldsymbol{\alpha}_r,\boldsymbol{\beta}_r,\boldsymbol{A}_{\text{SO},\boldsymbol{r}},\boldsymbol{B}_{\text{SO},\boldsymbol{r}}} c(\boldsymbol{v}_r, \boldsymbol{w}_r, \boldsymbol{\alpha}_r, \boldsymbol{\beta}_r, \boldsymbol{A}_{\text{SO},\boldsymbol{r}}, \boldsymbol{B}_{\text{SO},\boldsymbol{r}}) = c(\text{HB}(k,s,p)).$$

In the optimization formulation with any feasible initial data, the ratio r becomes the variable r which satisfies the equations in three variables $\alpha_{ij}, r, \beta_{ij}$,

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

together with the two conditions (2.1.73) which is (2.1.82) and (2.1.73) which is (2.1.83).

Hence, the problem of optimizing the canonical HB(k, s, p) can be formulated as

$$c(\text{HB}(k,s,p)) = \max_{\boldsymbol{v}_\text{B},\boldsymbol{w}_\text{B},\boldsymbol{\beta}_\text{B},\boldsymbol{A}_\text{B},\boldsymbol{B}_\text{B}} r, \tag{2.1.75}$$

subject to the component-wise inequalities

$$(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\,\boldsymbol{v}_{\mathrm{B}} \geq 0 \tag{2.1.76}$$

$$(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\,\boldsymbol{w}_{\mathrm{B}} \geq 0 \tag{2.1.77}$$

$$\boldsymbol{\beta}_{\mathrm{B}}\,(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1} \geq 0 \tag{2.1.78}$$

$$(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\,\boldsymbol{A}_{\mathrm{B}} \geq 0 \tag{2.1.79}$$

$$(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\,\boldsymbol{B}_{\mathrm{B}} \geq 0 \tag{2.1.80}$$

$$r\boldsymbol{\beta}_{\mathrm{B}}\,(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\,\boldsymbol{e}_{s+1} + (\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\,\boldsymbol{A}_{\mathrm{B}}\boldsymbol{e}_{\mathrm{back}} \leq \boldsymbol{e}_{s+1}, \tag{2.1.81}$$

$$(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\,(-\boldsymbol{v}_{\mathrm{B}}+r\boldsymbol{w}_{\mathrm{B}}) \leq 0, \tag{2.1.82}$$

$$(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\,(-\boldsymbol{A}_{\mathrm{B}}+r\boldsymbol{B}_{\mathrm{B}}) \leq 0, \tag{2.1.83}$$

together with the set of order conditions (2.1.4)–(2.1.10).

Inequalities (2.1.76)–(2.1.80) ensure the coefficient $\boldsymbol{v}_r, \boldsymbol{w}_r, \boldsymbol{\alpha}_r, \boldsymbol{\beta}_r, \boldsymbol{A}_{\mathrm{SO},\boldsymbol{r}}, \boldsymbol{B}_{\mathrm{SO},\boldsymbol{r}}$ are nonnegative (by using relations (2.1.61)–(2.1.65)).

Inequalities (2.1.82) and (2.1.83) follow Theorem 2.1.11 to obtain the SSP coefficient from many feasible SSP coefficients.

For the MATLAB optimization toolbox, to avoid trouble, we use inequality (2.1.81) instead of the consistency condition (2.1.71) (or (2.1.69)). In fact, (2.1.81) guarantees that (2.1.71) (or (2.1.69)) is always satisfied for all output r because the inputs are in Butcher forms (2.1.50)–(2.1.54) with $\boldsymbol{v}_{\mathrm{B}}$ and $\boldsymbol{A}_{\mathrm{B}}$ always satisfy (2.1.49). Then we have:

$$\boldsymbol{v}_{\mathrm{B}} + \boldsymbol{A}_{\mathrm{B}}\boldsymbol{e}_{\mathrm{back}} = \boldsymbol{e}_{s+1},$$

$$\boldsymbol{v}_{\mathrm{B}} + r\boldsymbol{\beta}_{\mathrm{B}}\boldsymbol{e}_{s+1} + \boldsymbol{A}_{\mathrm{B}}\boldsymbol{e}_{\mathrm{back}} = \boldsymbol{e}_{s+1} + r\boldsymbol{\beta}_{\mathrm{B}}\boldsymbol{e}_{s+1},$$

$$\boldsymbol{v}_{\mathrm{B}} + r\boldsymbol{\beta}_{\mathrm{B}}\boldsymbol{e}_{s+1} + \boldsymbol{A}_{\mathrm{B}}\boldsymbol{e}_{\mathrm{back}} = (\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})\boldsymbol{e}_{s+1},$$

$$(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\boldsymbol{v}_{\mathrm{B}} + r(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\boldsymbol{\beta}_{\mathrm{B}}\boldsymbol{e}_{s+1} + (\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})^{-1}\boldsymbol{A}_{\mathrm{B}}\boldsymbol{e}_{\mathrm{back}} = \boldsymbol{e}_{s+1}.$$

The matrix $(\boldsymbol{I}+r\boldsymbol{\beta}_{\mathrm{B}})$ is invertible by Remark 2.1.7 and the last equation above is (2.1.71). It is to be noted that condition (2.1.78) implies condition (2.1.77).

Following the optimization problem, in the next section we shall obtain the SSP coefficients c and the effective coefficients c_{eff} of the canonical Shu–Osher form of s-stage HB(k,s,p) methods.

2.2 Effective SSP coefficients and their percentage efficiency gains

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 $c(\text{HB}(k,s,p))$ for different values of k. Several authors [56, 57, 10] have successfully used this technique to find optimal RK methods. In this work, the MATLAB Optimization Toolbox was used to tolerance 10^{-12} on the objective function $c(\text{HB}(k,s,p))$ provided all the constraints were satisfied to tolerance 10^{-14}.

**** NEW SENTENCE*** However, because of the limitation of fmincon function, it is not guaranteed that the obtained result are global. **** END******

Gottlieb [7] pointed out that one looks for high-order SSP methods with c as large as possible, taking their computational costs and orders into account. The effective coefficients c_{eff} provide a fair comparison between methods of the same order, although, in practice, starting methods, storage issues and order reduction may also be important.

Definition 2.2.1 *(See [47]) The effective SSP coefficients of an SSP method M, $c_{\mathit{eff}}(M)$, is defined by*

$$c_{\mathit{eff}}(M) = \frac{c(M)}{\ell}, \tag{2.2.1}$$

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

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

Definition 2.2.2 *(See [56]) The percentage efficiency gain (PEG) of the effective SSP coefficients $\mathrm{c}_{\mathit{eff}}$(M2) of method 2 over $\mathrm{c}_{\mathit{eff}}$(M1) of method 1 is evaluated by*

$$PEG(c_{\mathit{eff}}(\mathrm{M2}), \mathrm{c}_{\mathit{eff}}(\mathrm{M1})) = \frac{\mathrm{c}_{\mathit{eff}}(\mathrm{M2}) - \mathrm{c}_{\mathit{eff}}(\mathrm{M1})}{\mathrm{c}_{\mathit{eff}}(\mathrm{M1})}. \tag{2.2.2}$$

In Tables 2.1–2.9, for each stage value s, the row-wise maximum, $\max_k c_{\text{eff}}(\mathrm{HB}(k,s,p))$, is listed with an asterisk. The largest c_{eff} for each order p is in boldface. This data is summarized in Table 2.10 and Fig. 2.9.

Remark 2.2.3 *From Tables 2.1–2.9, it is generally seen that:*

- *For a given k, generally $c_{\mathit{eff}}(HB(k,s,p))$ first increases with s and then decreases.*

  ****** CORRECTION FOLLOWED THE REPORT *******

  As s increases, the set of feasible solutions is larger. It means that SSP coefficient, c increases with increasing s. However, $c_{\mathit{eff}} = \frac{c}{s}$, then it does not guarantee c_{eff} increases with increasing s.

  ********END*********

- *For fixed stage s, the effective SSP coefficients $c_{\mathit{eff}}(HB(k,s,p))$ first increase as the number of steps k increases and then stabilize.*

- *Empty entries in the tables correspond either to existing methods with smaller c_{eff}.*

The next subsections 2.2.1–2.2.9 follow Section 5 in [39].

2.2.1 Fourth-order methods

Spiteri and Ruuth [56] found a 5-stage SSP RK method of order 4, called RK(5,4), with c(RK(5,4)) $= 1.508$ and c_{eff}(RK(5,4)) $= 0.302$. Other fourth-order SSP RK methods with more stages can be found in [57] and [20]. Gottlieb, Shu and Tadmor [12] proved that there are no HM(2,4) with nonnegative coefficients. Huang [17] found k-step HM(k,4) of order 4:

- HM(3,4) with c(HM(3,4)) $= 0.494$ and c_{eff}(HM(3,4)) $= 0.247$,
- HM(4,4) with c(HM(4,4)) $= 0.682$ and c_{eff}(HM(4,4)) $= 0.341$,
- HM(5,4) with c(HM(5,4)) $= 0.793$ and c_{eff}(HM(5,4)) $= 0.396$,
- HM(6,4) with c(HM(6,4)) $= 0.879$ and c_{eff}(HM(6,4)) $= 0.439$,
- HM(7,4) with c(HM(7,4)) $= 0.938$ and c_{eff}(HM(7,4)) $= 0.469$.

Recently, Constantinescu and Sandu [4] obtained optimal 2-step general linear SSP methods of order 4, with certificates of optimality for some of them. Ketcheson, Gottlieb and Macdonald [23] found 2-step RK (TSRK) methods of order 4 with nonnegative coefficients (see also [10]). Among these, the 10-stage method has the best effective SSP coefficient, c_{eff}(TSRK(10,4)) $= 0.610$.

In our research, we have already found the SSP coefficients of the optimal non-canonical HB$(k, s, 4)$ with stage number $s = 4, 5, \ldots, 10$ [35]. Moreover, we numerically obtained optimal canonical HB$(k, s, 4)$, $s = 4, 5, \ldots, 12$, the c_{eff} of which are listed in Table 2.1.

Remark 2.2.4 *From Table 2.1, it is seen that:*

(1) HB(3,12,4) has largest c_{eff}(HB(3,12,4)) $= 0.656$.

(2) All our new methods (except HB(2,4,4) and HB(3,4,4)) have greater c_{eff} than those of the hybrid methods listed above. Actually, even with only 4 steps,

Table 2.1: $c_{\text{eff}}(\text{HB}(k,s,4))$ as function of k and s.

$s\backslash k$	2	3	4	5	6	7	RK$(s,4)$	TSRK$(s,4)$
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	

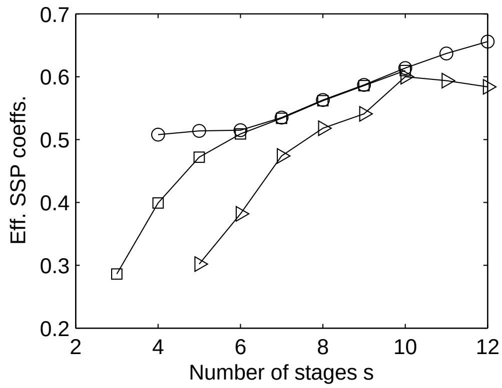
HB(4,4,4) has larger c_{eff} than Huang's best 7-step, HM(7,4), that is, c_{eff}(HB(4,4,4)) $=$ $0.483 >$ *c_{eff}(HM(7,4))* $= 0.469$.

(3) For the same stage number s, $c_{\mathit{eff}}(HB(k,s,4)) > c_{\mathit{eff}}(RK(s,4))$ especially when s is small.

(4) Although $c_{\mathit{eff}}(HB(2,s,4)) \approx c_{\mathit{eff}}(TSRK(s,4))$, $c_{\mathit{eff}}(HB(k,s,4)) \geq c_{\mathit{eff}}(TSRK(s,4))$ for $k \geq 3$.

(5) $c_{\mathit{eff}}(HB(2,s,4)) = c_{\mathit{eff}}(TSRK(s,4))$, $s = 9, 10$.

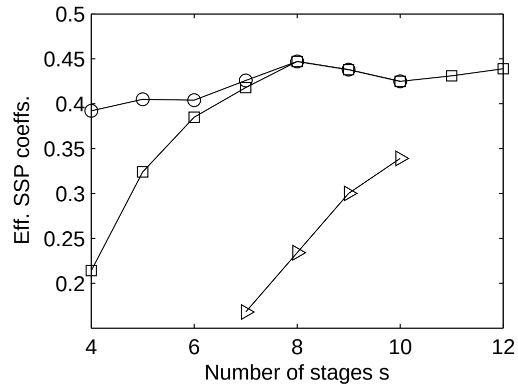
HB, TSRK and RK methods of order 4, including Ketcheson RK(10,4), are compared in Fig. 2.1 on the basis of $\max_k c_{\text{eff}}(\text{HB}(k,s,4))$ as a function of the number of stages s. In this figure, it is noted that $\max_k c_{\text{eff}}(\text{HB}(k,s,4))$ increases slightly and $c_{\text{eff}}(\text{RK}(s,4))$ increases dramatically with $s \leq 10$. However, when $s \geq 11$, $\max_k c_{\text{eff}}(\text{HB}(k,s,4))$ continues to increase while $c_{\text{eff}}(\text{RK}(s,4))$ decreases. At stage $s = 7, 8, 9$, Fig. 2.1 shows the c_{eff} of HB methods and TSRK methods are almost equal. Moreover, the figure confirms the third statement in Remark 2.2.4.



HB(k, s,4) of order 4 $\circ$, RK(s,4) of order 4 $\triangleright$

TSRK(s,4) of order 4 $\square$

Figure 2.1: $\max_k c_{\text{eff}}(\text{HB}(k, s, 4))$, $c_{\text{eff}}(\text{RK}(s, 4))$, $c_{\text{eff}}(\text{TSRK}(s, 4))$ as functions of s.



HB(k, s,5) of order 5 $\circ$, RK(s,5) of order 5 $\triangleright$

TSRK(s,5) of order 5 $\square$

Figure 2.2: $\max_k c_{\text{eff}}(\text{HB}(k, s, 5))$, $c_{\text{eff}}(\text{RK}(s, 5))$, $c_{\text{eff}}(\text{TSRK}(s, 5))$ as functions of s.

2.2.2 Fifth-order methods

Ruuth and Spiteri [46] proved that there are no fifth-order SSP RK methods with nonnegative coefficients. In [44, 47], they recently considered fifth-order methods with negative coefficients,

- RK(7,5) with $c(\text{RK}(7{,}5)) = 1.1785$, $c_{\text{eff}}(\text{RK}(7{,}5)) = 0.168$,
- RK(8,5) with $c(\text{RK}(8{,}5)) = 1.8757$, $c_{\text{eff}}(\text{RK}(8{,}5)) = 0.234$,
- RK(9,5) with $c(\text{RK}(9{,}5)) = 2.696$, $c_{\text{eff}}(\text{RK}(9{,}5)) = 0.300$,
- RK(10,5) with $c(\text{RK}(10{,}5)) = 3.395$, $c_{\text{eff}}(\text{RK}(10{,}5)) = 0.339$.

Ruuth and Hundsdorfer [45] pointed out that fifth-order linear multistep (LM) methods with nonnegative coefficients require at least $k = 7$ steps with $c_{\text{eff}}(\text{LM}(7{,}5)) = 0.038$. In [17], one finds the following HM(k, 5) with nonnegative coefficients:

- HM(4,5) with $c(\text{HM}(4{,}5)) = 0.371$ and $c_{\text{eff}}(\text{HM}(4{,}5)) = 0.185$,
- HM(5,5) with $c(\text{HM}(5{,}5)) = 0.525$ and $c_{\text{eff}}(\text{HM}(5{,}5)) = 0.262$,

Table 2.2: $c_{\text{eff}}(\text{HB}(k, s, 5))$ as function of k and 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

- HM(6,5) with $c(\text{HM(6,5)}) = 0.657$ and $c_{\text{eff}}(\text{HM(6,5)}) = 0.328$,
- HM(7,5) with $c(\text{HM(7,5)}) = 0.746$ and $c_{\text{eff}}(\text{HM(7,5)}) = 0.373$.

Two-step RK methods of order 5 with nonnegative coefficients are found in [23]. Their formulae and SSP coefficients are also listed in [10]. Among these, the 8-stage method has the best $c_{\text{eff}}(\text{TSRK(8,5)}) = 0.447$.

In our work, optimal canonical HB$(k, s, 5)$ with stage number $s = 4, 5, \ldots, 10$ are found and their c_{eff} are listed in Table 2.2 with the largest $c_{\text{eff}}(\text{HB(2,8,5)}) = 0.447$.

The $\max_k c_{\text{eff}}(\text{HB}(k, s, 5))$, for $s = 4, 5, \ldots, 10$, TSRK$(s, 5)$ for $s = 4, 5, \ldots, 12$ and RK$(s, 5)$, for $s = 7, 8, 9, 10$, are plotted in Fig. 2.2. The figure shows that the new methods have larger effective SSP coefficients when $s > 6$.

Remark 2.2.5 *From Table 2.2, it is observed that:*

- *Unlike the fourth order, the fifth order methods present an unusual phenomenon: for all the step numbers, as the number of stages is greater than eight, it is not possible to obtain larger c_{eff} than the 8-stage method. This phenomenon, which will happen differently at different orders, will be seen clearly in the next Subsections.*

- *For the same step number k, HB($k, s, 5$) methods have larger c_{eff} than those of hybrid methods (HM). Moreover, even with the lowest stage $s = 4$, our method is better than the best HM method, that is, c_{eff}(HB(4,4,5)) $= 0.384 >$ c_{eff}(HM(7,5)) $= 0.373$.*

- *With $k = 2$, although c_{eff}(HB(2,s,5)) are slightly smaller than c_{eff}(TSRK(s,5)), they are equal when $s \geq 6$. However, as $k > 2$, c_{eff}(HB((k,s,5))) $>$ c_{eff}(TSRK(s,5)).*

- *Except for HB(2,4,5) and HB(2,5,5), all the HB methods have larger c_{eff} than that of the best RK method. In fact, c_{eff}(HB(3,4,5)) $= 0.341 >$ c_{eff}(RK(10,5)) $=$ 0.339.*

2.2.3 Sixth-order methods

Ketcheson [21] pointed out that LM methods of order 6 with nonnegative coefficients require at least $k = 10$ steps with c_{eff}(LM(10,6)) $= 0.052$. Moreover, the family of k-step HM(k,6) with $k = 5, 6, 7$ was found in [17]:

- HM(5,6) with c(HM(5,6)) $= 0.209$ and c_{eff}(HM(5,6)) $= 0.104$,

- HM(6,6) with c(HM(6,6)) $= 0.362$ and c_{eff}(HM(6,6)) $= 0.181$,

- HM(7,6) with c(HM(7,6)) $= 0.440$ and c_{eff}(HM(7,6)) $= 0.220$.

Furthermore, two-step RK methods of order 6 with nonnegative coefficients are found in [23] (see more in [10]). Among these, the 12-stage method has the best effective SSP coefficient c_{eff}(TSRK(12,6)) $= 0.365$.

Optimal canonical HB($k, s, 6$) were found numerically with stage number $s = 4, \dots, 10$ in our study. Their c_{eff} are listed in Table 2.3 with largest c_{eff}(HB(5,7,6)) $=$ 0.351.

Remark 2.2.6 *From Table 2.3, we notice that:*

Table 2.3: $c_{\text{eff}}(\text{HB}(k, s, 6))$ as function of k and s.

$s \backslash k$	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

- *The phenomenon, which is mentioned in Remark 2.2.5, also happens with sixth order methods. Yet,* c_{eff} *falls off when* $s = 7$ *and* $s = 9$ *for* $k \geq 3$ *and* $k = 2$*, respectively.*

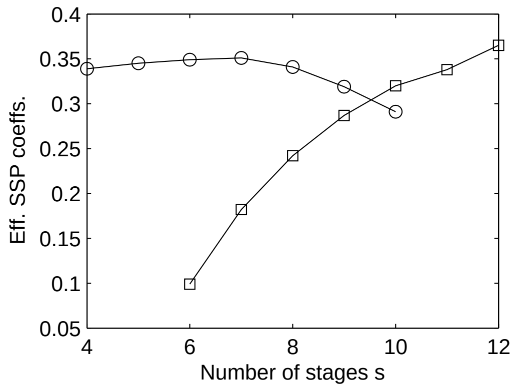
- *All HB methods, excluding HB(2,7,6) and HB(3,4,6), have larger* c_{eff} *than those of the best HM method, HM(7,6), with* $c_{\mathit{eff}}(HM(7,6)) = 0.220$.

- *As* $s = 6, 7$*, HB methods have significantly better* c_{eff} *when compared to TSRK methods. For instance,* $PEG(c_{\mathit{eff}}(HB(3,6,6)), c_{\mathit{eff}}(TSRK(6,6))) = 226\%$ *(by* (2.2.2)*).*

In Fig. 2.3, $\max_k c_{\text{eff}}(\text{HB}(k, s, 6))$ and $c_{\text{eff}}(\text{TSRK}(s, 6))$ 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 small.

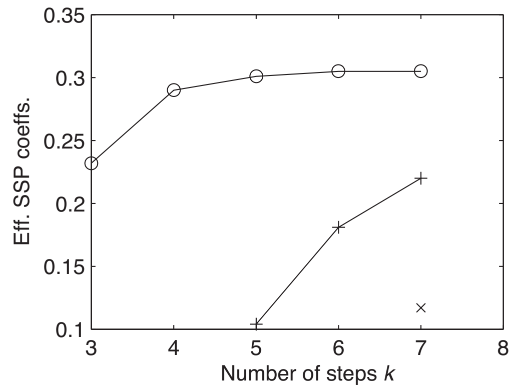
2.2.4 Seventh-order methods

LM methods of order 7 with nonnegative coefficients require at least $k = 12$ steps with $c_{\text{eff}}(\text{LM}(12,7)) = 0.018$ [21].



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

Figure 2.3: $\max_k c_{\text{eff}}(\text{HB}(k, s, 6))$ and $c_{\text{eff}}(\text{TSRK}(s, 6))$ versus stage number s.



HB(k,6,7) ∘, HM(7,7) ×, HM(k,6) +

Figure 2.4: 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.

In [17], Huang introduced the 7-step HM(7,7) of order 7 with $c(\text{HM}(7,7)) = 0.234$ and $c_{\text{eff}}(\text{HM}(7,7)) = 0.117$.

Two-step RK methods of order 7 with nonnegative coefficients are found by Gottlieb, Ketcheson and McDonald ([23], [10]). Among these, the 12-stage method has the best $c_{\text{eff}}(\text{TSRK}(12,7)) = 0.231$.

For HB methods, we also obtained the optimal methods of order 7, HB(k,s,7) with stage number $s = 4, 5, \ldots, 10$. Their c_{eff} are listed in Table 2.4 with largest $c_{\text{eff}}(\text{HB}(6,6,7)) = 0.305$.

Remark 2.2.7 *From Table 2.4, we notice that:*

- *All HB methods have larger c_{eff} than the HM method HM(7,7) with $c_{\mathit{eff}}(HM(7,7)) = 0.117$.*
- *The c_{eff} of all HB methods of order 7 drop-off with increasing $s > 6$.*
- *For the same number of stages, the HB methods have better c_{eff} than the TSRK methods in row-wise comparison.*

Table 2.4: $c_{\text{eff}}(\text{HB}(k,s,7))$ as function of k and s.

$s\backslash k$	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

In Fig. 2.4, the c_{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_{eff} than HM(7,7) and HM(k,6), for $k = 5, 6, 7$. Even with a smaller step number $k = 3$, HB(3,6,7) has larger c_{eff} than HM(7,7) and HM(k,6) which require more steps, namely, $k = 5, 6, 7$.

2.2.5 Eighth-order methods

The necessity for LM methods of order 8 with nonnegative coefficients exists is $k \geq 15$ and $c_{\text{eff}}(\text{LM}(15,8)) = 0.012$ [21].

Two-step RK methods of order 8 with nonnegative coefficients are found in [23]. Among these, the 12-stage method has the best $c_{\text{eff}}(\text{TSRK}(12,8)) = 0.078$.

The optimal canonical HB$(k, s, 8)$ with stage number $s = 4, 5, \ldots, 10$ were numerically found in our research. Their c_{eff} are listed in Table 2.5 with largest $c_{\text{eff}}(\text{HB}(8,6,8)) =$ 0.261.

From Table 2.5, we see that these new methods are better than HM(7,7) even with the smallest step number $k = 4$ and are competitive with TSRK(12,8) with lowest

Table 2.5: $c_{\text{eff}}(\text{HB}(k, s, 8))$ as function of k and s.

$s\backslash k$	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

stage number $s = 4$. For example, $c_{\text{eff}}(\text{HB}(4,5,8)) = 0.121 > c_{\text{eff}}(\text{HM}(7,7)) = 0.117$ and $c_{\text{eff}}(\text{HB}(5,4,8)) = 0.123 > c_{\text{eff}}(\text{TSRK}(12,8)) = 0.078$.

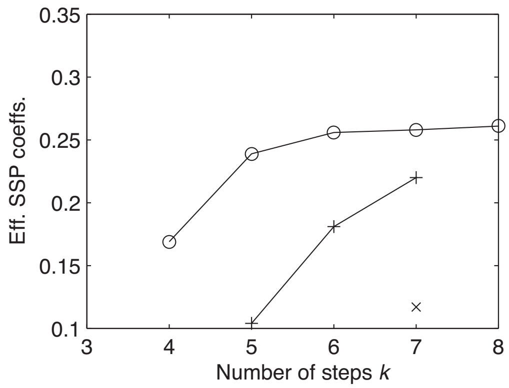
In Fig. 2.5, the c_{eff} of HB(k,6,8), HM(7,7) of order 7 and HM(k,6) of order 6 are compared as functions of k. It is seen that HB(k,6,8) have larger c_{eff} than HM(7,7) and HM(k,6) for $k = 5, 6, 7$ even though it has larger order than HM.

2.2.6 Ninth-order methods

Although LM methods with nonnegative coefficients require at least $k = 18$ steps to obtain order 9, their c_{eff} are not high. Indeed, in [21], Ketcheson presented the table of c_{eff} of all optimal explicit linear multistep methods. The table shows that $c_{\text{eff}}(\text{LM}(18,9)) = 0.003$ and the best one is $c_{\text{eff}}(\text{LM}(50,9)) = 0.261$.

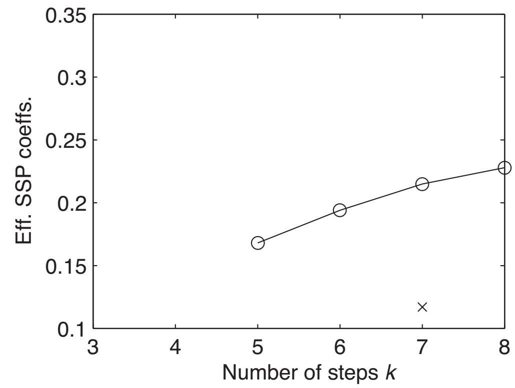
However, HB($k, s, 9$) exist even with only small k and s. A family of optimal HB methods of order 9 was found numerically with stage number $s = 4, 5, \ldots, 10$ and their c_{eff} are listed in Table 2.6 with largest $c_{\text{eff}}(\text{HB}(8,6,9)) = 0.228$. All c_{eff} of HB methods in the table decrease as $s > 6$, except for HB(6,s,9) that drop-off as $s > 7$.

Even with only 5 steps, these new methods are competitive with HM(7,7) of



HB(k,6,8) $\circ$, HM(7,7) $\times$, HM(k,6) $+$

Figure 2.5: 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, respectively.



HB(k,6,9) $\circ$, HM(7,7) $\times$

Figure 2.6: $c_{\text{eff}}(\text{HB}k, 6, 9)$ of order 9 as function of k and HM(7,7) of order 7.

order 7. For instance, c_{eff}(HB(5,6,9)) $= 0.168 > c_{\text{eff}}$(HM(7,7)) $= 0.117$.

In Fig. 2.6, it is seen that, for all k, HB(k,6,9) have larger c_{eff} than HM(7,7).

2.2.7 Tenth-order methods

LM methods of order 10 with nonnegative coefficients require at least $k = 22$ steps with c_{eff}(LM(22,10)) $= 0.010$ and the largest c_{eff} is c_{eff}(LM(50,10)) $= 0.218$ [21].

For HB methods, the step number required is $k = 6$ and we numerically found optimal HB($k, s, 10$) with stage number $s = 4, 5, \dots, 10$. Their c_{eff} are listed in Table 2.7 with largest c_{eff}(HB(8,6,10)) $= 0.185$.

Despite low step number $k = 6$, we have c_{eff}(HB(6,6,10)) $= 0.126 > 0.117 = c_{\text{eff}}$(HM(7,7)), the best method among HM methods.

In Fig. 2.7, the c_{eff} of HB(k,6,10) of order 10 and HM(7,7) of order 7 are compared as functions k. It is observed that all HB(k,6,10) have larger c_{eff} than HM(7,7).

Table 2.6: c_{eff}(HB(k,s,9)) as function of k and s.

$s\backslash k$	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	**0.228**
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

Table 2.7: $c_{\text{eff}}(\text{HB}(k, s, 10))$ as function of k and s.

$s\backslash k$	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	0.141	0.170	*0.176
9	0.128	0.154	* 0.159
10	0.117	0.140	*0.144

2.2.8 Eleventh-order methods

In [21], Ketcheson showed that LM methods of order 11 with nonnegative coefficients need at least $k = 26$ steps with c_{eff}(LM(26,11)) $= 0.012$.

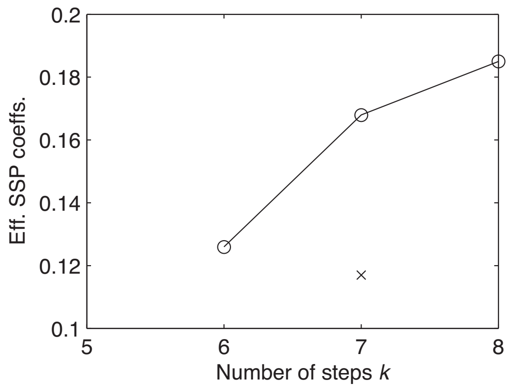
The optimal canonical $\text{HB}(k, s, 11)$ with stage number $s = 4, 5, \ldots, 10$ were found and presented in [40]. Their c_{eff} are listed in Table 2.8.

Table 2.8: c_{eff}(HB(k,s,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

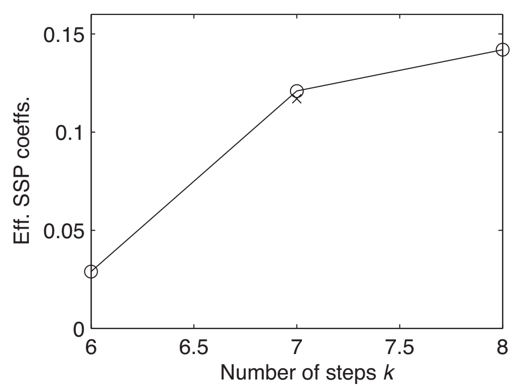
Table 2.9: c_{eff}(HB(k,s,12)) as function of k and s.

$s\backslash k$	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



HB(k,6,10) $\circ$, HM(7,7) $\times$

Figure 2.7: c_{eff}(HBk,6,10) of order 10 as function of k and HM(7,7) of order 7.



HB(k,7,11) $\circ$, HM(7,7) $\times$

Figure 2.8: Effective SSP coefficients versus number of steps k of 7-stage HB(k,7,11) of order 11 and HM(7,7) of order 7.

Remark 2.2.8 *From Table 2.8, we see that:*

- *The best HB method have larger c_{eff} than the best HM method, HM(7,7), that is, c_{eff}(HB(8,6,11)) $= 0.142 > c_{\mathit{eff}}$(HM(7,7)) $= 0.117$.*

- *The c_{eff} of HB(k, s,11) methods are equal at $s = 6$ and $s = 7$ when $k = 6$ and $k = 8$, that is, c_{eff}(HB(8,6,11)) $= c_{\mathit{eff}}$(HB(8,7,11)) $= 0.142$ and they are both the largest values.*

Figure 2.8 shows that c_{eff}(HB(8,7,11)) $>$ c_{eff}(HB(7,7,11)) $>$ c_{eff}(HM(7,7)) $=$ 0.117.

2.2.9 Twelfth-order methods

In [21], LM methods of order 12 with nonnegative coefficients require at least $k = 30$ steps with c_{eff}(LM(30,12)) $= 0.002$.

We numerically found optimal HB(k, s,12) with stage number $s = 5, 6, \dots, 10$ with their formulae and numerical results listed in [42]. Their c_{eff} are listed in Table 2.9 with largest c_{eff}(HB(8,7,12)) $= 0.096$.

Table 2.10: $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$ as function of stage number s and order p, and $c_{\text{eff}}(\text{RK}(s,4))$ of the s-stage RK(s,4) of order 4.

$p \backslash s$	4	5	6	7	8	9	10
4	HB(7,4,4) 0.508	HB(7,5,4) 0.514	HB(5,6,4) 0.515	HB(4,7,4) 0.535	HB(3,8,4) 0.554	HB(3,9,4) 0.587	**HB(3,10,4)** **0.614**
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) 0.341	HB(6,9,6) 0.319	HB(4,10,6) 0.290
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(5,8,7) 0.285	HB(5,9,7) 0.277	HB(6,10,7) 0.260
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(6,8,8) 0.233	HB(7,9,8) 0.212	HB(6,10,8) 0.193
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) 0.210	HB(8,9,9) 0.191	HB(8,10,9) 0.174
10	HB(8,4,10) 0.117	HB(8,5,10) 0.172	**HB(8,6,10)** **0.185**	HB(8,7,10) 0.182	HB(8,8,10) 0.176	HB(8,9,10) 0.159	HB(8,10,10) 0.144
11	HB(8,4,11) 0.053	HB(8,5,11) 0.126	**HB(8,6,11)** **0.142**	**HB(8,7,11)** **0.142**	HB(8,8,11) 0.127	HB(8,9,11) 0.114	HB(8,10,11) 0.104
12		HB(8,5,12) 0.057	HB(8,6,12) 0.091	**HB(8,7,12)** **0.096**	HB(8,8,12) 0.091	HB(8,9,12) 0.083	HB(8,10,12) 0.076

Table 2.10 lists the $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$ which are the numbers marked with an asterisk and the boldface numbers in Tables 2.1–2.9.

In Table 2.10, for a given s, $c_{\text{eff}}(\text{HB}(k,s,p))$ decreases with increasing p because the number of order conditions increases, which makes the set of feasible solutions of the optimization problem smaller. Thus, the SSP coefficient decreases, and hence c_{eff} also declines. In addition, $c_{\text{eff}}(\text{HB}(k,s,p))$ of orders $p = 6, 7, \ldots, 12$ are among the highest values when $s \in [6, 8]$. Hence, based on the c_{eff}, it seems that there are only 3 HB families which can have methods up to order 12 with good c_{eff}, namely, the 6-, 7- and 8-stage HB methods of order 4 to 12, among the most efficient methods on hand.

In Fig. 2.9, $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$, $p = 4, 5, \ldots, 12$, is plotted as a function of the stage number s. We note that, for a given $p \geq 5$, $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$ first increases with s and then decreases, which confirms again the first item in Remark 2.2.3. Besides, the smallest order HB methods have, the largest c_{eff} they achieve.

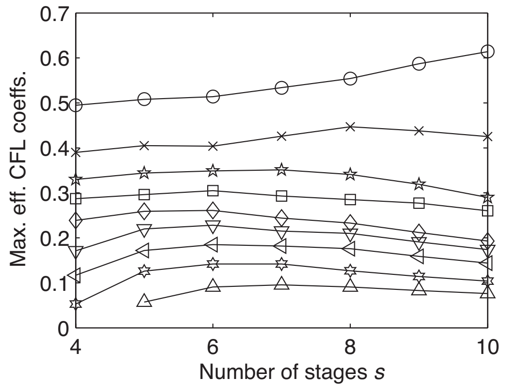


Figure 2.9: $\max_k c_{\text{eff}}(\text{HB}(k, s, p))$ as functions of s for orders $p = 4, 5, \ldots, 12$.

HB order 4 $\circ$, HB order 5 $\times$, HB order 6 $\star$

HB order 7 $\Box$, HB order 8 $\diamond$, HB order 9 $\bigtriangledown$

HB order 10 $\triangleleft$, HB order 11 $*$, HB order 12 $\bigtriangleup$

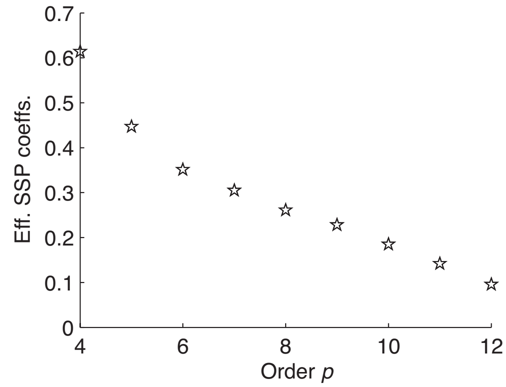


Figure 2.10: The figure plots $\max_{k,s} c_{\text{eff}}(\text{HB}(k, s, p))$ versus order p.

Figure 2.10 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.

Chapter 3

SSP s-Stage HB Methods Based on Combining k-Step with RK5 Methods

In 2002, Ruuth and Spiteri [46] have shown that there is no fifth-order SSP Runge–Kutta methods with nonnegative coefficients. In our research, we have been able to construct optimal SSP HB(k, s, p) methods with nonnegative coefficients, which have order conditions analogous to order conditions of s-stage RK of order 5 for $p = 5, 6, \dots, 12$. In addition, throughout our experiments, it is shown that the SSP effective coefficient, c_{eff} also depends on the order of RK methods which order conditions of HB methods are analogous to. Specifically, higher order RK methods lead to larger c_{eff} for HB(k, s, p). Therefore, we expect to construct HB(k, s, p) with nonnegative coefficients and larger c_{eff} based on RK methods of order 5 than with RK methods of order 4.

3.1 Order conditions for HB(k, s, p)

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

$$B_i(j) = \sum_{\ell=1}^{k-1} A_{\mathrm{B},i\ell}\,\frac{(-\ell)^j}{j!} + \sum_{\ell=1}^{k-1} B_{\mathrm{B},i\ell}\,\frac{(-\ell)^{j-1}}{(j-1)!}, \qquad \begin{cases} i = 2, 3, \ldots, s, \\ j = 1, 2, \ldots, p. \end{cases} \tag{3.1.1}$$

As in Subsection (2.1.2), expanding the numerical solutions produced by formulae (2.1.1)–(2.1.2) and the exact solution in Taylor series, we have following multistep- and several RK-type order conditions, respectively:

$$v_{B,i} + \sum_{j=1}^{k-1} A_{B,ij} = 1, \qquad i = 2, 3, \ldots, s+1, \tag{3.1.2}$$

$$\sum_{j=1}^{i-1} a_{ij} c_j^m + m! B_i(m+1) = \frac{1}{m+1}\, c_i^{m+1}, \qquad \begin{cases} i = 2, 3, \ldots, s, \\ m = 0, 1, \ldots, p-5. \end{cases} \tag{3.1.3}$$

However, since we reduce one simplifying assumption in (2.1.5) in the case of RK4 , the original set of order conditions for HB methods to obtain order p now is reduced to following equations, which are solved in the case of order $p > 5$,

$$\sum_{i=1}^{s} b_i c_i^m + m! B(m+1) = \frac{1}{m+1}, \qquad m = 0, 1, \ldots, p-1, \tag{3.1.4}$$

$$\sum_{i=2}^{s} b_i \left[\sum_{j=1}^{i-1} a_{ij}\, \frac{c_j^{p-4}}{(p-4)!} + B_i(p-3) \right] + B(p-2) = \frac{1}{(p-2)!}, \tag{3.1.5}$$

$$\sum_{i=2}^{s} b_i \frac{c_i}{p-2} \left[\sum_{j=1}^{i-1} a_{ij}\, \frac{c_j^{p-4}}{(p-4)!} + B_i(p-3) \right] + B(p-1) = \frac{1}{(p-1)!}, \tag{3.1.6}$$

$$\sum_{i=2}^{s} b_i \left[\sum_{j=1}^{i-1} a_{ij}\, \frac{c_j^{p-3}}{(p-3)!} + B_i(p-2) \right] + B(p-1) = \frac{1}{(p-1)!}, \tag{3.1.7}$$

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

$$= \frac{1}{(p-1)!}, \tag{3.1.8}$$

$$\sum_{i=2}^{s} b_i \frac{c_i^2}{(p-2)(p-1)} \left[\sum_{j=1}^{i-1} a_{ij} \, \frac{c_j^{p-4}}{(p-4)!} + B_i(p-3) \right] + B(p) = \frac{1}{p!}, \tag{3.1.9}$$

$$\sum_{i=2}^{s} b_i \frac{c_i}{p-1} \left[\sum_{j=1}^{i-1} a_{ij} \, \frac{c_j^{p-3}}{(p-3)!} + B_i(p-2) \right] + B(p) = \frac{1}{p!}, \tag{3.1.10}$$

$$\sum_{i=2}^{s} b_i \frac{c_i}{p-1} \left[\sum_{j=1}^{i-1} a_{ij} \left[\sum_{k=1}^{j-1} a_{jk} \, \frac{c_k^{p-4}}{(p-4)!} + B_j(p-3) \right] + B_i(p-2) \right] + B(p) = \frac{1}{p!}, \tag{3.1.11}$$

$$\sum_{i=2}^{s} b_i \left[\sum_{j=1}^{i-1} a_{ij} \, \frac{c_j^{p-2}}{(p-2)!} + B_i(p-1) \right] + B(p) = \frac{1}{p!}, \tag{3.1.12}$$

$$\sum_{i=2}^{s} b_i \left[\sum_{j=1}^{i-1} a_{ij} \frac{c_j}{p-2} \left[\sum_{k=1}^{j-1} a_{jk} \, \frac{c_k^{p-4}}{(p-4)!} + B_j(p-3) \right] + B_i(p-1) \right] + B(p) = \frac{1}{p!}, \tag{3.1.13}$$

$$\sum_{i=2}^{s} b_i \left[\sum_{j=1}^{i-1} a_{ij} \left[\sum_{k=1}^{j-1} a_{jk} \, \frac{c_k^{p-3}}{(p-3)!} + B_j(p-2) \right] + B_i(p-1) \right] + B(p) = \frac{1}{p!}, \tag{3.1.14}$$

$$\sum_{i=2}^{s} b_i \left\{ \sum_{j=1}^{i-1} a_{ij} \left[\sum_{k=1}^{j-1} a_{jk} \left(\sum_{\ell=1}^{k-1} a_{k\ell} \, \frac{c_\ell^{p-4}}{(p-4)!} + B_k(p-3) \right) + B_j(p-2) \right] + B_i(p-1) \right\} + B(p) = \frac{1}{p!}, \tag{3.1.15}$$

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

$$B(j) = \sum_{i=1}^{k-1} A_{B,s+1,i} \, \frac{(-i)^j}{j!} + \sum_{i=1}^{k-1} B_{B,s+1,i} \, \frac{(-i)^{j-1}}{(j-1)!}, \qquad j = 1, \ldots, p+1. \tag{3.1.16}$$

These order conditions are simply RK order conditions with backstep parts $B_i(\cdot)$ and $B(\cdot)$.

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

$$\sum_{i=2}^{s} \frac{b_i}{6} \left[\sum_{j=1}^{i-1} a_{ij} \, c_j + B_i(2) \right]^2 + B(5) = \frac{1}{5!}, \tag{3.1.17}$$

besides the order conditions (3.1.2)–(3.1.15).

**************** CORRECTIONS FOLLOWED REPORTS ***************

In fact, when expanding Taylor up to order 5 for numerical solution and exact solution, we obtain:

$$3\sum_{j=1}^{k-1} A_{B,s+1,j}\,\frac{(-j)^5}{5!} + \sum_{i=2}^{s}\frac{b_i}{2}\left[\sum_{j=1}^{k-1} A_{B,ij}\,\frac{(-j)^2}{2!} + \sum_{j=1}^{i-1} a_{ij}\,c_j + \sum_{j=1}^{k-1} B_{B,ij}\,(-j)\right]^2 \tag{3.1.18}$$
$$+\,3\sum_{j=1}^{k-1} B_{B,s+1,j}\,\frac{(-j)^4}{4!} = \frac{3}{5!},$$

which corresponds to elementary differential $\{\{f\}^2\}$. Equation (3.1.18) becomes (3.1.17) by using (3.1.1) and (3.1.16).

However, as $p = 6$, there is one more simplifying assumption in (3.1.3), that is:

$$\sum_{j=1}^{i-1} a_{ij}c_j + B_i(2) = \frac{1}{2}\,c_i^2. \tag{3.1.19}$$

Substitute (3.1.19) into (3.1.17), we have (3.1.4). Therefore, as $p \geq 6$, there is no additional condition (3.1.17).

**************** END ***************

3.2 Comparing effective SSP coefficients of HB with other methods

Following closely Subsection 2.1.8, to obtain the largest SSP coefficients c, we maximize r mentioned in (2.1.75) that is subject to the component-wise inequalities (2.1.76)–(2.1.83) together with the order conditions (3.1.2)–(3.1.15). The SSP effective coefficients c_{eff} obtained in what follows are computed by (2.2.1).

In Tables 3.1–3.7, for each stage value s, the row-wise maxima, $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$ are listed with an asterisk. The largest c_{eff} for each order p is in boldface. This data is

Table 3.1: c_{eff}(HB(k,s,6)) as function of k and s.

				HM(5,6) 0.104	HM(6,6) 0.181	HM(7,6) 0.220	
$s\backslash k$	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

summarized in Table 3.8 and Fig. 3.2. In Tables 3.1–3.8, the SSP effective coefficients c_{eff}, which are identical to the c_{eff} of HB for k-step methods combined with RK4, are put inside parenthesis.

It is noted that, in Tables 3.1–3.7, for a given k, c_{eff}(HB(k,s,p)) first increases with s and then decreases. On the other hand, for a given s, c_{eff}(HB(k,s,p)) first increases with k and then stabilizes. Therefore, empty entries in the tables correspond either to existing methods with smaller c_{eff}. These facts confirm again Remark 2.2.3 in Section 2.2.

3.2.1 Sixth-order methods

Table 3.1 shows c_{eff} of HB as well as c_{eff} of HM [17] and of TSRK ([23],[10]) 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 Ketcheson, Gottlieb and Macdonald [23] that 4- and 5-stage TSRK methods of order 6 exist. We found 3-step 4-stage HB(3,4,6) with good $c_{\text{eff}}(\text{HB}(3,4,6)) = 0.179$.

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 $\text{PEG}(c_{\text{eff}}(\text{HB}(5,7,6)), c_{\text{eff}}(\text{HM}(5,6))) = 238\%$ (by (2.2.2)).

Table 3.1 also gives a new phenomenon, which did not happen with k-step methods combined with RK4. That is, c_{eff} increases again when $s > 8$ after it has decreased for $k = 3, 4, 5, 6$.

3.2.2 Seventh-order methods

Table 3.2 lists c_{eff} of HB methods of order 7 together with c_{eff} of HM(7,7) [17] and TSRK ([23], [10]) of the same order. 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 $k = 3, 4, \ldots, 7$, we found HB(k,s,7), $s = 4, 5, \ldots, 10$, 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, Gottlieb and Macdonald [23] found a two-step, 8-stage RK method of order 7 with $c_{\text{eff}}(\text{TSRK}(8,7)) = 0.071$ with the best $c_{\text{eff}}(\text{TSRK}(12,7)) = 0.231$. However, they did not mention that with lower step number $s < 8$, two-step, s-stage RK 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 $c_{\text{eff}}(\text{TSRK}(12,7)) = 0.231$ of the best 12-stage

Table 3.2: c_{eff}(HB(k,s,7)) as function of k and s.

$s\backslash k$	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	”

method TSRK(12,7).

Compared with hybrid methods, despite the lower step number, $k = 4$, our optimal 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(7,7) is nonnegligible with PEG(c_{eff}(HB(6,6,7)), c_{eff}(HM(7,7))) = 161% (by (2.2.2)).

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

3.2.3 Eighth-order methods

The c_{eff} of optimal HB(k,s,8) with stage number $s = 4, 5, \ldots, 10$ and $k = 3, 4, \ldots, 8$ are presented in Table 3.3 with largest c_{eff}(HB(8,6,8)) = 0.261. Ketcheson, Gottlieb, Macdonald and Shu found c_{eff} of 11- and 12-stage TSRK ([23], [10]) of order 8. The best of these has c_{eff}(TSRK(12,8)) = 0.078. It is not mentioned in Ketcheson, Gottlieb and Macdonald [23] 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 HB(8,s,8) with good c_{eff}(HB(8,s,8)) $\geq$ 0.237 with stage number

Table 3.3: c_{eff}(HB(k,s,8)) as function of k and s.

$s\backslash k$	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

$s = 4, 5, \ldots, 10$.

Though general linear multistep, multistage SSP methods of order 9 to 12 with nonnegative coefficients have not been found in the literature, similar to the case of HB methods combining k-step and RK4 considered in Subsection 3.2.5 of Chapter 3, we discovered HB(k,s,p) of these high orders with good effective SSP coefficients, described in the following subsection 3.2.4.

3.2.4 High order methods

We numerically found optimal HB(k,s,9) with stage number $s = 4, 5, \ldots, 10$. Their c_{eff} are listed in Table 3.4 with largest c_{eff}(HB(8,6,9)) = 0.228.

In addition to the above results, the optimal HB(k,s,10) with stage number $s = 4, 5, \ldots, 10$ are found numerically and Table 3.5 lists all the c_{eff} of our optimal methods with largest c_{eff}(HB(8,6,10)) = 0.186.

The optimal HB(k,s,11) as well as HB(k,s,12) with stage number $s = 4, 5, \ldots, 10$ and their c_{eff} are listed in Table 3.6 and 3.7, respectively (see more in [40], [42]).

We see in Tables 3.6 and 3.7 that c_{eff}(HB(8,8,11)) = 0.156 and c_{eff}(HB(8,8,12)) =

Table 3.4: $c_{\text{eff}}(\text{HB}(k,s,9))$ as function of k and s.

$s\backslash k$	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 3.5: $c_{\text{eff}}(\text{HB}(k,s,10))$ as function of k and s.

$s\backslash k$	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

0.116 are largest for the values of k and s on hand, corresponding to order 11 and 12.

Table 3.8 lists $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$, which are the numbers with an asterisk and the boldface numbers in Tables 3.1–3.7.

In Table 3.8, as expected, for a given s, $c_{\text{eff}}(\text{HB}(k,s,p))$ decreases with increasing p. Moreover, the data from this table shows the phenomenon clearer than in the case of combining k-step and RK4. It is also seen that $c_{\text{eff}}(\text{HB}(k,s,p))$ of orders $p = 5, 6, \dots, 12$ 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. In chapter 5, numerical results about 8-stage HB methods, which combine k-step and RK5, will be presented.

In Fig. 3.1, $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$, $p = 4, 5, \dots, 12$, is plotted as a function of the stage number s. We note that, for a given $p \geq 5$, generally, $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$ first increases with s and then decreases.

Figure 3.2 plots $\max_{k,s} c_{\text{eff}}(\text{HB}(k,s,p))$ as a function of the order p. We note that,

Table 3.6: c_{eff}(HB(k,s,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	0.086	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 3.7: c_{eff}(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	0.062	*0.097
8	0.100	**0.116**
9	0.097	*0.112
10	0.089	*0.103

as expected, $\max_{k,s} c_{\text{eff}}(\text{HB}(k,s,p))$ decreases with increasing p.

Furthermore, as we see in Tables 3.1–3.8, most of the c_{eff} of HB(k,s,p) based on RK5 in this section when $s \geq 8$ are not identical to c_{eff} of HB methods based on RK4 in Section 2.2. Therefore, in the next section we shall concentrate on these stages to make comparison.

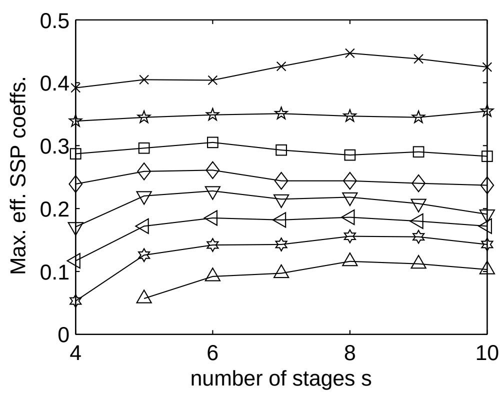
3.3 Comparing HB(k, s, p) based on combining k-step with RK2, RK3, RK4 and RK5 methods

Notation 3.3.1 *We denote the SSP HB methods used in this section as HB$_{RKq}$(k,s,p) for Hermite–Birkhoff methods of order p combining k-step methods and s-stage RKq of order q for $q = 2, 3, 4, 5$.*

The effective SSP coefficients c_{eff}(HB(k,s,p)) of HB(k,s,p) of order $p = 5, 6, \dots, 12$ are listed in Tables 3.9, 3.11 and 3.13 for stages $s = 8, 9, 10$, respectively. In these tables, the effective SSP coefficients are shown as a function of the Runge–Kutta methods RKq, $q = 2, 3, 4, 5$, which are combined with a k-step method to obtain HB(k,s,p).

Table 3.8: $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$ of HB(k,s,p) for k-step methods combined with RK5 as function of s and p.

$p\backslash s$	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) (0.117)	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) 0.156**	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



HB order 5 ×, HB order 6 ⋆

HB order 7 □, HB order 8 ⋄, HB order 9 ▽

HB order 10 ◃, HB order 11 ∗, HB order 12 △

Figure 3.1: $\max_k c_{\text{eff}}(\text{HB}(k,s,p))$ as function of s for orders $p = 5, 6, \ldots, 12$.

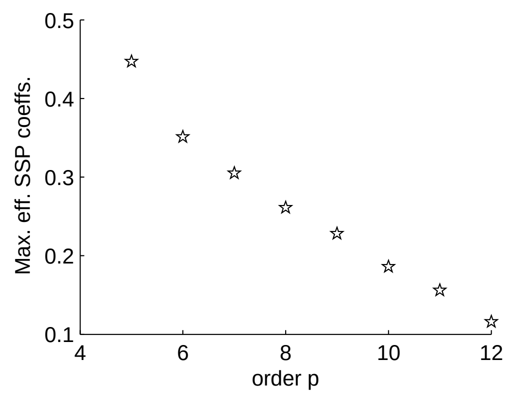


Figure 3.2: $\max_{k,s} c_{\text{eff}}(\text{HB}(k,s,p))$ versus order p.

Table 3.9: $c_{\text{eff}}(\text{HB}_{\text{RK}q}(k{,}8{,}p))$ for $p = 5, 6, \dots, 12$, as a function of RKq, $q = 2, 3, 4, 5$, which combine a k-step method to obtain $\text{HB}_{\text{RK}q}(k{,}8{,}p)$ for the listed k, p taken row-wise.

		c_{eff} of 8-stage HB combining k-step and:			
p	k	RK2	RK3	RK4	RK5
5	3	0.236	0.356	0.447	0.447
6	5	0.237	0.312	0.339	0.345
7	6	0.193	0.236	0.285	0.286
8	7	0.173	0.207	0.233	0.243
9	8	0.128	0.178	0.210	0.218
10	8	0.093	0.127	0.176	0.186
11	8	0.020	0.093	0.127	0.156
12	8		0.020	0.091	0.116

Following Definition 2.2.2 and formula (2.2.2), the percentage efficiency gain (PEG) of c_{eff} of $\text{HB}_{\text{RK5}}((k{,}s{,}p)$ over $\text{HB}_{\text{RK}q}(k{,}s{,}p)$, $q = 2, 3, 4$, for each order p are listed in Tables 3.10, 3.12 and 3.14 for stages $s = 8, 9, 10$, respectively. Here $\text{HB}_{\text{RK2}}(k{,}2{,}p)$ are Huang's hybrid methods [17].

The methods $\text{HB}_{\text{RKq}}(k{,}s{,}p)$, $q = 2, 3, 4, 5$, are compared in Fig. 3.3 on the basis of their effective SSP coefficients c_{eff} as a function of their order $p \geq 5$.

Remark 3.3.2 *From these tables and Fig. 3.3, it is observed that:*

- *For the same stage s, same order p and same step number k, if the order of RK, which is combined with a k-step method, is higher, the c_{eff} of the corresponding HB method is higher. For example, we consider the cases of RK4 and RK5, to obtain HB(k, s, p) methods in both cases, we agree Taylor expansions of exact and numerical solutions. This step will give the same number of conditions. However, after this step, we will use different number of simplifying assumptions*

Table 3.10: PEG($c_{\text{eff}}(\text{HB}_{\text{RK5}}(k,8,p))$, $c_{\text{eff}}(\text{HB}_{\text{RK}q}(k,8,p))$), $q = 2, 3, 4$, for the listed k, p taken row-wise.

		PEG of $c_{\text{eff}}(\text{HB}_{\text{RK5}}(k,8,p))$ over:		
p	k	$c_{\text{eff}}(\text{HB}_{\text{RK2}}(k,8,p))$	$c_{\text{eff}}(\text{HB}_{\text{RK3}}(k,8,p))$	$c_{\text{eff}}(\text{HB}_{\text{RK4}}(k,8,p))$
5	3	89 %	26 %	0 %
6	5	46 %	11 %	2 %
7	6	48 %	21 %	0 %
8	7	40 %	17 %	4 %
9	8	70 %	22 %	4 %
10	8	100 %	46 %	6 %
11	8	680 %	68 %	23 %
12	8		480 %	27 %

Table 3.11: $c_{\text{eff}}(\text{HB}_{\text{RK}q}(k,9,p))$, $q = 2, 3, 4, 5$, for $p = 5, 6, \ldots, 12$, respectively, as a function of RKq, which combine a k-step method to obtain $\text{HB}_{\text{RK}q}(k,9,p)$ for the listed k, p taken row-wise.

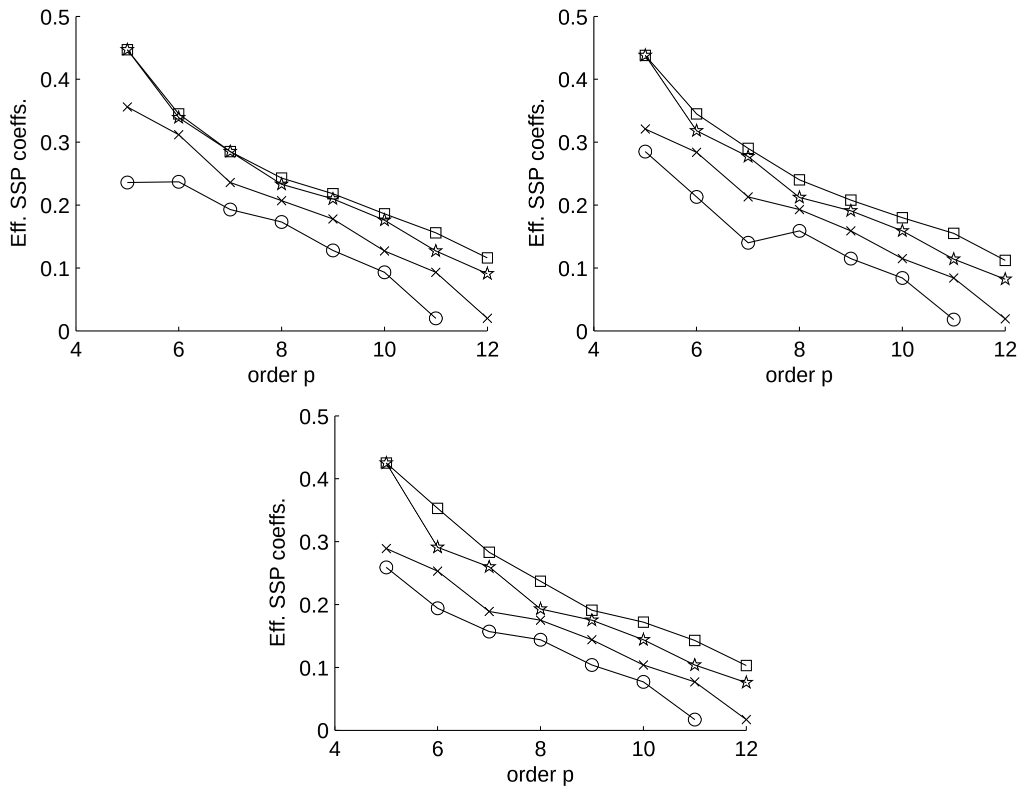
		c_{eff} of 9-stage HB combining k-step and:			
p	k	RK2	RK3	RK4	RK5
5	5	0.285	0.321	0.438	0.438
6	5	0.213	0.284	0.318	0.345
7	5	0.140	0.213	0.277	0.290
8	8	0.159	0.193	0.212	0.240
9	8	0.115	0.159	0.191	0.208
10	8	0.084	0.115	0.159	0.180
11	8	0.018	0.084	0.114	0.155
12	8		0.019	0.082	0.112

Table 3.12: PEG of $c_{\text{eff}}(\text{HB}_{\text{RK5}}(k,9,p))$ over $c_{\text{eff}}(\text{HB}_{\text{RK}q}(k,9,p))$, $q = 2, 3, 4$, respectively, for the listed k, p taken row-wise.

		PEG of $c_{\text{eff}}(\text{HB}_{\text{RK5}}(k,9,p))$ over:		
p	k	$c_{\text{eff}}(\text{HB}_{\text{RK2}}(k,9,p))$	$c_{\text{eff}}(\text{HB}_{\text{RK3}}(k,9,p))$	$c_{\text{eff}}(\text{HB}_{\text{RK4}}(k,9,p))$
5	5	54 %	36 %	0 %
6	5	62 %	21 %	8 %
7	5	107 %	36 %	5 %
8	8	51 %	24 %	13 %
9	8	81 %	31 %	9 %
10	8	114 %	57 %	13 %
11	8	761 %	85 %	36 %
12	8		489 %	37 %

Table 3.13: $c_{\text{eff}}(\text{HB}_{\text{RK}q}(k, 10, p))$ for $p = 5, 6, \ldots, 12$ as a function of RKq, which combine a k-step method to obtain $\text{HB}_{\text{RK}q}(k, 10, p)$, $q = 2, 3, 4, 5$, for the listed k, p taken row-wise.

		c_{eff} of 10-stage HB combining k-step and:			
p	k	RK2	RK3	RK4	RK5
5	5	0.259	0.289	0.425	0.425
6	5	0.194	0.253	0.291	0.353
7	6	0.157	0.189	0.260	0.283
8	8	0.144	0.175	0.193	0.237
9	8	0.104	0.144	0.175	0.191
10	8	0.077	0.104	0.144	0.172
11	8	0.017	0.077	0.104	0.143
12	8		0.017	0.076	0.103



$\mathrm{HB}_{\mathrm{RK2}}(k,s,p)$ $\circ$, $\mathrm{HB}_{\mathrm{RK3}}(k,s,p)$ $\times$, $\mathrm{HB}_{\mathrm{RK4}}(k,s,p)$ $\star$, $\mathrm{HB}_{\mathrm{RK5}}(k,s,p)$ $\square$

Figure 3.3: Effective SSP coefficients c_{eff} of 8-stage HB(k,8,p) (top left), 9-stage HB(k,9,p) (top right) and 10-stage HB(k,10,p) (bottom) versus their order $p = 5, 6, \ldots, 12$.

Table 3.14: PEG(c_{eff}(HB$_{\text{RK5}}$(k,10,p)), c_{eff}(HB$_{\text{RK}q}$(k,10,p))), $q = 2, 3, 4$, for the listed k, p taken row-wise.

		PEG of c_{eff}(HB$_{\text{RK5}}$(k,10,p)) over:		
p	k	c_{eff}(HB$_{\text{RK2}}$(k,10,p))	c_{eff}(HB$_{\text{RK3}}$(k,10,p))	c_{eff}(HB$_{\text{RK4}}$(k,10,p))
5	5	64 %	47 %	0 %
6	5	82 %	40 %	21 %
7	6	80 %	50 %	9 %
8	8	65 %	35 %	23 %
9	8	84 %	33 %	9 %
10	8	123 %	65 %	19 %
11	8	740 %	86 %	38 %
12	8		506 %	36 %

to reduce these conditions. We use $(p-3)$ *and* $(p-4)$ *equations for RK4 and RK5, respectively (see* (2.1.5) *and* (3.1.3)*). The order of k-step methods combined now are* $(p-3)$ *and* $(p-4)$ *for RK4 and RK5, respectively. Therefore, the number of constraints in optimization problem* (2.1.75) *in the case of RK4 are more than in the case of RK5. It leads to larger* c_{eff} *in the case of RK5.*

- *HB$_{RK5}$(k,s,p) compare favorably with the corresponding HB$_{RKq}$(k,s,p),* $q = 2, 3, 4$, *for stages* $s = 8, 9, 10$ *on the basis of* c_{eff}*, especially for the higher order such as* $p = 10, 11, 12$. *For example, the PEG of* c_{eff}*(HB$_{RK5}$(8,9,11)) is* 761% *over* c_{eff}*(HB$_{RK2}$(8,9,11)), the PEG of* c_{eff}*(HB$_{RK5}$(8,10,12)) is* 506% *over* c_{eff}*(HB$_{RK3}$(8,10,12)), and the PEG of* c_{eff}*(HB$_{RK5}$(k,10,p)) is* 38% *over* c_{eff}*(HB$_{RK4}$(8,10,11)) according to Tables 3.12 and 3.14, respectively.*

Chapter 4

Numerical Results for Some SSP HB Methods Based on Combining k-Step with RK4 Methods

This chapter presents some HB methods in noncanonical as well as canonical forms with fixed stage number or fixed order as typical examples when combining k-step methods with RK4. These new methods are combined with a spatial discretization such as difference quotient and WENO5 to solve Burgers' equation and linear advection equation. The obtained numerical results presented in this chapter show the efficiency of our methods.

4.1 Non-canonical SSP 4-stage HB methods and difference quotients

In this section, we shall consider explicit, k-step, 4-stage, SSP general linear methods of order p, $p = 5, 6, \ldots, 8$, with nonnegative coefficients as a combination of linear k -step methods of order $p-3$ and a 4-stage RK method of order 4 (see Section 5 and

6 in [38] for details).

The family of SSP HB methods that combine linear k-step methods of order $p-3$ and 4-stage RK method considered in this section, are 4-stage methods of order 4–8 with low step number.

The 4 formulae of these 4-stage HB methods to perform integration from t_n to t_{n+1} are defined in Section 2.1 by (2.1.1) and (2.1.2) with $s = 4$. Their order conditions are determined from (2.1.4)–(2.1.10) with $s = 4$.

The Shu–Osher and Butcher forms of these noncanonical SSP HB methods together with Theorem 2.1.4 to compute their feasible SSP coefficients are studied from Subsections 2.1.3–2.1.6 in Chapter 2 with $s = 4$.

Subsection 4.1.1 is about the construction of 4-stage SSP HB methods and a comparison of the effective SSP coefficients of our new methods to other methods. The numerical results are presented in Subsection 4.1.2 including the validating of the order preservation property, and the comparison when applied to Burgers' equation. The formulae of eleven noncanonical HB($k, 4, p$) methods are listed in the Appendix A.1.

4.1.1 Construction of 4-stage SSP HB methods

Since there are many free parameters in HB(k,s,p) when the number of steps, k, is sufficiently large, we use the MATLAB Optimization Toolbox to search for the methods with largest c for different k and different order p, see more in [38] for the complete families of 4-stage HB method of order p. The new HB(k,4,p) have larger effective SSP coefficients than known SSP hybrid methods (HM(k,p)) with the same k and p, especially when k is small.

There are many optimal SSP methods and results related to order 4 such as the family of SSP RK methods of Spiteri and Ruuth, Huang's hybrid methods [17], and Gottlieb, Shu and Tadmor [12] with the result about the non-existence of two-step

HM methods of order four with nonnegative coefficients.

Note that the new HB(2,4,4) requires one step less than HM(3,4) while both are fourth order. Also, the 4-stage HB(2,4,4) uses one fewer function evaluation than the 5-stage RK(5,4), both being of order 4.

Ruuth and Spiteri recently considered in [44, 47] fifth-order methods with negative coefficients. In case of linear multistep methods, Ruuth and Hundsdorfer [45] pointed out that fifth-order methods of this type need at least $k = 7$ steps. Huang [17] constructed a hybrid four-step, fifth-order SSP method with nonnegative coefficients, called HM(4,5), with $c(\mathrm{HM}(4,5)) = 0.371$ and $c_{\mathrm{eff}}(\mathrm{HM}(4,5)) = 0.185$.

Some authors found optimal SSP schemes of order 7 such as Huang [17] with hybrid methods, Ketcheson, Gottlieb, and Shu [10] with TSRK methods.

Table 4.1 lists $c(\mathrm{HB}(k,4,p))$, $c_{\mathrm{eff}}(\mathrm{HB}(k,4,p))$, $c(\mathrm{OM}(k,p))$, and $c_{\mathrm{eff}}(\mathrm{OM}(k,p))$ of HB(k,4,p) and known methods of order p in columns 3, 4, 6, and 7, respectively. Column 8 lists $\mathrm{PEG}(c_{\mathrm{eff}}(\mathrm{HB}(k,4,p)), c_{\mathrm{eff}}(\mathrm{OM}(k,p)))$ of HB methods over other known methods. It is seen that the $\mathrm{PEG}(c_{\mathrm{eff}}(\mathrm{HB}(k,4,p)), c_{\mathrm{eff}}(\mathrm{OM}(k,p)))$ is not negligible.

****************** CORRECTIONS **********************

For example, $\mathrm{PEG}(c_{\mathrm{eff}}(\mathrm{HB}(5,4,4)), c_{\mathrm{eff}}(\mathrm{RK}(4,4)))$ is 197% and $\mathrm{PEG}(c_{\mathrm{eff}}(\mathrm{HB}(5,4,6)), c_{\mathrm{eff}}(\mathrm{HM}(5,6)))$ is 202%. It is also noted that for given p, $\mathrm{PEG}(c_{\mathrm{eff}}(\mathrm{HB}(k,4,p)), c_{\mathrm{eff}}(\mathrm{HM}(k,p)))$ decreases as k increases.

************** END ***************************

Table 4.1 also shows that the new methods are generally competitive with known methods. As a first example, HB(5,4,4) has $c_{\mathrm{eff}}(\mathrm{HB}(5,4,4)) = 0,494$ larger than every k-step method of order 4 on hand including the seven-step SSP hybrid HM(7,4) with large $c_{\mathrm{eff}}(\mathrm{OM}(k,p)) = 0.469$. As a second example, these new methods are competitive with fifth-order hybrid methods given by Huang [17] based on the same number of steps, and with fifth-order RK methods with ten stages given by Ruuth [44]. This ten-stage method has $c_{\mathrm{eff}}(\mathrm{OM}(k,p)) = 3.395/10 \approx 0.339$, which is less than $c_{\mathrm{eff}}(\mathrm{HB}(5,4,5)) = 0.390$ of HB(5,4,5).

Table 4.1: PEG(c_{eff}(HB(k,4,p)),c_{eff}(OM(k,p))) for k-step HB(k,4,p), HM(k,p), LM(k,p) and GL(k,p) and s-stage RK(s,p) all of order p. Comparison is row-wise.

p	Meth.	c(HB(k,4,p))	c_{eff}(HB(k,4,p))	Meth.	c(OM(k,p))	c_{eff}(OM(k,p))	PEG
4	HB(2,4,4)	1.593	0.398	GL(2,4)	1.59	0.398	0 %
	HB(3,4,4)	1.843	0.461	HM(3,4)	0.494	0.247	87 %
	”			GL(3,4)	1.84	0.461	0 %
	HB(4,4,4)	1.932	0.483	HM(4,4)	0.682	0.341	42 %
	”			GL(4,4)	1.93	0.483	0 %
	HB(5,4,4)	1.979	0.494	HM(5,4)	0.793	0.396	25 %
	”			HM(7,4)	0.938	0.469	5 %
	”			RK(10,4)	6.000	0.600	-18 %
	”			RK(5,4)	1.508	0.302	64 %
	”			RK(4,4)	0.667	0.167	197 %
5	HB(4,4,5)	1.537	0.384	HM(4,5)	0.371	0.185	108 %
	HB(5,4,5)	1.562	0.390	HM(5,5)	0.525	0.262	49 %
	”			RK(10,5)	3.395	0.339	15 %
	HB(6,4,5)	1.569	0.392	HM(6,5)	0.657	0.328	20 %
6	HB(5,4,6)	1.265	0.316	HM(5,6)	0.209	0.104	202 %
	HB(6,4,6)	1.321	0.330	HM(6,6)	0.362	0.181	82 %
7	HB(7,4,7)	1.148	0.287	HM(7,7)	0.234	0.117	145 %

4.1.2 Numerical results

A. Validating order preservation

In many problems, the order of time discretizations is smaller than the conventional order of method formulae. This phenomenon is called order reduction phenomenon, see [49]. To illustrate the boundary/source order reduction phenomenon we consider a classic test problem described in [49]:

$$u_t(x,t) = -u_x(x,t) + b(x,t), \tag{4.1.1}$$

over $0 \leq x \leq 1$ and $0 \leq t \leq 1$ with initial condition $u(x,0) = 1 + x$, boundary conditions $u(0,t) = 1/(1+t)$ and source term $b(x,t) = (t-x)/(1+t)^2$. The exact solution, $u(x,t) = (1+x)/(1+t)$, is linear in space, allowing the use of first-order upwind space discretization without introducing discretization errors:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{u_i^n - u_{i-1}^n}{\Delta x} = 0,$$

where solution $u_i^n \approx u(t_i, x_n)$ for $t_i = i\Delta t$ and $x_n = n\Delta t$.

For the time integration, the SSP 5-stage RK method of order 4 and the classic RK method of order 4 are used. All considered explicit RK methods have stage order equal to one. Sanz-Serna *et al.* [49] show that explicit RK methods with $p \geq 3$ suffer from order reduction on problems with nonhomogeneous boundary conditions or nonzero source terms such as (4.1.1).

For the test problem (4.1.1), we distinguish two cases, one that illustrates the order reduction phenomenon, and for validation purposes, one that does not. Specifically, if the spatial and temporal grids are refined simultaneously, one notices that low stage order methods suffer from order reduction [49]. If the space grid is kept fixed, that is the ODE problem is fixed, then the (classic) order of consistency is preserved.

In the cases of RK(4,4) and RK(5,4), Table 4.2 shows the discretization error versus the time step without order reduction (when $\Delta x = 1/10$) and with order

Table 4.2: L_∞-error at $t = 1$ for the listed methods applied to Problem (4.1.1).

	HB(4,4,5)		HB(4,4,6)		HB(5,4,5)		HB(5,4,6)	
$\Delta t/\Delta x$	1/10	1/20	1/10	1/20	1/10	1/20	1/10	1/20
1/20	2.04e-8	2.33e-8	1.46e-9	1.90e-9	2.08e-8	2.25e-8	2.19e-9	2.81e-9
1/40	1.29e-9	1.60e-9	4.85e-11	6.36e-11	1.32e-9	1.62e-9	6.85e-11	8.98e-11
1/80	5.13e-11	7.41e-11	1.01e-12	1.53e-12	5.26e-11	7.49e-11	1.54e-12	2.13e-12
	HB(6,4,6)		HB(5,4,7)		RK(4,4)		RK(5,4)	
$\Delta t/\Delta x$	1/10	1/20	1/10	1/20	1/10	1/20	1/10	1/20
1/20	3.07e-9	3.86e-9	2.41e-10	5.98e-10	2.62e-6	1.63e-5	1.14e-6	5.89e-6
1/40	9.80e-11	1.25e-10	4.44e-12	5.78e-12	1.27e-7	6.55e-7	6.08e-8	2.89e-7
1/80	2.11e-12	2.97e-12	5.21e-14	7.66e-14	6.91e-9	3.24e-8	3.47e-9	1.56e-8

reduction (when $\Delta x = 1/20$). In the former case, the order of the RK methods is preserved (if Δx is maintained fixed at $\Delta x = 1/10$), whereas in the later case, the order clearly drops for all RK methods. A special boundary/source treatment can be used to alleviate this problem, but with great effort and limited success [2, 48, 49]. This discussion also applies to implicit RK methods with low stage orders such as DIRK [33].

The HB(k,4,p) methods listed in Table 4.2 maintain well their consistency orders compared to RK(4,4) and RK(5,4), in particular when space and time are refined simultaneously.

In the next parts, we present some numerical results to confirm the validity of our new optimal schemes on some test problems mentioned in Laney [27].

From now on we shall use the total variation semi-norm $\|y_n\| = TV(y_n)$ where

$$TV(y_n) = \sum_j |y_{n,j+1} - y_{n,j}|, \tag{4.1.2}$$

where $y_{n,j} \approx y(t_n, x_j)$ for $t_n = n\Delta t$ and $x_j = j\Delta t$, and say that a method is total variation diminishing (TVD) if

$$TV(y_{n+1}) \leq TV(y_n). \tag{4.1.3}$$

The following two definitions will help compare different methods with different computational costs more easily and fairly (See more in [17]).

Definition 4.1.1 *The largest effective CFL number of method M denoted by $num_{eff}(M)$, for error ϵ,*

$$|TV(u(x, t_{final})) - TV(u(x, t_0))| \leq \epsilon, \tag{4.1.4}$$

is defined by

$$num_{eff}(M) = \max_{\Delta t} \left\{ \frac{\Delta t}{\Delta x} \frac{1}{\ell} \right\}, \tag{4.1.5}$$

with time stepsize Δt, space stepsize Δx and ℓ is the number of function evaluations of the method per time step.

Then $\max \Delta t_{num} = \ell \Delta x \, num_{eff}(M)$ is called the maximum numerical stepsize. We let $\max\{\Delta t_{theor}\}$ be the maximum theoretical time step taken as

$$\max \Delta t_{theor} = c(M) \Delta t_{FE}, \tag{4.1.6}$$

and $R_{num/theor}$ be the ratio of the maximum numerical to theoretical stepsizes

$$R_{num/theor} = \frac{\max \Delta t_{num}}{\max \Delta t_{theor}}. \tag{4.1.7}$$

Definition 4.1.2 *The percentage efficiency gain, $PEG(num_{eff})$, of num_{eff} of method 2 over method 1, is defined by*

$$PEG(num_{eff}(M_2), num_{eff}(M_1)) = \frac{num_{eff}\,(M2) - num_{eff}\,(M1)}{num_{eff}\,(M1)}. \tag{4.1.8}$$

For the same method, $\mathrm{num}_{\mathrm{eff}}(M)$ and $R_{\mathrm{num/theor}}$ will be different to different test problems. There are many illustrations shown in Chapter 4 and 5.

*************** CORRECTIONS *******************

To apply the HB schemes, we need some starting values $t_0, t_1, t_3, \dots, t_{k-1}$ with $\Delta t = \ell \Delta x \, \mathrm{num}_{\mathrm{eff}}(M)$. These values are computed by using the optimal RK(5,4) scheme [46] with a small initial step size $h \approx 1.0\,$e-04.

************* END ***********************

B. Comparing SSP HB with other methods on Burgers' equation with unit-step initial condition

As a first comparison of our new methods with RK methods, following Huang [17], we consider Burgers' equation in Problem 1.

Problem 1 *Burgers' equation with unit-step initial condition:*

$$\frac{\partial}{\partial t} u(x,t) + \frac{\partial}{\partial x}\left[\frac{1}{2}\, u(x,t)^2\right] = 0, \quad u(x,0) = \begin{cases} 1, & -1 \le x < 0, \\ 0, & \quad 0 < x \le 1, \end{cases} \tag{4.1.9}$$

and boundary condition $u(-1,t) = 1$ for $t \ge 0$.

By using characteristic methods and the Rankine–Hugoniot jump condition, we can easily find the weak solution:

$$u(x,t) = \begin{cases} 1, & -1 \le x < t/2, \\ 0, & t/2 < x \le 1, \end{cases} \tag{4.1.10}$$

where the shock curve moves along $x = t/2$ (see Figures 4.1 and 4.2).

We discretize the spatial derivative by the difference quotient

$$\frac{1}{\Delta x}\left[\frac{1}{2}(u_j(t))^2 - \frac{1}{2}(u_{j-1}(t))^2\right], \tag{4.1.11}$$

with space stepsize $\Delta x = 1/150$, where $u_j(t)$ is an approximation to $u(x_j, t)$ with $x_j = j\Delta x$, $j = \dots, -2, -1, 0, 1, 2, \dots$. This leads to the semi-discrete system

$$\frac{d}{dt} u_j(t) = -\frac{1}{\Delta x}\left[\frac{1}{2}(u_j(t))^2 - \frac{1}{2}(u_{j-1}(t))^2\right], \tag{4.1.12}$$

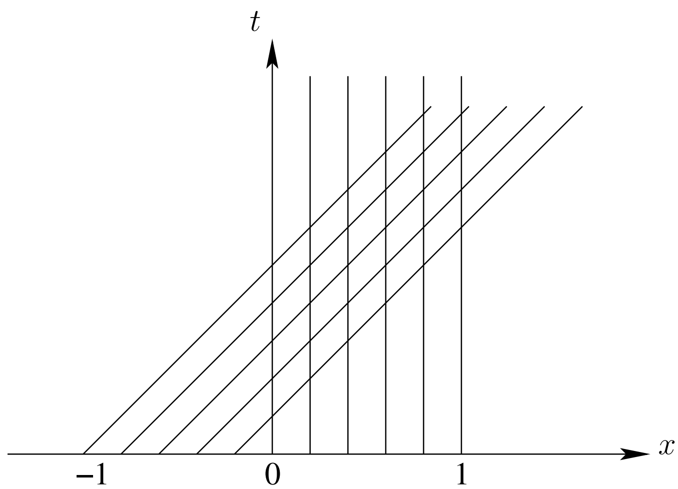


Figure 4.1: Characteristic curves associated with the initial-value Problem 1.

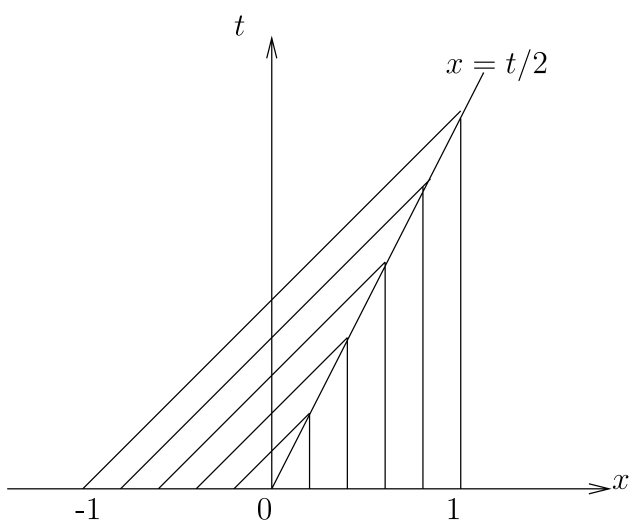


Figure 4.2: Characteristic curves associated with the solution of Problem 1.

to which a time discretization can be applied.

We consider the total variation norm of the numerical solution for this problem at $t_{\text{final}} = 1.8$ and take Δt sufficiently small such that (4.1.4) holds with $\epsilon = 5.0\,\text{e-}02$.

In Table 4.3, we list the maximum effective CFL number, num_{eff}, and the ratio $\max \Delta t_{\text{num}} / \max \Delta t_{\text{theor}}$ of SSP HB and other methods for Problems 1 on page 72. Column 8 shows the PEG(num_{eff}) of HB methods over hybrid and other known methods.

It is seen that:

- Generally, the k-step HB methods of orders 4 to 7 have higher num_{eff} than k-step hybrid methods, for the same k and RK methods with the same stage number s.
- An increase in the step number k improves the num_{eff} for the same order.
- HB(2,4,4), HB(3,4,4) and HB(4,4,4) behave almost like GL(2,4), GL(3,4) and GL(4,4), respectively, since their coefficients are almost identical.
- In Table 4.3, num_{eff} of HB(5,4,4), HB(4,4,5), HB(6,4,6) and HB(7,4,7) compare favorably with num_{eff} of most of the other methods of the same order.
- PEG(num_{eff}) between HB method and HM decreases as the step number k increases. For the same order, most of the new methods have larger PEG(num_{eff}) than Huang's hybrid methods when k is small.

C. Comparing SSP 4-stage HB and other methods on Burgers' equation with a square-wave initial condition

With the second comparison, we shall consider Burgers' equation with a square-wave initial value in Problem 2, which is one of Laney's five test problems [27].

Table 4.3: PEG of $\mathrm{num}_{\mathrm{eff}}$ for HB(k,4,p) over HM(k,p) and RK(s,p), and ratio $R_{\mathrm{num/theor}}$ applied to Problem 1.

p	Meth.	$\mathrm{num}_{\mathrm{eff}}$	$R_{\mathrm{num/theor}}$	Meth.	$\mathrm{num}_{\mathrm{eff}}$	$R_{\mathrm{num/theor}}$	PEG($\mathrm{num}_{\mathrm{eff}}$)
4	HB(2,4,4)	0.517	1.111	GL(2,4)	0.517	1.111	0 %
	HB(3,4,4)	0.572	1.065	HM(3,4)	0.302	1.049	89 %
	”		”	GL(3,4)	0.572	1.065	0 %
	HB(4,4,4)	0.610	1.083	HM(4,4)	0.408	1.026	50 %
	”		”	GL(4,4)	0.610	1.083	0 %
	HB(5,4,4)	0.636	1.102	HM(5,4)	0.486	1.051	31 %
	HB(5,4,4)	0.636	1.102	RK(10,4)	0.662	0.946	-4 %
	”		”	RK(5,4)	0.496	1.410	28 %
	”		”	RK(4,4)	0.414	2.130	54 %
5	HB(2,4,5)	0.385	1.547				
	HB(3,4,5)	0.496	1.246				
	HB(4,4,5)	0.538	1.201	HM(4,5)	0.342	1.581	57 %
	HB(5,4,5)	0.516	1.133	HM(5,5)	0.430	1.405	20 %
6	HB(3,4,6)	0.325	1.557				
	HB(4,4,6)	0.378	1.194				
	HB(5,4,6)	0.396	1.074	HM(5,6)	0.292	2.396	36 %
	HB(6,4,6)	0.422	1.096	HM(6,6)	0.258	1.222	64 %
7	HB(4,4,7)	0.316	1.922				
	HB(5,4,7)	0.368	1.439				
	HB(6,4,7)	0.408	1.368				
	HB(7,4,7)	0.410	1.225	HM(7,7)	0.208	1.525	97 %
8	HB(5,4,8)	0.244	1.708				
	HB(6,4,8)	0.294	1.397				
	HB(7,4,8)	0.310	1.248				

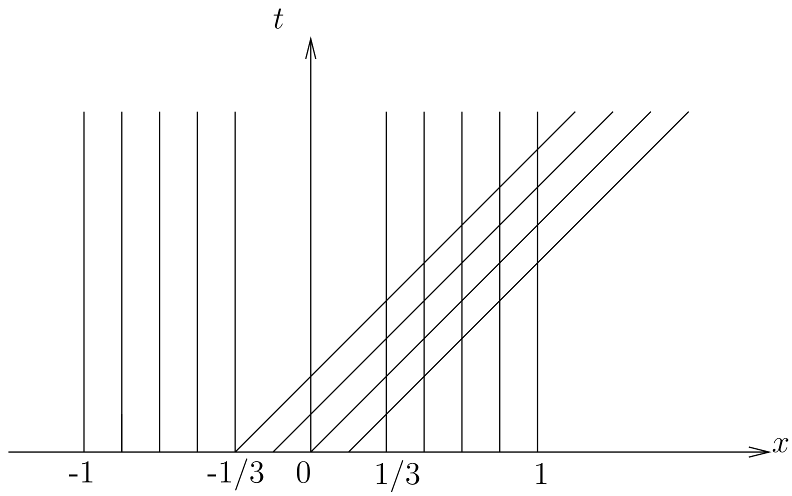


Figure 4.3: Characteristic curves associated with the initial-value Problem 2.

Problem 2 *Burgers' equation with a square wave initial condition:*

$$\frac{\partial}{\partial t}u(x,t) + \frac{\partial}{\partial x}\left[\frac{1}{2}\,u(x,t)^2\right] = 0, \quad u(x,0) = \begin{cases} 1, & |x| \le \frac{1}{3}, \\ 0, & \frac{1}{3} < |x| \le 1. \end{cases} \tag{4.1.13}$$

Here the jump at $x = -\frac{1}{3}$ creates an expansion fan and the jump at $x = \frac{1}{3}$ creates a shock. Using the method of characteristics and the Rankine–Hugoniot jump condition, the exact solution of the problem (see Figures 4.3 and 4.4) on domain $[-1,1]$ is as follow:

$$u(x,t) = \begin{cases} 0, & -1 \le x < -\frac{1}{3}, \\ \frac{x-\frac{1}{3}}{t}, & -\frac{1}{3} \le x < t - \frac{1}{3}, \\ 1, & t - \frac{1}{3} \le x < \frac{t}{2} + \frac{1}{3}, \\ 0, & \frac{t}{2} + \frac{1}{3} \le x \le 1, \end{cases} \tag{4.1.14}$$

We notice that solution (4.1.14) is the solution until the expansion fan $x = t - \frac{1}{3}$ and the shock $x = \frac{t}{2} + \frac{1}{3}$ intersect at the point $(1, \frac{4}{3})$.

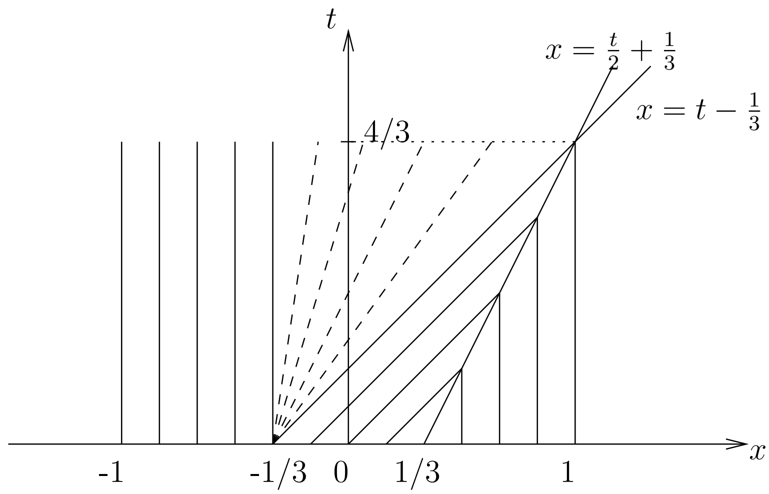


Figure 4.4: Characteristic curves associated with the solution of Problem 2 for $t \leq 4/3$.

If we continue consider $x > 1$, then the solution of Problem 2 also includes:

$$u(x,t) = \begin{cases} 0, & -1 \leq x < -\frac{1}{3}, \\ \frac{x-\frac{1}{3}}{t}, & -\frac{1}{3} \leq x < \frac{\sqrt{3t}+1}{3}, \\ 0, & \frac{\sqrt{3t}+1}{3} \leq x, \end{cases}$$

for $t > \frac{4}{3}$.

We discretize the spatial derivative of Problem 2 with periodic boundary condition $u(-1,t) = u(1,t)$ for $t \geq 0$ by the difference quotient (4.1.11) and compute the total variation of the numerical solution as a function of the effective CFL number, $\Delta t/(\ell \Delta x)$ at $t_{\text{final}} = 0.6$.

The num_{eff} of HB methods and hybrid methods applied to Problem 2 are listed in columns 3 and 6 of Table 4.4, respectively. The last column lists the $\text{PEG}(\text{num}_{\text{eff}})$ of HB methods over hybrid methods and other known methods.

It is seen that

- For the same order, $\text{PEG}(\text{num}_{\text{eff}})$ decreases as k increases but a simultaneous increase of k and p improves $\text{PEG}(\text{num}_{\text{eff}})$. In other words, Problem 2 confirms again that the new methods have larger PEG(num_{eff}) than Huang's hybrid methods when k is small.

- In Table 4.4, num_{eff} of HB(5,4,4) compares favorably with num_{eff} of other methods of the same order, including RK(10,4),
- num_{eff} of HB(4,4,5), HB(6,4,6) and HB(7,4,7) compare favorably with num_{eff} of other methods of the same order.

We observe that, as with RK methods [17], the ratio $\max \Delta t_{\text{num}} / \max \Delta t_{\text{theor}}$ of SSP HB for Problems 1 (page 72) and 2 (page 76) are greater than 1. The theoretical strong stability bounds of SSP HB methods are then verified in the numerical comparison of maximum time steps for Problem 1 and confirmed again in Problem 2. Moreover, generally, from Tables 4.3 and 4.4, HB methods have $\max \Delta t_{\text{num}} \geq \max \Delta t_{\text{FE}}$. Besides, these tables suggest the maximum step size we can take for each HB time discretizations to obtain good numerical solutions.

In conclusion, a collection of new SSP explicit 4-stage k-step Hermite–Birkhoff methods, HB(k,4,p), of orders $p = 4, \ldots, 8$ with nonnegative coefficients are constructed as k-step analogues of fourth-order Runge–Kutta methods, incorporating function evaluations at three off-step points. The new methods tend to have larger effective CFL coefficients than hybrid methods [17] with the same number of steps and other frequently used methods. Most of the proposed general linear methods can attain high stage orders, a property that alleviates the order reduction phenomenon encountered in the classic explicit RK schemes due to nonhomogeneous boundary/source terms (see [4]). Similar to [17], finding more efficient generalized SSP methods appears to be promising in the light of the present work.

Table 4.4: PEG of $\mathrm{num}_{\mathrm{eff}}$ of HB(k,4,p) over HM(k,p) and other known methods, and the ratio $R_{\mathrm{num/theor}}$ for Problem 2.

p	Meth.	$\mathrm{num}_{\mathrm{eff}}$	$R_{\mathrm{num/theor}}$	Meth.	$\mathrm{num}_{\mathrm{eff}}$	$R_{\mathrm{num/theor}}$	PEG($\mathrm{num}_{\mathrm{eff}}$)
4	HB(2,4,4)	0.540	1.141	GL(2,4)	0.540	1.141	0 %
	HB(3,4,4)	0.594	1.085	HM(3,4)	0.310	1.056	92 %
	”	”	”	GL(3,4)	0.594	1.085	0 %
	HB(4,4,4)	0.634	1.105	HM(4,4)	0.406	1.002	56 %
	”	”	”	GL(4,4)	0.634	1.105	0 %
	HB(5,4,4)	0.664	1.130	HM(5,4)	0.470	0.998	41 %
	”	”	”	RK(10,4)	0.618	0.867	7 %
	”	”	”	K(5,4)	0.442	1.234	50 %
	”	”	”	RK(4,4)	0.348	1.758	91 %
5	HB(2,4,5)	0.369	1.455				
	HB(3,4,5)	0.504	1.242				
	HB(4,4,5)	0.538	1.179	HM(4,5)	0.294	1.334	83 %
	HB(5,4,5)	0.532	1.147	HM(5,5)	0.382	1.225	39 %
6	HB(3,4,6)	0.325	1.528				
	HB(4,4,6)	0.394	1.221				
	HB(5,4,6)	0.412	1.097	HM(5,6)	0.252	2.030	63 %
	HB(6,4,6)	0.430	1.096	HM(6,6)	0.274	1.274	57 %
7	HB(4,4,7)	0.316	1.886				
	HB(5,4,7)	0.384	1.474				
	HB(6,4,7)	0.424	1.395				
	HB(7,4,7)	0.424	1.244	HM(7,7)	0.232	1.669	83 %
8	HB(5,4,8)	0.260	1.787				
	HB(6,4,8)	0.310	1.446				
	HB(7,4,8)	0.326	1.288				

4.2 Non-canonical SSP HB methods of order 4 and WENO5

In this section, to solve system (1.1.2), we construct non-canonical optimal, 4- to 10-stage, explicit SSP HB methods of order 4, denoted by HB(k,s,4) with nonnegative coefficients by combining linear k-step methods of order 1 with a 4- to 10-stage RK method of order 4 (see [35] for details).

The s formulae of these s-stage HB methods of order 4, defined by (2.1.1) and (2.1.2) in Section 2.1 with $s = 4, 5, \ldots, 10$, perform integration from t_n to t_{n+1}. Their order conditions are (2.1.4)–(2.1.10) with $p = 4$. The Shu–Osher and Butcher form of these non-canonical SSP HB methods using Theorem 2.1.4 to compute their feasible SSP coefficients are studied in (3.1.3)–(3.1.7) with $p = 4$. Their optimization problem can be formulated as (2.1.35)–(2.1.37) subject to all the constraints listed in Subsection 2.1.4 and the order conditions (2.1.4)–(2.1.10) for $p = 4$ (see also [35]).

In Subsection 4.2.1, we compare the effective SSP coefficients of our methods with those of other methods. The numerical results on the efficiency of the new methods tested on Burgers' equation are presented in Subsection 4.2.2. The list of thirteen noncanonical HB($k, s, 4$) formulae is in the Appendix A.2.

4.2.1 Comparing our new HB(k,s,4) with other SSP methods

The c_{eff} coefficients of HB(k,s,4) methods are listed in Table 4.5

Remark 4.2.1 *From Table 4.5, we observe that:*

- *We have the same phenomenon described in Remark 2.2.3 of Section 2.2, that is, c_{eff} increases with s or with k.*
- *The 3-step, 10-stage HB method has the largest effective SSP coefficient, listed in boldface, among the 4th-order HB methods on hand.*

Table 4.5: $c_{\text{eff}}(\text{HB}(k,s,4))$ for $k = 2, 3, 4, 5$ and $s = 4, 5, \ldots, 10$.

s/k	HB(2,s,4)	HB(3,s,4)	HB(4,s,4)	HB(5,s,4)
4	0.398	0.461	0.483	0.494
5	0.452	0.504	0.508	
6	0.488	0.512	0.514	0.515
7	0.532	0.534	0.536	
8	0.553	0.554	0.554	
9	0.586	0.587		
10	0.610	**0.614**		

- *All of our new methods (except HB(2,4,4)) have greater* c_{eff} *than those of the hybrid methods listed in Table 4.6.*
- *As shown in Tables 4.5 and 4.6, RK(5,4) and RK(6,4) have smaller* c_{eff} *than those of HB(k,s,4) methods.*
- *For the same stage s,* $s = 5, \ldots, 10$, $c_{\mathit{eff}}(HB(k,s,4)) > c_{\mathit{eff}}(RK(s,4))$.

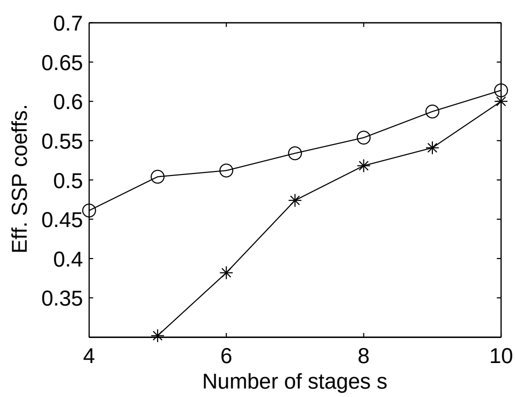
In Table 4.6, we compare the efficiency of our methods computed by (2.2.2) in Section 2.2 with some other methods. Although we do not compute the PEG between HB methods and GL methods of the same order in the table, we saw that their c_{eff} are the same, and hence the PEG will be zero.

Figure 4.5 compares HB(3,s,4) and RK(s,4) on the basis of their effective SSP coefficients as functions of their number of stages. Clearly, the new methods, generally, have larger effective SSP coefficients, especially when the number of stages of both methods is small.

From these tables and figure, our investigation to obtain HB(k,s,4) methods by combining linear k-step methods and 4- to 10-stage RK methods of order 4, shows that these new SSP methods have good SSP coefficients.

Table 4.6: Lower right block: PEG(c_{eff}) of HB(k,s,4) over HM(k,4) and RK(s,4).

			HB(5,4,4)	HB(3,5,4)	HB(5,6,4)	HB(3,7,4)	HB(2,8,4)	HB(3,9,4)	HB(2,10,4)
	c		1.979	2.520	3.093	3.741	4.424	5.279	6.102
		c_{eff}	0.494	0.504	0.515	0.534	0.553	0.587	0.610
HM(3,4)	0.494	0.247	80%	104%	109%				147%
HM(4,4)	0.682	0.341	45%	48%	51%	57%			79%
HM(5,4)	0.793	0.396	25%	27%	30%	35%	40%		54%
HM(6,4)	0.879	0.439	13%	15%	17%	22%	26%	34%	39%
RK(5,4)	1.508	0.302	64%	67%	71%	77%	83%	94%	102%
RK(6,4)	2.295	0.382	29%	32%	35%	40%	45%	54%	60%
RK(7,4)	3.321	0.474	4%	6%	9%	13%	17%	24%	29%
RK(8,4)	4.146	0.518	-5%	-3%	-1%	3%	7%	13%	18%
RK(9,4)	4.869	0.541	-9%	-7%		-1%	2%	9%	13%
RK(10,4)	6.000	0.600					-8%	-2%	2%



HB(3,s,4) $\circ$, RK(s,4) $*$

Figure 4.5: Effective SSP coefficients, c_{eff}, versus number of stages, s, of 3-step HB(3,s,4) methods and RK(s,4) methods, including Ketcheson's RK(10,4).

In the next parts, we shall present some numerical results to confirm the validity of our new optimal schemes on two problems of inviscid Burgers' equation with different initial conditions: the first problem with a unit downstep initial condition and the second with a square-wave initial condition.

However, instead of using the difference quotient (4.1.11) as a spatial discretization, we shall use Weighted Essentially Non-Oscillatory (WENO) schemes.

In our research, we use WENO of order 5 (WENO5), which was suggested by Jiang and Shu in [19], and combine this finite difference scheme with SSP time discretization methods when we compare our SSP HB methods to other methods on Burgers' equation. The reason of using WENO5 is the compatibility of orders between our methods as time discretization methods and WENO5 as a spatial discretization method. Furthermore, this method is a very good choice as Shu suggested in [52].

**************** CORRECTIONS FOLLOWED REPORTS ***********************
There are many studying about finite volume and finite difference WENO5 when combining with SSP methods (see [32, 19, 52, 61]). Recently, Wang and Spiteri in [60] proved theoretically and numerically the linear instability of first- and second-order SSP RK methods when coupled with WENO5. Moreover, they showed that it is sufficient to include the part of imaginary axis in the linear stability domain of explicit RK methods such as SSP RK of order three. However, in 2011, Motamed, Macdonald and Ruuth in [34] pointed out that inclusion of imaginary axis is not a necessary condition. They also illustrated that the time discretization methods, which do not satisfy this condition, are suitable when combining with WENO5.

*************** END *******************

4.2.2 Numerical results with WENO5 spatial discretization

A. Burgers' equation with a unit downstep initial condition

Consider Problem 1 with (4.1.9) (page 72). First we discretize the spatial derivative of the flux function $f(u) = u(x,t)^2/2$ by WENO5 of Jiang and Shu [19] with the spatial step size $\Delta x = 1/150$ to obtain the semi-discrete system

$$\frac{d}{dt}u_j(t) = -\frac{1}{\Delta x}\left[f_{j+(1/2)} - f_{j-(1/2)}\right], \tag{4.2.1}$$

where $u_j(t) \approx u(x_j,t)$ with $x_j = j\Delta x,\ j = -150, -149, \ldots, 149, 150,$ and $f_{j+(1/2)}$ is the numerical flux, which typically is a Lipschitz continuous function of several neighboring values $u_j(t)$ (see [19] for details). Now a time discretization can be applied to (4.2.1). For Problem 1, we consider the total variation norm of the numerical solution at $t_{\text{final}} = 1.8$ and take Δt sufficiently small such that (4.1.4) holds with $\epsilon = 5.0\,\text{e-02}$.

The numerical results show that the FE method satisfies the TVD property (4.1.3) under the time step restriction

$$\Delta t \leq \Delta t_{\text{FE}} = 0.325\Delta x. \tag{4.2.2}$$

The num_{eff}(HB(k,s,4)), for $s = 4, 5, \ldots, 10$, as a function of s for this problem are listed in Table 4.7.

The largest effective CFL numbers, num_{eff}, of several HB(k,s,4) and HM(k,4) for $k = 3, \ldots, 6$ and RK(10,4) applied to Problem 1 (page 72) are listed and compared in Table 4.8. The lower right block lists the PEG(c_{eff}) of HB(k,s,4) over the other methods on hand.

Remark 4.2.2

- *HB(k,s,4) have larger num$_{\text{eff}}$ than HM methods and RK(10,4), thus every percentage efficiency gain in Table 4.9 is positive.*

Table 4.7: num_{eff}(HB(k,s,4)) for HB(k,s,4) applied to Problem 1.

s/k	HB(2,s,4)	HB(3,s,4)	HB(4,s,4)	HB(5,s,4)
4	0.390	0.365	0.380	0.380
5	0.385	0.405	0.395	
6	0.430	**0.440**	0.420	0.421
7	0.421	0.426	0.421	
8	0.370	0.375	0.377	
9	0.360	0.365		
10	0.350	0.360		

- *Among HB schemes, although HB(2,10,4) has the largest* $c_{\text{eff}} = 0.610$ *(see Table 4.5), it has the smallest num*$_{\text{eff}}$ *when applied to Problem 1.*
- *HB(3,6,4) has the greatest num*$_{\text{eff}}$ *among the HB(k,s,4) methods listed in Table 4.7.*

B. Burgers' equation with a square-wave initial condition

In the next comparison, we consider again the fourth of Laney's five test problems [27, p. 312], that is Problem 2 (page 76).

We use the same procedure as in Problem 1, that is we discretize the spatial derivative of Problem 2 by WENO5 and compute the total variation of the numerical solution as a function of the effective CFL number, (4.1.5) at t_{final}. However, for Problem 2, $t_{\text{final}} = 0.6$ and obtained num_{eff}(FE)=0.183 in (4.2.2) instead of 0.325.

In Table 4.9, we list num_{eff}(HB(k,s,4)) for $s = 4, 5, \ldots, 10$ and $k = 2, \ldots, 5$ for HB(k,s,4) applied to Problem 2.

The num_{eff} of HB(k,s,4), HM(k,4) and RK(10,4) applied to Problem 2 are listed in Table 4.10. The lower right block shows PEG(c_{eff}) of HB(k,s,4) over the other

Table 4.8: Lower right block: PEG(num_{eff}) of HB(k,s,4) over HM(k,4) and RK(10,4) and ratio $R_{\text{num/theor}}$ for HB(k,s,4), HM(k,4) and RK(10,4) applied to Problem 1.

			HM(3,4)	HM(4,4)	HM(5,4)	HM(6,4)	RK(10,4)
	num_{eff}		0.214	0.264	0.329	0.274	0.346
		$R_{\text{num/theor}}$	2.666	2.382	2.553	1.918	1.774
HB(2,4,4)	0.390	3.013	82%	48%	19%	42%	13%
HB(3,4,4)	0.365	2.437	71%	38%	11%	33%	5%
HB(2,5,4)	0.385	2.623	80%	46%	17%	41%	11%
HB(3,6,4)	0.440	2.647	101%	63%	31%	57%	24%
HB(4,7,4)	0.421	2.434	97%	60%	28%	54%	22%
HB(4,8,4)	0.377	2.092	76%	43%	15%	38%	9%
HB(2,9,4)	0.360	1.891	68%	36%	9%	31%	4%
HB(2,10,4)	0.350	1.765	64%	33%	6%	28%	1%

Table 4.9: num_{eff}(HB(k,s,4)) for HB(k,s,4) applied to Problem 2.

s/k	HB(2,s,4)	HB(3,s,4)	HB(4,s,4)	HB(5,s,4)
4	0.405	0.350	0.375	0.375
5	0.410	0.405	0.395	
6	0.415	0.435	0.451	
7	0.446	0.441	0.450	
8	0.400	0.410	0.410	
9	0.400	0.405		
10	0.390	0.390		

Table 4.10: Lower right block: PEG(num$_{\text{eff}}$) of HB(k,s,4) over HM(k,4) and RK(10,4) and ratio $R_{\text{num/theor}}$ for HB(k,s,4), HM(k,4) and RK(10,4) applied to Problem 2.

			HM(3,4)	HM(4,4)	HM(5,4)	HM(6,4)	RK(10,4)
	num$_{\text{eff}}$ \ num$_{\text{eff}}$		0.210	0.280	0.310	0.204	0.371
		$R_{\text{num/theor}}\backslash R_{\text{num/theor}}$	4.638	4.480	4.265	2.532	3.373
HB(2,4,4)	0.405	5.548	93%	45%	31%	99%	9%
HB(3,4,4)	0.350	4.144	67%	25%	13%	72%	-0.1%
HB(2,5,4)	0.410	4.953	95%	46%	32%	101%	11%
HB(3,6,4)	0.435	4.640	107%	55%	40%	113%	17%
HB(4,7,4)	0.450	4.584	114%	61%	45%	121%	21%
HB(2,8,4)	0.400	3.946	91%	43%	29%	96%	8%
HB(2,10,4)	0.390	3.487	86%	39%	26%	91%	5%

methods on hand.

Remark 4.2.3

- *For Problem 2, the num$_{\textit{eff}}$(HB(k,s,4)) listed in Table 4.8, except for HB(3,4,4)=0.350, are larger than the num$_{\textit{eff}}$ of HM(k,4) and RK(10,4) listed in Table 4.10.*
- *Although, according to Table 4.5, HB(2,5,4) has smaller $c_{\textit{eff}}$ than HB(3,8,4), HB(4,8,4), it is shown in Table 4.8 that they have the same num$_{\textit{eff}}$ when applied to Problem 2. Similarly, although HB(3,5,4) has smaller $c_{\textit{eff}}$ than HB(3,9,4), they also have the same num$_{\textit{eff}}$ when applied to Problem 2.*
- *Among the HB(k,s,4) methods, HB(3,6,4) and HB(4,6,4) have the highest num$_{\textit{eff}}$ for Problems 1 and 2, respectively.*

To sum up, we extend the Shu–Osher form for Runge–Kutta methods [53] to a Shu–Osher form for HB methods. Moreover, under this form, new series of optimal, explicit, k-step, s-stage, SSP Hermite–Birkhoff methods, HB(k,s,4), of order 4 for

$s = 4, 5, \ldots, 10$, with nonnegative coefficients are obtained by combining linear k-step methods with 4- to 10-stage Runge–Kutta methods of order 4. Although some methods, such as HM, GL, and RK methods of the same order, have been found in the literature, HB methods have better SSP coefficients and larger maximum effective CFL numbers when tested on Burgers' equation.

4.3 Canonical SSP 8-stage HB methods of order p and WENO5

In this subsection, we construct canonical optimal, 8-stage, explicit SSP HB methods of orders 4 to 12, HB(k,8,p), with nonnegative coefficients by combining linear k-step methods of order $(p-3)$ with an 8-stage RK method of order 4 (see also [41] for the case of non-canonical, 7-stage SSP HB methods) .

We perform an integration from t_n to t_{n+1} by a set of 8 formulae of 8-stage HB methods defined by (2.1.1)–(2.1.2) in Section 2.1 with $s = 8$.

Using the optimization problem (2.1.75) and the inequalities (2.1.76)–(2.1.83) together with the order conditions (2.1.4)–(2.1.10) corresponding to $s = 8$, we obtain optimal HB schemes.

The first part of this section, Subsection 4.3.1, presents the construction of the new methods as well as comparing the SSP coefficients and effective SSP coefficients of the new methods with other methods. The numerical verification of the order of the new methods is presented in the next subsection. Subsection 4.3.3 gives the numerical results when the new methods are applied on Burgers' equation and linear advection equation to confirm their efficiency. The Appendix A.3 lists the canonical Shu–Osher form of nine of the 29 new 8-stage HB(k,8,p) methods with lowest k for given p (except for HB(8,8,11) and HB(8,8,12)), their c(HB(k,8,p)), c_{eff}(HB(k,8,p)) and abscissa vector $\sigma = [c_1, c_2, \ldots]$.

4.3.1 Effective SSP coefficients, c_{eff}, of 8-stage HB(k,8,p)

In [23], Ketcheson, Gottlieb and Macdonald found two-step 8-stage RK methods of order 6 with c_{eff}(TSRK(8,6)) = 0.242. We found the best HB(k,8,6) with $k = 2, 3, 4, 5, 6$. Moreover, HB(6,8,6) has largest c_{eff}(HB(6,8,6)) = 0.341 among the 8-stage sixth-order HB methods.

Ketcheson, Gottlieb and Macdonald [23] found two-step 8-stage RK methods of order 7 with c_{eff}(TSRK(8,7)) = 0.071. We have not found HB(2,8,7) since there is no feasible solution the optimization problem with fmincon function of Matlab Optimization Toolbox. However, increasing the step number to $k = 3, 4, 5$, we find HB(k,8,7) with larger SSP coefficients.

Two-step RK methods of order 6 to 8 with nonnegative coefficients with more stages are found in [23]. Among these, the following methods have the best effective SSP coefficients, c_{eff}(TSRK(12,6)) = 0.365, c_{eff}(TSRK(12,7)) = 0.231, and c_{eff}(TSRK(12,8)) = 0.078,

It is not mentioned in [23] that two-step 8- to 10-stage RK methods of order 8 exist. Our investigation shows that a 4-step, 8-stage HB method of order 8 exists and has a fairly good effective SSP coefficient, c_{eff}(HB(4,8,8)) = 0.192.

Although we have not found any SSP general linear methods of order 9 to 12 with nonnegative coefficients in the literature, our study indicates that HB(5,8,9), HB(6,8,10), HB(7,8,11) and HB(8,8,12) exist with a low step number k and have fairly good SSP coefficients, c_{eff}(HB(5,8,9)) = 0.153, c_{eff}(HB(6,8,10)) = 0.141, c_{eff}(HB(7,8,11)) is 0.110 and c_{eff}(HB(8,8,12)) = 0.091, respectively.

According to our numerical search, it seems that HB(k,8,p) methods of order 6 to 12 with nonnegative coefficients require at least $k = 2, 3, 4, 5, 6, 7$ steps with c_{eff}(HB(2,8,6)) = 0.240, c_{eff}(HB(3,8,7)) = 0.229, c_{eff}(HB(4,8,8)) = 0.192, c_{eff}(HB(5,8,9)) is 0.153, c_{eff}(HB(6,8,10)) = 0.141, c_{eff}(HB(7,8,11)) = 0.110 and c_{eff}(HB(7,8,12)) = 0.055, respectively.

Our best k-step methods of orders 6 to 12 are with $k = 2, 3, \ldots, 6$, $k = 3, 4, 5, 6$, $k = 4, 5, \ldots, 8$, $k = 5, 6, 7, 8$, $k = 7, 8$, $k = 7, 8$ and $k = 7, 8$, respectively.

Table 4.11 lists c(HB(k,8,p)), c_{eff}(HB(k,8,p)), and c(OM(k,p)), c_{eff}(OM(k,p)) for the other methods on hand, and column 8 shows the PEG(c_{eff}(HB(k,8,p)), c_{eff}(OM(k,8,p))) computed by (2.2.2).

Remark 4.3.1 *From Table 4.11, we observe that:*

- *Our best methods of order 4 are HB(2,8,4) and HB(3,8,4) and of order 5 is HB(2,8,5) with* c_{eff}*(HB(2,8,5))* $=$ c_{eff}*(TSRK(8,5)).*

- *The characteristic of* c_{eff} *follows Remark 2.2.3 in Section 2.2. Therefore, among the obtained HB(k,8,p), the methods, which have the largest and smallest* c_{eff} *are HB(3,8,4) and HB(7,8,12), respectively.*

- *All of the HB methods have greater* c_{eff} *than those of GL and HM methods of the same order, which implies that the corresponding PEG are positive.*

- *We have not found any SSP general linear methods of order 9 to 12 with non-negative coefficients in the literature. But our study indicates that there are SSP HB methods of order 9 to 12 with low step number and fairly good effective SSP coefficients (see Table 4.11).*

- *For the same step number, the same order and the same stage number, TSRK methods are slightly better than HB methods. However, if we increase the step number* $k = 3, 4, 5, 6$*, we find that HB(k,8,p) have larger effective SSP coefficients* c_{eff}*. This is the advantage of increasing the step number. For instance,* c_{eff}*(HB(2,8,6))* $= 0.240$ *is smaller than* c_{eff}*(TSRK(8,6))* $= 0.242$*, yet when k increases,* c_{eff}*(HB(k,8,6))) increase and are larger than* c_{eff}*(TSRK(8,6)).*

- *The last column of Table 4.11 shows that our methods are better than others except for RK(10,4) and TSRK(8,4).*

Table 4.11: PEG(c_{eff}(HB(k,8,p)), c_{eff}(OM(k,p))) for HB(k,8,p) and OM(k,p) taken row-wise.

p	HB(k,8,p)	c(HB(k,8,p))	c_{eff}(HB(k,8,p))	OM(k,p)	c(OM(k,p))	c_{eff}(OM(k,p))	PEG
4	HB(2,8,4)	4.424	0.561	GL(2,4)	1.590	0.398	41 %
	HB(3,8,4)	4.431	0.562	GL(3,4)	1.840	0.461	22 %
	”	”	”	GL(4,4)	1.930	0.483	16 %
	”	”	”	HM(3,4)	0.494	0.247	127 %
	”	”	”	HM(4,4)	0.682	0.341	65 %
	”	”	”	HM(5,4)	0.793	0.396	42 %
	”	”	”	HM(6,4)	0.879	0.439	28 %
	”	”	”	HM(7,4)	0.938	0.469	20 %
	”	”	”	RK(5,4)	1.508	0.302	86 %
	”	”	”	RK(8,4)	4.146	0.518	8 %
	”	”	”	RK(10,4)	6.000	0.600	-6 %
	”	”	”	TSRK(8,4)	4.496	0.562	0 %
5	HB(2,8,5)	3.579	0.447	HM(4,5)	0.371	0.185	142 %
	”	”	”	HM(5,5)	0.525	0.262	71 %
	”	”	”	HM(6,5)	0.657	0.328	32 %
	”	”	”	HM(7,5)	0.746	0.373	20 %
	”	”	”	RK(9,5)	2.696	0.300	49 %
	”	”	”	RK(10,5)	3.395	0.339	32 %
	”	”	”	TSRK(8,5)	3.576	0.447	0 %
6	HB(2,8,6)	1.924	0.240	HM(5,6)	0.209	0.104	131 %
	HB(3,8,6)	2.621	0.328	”	”	”	215 %
	HB(4,8,6)	2.687	0.336	”	”	”	223 %
	HB(5,8,6)	2.714	0.339	”	”	”	226 %
	HB(6,8,6)	2.727	0.341	”	”	”	229 %
	”	”	”	HM(6,6)	0.362	0.181	88 %
	”	”	”	HM(7,6)	0.440	0.220	55 %
	”	”	”	TSRK(8,6)	1.936	0.242	41 %
7	HB(3,8,7)	1.828	0.229	HM(7,7)	0.234	0.117	96 %
	HB(4,8,7)	2.243	0.280	”	”		139 %
	HB(5,8,7)	2.279	0.285	”	”	”	144 %
	HB(6,8,7)	2.284	0.285	”	”	”	144 %
	”	”	”	TSRK(8,7)	0.568	0.071	302 %
8	HB(4,8,8)	1.538	0.192	HM(7,7)	0.234	0.117	64 %
	HB(5,8,8)	1.851	0.231	”	”	”	97 %
	HB(6,8,8)	1.863	0.233	”	”	”	99 %
	HB(7,8,8)	1.866	0.233	”	”	”	99 %
	HB(8,8,8)	1.867	0.233	”	”	”	99 %
	”	”	”	TSRK(12,8)	0.936	0.078	199 %
9	HB(5,8,9)	1.223	0.153	HM(7,7)	0.234	0.117	31 %
	HB(6,8,9)	1.527	0.191	”	”	”	63 %
	HB(7,8,9)	1.646	0.206	”	”	”	76 %
	HB(8,8,9)	1.682	0.210	”	”	”	79 %
10	HB(6,8,10)	1.129	0.141	HM(7,7)	0.234	0.117	21 %
	HB(7,8,10)	1.365	0.170	”	”	”	45 %
	HB(8,8,10)	1.411	0.176	”	”	”	50 %
11	HB(7,8,11)	0.878	0.110				
	HB(8,8,11)	1.014	0.127				
12	HB(7,8,12)	0.442	0.055				
	HB(8,8,12)	0.725	0.091				

- *c_{eff}(HB(k,8,p)) for $p = 11, 12$ are not high when compare to other methods in the same family because of their orders are very high. In fact, as the order p increases, the number of constraints in optimization problem* (2.1.36) *or* (2.1.75)*, which leads effective SSP coefficients, c_{eff} decreases. However, they are better than c_{eff}(TSRK(12,8)) $= 0.078$ except HB(7,8,12), even though they have higher order.*

4.3.2 Numerical verification of the order p of HB(k,8,p)

To show the relevance of the theoretical order of HB(k,8,p) when solving ODEs, we apply these methods with various constant stepsizes on the following system of five equations over $t \in [0, t_n]$ with the given initial value at $t_0 = 0$ and exact solution $y_i(t)$:

$$\begin{aligned}
y_1' &= -y_1, & y_1(0) &= 1, & y_1(t) &= e^{-t},\\
y_2' &= y_3, & y_2(0) &= 0, & y_2(t) &= \sin t,\\
y_3' &= -y_2, & y_3(0) &= 1, & y_3(t) &= \cos t,\\
y_4' &= 1, & y_4(0) &= 0, & y_4(t) &= t,\\
y_5' &= -y_1 + (y_2 + y_4 y_3), & y_5(0) &= 1, & y_5(t) &= e^{-t} + t\sin t.
\end{aligned} \tag{4.3.1}$$

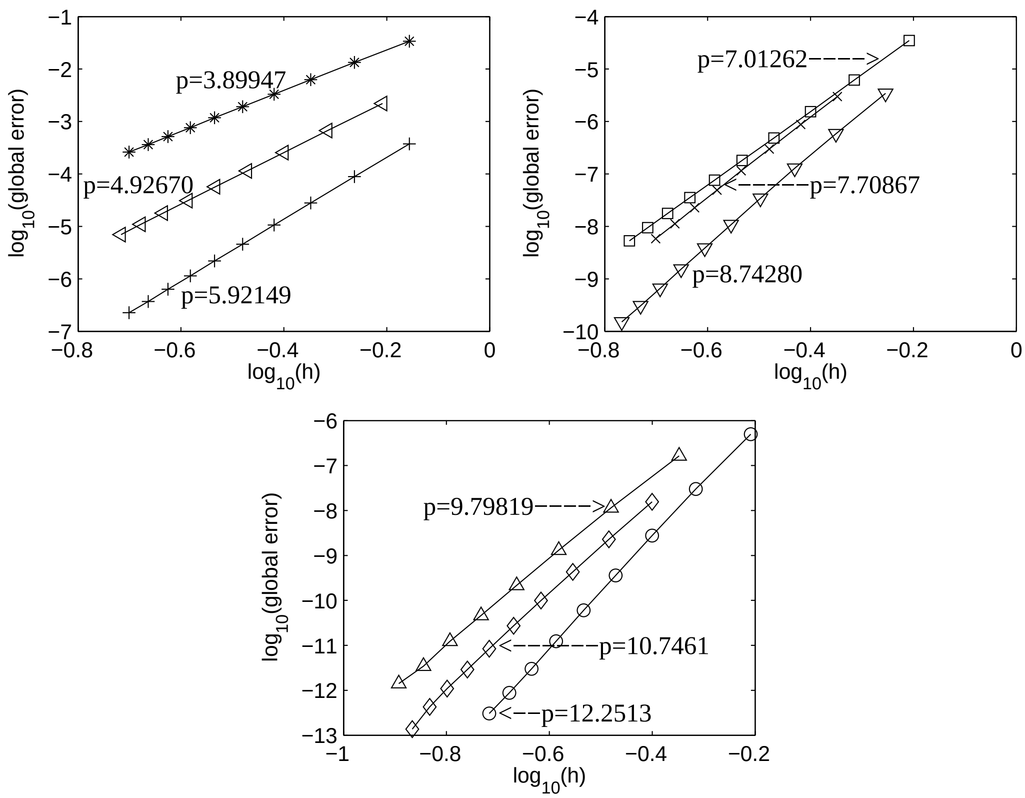
In Fig. 4.6, the error at $t_n = 4\pi$ for the first two graphs and $t_n = 8+\pi$ for the last graph, is plotted for different stepsizes h in a log-log scale so that the curve appears as a straight line with slope p whenever the leading term of the error of y_2 and y_5 is of order p, that is,

$$\max\{|y_{2,n} - y_2(t_n)|, |y_{5,n} - y_5(t_n)|\} = O(h^p),$$

in the maximum norm.

********************CORRECTION FOLLOWED THE REPORTS********************

The equations of these straight lines with their slopes are shown in Table 4.12.



HB(2,8,4) $*$, HB(2,8,5) $\triangleleft$, HB(2,8,6) $+$

HB(3,8,7) $\square$, HB(4,8,8) $\times$, HB(5,8,9) $\bigtriangledown$

HB(7,8,10) $\triangle$, HB(7,8,11) $\diamondsuit$, HB(7,8,12) $\circ$

Figure 4.6: $\log_{10}$(error) versus $\log_{10} h$ at t_n for the listed HB(k,8,p) methods applied to Problem (4.3.1) over $t \in [0, t_n]$ with constant stepsizes.

Table 4.12: Slope and Equations of lines corresponding to method HB(k,8,p) in Figure 4.6

Method HB(k,8,p)	Slope	Equations of lines
HB(2,8,4)	3.89947	$y = 3.89947x - 0.84744$
HB(2,8,5)	4.92670	$y = 4.92670x - 1.62155$
HB(2,8,6)	5.92149	$y = 5.92149x - 2.49456$
HB(3,8,7)	7.01262	$y = 7.01262x - 3.00300$
HB(4,8,8)	7.70867	$y = 7.70867x - 2.82587$
HB(5,8,9)	8.74280	$y = 8.74280x - 3.21337$
HB(7,8,10)	9.79819	$y = 9.79819x - 3.37169$
HB(7,8,11)	10.7461	$y = 10.7461x - 3.41112$
HB(7,8,12)	12.2513	$y = 12.2513x - 3.60680$

As in Fig. 4.6 and Table 4.12, the slopes of the straight lines which approximate the data in the least-squares sense are very close to p of HB(k,8,p) for $p = 4, 5, \ldots, 12$, which confirms the orders of the methods.

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4.3.3 Numerical results

A. Burgers' equation with a unit downstep initial condition

We continue to consider Problem 1 (page 72). Discretizing the spatial derivative by WENO5 first, then we apply our new methods as time discretization. We take Δt sufficiently small, $\Delta t \leq \max \Delta t_{\text{num}}$ such that (4.1.4) holds with error $\epsilon = 5.0$ e-02 at $t_{\text{final}} = 1.8$.

The numerical results show that the FE method satisfies the TVD property (4.1.3) under time step restriction (4.2.2): $\Delta t \leq \Delta t_{\text{FE}} = 0.325\Delta x$.

Table 4.13 presents $\text{num}_{\text{eff}}(\text{HB}(k,8,p))$ of HB methods and $\text{num}_{\text{eff}}(\text{OM}(k,p))$ for other methods (OM) on hand applied to Problem 1 and the $\text{PEG}(\text{num}_{\text{eff}}(\text{HB}(k,8,p)), \text{num}_{\text{eff}}(\text{OM}(k,p)))$ is shown in column 8.

Remark 4.3.2 *From Table 4.13, it is seen that:*

- *Generally, HB methods have larger* num_{eff}*(HB(k,8,p) than other methods of the same order, so most PEG in the last column are positive.*
- *Quite remarkably, although* c_{eff}*(HB(3,8,4) is smaller than* c_{eff}*(RK(10,4)), its* num_{eff} *is larger than that of RK(10,4).*
- *Similarly,* c_{eff}*(HB(7,8,11) is smaller than* c_{eff}*(HM(7,7), but its* num_{eff} *is larger than that of HM(7,7).*

B. Burgers' equation with a square-wave initial condition

In the next comparison, our Problem 2 (page 76) is the fourth of Laney's five test problems [27, p. 312], that is, Burgers' equation with a square-wave initial condition,

We discretize the spatial derivative of Problem 2 by WENO5 and compute the total variation of the numerical solution as a function of the effective CFL number at $t_{\text{final}} = 0.6$. In this case, num_{eff}(FE)=0.325 in the time step restriction (4.2.2) is replaced by num_{eff}(FE)=0.183.

Remark 4.3.3 *Table 4.14 has the same characteristics as in Remark 4.3.2 for Table 4.13. Moreover:*

- *For* $p = 12$*, HB(7,8,12) has the largest ratio* $R_{num/theor}$*, despite its small* num_{eff}*.*
- *For Problem 1,* $\text{num}_{\text{eff}}(HB(2,8,4)) < \text{num}_{\text{eff}}(GL(2,4))$*, but* $\text{num}_{\text{eff}}(HB(2,8,4)) > \text{num}_{\text{eff}}(GL(2,4))$ *for Problem 2.*

Table 4.13: PEG($\mathrm{num_{eff}}$(HB(k,8,p)), $\mathrm{num_{eff}}$(OM(k,p))) and ratio $R_{\mathrm{num/theor}}$ for Problem 1.

p	HB(k,8,p)	$\mathrm{num_{eff}}$(HB(k,8,p))	$R_{\mathrm{num/theor}}$	OM(k,p)	$\mathrm{num_{eff}}$(OM(k,p))	$R_{\mathrm{num/theor}}$	PEG
4	HB(2,8,4)	0.384	2.104	GL(2,4)	0.390	3.019	-2 %
	HB(3,8,4)	0.389	2.128	GL(3,4)	0.365	2.442	7 %
	”	”	”	GL(4,4)	0.380	2.423	2 %
	”	”	”	HM(3,4)	0.214	2.666	82 %
	”	”	”	HM(4,4)	0.264	2.382	47 %
	”	”	”	HM(5,4)	0.329	2.553	18 %
	”	”	”	HM(6,4)	0.274	1.918	42 %
	”	”	”	HM(7,4)	0.299	1.962	30 %
	”	”	”	RK(5,4)	0.311	3.173	25 %
	”	”	”	RK(10,4)	0.346	1.774	12 %
5	HB(2,8,5)	0.334	2.297	HM(4,5)	0.182	3.019	84 %
	”	”	”	HM(5,5)	0.277	3.247	21 %
	”	”	”	HM(6,5)	0.277	2.594	21 %
	”	”	”	HM(7,5)	0.317	2.615	5 %
	”	”	”	RK(10,5)	0.324	2.933	3 %
6	HB(2,8,6)	0.305	3.902	HM(5,6)	0.174	5.123	75 %
	HB(3,8,6)	0.315	2.958	”	”	”	81 %
	HB(4,8,6)	0.300	2.748	”	”	”	72 %
	HB(5,8,6)	0.285	2.585	”	”	”	64 %
	”	”	”	HM(6,6)	0.169	2.873	69 %
	”	”	”	HM(7,6)	0.189	2.643	51 %
7	HB(3,8,7)	0.295	3.972	HM(7,7)	0.127	3.340	132 %
	HB(4,8,7)	0.270	2.963	”	”	”	113 %
	HB(5,8,7)	0.230	2.484	”	”	”	81 %
	HB(6,8,7)	0.250	2.694	”	”	”	97 %
	HB(7,8,7)	0.230	2.479	”	”	”	81 %
8	HB(4,8,8)	0.230	3.681	HM(7,7)	0.127	3.340	81 %
	HB(5,8,8)	0.280	3.724	”	”	”	120 %
	HB(6,8,8)	0.260	3.435	”	”	”	105 %
	HB(7,8,8)	0.270	3.667	”	”	”	113 %
	HB(8,8,8)	0.290	3.823	”	”	”	128 %
9	HB(5,8,9)	0.240	2.516	HM(7,7)	0.127	3.340	89 %
	HB(6,8,9)	0.260	4.191	”	”	”	105 %
	HB(7,8,9)	0.275	4.113	”	”	”	117 %
	HB(8,8,9)	0.270	3.951	”	”	”	113 %
10	HB(7,8,10)	0.215	3.877	HM(7,7)	0.127	3.340	69 %
	HB(8,8,10)	0.235	4.099	”	”	”	85 %
11	HB(7,8,11)	0.200	5.607	HM(7,7)	0.127	3.340	57 %
	HB(8,8,11)	0.195	4.734	”	”	”	54 %
12	HB(7,8,12)	0.105	5.848				
	HB(8,8,12)	0.125	4.244				

Table 4.14: PEG($\mathrm{num}_{\mathrm{eff}}(\mathrm{HB}(k,8,p)), \mathrm{num}_{\mathrm{eff}}(\mathrm{OM}(k,p))$, and ratio $R_{\mathrm{num/theor}}$ for Problem 2.

p	HB(k,8,p)	$\mathrm{num}_{\mathrm{eff}}$(HB($k$,8,$p$))	$R_{\mathrm{num/theor}}$	OM(k,p)	$\mathrm{num}_{\mathrm{eff}}$(OM($k$,$p$))	$R_{\mathrm{num/theor}}$	PEG
4	HB(2,8,4)	0.426	4.143	GL(2,4)	0.405	5.559	5 %
	HB(3,8,4)	0.421	4.087	GL(3,4)	0.350	4.151	20 %
	”			GL(4,4)	0.375	4.240	12 %
	”			HM(3,4)	0.210	4.638	100 %
	”			HM(4,4)	0.280	4.480	50 %
	”			HM(5,4)	0.310	4.265	36 %
	”			HM(6,4)	0.305	3.786	38 %
	”			HM(7,4)	0.330	3.839	28 %
	”			RK(5,4)	0.306	5.535	38 %
	”			RK(10,4)	0.371	3.373	13 %
5	HB(2,8,5)	0.345	4.207	HM(4,5)	0.192	5.647	80 %
	”			HM(5,5)	0.292	6.069	18 %
	”			HM(6,5)	0.287	4.766	20 %
	”			HM(7,5)	0.312	4.563	11 %
	”			RK(10,5)	0.324	5.200	6 %
6	HB(2,8,6)	0.265	6.011	HM(5,6)	0.179	9.345	48 %
	HB(3,8,6)	0.335	5.578	”	”	”	87 %
	HB(4,8,6)	0.285	2.030	”	”	”	59 %
	HB(5,8,6)	0.300	4.824	”	”	”	68 %
	”			HM(6,6)	0.174	5.245	72 %
	”			HM(7,6)	0.194	4.811	55 %
7	HB(3,8,7)	0.295	7.043	HM(7,7)	0.124	5.782	138 %
	HB(4,8,7)	0.265	4.304	”	”	”	114 %
	HB(5,8,7)	0.227	4.347	”	”	”	83 %
	HB(6,8,7)	0.243	4.643	”	”	”	96 %
	HB(7,8,7)	0.245	4.682	”	”	”	98 %
8	HB(4,8,8)	0.219	6.215	HM(7,7)	0.124	5.782	77 %
	HB(5,8,8)	0.279	6.578	”	”	”	125 %
	HB(6,8,8)	0.254	5.950	”	”	”	105 %
	HB(7,8,8)	0.249	5.824	”	”	”	101 %
	HB(8,8,8)	0.255	5.961	”	”	”	106 %
9	HB(5,8,9)	0.229	8.172	HM(7,7)	0.124	5.782	85 %
	HB(6,8,9)	0.224	6.402	”	”	”	81 %
	HB(7,8,9)	0.260	6.894	”	”	”	110 %
	HB(8,8,9)	0.254	6.591	”	”	”	105 %
10	HB(6,8,10)	0.115	4.446	HM(7,7)	0.124	5.782	-7 %
	HB(7,8,10)	0.214	6.842	”	”	”	73 %
	HB(8,8,10)	0.232	7.176	”	”	”	87 %
11	HB(7,8,11)	0.169	8.401	HM(7,7)	0.124	5.782	36 %
	HB(8,8,11)	0.204	8.781	”	”	”	65 %
12	HB(7,8,12)	0.114	11.257				
	HB(8,8,12)	0.110	6.622				

- *Most of the HB methods have larger* num_{eff}*(HB(k,8,p)) than those of other methods of the same order, so most PEG in the last column are positive. This confirms the results shown in Table 4.13.*

- *The ratio* $R_{num/theor}$ *of HB(k,8,p) for Problems 1 and 2 shown in Tables 4.13 and 4.14, respectively, are all much greater than 1. Therefore, the theoretical strong stability bounds of HB(k,8,p) are verified in the numerical comparison of the maximum time steps for the two problems.*

C. Linear advection equation with a square-wave initial condition

In this part, the last problem we use as test problem is the second of Laney's five test problems [27, p. 311].

Problem 3 *Linear advection equation with a square-wave initial condition,*

$$\frac{\partial}{\partial t}u(x,t)+\frac{\partial}{\partial x}u(x,t)=0, \quad u(x,0)=\begin{cases}1, & |x|\leq \frac{1}{3},\\ 0, & \frac{1}{3}<|x|\leq 1,\end{cases} \tag{4.3.2}$$

and periodic boundary condition $u(-1,t)=u(1,t)$ *for* $t\geq 0$.

Similar to Problems 1 and 2, we use WENO5 as spatial discretization for the flux function $f(u)=u(x,t)$ and compute the total variation of the numerical solution as a function of the effective CFL number at $t_{\text{final}}=4$ and num_{eff}(FE)=0.033. At $t=4$, the initial condition moves around the periodic domain $[-1,1]$ twice so that $u(x,4)=u(x,0)$. Results are in Table 4.15.

Remark 4.3.4 *From Table 4.15, we observe that:*

- *At first glance, we see that the ratios* $R_{num/theor}$ *are especially large since* num_{eff}*(FE) is so small (0.033).*

Table 4.15: PEG($\mathrm{num_{eff}}$(HB(k,8,p)), $\mathrm{num_{eff}}$(OM(k,8,p)) and ratio $R_{\mathrm{num/theor}}$ for Problem 3.

p	HB(k,8,p)	$\mathrm{num_{eff}}$(HB(k,8,p))	$R_{\mathrm{num/theor}}$	OM(k,p)	$\mathrm{num_{eff}}$(OM(k,p))	$R_{\mathrm{num/theor}}$	PEG
4	HB(2,8,4)	0.380	20.507	GL(2,4)	0.350	26.682	9 %
	HB(3,8,4)	0.385	20.741	GL(3,4)	0.375	24.704	3 %
	”			GL(4,4)	0.395	24.808	-3 %
	”			HM(3,4)	0.225	27.604	71 %
	”			HM(4,4)	0.270	23.994	43 %
	”			HM(5,4)	0.335	25.603	15 %
	”			HM(6,4)	0.275	18.961	40 %
	”			HM(7,4)	0.300	19.384	28 %
	”			RK(5,4)	0.340	34.161	13 %
	”			RK(10,4)	0.345	17.424	12 %
5	HB(2,8,5)	0.340	23.030	HM(4,5)	0.150	24.504	127 %
	”			HM(5,5)	0.265	30.592	28 %
	”			HM(6,5)	0.150	13.837	127 %
	”			HM(7,5)	0.330	26.810	3 %
	”			RK(10,5)	0.319	28.473	7 %
6	HB(2,8,6)	0.325	40.950	HM(5,6)	0.150	43.497	117 %
	HB(3,8,6)	0.305	28.210	”	”	”	103 %
	HB(4,8,6)	0.335	30.224	”	”	”	123 %
	HB(5,8,6)	0.340	30.370	”	”	”	127 %
	”			HM(6,6)	0.185	30.973	84 %
	”			HM(7,6)	0.205	28.237	66 %
7	HB(3,8,7)	0.290	38.459	HM(7,7)	0.180	46.620	61 %
	HB(4,8,7)	0.315	34.045	”	”	”	75 %
	HB(5,8,7)	0.325	34.571	”	”	”	81 %
	HB(6,8,7)	0.320	33.965	”	”	”	78 %
	HB(7,8,7)	0.325	34.496	”	”	”	81 %
8	HB(4,8,8)	0.220	34.677	HM(7,7)	0.180	46.620	22 %
	HB(5,8,8)	0.305	39.946	”	”	”	69 %
	HB(6,8,8)	0.305	39.688	”	”	”	69 %
	HB(7,8,8)	0.300	38.975	”	”	”	67 %
	HB(8,8,8)	0.310	40.253	”	”	”	72 %
9	HB(5,8,9)	0.275	54.511	HM(7,7)	0.180	46.620	53 %
	HB(6,8,9)	0.295	46.834	”	”	”	64 %
	HB(7,8,9)	0.285	41.975	”	”	”	58 %
	HB(8,8,9)	0.285	41.077	”	”	”	58 %
10	HB(6,8,10)	0.235	50.460	HM(7,7)	0.180	46.620	31 %
	HB(7,8,10)	0.295	52.392	”	”	”	64 %
	HB(8,8,10)	0.290	49.825	”	”	”	61 %
11	HB(7,8,11)	0.210	57.983	HM(7,7)	0.180	46.620	17 %
	HB(8,8,11)	0.205	49.011	”	”	”	14 %
12	HB(8,8,12)	0.215	71.891	”	”	”	19 %

- *HB methods of order 12 have positive PEG for Problem 3, while they have negative PEG for Problem 1 and 2.*
- *Once again,* $\textit{num}_{\text{eff}}(\textit{HB}(k,8,p)) > \textit{num}_{\text{eff}}(\textit{RK}(s,p))$*, so their PEG is positive.*
- *For Tables 4.13 and 4.14, HB methods of order* 12 *have smaller* $\textit{num}_{\text{eff}}$ *than other methods because of their much higher order; however, their* $\textit{num}_{\text{eff}}$ *are better to Problem 3 (see Table 4.15).*

The new family of optimal, explicit, k-step, 8-stage, SSP HB methods of order p, HB(k,8,p), for $p = 4, 5, \ldots, 12$, with nonnegative coefficients are presented in their canonical Shu–Osher form. These new methods are constructed by combining linear k-step methods of order $(p-3)$ with 8-stage Runge–Kutta methods of order 4. The numerical results show that our methods are more efficient than others. These methods are shown as remarkable examples for chapter 4.

Chapter 5

SSP 8-Stage HB Methods Based on Combining k-Step with RK5 Methods

In this chapter, to solve system (1.1.2), we consider explicit, SSP, k-step, 8-stage, general linear methods of order p, $p = 5, 6, \ldots, 12$, with nonnegative coefficients based on combining linear k-step methods of order $(p-4)$ and an 8-stage RK method of order 5. This family is the best family in $\mathrm{HB}_{\mathrm{RK5}}(k, s, p)$ methods (see Table 3.8).

The 8 formulae of these 8-stage HB methods to perform the integration from t_n to t_{n+1} are defined in Chapter 2 by (2.1.1) and (2.1.2) with $s = 8$. Their order conditions are (3.1.2)–(3.1.15) with $s = 8$. In the case of $p = 5$, HB(k,s,5) has to satisfy the additional condition (3.1.17) in Chapter 4 with $s = 8$.

The Shu–Osher and Butcher form in vector notation of these canonical SSP HB methods together with Theorem 2.1.11 to compute their feasible SSP coefficients are studied in Subsections 2.1.6–2.1.8 with $s = 8$.

Section 5.1 presents the construction of several new HB(k,8,p) methods obtained by computer search and compares the effective SSP coefficients of our new methods with those of other methods. Section 5.2 considers the numerical verification of the order p of HB(k,8,p). In Section 5.3, we present numerical results for our new methods and other methods applied to Burgers' equations to confirm the efficiency of the new methods. The formulae of eight of the 24 new HB(k,8,p) methods are listed in their Shu–Osher representation together with their c(HB(k,8,p)), c_{eff}(HB(k,8,p)) and abscissa vector σ in Appendix A.4.

5.1 Construction of 8-stage HB(k,8,p)

The problem of optimizing HB(k,8,p) in Subsection (3.1.9) can be formulated from (2.1.75) to (2.1.83) together with the set of order conditions (3.1.2)–(3.1.15) with $s = 8$. Especially, when $p = 5$, HB(k,8,5) needs to satisfy the additional condition (3.1.17) in Chapter 4 with $s = 8$. We search for the methods with largest c(HB(k,8,p)) for different values of k. In this work, fmincon function in the MATLAB Optimization Toolbox was used to tolerance 10^{-12} on the objective function c(HB(k,8,p)) provided all the constraints were satisfied to tolerance 10^{-14}.

The effective SSP coefficients, c_{eff}(HB(k,8,p)), of the new methods and c_{eff}(OM(k,p)) of the other methods (OM) on hand are compared in Table 5.1. With the same order and the same stage, generally, any HB methods may need more storage than RK methods. These HB(k,8,p) have fairly good c_{eff}(HB(k,8,p)) and low step number k for reduced storage implementation.

With $p = 5$, our best method of order 5 is HB(2,8,5) with c(HB(2,8,5)) $= 3.579$ and c_{eff}(HB(2,8,5)) $= 0.447$.

In [23], Ketcheson, Gottlieb and Macdonald found a two-step 8-stage RK method of order 6 with c_{eff}(TSRK(8,6)) $= 0.242$. We found HB(2,8,6) with similar c_{eff}(HB(2,8,6)) $=$ 0.241. If we further increase the step number k, we can find HB(k,8,6) with larger SSP coefficients. We found the best HB(k,8,6) with $k = 2, 3, 4, 5$. Moreover, HB(5,8,6) has the largest c_{eff}(HB(5,8,6)) $= 0.345$ among the 8-stage sixth-order HB methods on hand. Here we note the advantage of increasing the step number k.

It is not mentioned in Ketcheson, Gottlieb and Macdonald [23] that two-step 8- to 10-stage RK methods of order 8 exist. We found HB(3,8,8) with good $c_{\text{eff}}(\text{HB}(3,8,8)) = 0.160$.

We have not found in the literature general linear SSP methods of order 9 to 12 with nonnegative coefficients. However, we found the following HB(k,8,p) with effective SSP coefficients:

$$c_{\text{eff}}(\text{HB}(4,8,9)) = 0.138, \quad c_{\text{eff}}(\text{HB}(5,8,10)) = 0.121,$$

$$c_{\text{eff}}(\text{HB}(7,8,11)) = 0.135, \quad c_{\text{eff}}(\text{HB}(7,8,12)) = 0.100.$$

According to our numerical search, it seems that HB(k,8,p) methods of order 9 to 12 with nonnegative coefficients require at least $k = 3, 4, 5, 6$ steps with

$$c_{\text{eff}}(\text{HB}(3,8,9)) = 0.035, \quad c_{\text{eff}}(\text{HB}(4,8,10)) = 0.043,$$

$$c_{\text{eff}}(\text{HB}(5,8,11)) = 0.060, \quad c_{\text{eff}}(\text{HB}(6,8,12)) = 0.025.$$

Our best k-step methods of orders 7 to 12 are with $k = 3, \dots, 6$, $k = 3, \dots, 7$, $k = 4, \dots, 8$, $k = 5, \dots, 8$, $k = 7, 8$, and $k = 7, 8$, respectively.

We compare our new methods with others based on the notion of percentage efficiency gain (Definition 2.2.2) mentioned in Section 2.2. Table 5.1 lists $c(\text{HB}(k,8,p))$, $c_{\text{eff}}(\text{HB}(k,8,p))$, and $c(\text{OM}(k,p))$, $c_{\text{eff}}(\text{OM}(k,p))$ for the other methods (OM) on hand. Column 8 lists $\text{PEG}(c_{\text{eff}}(\text{HB}(k,8,p)), c_{\text{eff}}(\text{OM}(k,p)))$ which is seen to be non negligible.

Table 5.1 also shows that the new HB(k,8,p) are generally competitive with the other methods on hand. For example,

- $c_{\text{eff}}(\text{HB}(2,8,5)) > c_{\text{eff}}(\text{HM}(k,5))$, for $k = 4, 5, 6, 7$.
- $c_{\text{eff}}(\text{HB}(2,8,5)) > c_{\text{eff}}(\text{RK}(s,5))$, for $s = 9, 10$.
- $c_{\text{eff}}(\text{HB}(k,8,8)) > c_{\text{eff}}(\text{HM}(7,7)) = 0.117$ for $k = 3, 4, 5, 6, 7$.

Table 5.1: PEG(c_{eff}(HB(k,8,p)), c_{eff}(OM(k,p))) taken row-wise.

p	HB(k,8,p)	c(HB(k,8,p))	c_{eff}(HB(k,8,p))	OM(k,p)	c(OM(k,p))	c_{eff}(OM(k,p))	PEG
5	HB(2,8,5)	3.579	0.447	HM(4,5)	0.371	0.185	141 %
	”	”	”	HM(5,5)	0.525	0.262	70 %
	”	”	”	HM(6,5)	0.657	0.328	36 %
	”	”	”	HM(7,5)	0.746	0.373	20 %
	”	”	”	RK(9,5)	2.696	0.300	49 %
	”	”	”	RK(10,5)	3.395	0.339	32 %
	”	”	”	TSRK(8,5)	3.576	0.447	0 %
6	HB(2,8,6)	1.928	0.241	HM(5,6)	0.209	0.104	131 %
	HB(3,8,6)	2.621	0.328	”	”	”	213 %
	HB(4,8,6)	2.732	0.341	”	”	”	227 %
	”	”	”	HM(6,6)	0.362	0.181	89 %
	”	”	”	HM(7,6)	0.440	0.220	55 %
	”	”	”	TSRK(8,6)	1.936	0.242	41 %
7	HB(3,8,7)	1.985	0.248	HM(7,7)	0.234	0.117	112 %
	HB(4,8,7)	2.273	0.284	”	”	”	143 %
	”	”	”	TSRK(8,7)	0.568	0.071	300 %
8	HB(3,8,8)	1.277	0.160	HM(7,7)	0.234	0.117	36 %
	HB(4,8,8)	1.588	0.198	”	”	”	70 %
	HB(5,8,8)	1.884	0.235	”	”	”	101 %
	HB(6,8,8)	1.930	0.241	”	”	”	106 %
	HB(7,8,8)	1.943	0.243	”	”	”	108 %
	”	”	”	TSRK(12,8)	0.936	0.078	211 %
9	HB(4,8,9)	1.107	0.138	HM(7,7)	0.234	0.117	18 %
	HB(5,8,9)	1.429	0.178	”	”	”	53 %
	HB(6,8,9)	1.623	0.203	”	”	”	73 %
	HB(7,8,9)	1.727	0.216	”	”	”	85 %
	HB(8,8,9)	1.741	0.218	”	”	”	86 %
10	HB(5,8,10)	0.971	0.121	HM(7,7)	0.234	0.117	4 %
	HB(6,8,10)	1.249	0.156	”	”	”	33 %
	HB(7,8,10)	1.453	0.182	”	”	”	55 %
	HB(8,8,10)	1.492	0.186	”	”	”	59 %
11	HB(7,8,11)	1.078	0.135	HM(7,7)	0.234	0.117	15 %
	HB(8,8,11)	1.247	0.156	”	”	”	33 %
12	HB(7,8,12)	0.801	0.100				
	HB(8,8,12)	0.930	0.116				

Table 5.2: c_{eff}(HB(k,8,p)) as function of step number k and order p.

$p\backslash k$	2	3	4	5	6	7	8
5	0.447						
6	0.241	0.328	0.341	0.345	0.347		
7	*0.040	0.248	0.284	0.285			
8		0.142	0.198	0.235	0.241	0.243	
9		*0.035	0.138	0.179	0.203	0.216	0.218
10			*0.043	0.121	0.156	0.182	0.186
11				*0.060	0.106	0.135	0.156
12					*0.025	0.100	0.116

- c_{eff}(HB(k,8,9)) $>$ c_{eff}(HM(7,7)) for $k = 4, 5, 6, 7, 8$.
- c_{eff}(HB(k,8,p)) $>$ c_{eff}(HM(7,7)) for $k = 5, 6, 7, 8$ and $p = 10, 11$.
- Generally, PEG(c_{eff}(HB(k,8,p)), c_{eff}(OM(k,p))) > 0.

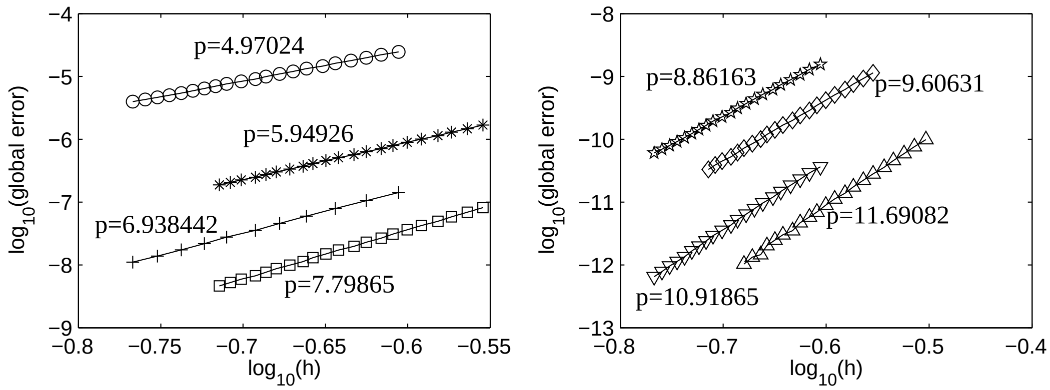
Table 5.2 lists c_{eff}(HB(k,8,p)) as a function of the step number k and the order p. The nonstarred methods are listed in Table 5.1 and are fairly good methods. The starred methods with rather small c_{eff}(HB(k,8,p)) are not listed in Table 5.1.

5.2 Numerical verification of the order p of HB(k,8,p)

To show the relevance of the theoretical order of HB(k,8,p) when solving ODEs, we have applied these methods with various constant stepsizes on the initial value problem (4.3.1) in Chapter 4 over $t \in [0, \pi + 8]$ with exact solution $y_i(t)$.

In Fig. 5.1, the error of y_2 and y_5 at $t_n = \pi + 8$ is plotted for different stepsizes h in a log-log scale so that the curves appear as straight lines with slope p whenever the leading term of the error is of order p, that is

$$\max\{|y_{2,n} - y_2(t_n)|, |y_{5,n} - y_5(t_n)|\} = O(h^p).$$



HB(2,8,5) $\circ$, HB(2,8,6) $*$, HB(3,8,7) $+$, HB(4,8,8) $\square$ (left figure)

HB(5,8,9) $\star$, HB(6,8,10) $\diamondsuit$, HB(7,8,11) $\triangledown$, HB(7,8,12) $\triangle$ (right figure)

Figure 5.1: $\log_{10}$(error) versus $\log_{10} h$ at $t_n = \pi + 8$ for the listed HB(k,8,p) methods applied to problem (4.3.1) over $t \in [0, \pi+8]$ with constant stepsizes.

*************CORRECTION FOLLOWED THE REPORTS**************

The equations of these straight lines with their slopes are shown in Table 5.3.

As in Fig. 5.1 and Table 5.3, the slopes of the straight lines which approximate the data in the least-squares sense are very close to p of HB(k,8,p) for $p = 5, 6, \ldots, 12$, which confirms the orders of the methods.

****

It is to be noted that HB(2,8,6) uses $t_n = 4\pi$ instead of $t_n = \pi + 8$.

Table 5.3: Slope and Equations of lines corresponding to method HB(k,8,p) in Figure 5.1

Method HB(k,8,p)	Slope	Equations of lines
HB(2,8,5)	4.97024	$y = 4.97024x - 1.59360$
HB(2,8,6)	5.94926	$y = 5.94926x - 2.4775$
HB(3,8,7)	6.93844	$y = 6.93844x - 2.63865$
HB(4,8,8)	7.79865	$y = 7.79865x - 2.76336$
HB(5,8,9)	8.86163	$y = 8.86163x - 3.43010$
HB(6,8,10)	9.60631	$y = 9.60631x - 3.61491$
HB(7,8,11)	10.91865	$y = 10.91865x - 3.80284$
HB(7,8,12)	11.69082	$y = 11.69082x - 4.35231$

5.3 Comparing HB(k,8,p) with other methods on Burgers' equation

5.3.1 Comparing HB(k,8,p) with other methods on Burgers' equation with unit downstep initial condition

As a first comparison of our new methods with RK methods, following Huang [17], we consider Burgers' equation in Problem 1 (page 72).

As in Sections 4.2 and 4.3 in Chapter 4, we use WENO5 as the spatial discretization and our methods as time discretization.

It is also numerically observed that the TVD property (4.1.4) holds with error $\epsilon = 5.0e-02$ for the methods listed in Table 5.4 with $\Delta t \leq \max \Delta t_{\text{num}}$. This confirms the result of Theorem 2.1.11 that HB methods are also TVD when combined with the WENO5 space discretization since these new methods are convex combinations of the forward Euler method. The same situation holds for Problem 2 (page 76) below.

For Problem 1, Table 5.4 lists num_{eff} in columns 3 and 6 and the ratio $R_{\text{num/theor}}$ (computed by (4.1.7)) for HB(k,8,p) in column 4 and OM(k,p) (other methods) in column 7. The PEG(num_{eff}) is in column 8.

It is seen that:

(a) $\text{num}_{\text{eff}}(\text{HB}(k,8,p)) > \text{num}_{\text{eff}}(\text{OM}(k,p))$ for methods of the same order p and all k,

(b) quite remarkably, even though $c_{\text{eff}}(\text{HB}(7,8,12))=0.100 < c_{\text{eff}}(\text{HM}(7,7)) = 0.117$ and $c_{\text{eff}}(\text{HB}(8,8,12))=0.116 < c_{\text{eff}}(\text{HM}(7,7)) = 0.117$, in this example, HB(7,8,12) and HB(8,8,12) allow for a larger time step since $\text{num}_{\text{eff}}(\text{HB}(7,8,12)) > \text{num}_{\text{eff}}(\text{HM}(7,7))$ and $\text{num}_{\text{eff}}(\text{HB}(8,8,12)) > \text{num}_{\text{eff}}(\text{HM}(7,7))$,

(c) $\text{PEG}(\text{num}_{\text{eff}}(\text{HB}(k,8,p)), \text{num}_{\text{eff}}(\text{OM}(k,8,p))) > 0$ for HB(k,8,p) and OM(k,p) taken row-wise in all cases on hand.

5.3.2 Comparing HB(k,8,p) and other methods on Burgers' equation with a square-wave initial condition

As a second comparison, we continue to consider Burgers' equation with a square-wave initial value in Problem 2 (page 76), which is one of Laney's five test problems [27, p. 312].

Discretizing the spatial derivative of Problem 2 by WENO5 and computing the total variation of the numerical solution as a function of the effective CFL number, $\text{num}_{\text{eff}} = \Delta t/(\ell \Delta x)$, at $t_{\text{final}} = 0.6$, we find $\text{num}_{\text{eff}} = 0.183$.

Table 5.5 lists num_{eff} in columns 3 and 6, and the ratio $R_{\text{num/theor}}$ in column 4 and column 7 for HB(k,8,p) and for OM(k,p) (other methods), respectively, applied to Problem 2. The PEG(num_{eff}) is in column 8.

It is seen that the results for Problem 2 listed in Table 5.5 confirm the observations (a)–(c) obtained for Problem 1 (page 72) as listed in Table 5.4.

Table 5.4: PEG(num_{eff}(HB(k,8,p)), num_{eff}(OM(k,8,p)) taken row-wise and $R_{\text{num/theor}}$ applied to Problem 1.

p	HB(k,8,p)	num_{eff}(HB(k,8,p))	$R_{\text{num/theor}}$	OM(k,p)	num_{eff}(OM(k,p))	$R_{\text{num/theor}}$	PEG
5	HB(2,8,5)	0.336	2.311	HM(4,5)	0.182	3.019	85 %
	”	”	”	HM(5,5)	0.277	3.247	21 %
	”	”	”	HM(6,5)	0.277	2.594	21 %
	”	”	”	HM(7,5)	0.317	2.615	6 %
	”	”	”	RK(10,5)	0.324	2.933	4 %
6	HB(2,8,6)	0.311	3.970	HM(5,6)	0.174	5.123	79 %
	HB(3,8,6)	0.316	2.968	”	”	”	82 %
	HB(4,8,6)	0.306	2.757	”	”	”	76 %
	”	”	”	HM(6,6)	0.169	2.873	81 %
	”	”	”	HM(7,6)	0.189	2.643	62 %
7	HB(3,8,7)	0.309	3.831	HM(7,7)	0.127	3.340	143 %
	HB(4,8,7)	0.304	3.292	”	”	”	139 %
8	HB(3,8,8)	0.203	3.914	HM(7,7)	0.127	3.340	60 %
	HB(4,8,8)	0.234	3.628	”	”	”	84 %
	HB(5,8,8)	0.249	3.253	”	”	”	96 %
	HB(6,8,8)	0.289	3.686	”	”	”	128 %
	HB(7,8,8)	0.319	4.041	”	”	”	151 %
9	HB(4,8,9)	0.148	3.290	HM(7,7)	0.127	3.340	17 %
	HB(5,8,9)	0.238	4.099	”	”	”	87 %
	HB(6,8,9)	0.268	4.063	”	”	”	111 %
	HB(7,8,9)	0.268	3.819	”	”	”	111 %
	HB(8,8,9)	0.293	4.142	”	”	”	131 %
10	HB(5,8,10)	0.253	6.413	HM(7,7)	0.127	3.340	99 %
	HB(6,8,10)	0.163	3.213	”	”	”	28 %
	HB(7,8,10)	0.288	4.879	”	”	”	127 %
	HB(8,8,10)	0.288	4.751	”	”	”	127 %
11	HB(7,8,11)	0.165	3.766	HM(7,7)	0.127	3.340	30 %
	HB(8,8,11)	0.245	4.835	”	”	”	93 %
12	HB(7,8,12)	0.170	5.224	HM(7,7)	0.127	3.340	34 %
	HB(8,8,12)	0.180	4.764	”	”	”	42 %

Table 5.5: $\mathrm{PEG}(\mathrm{num}_{\mathrm{eff}}(\mathrm{HB}(k,8,p)), \mathrm{num}_{\mathrm{eff}}(\mathrm{OM}(k,p)))$ taken row-wise and $R_{\mathrm{num/theor}}$ applied to Problem 2.

p	HB(k,8,p)	$\mathrm{num}_{\mathrm{eff}}$(HB($k$,8,$p$))	$R_{\mathrm{num/theor}}$	OM(k,p)	$\mathrm{num}_{\mathrm{eff}}$(OM($k$,$p$))	$R_{\mathrm{num/theor}}$	PEG
5	HB(2,8,5)	0.366	4.463	HM(4,5)	0.192	5.647	91 %
	”	”	”	HM(5,5)	0.292	6.069	25 %
	”	”	”	HM(6,5)	0.287	4.766	28 %
	”	”	”	HM(7,5)	0.312	4.563	17 %
	”	”	”	RK(10,5)	0.324	5.200	13 %
6	HB(2,8,6)	0.306	6.925	HM(5,6)	0.179	9.345	71 %
	HB(3,8,6)	0.331	5.512	”	”	”	85 %
	HB(4,8,6)	0.296	4.729	”	”	”	65 %
	”	”	”	HM(6,6)	0.174	5.244	70 %
	”	”	”	HM(7,6)	0.194	4.811	53 %
7	HB(3,8,7)	0.334	7.343	HM(7,7)	0.124	5.782	169 %
	HB(4,8,7)	0.289	5.549	”	”	”	133 %
8	HB(3,8,8)	0.198	6.785	HM(7,7)	0.124	5.782	60 %
	HB(4,8,8)	0.229	6.295	”	”	”	85 %
	HB(5,8,8)	0.234	5.421	”	”	”	89 %
	HB(6,8,8)	0.329	7.439	”	”	”	165 %
	HB(7,8,8)	0.309	6.940	”	”	”	149 %
9	HB(4,8,9)	0.148	5.853	HM(7,7)	0.124	5.782	20 %
	HB(5,8,9)	0.254	7.757	”	”	”	105 %
	HB(6,8,9)	0.269	7.230	”	”	”	117 %
	HB(7,8,9)	0.254	6.418	”	”	”	105 %
	HB(8,8,9)	0.284	7.119	”	”	”	129 %
10	HB(5,8,10)	0.248	11.169	HM(7,7)	0.124	5.782	100 %
	HB(6,8,10)	0.149	5.207	”	”	”	20 %
	HB(7,8,10)	0.279	8.381	”	”	”	125 %
	HB(8,8,10)	0.289	8.453	”	”	”	133 %
11	HB(7,8,11)	0.153	6.191	HM(7,7)	0.124	5.782	23 %
	HB(8,8,11)	0.233	8.153	”	”	”	88 %
12	HB(7,8,12)	0.163	8.907	HM(7,7)	0.124	5.782	32 %
	HB(8,8,12)	0.178	8.377	”	”	”	44 %

We observe that the ratio $R_{\mathrm{n}/t}$ of HB(k,8,p) for Problems 1 and 2 are greater than 1, as with hybrid methods in [17]. The theoretical strong stability bounds of HB(k,8,p) are thus verified in the numerical comparison of the maximum time steps for Problems 1 and 2.

To conclude, new explicit 8-stage, k-step SSP Hermite–Birkhoff methods, called HB(k,8,p), of orders $p = 4, 5, \dots, 12$, with nonnegative coefficients are constructed by combining linear k-step methods with an 8-stage Runge–Kutta (RK) method of order 5. We found no counterparts of HB(k,8,p) methods of order greater than 8 in the literature among hybrid and general linear multistep multistage methods. Our new HB(k,8,p) tend to have larger effective SSP coefficients than hybrid methods [17] of the same order and other frequently used methods. Based on the maximum effective CFL numbers, HB(2,8,5) compares favorably with other methods of the same order, including RK(10,5) of Ruuth. Following [17], finding more efficient generalized SSP methods appears to be promising in the light of the present work.

Chapter 6

Conclusion and Future Work

This thesis described the representation of Hermite–Birkhoff methods, HB(k,s,p), which are combinations of k-step methods and s-stage Runge–Kutta (RK) methods under the extended Shu–Osher form. Moreover, the vector formulation of the canonical Shu–Osher form for SSP RK methods was extended to SSP HB methods. These extensions are very helpful in setting up the optimization problems to obtain the SSP coefficients, c, and formulae of HB(k,s,p) methods. The following are important results which are derived from the coefficient c of HB(k,s,p):

- For the same order p, the same stage number s, when the step number k increases, the SSP coefficients increase.
- For the same step number k and the same stage number s, when the order p increases, the SSP coefficient decrease.
- If the order of RK methods combined with k-step methods increases, then the SSP coefficients of the HB methods increase.

There are many typical HB methods with specific stage number and order presented in this thesis such as:

- A collection of new SSP, explicit, 4-stage, noncanonical, k-step HB(k,4,p) ($p = 3, \ldots, 8$) by combining k-step methods of order $(p-3)$ with RK4.

- A family of new SSP, explicit, s-stage ($s = 4, 5, \ldots, 10$) noncanonical HB(k,s,4) methods of order 4 by combining k-step methods of order $(p-3)$ with RK4.

- A new series of SSP, explicit, 8-stage, canonical HB(k,8,p) methods by combining k-step methods of order $(p-3)$ with RK4.

- A new series of SSP, explicit, 8-stage, canonical HB(k,8,p) methods by combining k-step methods of order $(p-4)$ with RK5.

In general, the effective SSP coefficients, $c_{\text{eff}}(M)$ defined in (2.2.1), of these methods are much better than those of other methods such as hybrid methods, RK methods and general linear methods.

In addition, the largest effective CFL number, $\text{num}_{\text{eff}}(M)$ defined in (4.1.5) and the percentage efficiency gain, $\text{PEG}(\text{num}_{\text{eff}})$ defined in (4.1.8), which were obtained when tested on Burgers' equation, show numerically the good efficiency of the above HB methods over well-known methods.

The numerical results in this thesis also show that all the ratios of the maximum numerical to theoretical stepsize, $R_{\text{num/theor}}$ defined in (4.1.7) are greater than one, that is, as long as the forward Euler method satisfies the TVD property (4.1.3) with error (4.1.4) under its time step restriction, $\Delta t \leq \Delta t_{\text{FE}}$. In practice, it is possible to choose the stepsize $\Delta t \leq \max \Delta t_{\text{num}}$ instead of $\Delta t \leq \max \Delta t_{\text{theor}}$ as in Theorems 2.1.4 and 2.1.11 so that HB methods satisfy the TVD property (4.1.3) with error (4.1.4).

While many theoretical and numerical results on SSP HB methods were obtained and presented in this thesis, there are many other questions for future work. One obvious problem is the low storage requirements of the methods. Although the effective SSP coefficients, $c_{\text{eff}}(M)$, related to CPU time and the largest effective CFL number, $\text{num}_{\text{eff}}(M)$, are the basis to choose fairly good HB methods, in practice, it is more important to consider the memory used by the methods. Moreover, if the canonical Shu–Osher forms of the matrices $\boldsymbol{\alpha}_r$ and $\boldsymbol{\beta}_r$ are sparse and the step number, k, is low, the canonical Shu–Osher forms of k-step HB methods (2.1.68) will allow for reduced-storage implementation. In our planning, we will consider the low-storage of some chosen HB methods with low step number k.

Furthermore, there are other ideas which need further study:

- Albeit Chapter 3 just surveys the SSP coefficients of all families of HB methods based on combining k-step methods with RK5 and Chapter 5 presents a collection of HB methods as typical examples for Chapter 3, there are other good families of methods, which are worth to be considered; for instance, canonical 6-stage HB methods.

- In [52], Shu mentioned that WENO5 is usually the best choice, but our obtained methods have very high order ($p > 5$); therefore, combining them with other spatial time discretizations such as WENO7 or WENO11 may give good results when applied to other problems.

- All the test problems in this thesis are Burgers' equation and linear advection equation, so applying HB methods to more test problems such as nonconvex Buckley–Leverette flux or Burgers' equation with different initial conditions would also be interesting.

Appendix A

A.1 Eleven noncanonical HB$(k, 4, p)$ methods considered in the thesis

HB(2,4,4). Here $c = 1.593$, $c_{\text{eff}} = 0.398$, and
$\sigma = [0, 0.41402182360075634, 0.51006789128486130, 0.95950236308462156]^T$.

$$
\begin{aligned}
Y_2 &= 1.3137364256438025\,\text{e-}01 y_{n-1} + 8.6862635743561967\,\text{e-}01 y_n + 5.4539546616513657\,\text{e-}01 \Delta t f_n, \\
Y_3 &= 3.7611628586354845\,\text{e-}01 y_{n-1} + 2.3615691062661964\,\text{e-}01 \Delta t f_{n-1} + 6.2388371413645161\,\text{e-}01 Y_2 \\
&\quad + 6.2388371413645161\,\text{e-}01 Y_2 + 3.9172579348020337\,\text{e-}01 \Delta t F_2, \\
Y_4 &= 6.0575318286657687\,\text{e-}02 y_{n-1} + 4.3008189202816044\,\text{e-}02 y_n + 8.9641649251052635\,\text{e-}01 Y_3 \\
&\quad + 5.6284441132346308\,\text{e-}01 \Delta t F_3, \\
y_{n+1} &= 4.4524211403575709\,\text{e-}02 y_{n-1} + 3.8295387371954609\,\text{e-}01 y_n + 2.4045011377921155\,\text{e-}01 \Delta t f_n \\
&\quad + 1.6774221781036905\,\text{e-}01 Y_2 + 9.2083912086026398\,\text{e-}02 \Delta t F_2 + 4.0477969706650918\,\text{e-}01 Y_4 \\
&\quad + 2.5415417076166058\,\text{e-}01 \Delta t F_4.
\end{aligned}
$$

HB(3,4,4). Here $c = 1.843$, $c_{\text{eff}} = 0.461$, and
$\sigma = [0, 0.30622814192704767, 0.55930144311839380, 0.88515753145046949]^T$.

$$
\begin{aligned}
Y_2 &= 1.8162651927653470\,\text{e-}01 y_{n-1} + 8.1837348072346527\,\text{e-}01 y_n + 4.3925422184221165\,\text{e-}02 \Delta t f_{n-1} \\
&\quad + 4.4392923901936121\,\text{e-}01 \Delta t f_n, \\
Y_3 &= 2.2153848827415687\,\text{e-}01 y_{n-1} + 1.2017424174852812\,\text{e-}01 \Delta t f_{n-1} + 7.7846151172584321\,\text{e-}01 Y_2
\end{aligned}
$$

$$
\begin{aligned}
&+ 4.2227886734649689\,\text{e-}01\Delta t F_2,\\
Y_4 &= 6.7530828539879564\,\text{e-}04 y_{n-2} + 1.3756312556575984\,\text{e-}01 y_{n-1} + 7.4621545159975711\,\text{e-}02\Delta t f_{n-1}\\
&\quad + 8.6176156614884136\,\text{e-}01 Y_3 + 4.6746524085603702\,\text{e-}01\Delta t F_3,\\
y_{n+1} &= 1.0945244030080964\,\text{e-}02 y_{n-2} + 4.4070641867034777\,\text{e-}01 y_n + 2.3906256700586392\,\text{e-}01\Delta t f_n\\
&\quad + 5.4834833729957133\,\text{e-}01 Y_4 + 2.9745326043523995\,\text{e-}01\Delta t F_4.
\end{aligned}
$$

HB(2,4,5). Here $c = 0.854$, $c_{\text{eff}} = 0.213$, and
$\sigma = [0, 0.53932491626022294, 0.65240063351038347, 0.76547635076054232]^T$.

$$
\begin{aligned}
Y_2 &= 2.9087136529909646\,\text{e-}01 y_{n-1} + 7.0912863470090359\,\text{e-}01 y_n + 8.3019628155931935\,\text{e-}01\Delta t f_n,\\
Y_3 &= 1.7386041575857100\,\text{e-}01 y_{n-1} + 4.4327424061899495\,\text{e-}01 y_n + 1.7154130384111310\,\text{e-}01\Delta t f_{n-1}\\
&\quad + 3.8286534362243407\,\text{e-}01 Y_2 + 4.4823092603973058\,\text{e-}01\Delta t F_2,\\
Y_4 &= 1.0738138250177699\,\text{e-}01 y_{n-1} + 6.4165836289914413\,\text{e-}01 y_n + 4.2428460618156771\,\text{e-}01\Delta t f_n\\
&\quad + 6.9789004846984226\,\text{e-}03 Y_2 + 2.4398135411438043\,\text{e-}01 Y_3 + 2.8563564217231024\,\text{e-}01\Delta t F_3,\\
y_{n+1} &= 2.0843560497871033\,\text{e-}02 y_{n-1} + 3.7256984232963808\,\text{e-}01 y_n + 2.4401278765485472\,\text{e-}02\Delta t f_{n-1}\\
&\quad + 9.9464375557570234\,\text{e-}02\Delta t f_n + 1.9865525045683016\,\text{e-}01 Y_2 + 4.0793134671566084\,\text{e-}01 Y_4\\
&\quad + 4.7757638121279422\,\text{e-}01\Delta t F_4.
\end{aligned}
$$

HB(3,4,5). Here $c = 1.366$, $c_{\text{eff}} = 0.341$, and
$\sigma = [0, 0.49606471932245216, 0.45040838060150046, 0.90025795055268820]^T$.

$$
\begin{aligned}
Y_2 &= 6.7487162492609845\,\text{e-}02 y_{n-2} + 5.1463622662637439\,\text{e-}02 y_{n-1} + 8.8104921484475274\,\text{e-}01 y_n\\
&\quad + 3.7666033438306788\,\text{e-}02\Delta t f_{n-1} + 6.4483663353200249\,\text{e-}01\Delta t f_n,\\
Y_3 &= 5.0435237298896751\,\text{e-}01 y_{n-1} + 4.6382691456699904\,\text{e-}02 y_n + 3.6913362027045182\,\text{e-}01\Delta t f_{n-1}\\
&\quad + 3.3947318843433938\,\text{e-}02\Delta t f_n + 4.4926493555433245\,\text{e-}01 Y_2 + 3.2881533031940274\,\text{e-}01\Delta t F_2,\\
Y_4 &= 3.4089035733282883\,\text{e-}02 y_{n-2} + 1.1966629872952983\,\text{e-}01 y_{n-1} + 8.7583317617032308\,\text{e-}02\Delta t f_{n-1}\\
&\quad + 8.4624466553718747\,\text{e-}01 Y_3 + 6.1936331373448850\,\text{e-}01\Delta t F_3,\\
y_{n+1} &= 1.7929870801754462\,\text{e-}02 y_{n-2} + 2.1701226168846510\,\text{e-}07 y_{n-1} + 4.2335763047475578\,\text{e-}01 y_n\\
&\quad + 1.3122805551224935\,\text{e-}02\Delta t f_{n-2} + 1.5883046480813512\,\text{e-}07\Delta t f_{n-1} + 1.8492270511436729\,\text{e-}01\Delta t f_n\\
&\quad + 1.7607534416799414\,\text{e-}01 Y_2 + 1.2886888753573725\,\text{e-}01\Delta t F_2 + 2.4724918308539948\,\text{e-}03 Y_3\\
&\quad + 3.8016444571237995\,\text{e-}01 Y_4 + 2.7824093958806490\,\text{e-}01\Delta t F_4.
\end{aligned}
$$

HB(3,4,6). Here $c = 0.716$, $c_{\text{eff}} = 0.179$, and
$\sigma = [0, 0.30133930954368343, 0.67073091427861631, 0.78922095936386205]^T$.

$$
Y_2 = 4.7770452064870433\,\text{e-}02 y_{n-2} + 5.1822440739673215\,\text{e-}01 y_{n-1} + 4.3400514053839745\,\text{e-}01 y_n
$$

$$+\,3.0925041808997500\,\text{e-}01\Delta t f_{n-1} + 6.0585420298018144\,\text{e-}01\Delta t f_n,$$

$$\begin{aligned}
Y_3 &= 1.7881046936624978\,\text{e-}01 y_{n-2} + 3.1435205819021794\,\text{e-}01 y_{n-1} + 4.3625387781624295\,\text{e-}02\Delta t f_{n-2} \\
&\quad + 4.3882317945301935\,\text{e-}01\Delta t f_{n-1} + 5.0683747244353228\,\text{e-}01 Y_2 + 7.0752528996969044\,\text{e-}01\Delta t F_2, \\
Y_4 &= 2.9550265031416362\,\text{e-}02 y_{n-2} + 7.2551231803535421\,\text{e-}01 y_n + 1.6050124780249204\,\text{e-}02\Delta t f_{n-2} \\
&\quad + 3.2606121209759092\,\text{e-}01\Delta t f_n + 2.4493741693322948\,\text{e-}01 Y_3 + 3.4192305494818703\,\text{e-}01\Delta t F_3, \\
y_{n+1} &= 1.2753583942514621\,\text{e-}02 y_{n-2} + 2.8933666952256465\,\text{e-}01 y_{n-1} + 3.7340911321864906\,\text{e-}01 y_n \\
&\quad + 1.2858329242989275\,\text{e-}01\Delta t f_{n-1} + 4.7739129368719369\,\text{e-}01\Delta t f_n + 1.1871654869920525\,\text{e-}04 Y_2 \\
&\quad + 3.2438191676757244\,\text{e-}01 Y_4 + 4.5282446977609897\,\text{e-}01\Delta t F_4.
\end{aligned}$$

HB(4,4,6). Here $c = 1.086$, $c_{\text{eff}} = 0.271$, and
$\sigma = [0, 0.24121065330980895, 0.52911058180223902, 0.84576677386391186]^T$.

$$\begin{aligned}
Y_2 &= 3.1178857109809961\,\text{e-}02 y_{n-3} + 4.4689624054579768\,\text{e-}01 y_{n-1} + 5.2192490234439237\,\text{e-}01 y_n \\
&\quad + 1.6598587642875223\,\text{e-}02\Delta t f_{n-3} + 2.8486592470334560\,\text{e-}01\Delta t f_{n-1} + 4.8017895283881568\,\text{e-}01\Delta t f_n, \\
Y_3 &= 5.1959540622281350\,\text{e-}02 y_{n-3} + 3.5941507823114022\,\text{e-}01 y_{n-1} + 3.0209737556498341\,\text{e-}02\Delta t f_{n-3} \\
&\quad + 3.3066741043451991\,\text{e-}01\Delta t f_{n-1} + 5.8862538114657859\,\text{e-}01 Y_2 + 5.4154442116810342\,\text{e-}01\Delta t F_2, \\
Y_4 &= 8.0231772899364701\,\text{e-}03 y_{n-3} + 1.3131587577573756\,\text{e-}01 y_{n-1} + 2.5397806261967282\,\text{e-}01 y_n \\
&\quad + 1.1796160318280763\,\text{e-}03\Delta t f_{n-3} + 1.2081262924584257\,\text{e-}01\Delta t f_{n-1} + 6.0668288431465323\,\text{e-}01 Y_3 \\
&\quad + 5.5815760234260159\,\text{e-}01\Delta t F_3 \\
y_{n+1} &= 1.3097096111310189\,\text{e-}02 y_{n-3} + 7.4923370275830570\,\text{e-}02 y_{n-2} + 5.5794585649361489\,\text{e-}02 y_{n-1} \\
&\quad + 4.5776927884707702\,\text{e-}01 y_n + 6.8930655196950130\,\text{e-}02\Delta t f_{n-2} + 5.1331878572652812\,\text{e-}02\Delta t f_{n-1} \\
&\quad + 4.2115479060534788\,\text{e-}01\Delta t f_n + 3.9841566911642062\,\text{e-}01 Y_4 + 3.6654855503457545\,\text{e-}01\Delta t F_4.
\end{aligned}$$

HB(4,4,7). Here $c = 0.564$, $c_{\text{eff}} = 0.141$, and
$\sigma = [0, 0.47253084193946687, 0.62298379770112466, 0.77343675346274787]^T$.

$$\begin{aligned}
Y_2 &= 1.4181171301608114\,\text{e-}01 y_{n-3} + 2.6746986944809459\,\text{e-}01 y_{n-2} + 8.8729483281577440\,\text{e-}02 y_{n-1} \\
&\quad + 5.0198893425424684\,\text{e-}01 y_n + 4.7424507571486046\,\text{e-}01\Delta t f_{n-2} + 1.5732433938761134\,\text{e-}01\Delta t f_{n-1} \\
&\quad + 8.9006578806300507\,\text{e-}01\Delta t f_n, \\
Y_3 &= 5.6455583476077723\,\text{e-}02 y_{n-3} + 1.7475976037994695\,\text{e-}01 y_{n-2} + 3.7086510533962463\,\text{e-}01 y_{n-1} \\
&\quad + 1.8183631650368465\,\text{e-}01 y_n + 4.7513634361493660\,\text{e-}02\Delta t f_{n-3} + 6.5757294578528802\,\text{e-}01\Delta t f_{n-1} \\
&\quad + 3.2241006385482263\,\text{e-}01\Delta t f_n + 2.1608323430066603\,\text{e-}01 Y_2 + 3.8313253759417537\,\text{e-}01\Delta t F_2, \\
Y_4 &= 2.4221142166745917\,\text{e-}02 y_{n-3} + 4.8697070969724393\,\text{e-}02 y_{n-2} + 1.9256679584245262\,\text{e-}12 y_{n-1} \\
&\quad + 7.1071176389436097\,\text{e-}01 y_n + 8.6343729694796853\,\text{e-}02\Delta t f_{n-2} + 3.4143798899322064\,\text{e-}12\Delta t f_{n-1} \\
&\quad + 3.6397677596282374\,\text{e-}01\Delta t f_n + 1.3133260011104431\,\text{e-}02 Y_2
\end{aligned}$$

$$
\begin{aligned}
&+ 2.0323676295613866\,\text{e-}01 Y_3 + 3.6035473541396956\,\text{e-}01 \Delta t F_3,\\
y_{n+1} &= 3.3921902937070918\,\text{e-}02 y_{n-3} + 2.5714116547015001\,\text{e-}02 y_{n-2} + 3.9501177301951948\,\text{e-}02 y_{n-1}\\
&+ 5.3391509806078963\,\text{e-}01 y_n + 1.3755767756843626\,\text{e-}02 \Delta t f_{n-3} + 4.5593147272786197\,\text{e-}02 \Delta t f_{n-2}\\
&+ 7.0038688316725384\,\text{e-}02 \Delta t f_{n-1} + 3.0756492028491300\,\text{e-}01 \Delta t f_n + 8.6160403455941698\,\text{e-}02 Y_2\\
&+ 2.8078730169723076\,\text{e-}01 Y_4 + 4.9785792855077493\,\text{e-}01 \Delta t F_4.
\end{aligned}
$$

HB(5,4,7). Here $c = 0.877$, $c_{\text{eff}} = 0.219$, and
$\sigma = [0, 0.24952030418221310, 0.53315370185373812, 0.81678709952540329]^T$.

$$
\begin{aligned}
Y_2 &= 2.3982101438859836\,\text{e-}02 y_{n-4} + 8.7678139889331416\,\text{e-}02 y_{n-3} + 5.3701393015570177\,\text{e-}02 y_{n-2}\\
&+ 3.8841208288909290\,\text{e-}01 y_{n-1} + 4.4622628276714571\,\text{e-}01 y_n + 9.9887959665517417\,\text{e-}02 \Delta t f_{n-3}\\
&+ 6.1179703245210756\,\text{e-}02 \Delta t f_{n-2} + 4.3486379190199109\,\text{e-}01 \Delta t f_{n-1} + 5.0836654371316070\,\text{e-}01 \Delta t f_n,\\
Y_3 &= 1.1796058355794571\,\text{e-}02 y_{n-4} + 8.3827812174208732\,\text{e-}02 y_{n-3} + 4.0125168106181686\,\text{e-}01 y_{n-1}\\
&+ 7.7216192941462425\,\text{e-}02 \Delta t f_{n-3} + 4.5712890104892312\,\text{e-}01 \Delta t f_{n-1} + 5.0312444840817983\,\text{e-}01 Y_2\\
&+ 5.7318819346265659\,\text{e-}01 \Delta t F_2,\\
Y_4 &= 1.4755308341935032\,\text{e-}02 y_{n-4} + 6.1776665970132170\,\text{e-}02 y_{n-3} + 3.0637732023705277\,\text{e-}01 y_{n-1}\\
&+ 1.5743252991886703\,\text{e-}01 y_n + 7.0379516792679092\,\text{e-}02 \Delta t f_{n-3} + 3.4904259425320944\,\text{e-}01 \Delta t f_{n-1}\\
&+ 1.7935615671620367\,\text{e-}01 \Delta t f_n + 4.5965817553201299\,\text{e-}01 Y_3 + 5.2366892540627263\,\text{e-}01 \Delta t F_3,\\
y_{n+1} &= 1.1895330671295582\,\text{e-}02 y_{n-4} + 7.4076433114412518\,\text{e-}02 y_{n-2} + 1.2066305045361436\,\text{e-}02 y_{n-1}\\
&+ 5.4016773987737765\,\text{e-}01 y_n + 6.0405726702878262\,\text{e-}03 \Delta t f_{n-4} + 8.4392116124240218\,\text{e-}02 \Delta t f_{n-2}\\
&+ 1.3746625934402956\,\text{e-}02 \Delta t f_{n-1} + 3.9593568274754259\,\text{e-}01 \Delta t f_n\\
&+ 3.6179419129155271\,\text{e-}01 Y_4 + 4.1217666835272870\,\text{e-}01 \Delta t F_4.
\end{aligned}
$$

HB(5,4,8). Here $c = 0.490$, $c_{\text{eff}} = 0.123$, and
$\sigma = [0, 0.43719711625027513, 0.61523315185784544, 0.79326918746546093]^T$.

$$
\begin{aligned}
Y_2 &= 1.1240806184358765\,\text{e-}01 y_{n-4} + 2.3425521053653969\,\text{e-}01 y_{n-2} + 2.2640298225573424\,\text{e-}01 y_{n-1}\\
&+ 4.2693374536413853\,\text{e-}01 y_n + 6.5470343019684962\,\text{e-}02 \Delta t f_{n-4} + 4.7749624431538534\,\text{e-}01 \Delta t f_{n-2}\\
&+ 1.6853188701135904\,\text{e-}01 \Delta t f_{n-1} + 8.7024429260701008\,\text{e-}01 \Delta t f_n,\\
Y_3 &= 7.6866971450876870\,\text{e-}02 y_{n-4} + 1.9188166805763143\,\text{e-}01 y_{n-3} + 3.8225805090004583\,\text{e-}01 y_{n-1}\\
&+ 1.4490725338067179\,\text{e-}01 y_n + 3.0082537934918074\,\text{e-}01 \Delta t f_{n-3} + 7.7917918344710779\,\text{e-}01 \Delta t f_{n-1}\\
&+ 2.9537302117997444\,\text{e-}01 \Delta t f_n + 2.0408605621077405\,\text{e-}01 Y_2 + 4.1600067351578807\,\text{e-}01 \Delta t F_2,\\
Y_4 &= 1.3379640088295723\,\text{e-}02 y_{n-4} + 1.5102357622019259\,\text{e-}02 y_{n-3} + 4.9961391525236702\,\text{e-}02 y_{n-2}\\
&+ 6.1124255630347346\,\text{e-}03 y_{n-1} + 7.1696847190691049\,\text{e-}01 y_n + 8.4163142856899329\,\text{e-}03 \Delta t f_{n-4}\\
&+ 1.0183925795900226\,\text{e-}01 \Delta t f_{n-2} + 1.2459318378965911\,\text{e-}02 \Delta t f_{n-1} + 3.4874152013934234\,\text{e-}01 \Delta t f_n
\end{aligned}
$$

$$+ 1.9847571329450317\,\text{e-}01 Y_3 + 4.0456477987779804\,\text{e-}01 \Delta t F_3,$$

$$\begin{aligned} y_{n+1} = {} & 5.6758862391967811\,\text{e-}03 y_{n-4} + 1.6498330025689711\,\text{e-}01 y_{n-3} + 1.2555868880225157\,\text{e-}01 y_{n-2} \\ & + 1.7392006935005835\,\text{e-}01 y_{n-1} + 2.9860166752988093\,\text{e-}01 y_n + 6.8744743680103665\,\text{e-}02 \Delta t f_{n-3} \\ & + 2.5593369815305611\,\text{e-}01 \Delta t f_{n-2} + 3.5451155914745591\,\text{e-}01 \Delta t f_{n-1} + 6.0865743163304931\,\text{e-}01 \Delta t f_n \\ & + 6.0865743163304931\,\text{e-}01 \Delta t f_n + 2.3126038782171532\,\text{e-}01 Y_4 + 4.7139172012809527\,\text{e-}01 \Delta t F_4. \end{aligned}$$

HB(6,4,8). Here $c = 0.722$, $c_{\text{eff}} = 0.180$, and
$\sigma = [0, 0.33085734752000873, 0.57058367833569879, 0.81031000915165174]^T$.

$$\begin{aligned} Y_2 = {} & 4.6472690717261362\,\text{e-}03 y_{n-5} + 1.7617740666490314\,\text{e-}02 y_{n-2} + 5.1087509618159122\,\text{e-}01 y_{n-1} \\ & + 4.6685989408019241\,\text{e-}01 y_n + 4.0074586314538660\,\text{e-}03 \Delta t f_{n-5} + 2.4400693250375298\,\text{e-}02 \Delta t f_{n-2} \\ & + 2.2519192095834503\,\text{e-}01 \Delta t f_{n-1} + 6.4660419755303700\,\text{e-}01 \Delta t f_n, \\ Y_3 = {} & 6.3437465306319159\,\text{e-}03 y_{n-5} + 3.8280022711921196\,\text{e-}03 y_{n-4} + 1.3378083962303952\,\text{e-}01 y_{n-3} \\ & + 4.0276427099509055\,\text{e-}01 y_{n-1} + 1.0731673311116895\,\text{e-}01 y_n + 5.3018097467378913\,\text{e-}03 \Delta t f_{n-4} \\ & + 1.1632225850184115\,\text{e-}01 \Delta t f_{n-3} + 5.5783131417384202\,\text{e-}01 \Delta t f_{n-1} + 1.4863442111273212\,\text{e-}01 \Delta t f_n \\ & + 3.4596640746887680\,\text{e-}01 Y_2 + 4.7916587849650372\,\text{e-}01 \Delta t F_2, \\ Y_4 = {} & 2.4354830266242293\,\text{e-}02 y_{n-5} + 1.0614148803253295\,\text{e-}01 y_{n-3} + 3.0848403901567312\,\text{e-}01 y_{n-1} \\ & + 2.1975355520489917\,\text{e-}01 y_n + 1.2996464181697261\,\text{e-}02 \Delta t f_{n-5} + 1.4700669851193610\,\text{e-}01 \Delta t f_{n-3} \\ & + 4.2725253772042082\,\text{e-}01 \Delta t f_{n-1} + 3.0436020104627681\,\text{e-}01 \Delta t f_n \\ & + 3.4126608748065268\,\text{e-}01 Y_3 + 4.7265590264986124\,\text{e-}01 \Delta t F_3, \\ y_{n+1} = {} & 7.0409864973861782\,\text{e-}03 y_{n-5} + 3.1910209804637511\,\text{e-}02 y_{n-4} + 1.1534180942145611\,\text{e-}01 y_{n-2} \\ & + 7.1301418909879871\,\text{e-}02 y_{n-1} + 4.6441610170111464\,\text{e-}01 y_n + 3.5260849749088656\,\text{e-}02 \Delta t f_{n-4} \\ & + 1.5974920756946681\,\text{e-}01 \Delta t f_{n-2} + 9.8752960670244611\,\text{e-}02 \Delta t f_{n-1} + 4.9054264305477624\,\text{e-}01 \Delta t f_n \\ & + 3.0998947366552543\,\text{e-}01 Y_4 + 4.2933757517186882\,\text{e-}01 \Delta t F_4. \end{aligned}$$

HB(7,4,8). Here $c = 0.852$, $c_{\text{eff}} = 0.213$, and
$\sigma = [0, 0.28645813613098242, 0.55824315714402994, 0.83002817815821284]^T$.

$$\begin{aligned} Y_2 = {} & 1.1033483152094540\,\text{e-}02 y_{n-6} + 2.1618741753910483\,\text{e-}02 y_{n-4} + 7.3164773446182038\,\text{e-}02 y_{n-3} \\ & + 8.9377315222374923\,\text{e-}02 y_{n-2} + 3.3052209858727233\,\text{e-}01 y_{n-1} + 4.7428358783816565\,\text{e-}01 y_n \\ & + 7.9271467501655368\,\text{e-}03 \Delta t f_{n-6} + 2.5357039226603571\,\text{e-}02 \Delta t f_{n-4} + 8.5816374116448504\,\text{e-}02 \Delta t f_{n-3} \\ & + 8.5816374116448504\,\text{e-}02 \Delta t f_{n-3} + 1.0483237710410760\,\text{e-}01 \Delta t f_{n-2} \\ & + 3.8767574517240444\,\text{e-}01 \Delta t f_{n-1} + 5.5629636906003022\,\text{e-}01 \Delta t f_n, \\ Y_3 = {} & 4.1673572573951061\,\text{e-}03 y_{n-6} + 4.4113926716232821\,\text{e-}02 y_{n-4} + 4.0105444119401153\,\text{e-}02 y_{n-3} \\ & + 4.2687049006597683\,\text{e-}01 y_{n-1} + 5.1742075598859100\,\text{e-}02 \Delta t f_{n-4} + 4.7040449037793017\,\text{e-}02 \Delta t f_{n-3} \\ & + 5.0068463208894975\,\text{e-}01 \Delta t f_{n-1} + 4.8474278184099362\,\text{e-}01 Y_2 + 5.6856415946279171\,\text{e-}01 \Delta t F_2, \end{aligned}$$

$$
\begin{aligned}
Y_4 &= 6.7610940286408298\,\text{e-}03 y_{n-6} + 1.1290295300529569\,\text{e-}02 y_{n-4} + 6.5520108757853551\,\text{e-}02 y_{n-3} \\
&\quad + 2.9888049430192454\,\text{e-}01 y_{n-1} + 1.8498138261618360\,\text{e-}01 y_n + 4.7303133989144205\,\text{e-}03 \Delta t f_{n-6} \\
&\quad + 1.3242605146698148\,\text{e-}02 \Delta t f_{n-4} + 7.6849799438662283\,\text{e-}02 \Delta t f_{n-3} + 3.5056269714262467\,\text{e-}01 \Delta t f_{n-1} \\
&\quad + 2.1696823194354331\,\text{e-}01 \Delta t f_n + 4.3256662499486692\,\text{e-}01 Y_3 + 5.0736573862494427\,\text{e-}01 \Delta t F_3, \\
y_{n+1} &= 2.5881604396226902\,\text{e-}03 y_{n-6} + 7.6357016234845469\,\text{e-}03 y_{n-5} + 1.6304328340768028\,\text{e-}02 y_{n-4} \\
&\quad + 1.2567327447111440\,\text{e-}01 y_{n-2} + 7.7112740468168656\,\text{e-}02 y_{n-1} + 4.3369750806348006\,\text{e-}01 y_n \\
&\quad + 8.9560617261325842\,\text{e-}03 \Delta t f_{n-5} + 1.9123661219807291\,\text{e-}02 \Delta t f_{n-4} + 1.4740460785250881\,\text{e-}01 \Delta t f_{n-2} \\
&\quad + 9.0447020792438215\,\text{e-}02 \Delta t f_{n-1} + 5.0648288653910711\,\text{e-}01 \Delta t f_n + 3.3698828659336139\,\text{e-}01 Y_4 \\
&\quad + 3.9526006181688789\,\text{e-}01 \Delta t F_4.
\end{aligned}
$$

A.2 Thirteen noncanonical HB($k, s, 4$) methods considered in the thesis

HB(4,4,4). Here $c = 1.932$, $c_{\text{eff}} = 0.483$, and
$\sigma = [0, 0.29550672532505878, 0.55487098371182864, 0.87509757670763788]^T$.

$$
\begin{aligned}
Y_2 &= 4.7524774508095377\,\text{e-}02 y_{n-2} + 1.2685090981790423\,\text{e-}01 y_{n-1} + 8.2562431567400041\,\text{e-}01 y_n \\
&\quad + 2.4589659756032358\,\text{e-}02 \Delta t f_{n-2} + 6.5633572056908576\,\text{e-}02 \Delta t f_{n-1} + 4.2718395234621287\,\text{e-}01 \Delta t f_n, \\
Y_3 &= 1.9918300748893264\,\text{e-}01 y_{n-1} + 1.0305871903720029\,\text{e-}01 \Delta t f_{n-1} \\
&\quad + 8.0081699251106719\,\text{e-}01 Y_2 + 4.1434846512195339\,\text{e-}01 \Delta t F_2, \\
Y_4 &= 1.2681476034277145\,\text{e-}01 y_{n-1} + 6.5614868058771342\,\text{e-}02 \Delta t f_{n-1} \\
&\quad + 8.7318523965722883\,\text{e-}01 Y_3 + 4.5179231610038256\,\text{e-}01 \Delta t F_3, \\
y_{n+1} &= 3.2258872667719520\,\text{e-}03 y_{n-3} + 1.4711725267828712\,\text{e-}02 y_{n-1} + 4.0081143477759190\,\text{e-}01 y_n \\
&\quad + 7.6119523449503096\,\text{e-}03 \Delta t f_{n-1} + 2.0738271584706414\,\text{e-}01 \Delta t f_n + 5.8125095268780758\,\text{e-}01 Y_4 \\
&\quad + 3.0074341872002397\,\text{e-}01 \Delta t F_4.
\end{aligned}
$$

HB(2,5,4). Here $c = 2.258$, $c_{\text{eff}} = 0.452$, and
$\sigma = [0, 0.43353487829608683, 0.49212970792955379, 0.51952905303075192, 0.95306393132683886]^T$.

$$
\begin{aligned}
Y_2 &= y_n + 4.3353487829608683\,\text{e-}01 \Delta t f_n, \\
Y_3 &= 2.6154930329164866\,\text{e-}01 y_{n-1} + 1.1339074537097120\,\text{e-}01 \Delta t f_{n-1} \\
&\quad + 7.3845069670835128\,\text{e-}01 Y_2 + 3.2014413292511562\,\text{e-}01 \Delta t F_2,
\end{aligned}
$$

$$
\begin{aligned}
Y_4 &= 4.1933308968746225\,\text{e-01} y_n + 1.0527799621252554\,\text{e-02} y_{n-1} + 2.2992686629013520\,\text{e-03}\Delta t f_{n-1}\\
&\quad + 5.7013911069128531\,\text{e-01} Y_3 + 2.4717518996538551\,\text{e-01}\Delta t F_3,\\
Y_5 &= Y_4 + 4.3353487829608683\,\text{e-01}\Delta t F_4,\\
y_{n+1} &= 2.3548942789448177\,\text{e-02} y_{n-1} + 2.1442551411227079\,\text{e-01} y_n + 9.2960939164239198\,\text{e-02}\Delta t f_n\\
&\quad + 2.4250812182244122\,\text{e-01} Y_2 + 1.0509003662565282\,\text{e-01}\Delta t F_2\\
&\quad + 5.1951742127583977\,\text{e-01} Y_4 + 2.2522892200551811\,\text{e-01}\Delta t F_4
\end{aligned}
$$

HB(3,5,4). Here $c = 2.520$, $c_{\text{eff}} = 0.504$, and
$\sigma = [0, 0.39667202894458992, 0.34733932541243928, 0.74401135435702903, 0.87211776033132926]^T$.

$$
\begin{aligned}
Y_2 &= y_n + 3.9667202894458869488\,\text{e-01}\Delta t f_n,\\
Y_3 &= 3.1933390462023281\,\text{e-01} y_{n-1} + 1.2667082785650549\,\text{e-01}\Delta t f_{n-1}\\
&\quad + 6.8066609537976719\,\text{e-01} Y_2 + 2.7000120108808318\,\text{e-01}\Delta t F_2,\\
Y_4 &= Y_3 + 3.9667202894458875\,\text{e-01}\Delta t F_3,\\
Y_5 &= 3.0842709893420334\,\text{e-01} y_n + 9.7477349638087907\,\text{e-02}\Delta t f_n + 1.9119743013194673\,\text{e-02} Y_2\\
&\quad + 6.7245315805260308\,\text{e-01} Y_4 + 2.6674335857492221\,\text{e-01}\Delta t F_4,\\
y_{n+1} &= 3.7295391119407718\,\text{e-03} y_{n-2} + 1.6897464146259084\,\text{e-01} y_n + 5.2526715235296312\,\text{e-02}\Delta t f_n\\
&\quad + 1.9426370492958658\,\text{e-01} Y_2 + 7.4688701847753544\,\text{e-02}\Delta t F_2\\
&\quad + 6.3303211449588204\,\text{e-01} Y_5 + 2.5110613324416470\,\text{e-01}\Delta t F_5.
\end{aligned}
$$

HB(2,6,4). Here $c = 2.930$, $c_{\text{eff}} = 0.488$, and
$\sigma = [0, 0.34131501751573518, 0.58493205600266185, 0.59078590110096663, 0.58032954089932975, 0.89749336077124797]^T$.

$$
\begin{aligned}
Y_2 &= y_n + 3.4131501751573518\,\text{e-01}\Delta t f_n,\\
Y_3 &= 7.2837460069414606\,\text{e-02} y_{n-1} + 2.4860518959393910\,\text{e-02}\Delta t f_{n-1}\\
&\quad + 9.2716253993058551\,\text{e-01} Y_2 + 3.1645449855634128\,\text{e-01}\Delta t F_2,\\
Y_4 &= 2.1165650044551004\,\text{e-01} y_{n-1} + 7.2241542156878474\,\text{e-02}\Delta t f_{n-1}\\
&\quad + 7.8834349955449001\,\text{e-01} Y_3 + 2.6907347535885678\,\text{e-01}\Delta t F_3\\
Y_5 &= 5.2217429737665433\,\text{e-01} y_n + 1.7822592945537952\,\text{e-01}\Delta t f_n + 7.3255243277284984\,\text{e-02} Y_2\\
&\quad + 4.0457045934606084\,\text{e-01} Y_4 + 1.3808597341804979\,\text{e-01}\Delta t F_4\\
Y_6 &= 4.1616350378895876\,\text{e-02} y_n + 1.4204285358513801\,\text{e-02}\Delta t f_n + 2.3181094241883033\,\text{e-10} Y_2\\
&\quad + 9.5838364938929321\,\text{e-01} Y_5 + 3.2711073207810087\,\text{e-01}\Delta t F_5,\\
y_{n+1} &= 1.3882061429735554\,\text{e-02} y_{n-1} + 1.0652255784084119\,\text{e-01} y_n + 3.6357748695267644\,\text{e-02}\Delta t f_n\\
&\quad + 1.8790001888305066\,\text{e-01} Y_2 + 5.6513205020659152\,\text{e-02}\Delta t F_2\\
&\quad + 6.9169536184637270\,\text{e-01} Y_6 + 2.3608601454414754\,\text{e-01}\Delta t F_6.
\end{aligned}
$$

HB(3,6,4). Here $c = 3.069$, $c_{\text{eff}} = 0.512$, and
$\sigma = [0, 0.32582165651383960, 0.37067798466591867, 0.69649964117975816, 0.66867140411649717, 0.82079730062345002]^T$.

$$
\begin{aligned}
Y_2 &= y_n + 3.2582165651383960\,\text{e-}01\Delta t f_n,\\
Y_3 &= 2.1191789029946936\,\text{e-}01 y_{n-1} + 6.9047438062291244\,\text{e-}02\Delta t f_{n-1}\\
&\quad + 7.8808210970053061\,\text{e-}01 Y_2 + 2.5677421845154841\,\text{e-}01\Delta t F_2,\\
Y_4 &= Y_3 + 3.2582165651383960\,\text{e-}01\Delta t F_3\\
Y_5 &= 5.0766128220635420\,\text{e-}01 y_n + 1.6540703991641412\,\text{e-}01\Delta t f_n + 9.1877548437183622\,\text{e-}05 Y_2\\
&\quad + 4.9224684024520876\,\text{e-}01 Y_4 + 1.6038468090239727\,\text{e-}01\Delta t F_4\\
Y_6 &= 2.5976250331144174\,\text{e-}01 y_n + 8.4636249129115701\,\text{e-}02\Delta t f_n + 3.2614058591337942\,\text{e-}09 Y_2\\
&\quad + 7.4023749342715239\,\text{e-}01 Y_5 + 2.4118540632208724\,\text{e-}01\Delta t F_5\\
y_{n+1} &= 1.7848294943323458\,\text{e-}03 y_{n-2} + 1.1378607462930097\,\text{e-}01 y_n + 2.6029211669753471\,\text{e-}02\Delta t f_n\\
&\quad + 6.5472471465212512\,\text{e-}02 Y_2 + 1.7176907587067886\,\text{e-}02\Delta t F_2\\
&\quad + 8.1895662441115424\,\text{e-}01 Y_6 + 2.6683380397862461\,\text{e-}01\Delta t F_6.
\end{aligned}
$$

HB(2,7,4). Here $c(\text{HB(2,7,4)}) = 3.726$, $c_{\text{eff}}(\text{HB(2,7,4)})) = 0.532$, and
$\sigma = [0, 0.26841980744987709, 0.36782834082903565, 0.63624814827891274,$
$0.67218202479193823, 0.60626599422072069, 0.87468580167059773]^T$.

$$
\begin{aligned}
Y_2 &= y_n + 2.6841980744987709\,\text{e-}01\Delta t f_n,\\
Y_3 &= 1.3324553359862062\,\text{e-}01 y_{n-1} + 3.5765740472097872\,\text{e-}02\Delta t f_{n-1}\\
&\quad + 8.6675446640137932\,\text{e-}01 Y_2 + 2.3265406697777921\,\text{e-}01\Delta t F_2,\\
Y_4 &= Y_3 + 2.6841980744987709\,\text{e-}01\Delta t F_3,\\
Y_5 &= 3.6364127191257684\,\text{e-}01 y_n + 9.7608520187602299\,\text{e-}02\Delta t f_n + 1.7600759196159160\,\text{e-}013 Y_2\\
&\quad + 6.3459865216780720\,\text{e-}01 Y_4 + 1.7033884802283433\,\text{e-}01\Delta t F_4,\\
Y_6 &= 4.9707943453901537\,\text{e-}01 y_n + 1.3342596610625629\,\text{e-}01\Delta t f_n + 3.0940611702902734\,\text{e-}04 Y_2\\
&\quad + 5.0261115934395562\,\text{e-}01 Y_5 + 1.3491079061326405\,\text{e-}01\Delta t F_5,\\
Y_7 &= Y_6 + 2.6841980744987703\,\text{e-}01\Delta t F_6,\\
y_{n+1} &= 7.4249746253942581\,\text{e-}03 y_{n-1} + 4.2619903069630594\,\text{e-}02 y_n + 1.0451108327339836\,\text{e-}02\Delta t f_n\\
&\quad + 1.4505253390564679\,\text{e-}01 Y_2 + 3.7950229482122844\,\text{e-}02\Delta t F_2 + 8.0490258839932849\,\text{e-}01 Y_7\\
&\quad + 2.1605179779405539\,\text{e-}01\Delta t F_7
\end{aligned}
$$

HB(3,7,4). Here $c(\text{HB(3,7,4)}) = 3.741$, $c_{\text{eff}}(\text{HB(3,7,4)}) = 0.534$, and
$\sigma = [0, 0.26730677262648872, 0.36663180051479927, 0.63393857314128788,$

$0.66822290349557856, 0.60553808135903842, 0.86781907493917998]^T$.

$$
\begin{aligned}
Y_2 &= y_n + 2.6730677262648872\,\text{e-}01\Delta t f_n,\\
Y_3 &= 1.3255018308632302\,\text{e-}01 y_{n-1} + 3.5431561651855202\,\text{e-}02\Delta t f_{n-1}\\
&\quad + 8.6744981691367695\,\text{e-}01 Y_2 + 2.3187521097463354\,\text{e-}01\Delta t F_2,\\
Y_4 &= Y_3 + 2.6730677262648872\,\text{e-}01\Delta t F_3,\\
Y_5 &= 7.8339201835586181\,\text{e-}02 y_n + 2.0940599212805666\,\text{e-}02\Delta t f_n + 2.8923969641243608\,\text{e-}01 Y_2\\
&\quad + 6.3242110175197763\,\text{e-}01 Y_4 + 1.6905044365020938\,\text{e-}01\Delta t F_4,\\
Y_6 &= 4.5282440752517999\,\text{e-}01 y_n + 1.2104303094205779\,\text{e-}01\Delta t f_n + 4.1010199215761101\,\text{e-}02 Y_2\\
&\quad + 5.0616539325905896\,\text{e-}01 Y_5 + 1.3530143768729652\,\text{e-}01\Delta t F_5,\\
Y_7 &= 1.4859000088371840\,\text{e-}02 Y_2 + 3.9719113580793941\,\text{e-}03\Delta t F_2\\
&\quad + 9.8514099991162807\,\text{e-}01 Y_6 + 2.6333486126840927\,\text{e-}01\Delta t F_6,\\
y_{n+1} &= 8.3965945879398759\,\text{e-}04 y_{n-2} + 4.8613008172801175\,\text{e-}02 y_n + 1.2874262041034118\,\text{e-}01 Y_2\\
&\quad + 3.4413774361365404\,\text{e-}02\Delta t F_2 + 8.2180471195806348\,\text{e-}01 Y_7 + 2.1967396528275113\,\text{e-}01\Delta t F_7.
\end{aligned}
$$

HB(2,8,4). Here c(HB(2,8,4)) $= 4.424$, c_{eff}(HB(3,8,4) $= 0.553$, and
$\sigma = [0, 0.22603296506803669, 0.45206593013607332, 0.57538108409035438,$
$0.40503033408031602, 0.53276080986754903, 0.75879377493558564, 0.92644778515340753]^T$.

$$
\begin{aligned}
Y_2 &= y_n + 2.2603296506803669\,\text{e-}01\Delta t f_n,\\
Y_3 &= Y_2 + 2.2603296506803669\,\text{e-}01\Delta t F_2,\\
Y_4 &= 2.0286172312623845\,\text{e-}02 y_{n-1} + 1.0803874178805883\,\text{e-}01 y_n + 4.5853436777034788\,\text{e-}03\Delta t f_{n-1}\\
&\quad + 8.7167508589931730\,\text{e-}01 Y_3 + 1.9702730424175827\,\text{e-}01\Delta t F_3,\\
Y_5 &= 4.9460539841339118\,\text{e-}01 y_n + 5.0539460158660887\,\text{e-}01 Y_4 + 1.1423584032600029\,\text{e-}01\Delta t F_4,\\
Y_6 &= 2.3834939846072800\,\text{e-}01 y_n + 5.3874821256261370\,\text{e-}02\Delta t f_n + 4.3546190149383168\,\text{e-}03 Y_2\\
&\quad + 4.3546190149383168\,\text{e-}03 Y_2 + 7.5729598252433372\,\text{e-}01 Y_5 + 1.7117385636408730\,\text{e-}01\Delta t F_5,\\
Y_7 &= Y_6 + 2.2603296506803666\,\text{e-}01\Delta t F_6,\\
Y_8 &= 3.3268281696016186\,\text{e-}02 Y_2 + 7.5197283544692212\,\text{e-}03\Delta t F_2 + 7.6309888786772917\,\text{e-}02 Y_3\\
&\quad + 8.9042182951721116\,\text{e-}01 Y_7 + +2.0126468628708105\,\text{e-}01\Delta t F_7,\\
y_{n+1} &= 3.0622000515870560\,\text{e-}03 y_{n-1} + 3.4396037347807322\,\text{e-}02 y_n + 2.2397284277651699\,\text{e-}01 Y_3\\
&\quad + 5.0625245747493351\,\text{e-}02\Delta t F_3 + 7.3856891982408845\,\text{e-}01 Y_8 + 1.6694092285493578\,\text{e-}01\Delta t F_8.
\end{aligned}
$$

HB(3,8,4). Here c(HB(3,8,4)) $= 4.431$, c_{eff}(HB(3,8,4)) $= 0.5538$, and
$\sigma = [0, 0.22569317768029287, 0.45138635536058574, 0.55305470898706099,$
$0.41140419740313083, 0.53185945085898290, 0.75755262853927563, 0.91830243658955979]^T$.

$$
Y_2 = y_n + 2.2569317768029287\,\text{e-}01\Delta t f_n,
$$

$$
\begin{aligned}
Y_3 &= Y_2 + 2.2569317768029287\,\text{e-01}\Delta t F_2,\\
Y_4 &= 1.8136891011337745\,\text{e-02} y_{n-1} + 1.4429794897581311\,\text{e-01} y_n + 4.0933725655899564\,\text{e-03}\Delta t f_{n-1}\\
&\quad + 8.3756516001284920\,\text{e-01} Y_3 + 1.8903274247760293\,\text{e-01}\Delta t F_3,\\
Y_5 &= 4.7171067241834541\,\text{e-01} y_n + 5.2828932758165470\,\text{e-01} Y_4 + 1.1923129707648883\,\text{e-01}\Delta t F_4,\\
Y_6 &= 2.2802085154938864\,\text{e-01} y_n + 5.1462750563548147\,\text{e-02}\Delta t f_n + 2.7780924146448754\,\text{e-02} Y_2\\
&\quad + 7.4419822430416260\,\text{e-01} Y_5 + 1.6796046206723791\,\text{e-01}\Delta t F_5,\\
Y_7 &= Y_6 + 2.2569317768029284\,\text{e-01}\Delta t F_6,\\
Y_8 &= 7.2741873790442308\,\text{e-04} Y_2 + 1.6417344646181553\,\text{e-04}\Delta t F_2 + 1.2137884359347230\,\text{e-01} Y_3\\
&\quad + 8.7789373766862333\,\text{e-01} Y_7 + 1.9813462732006101\,\text{e-01}\Delta t F_7,\\
y_{n+1} &= 4.3049458217011075\,\text{e-04} y_{n-2} + 4.4222997383088054\,\text{e-02} y_n + 1.9714726015247588\,\text{e-01} Y_3\\
&\quad + 4.4494791614775667\,\text{e-02}\Delta t F_3 + 7.5819924788226600\,\text{e-01} Y_8 + 1.7112039756935671\,\text{e-01}\Delta t F_8.
\end{aligned}
$$

HB(2,9,4). Here $c(\text{HB(2,9,4)}) = 5.271$, $c_{\text{eff}}(\text{HB(2,9,4)}) = 0.586$, and

$$
\begin{aligned}
\sigma = [&0, 0.18973510416279940, 0.37947020832559880, 0.52900811739988363, 0.33177283195412421,\\
&0.52150793611692348, 0.63723279555722223, 0.75047127700234584, 0.94020638116514521]^T.
\end{aligned}
$$

$$
\begin{aligned}
Y_2 &= y_n + 1.8973510416279943\,\text{e-01}\Delta t f_n,\\
Y_3 &= Y_2 + 1.8973510416279937\,\text{e-01}\Delta t F_2,\\
Y_4 &= 7.0619852286311971\,\text{e-02} y_n + 9.2938014771368804\,\text{e-01} Y_3 + 1.7633603913329446\,\text{e-01}\Delta t F_3,\\
Y_5 &= 5.3839866310977136\,\text{e-01} y_n + 4.6160133689022864\,\text{e-01} Y_4 + 8.7581977736554989\,\text{e-02}\Delta t F_4,\\
Y_6 &= Y_5 + 1.8973510416279937\,\text{e-01}\Delta t F_5,\\
Y_7 &= 1.4191585515183294\,\text{e-01} y_n + 2.6926419559585760\,\text{e-02}\Delta t f_n,\\
&\quad + 8.5808414484816709\,\text{e-01} Y_6 + 1.6280868460321360\,\text{e-01}\Delta t F_6,\\
Y_8 &= 1.7093368412148527\,\text{e-01} Y_2 + 3.2432120361721037\,\text{e-02}\Delta t F_2 + 9.3714265975099066\,\text{e-06} Y_3\\
&\quad + 8.2905694445191724\,\text{e-01} Y_7 + +1.5730120571247669\,\text{e-01}\Delta t F_7,\\
Y_9 &= Y_8 + 1.8973510416279937\,\text{e-01}\Delta t F_8,\\
y_{n+1} &= 3.7795761833689869\,\text{e-03} y_{n-1} + 1.2870630639322917\,\text{e-03} y_n + 1.3274175171758950\,\text{e-02} Y_4\\
&\quad + 2.0055779156521011\,\text{e-01} Y_3 + 3.8052853473286137\,\text{e-02}\Delta t F_3\\
&\quad + 7.8110139401572964\,\text{e-01} Y_9 + 1.4820235435528228\,\text{e-01}\Delta t F_9.
\end{aligned}
$$

HB(3,9,4). Here $c(\text{HB(3,9,4)}) = 5.279$, $c_{\text{eff}}(\text{HB(3,9,4)}) = 0.587$, and

$$
\begin{aligned}
\sigma = [&0, 0.18943721061280203, 0.37887442122560405, 0.51190473654655466, 0.33220975334717834,\\
&0.52164696395998034, 0.64258973999314262, 0.74627464684283940, 0.93064568637963851]^T.
\end{aligned}
$$

$$
\begin{aligned}
Y_2 &= y_n + 1.8943721061280203\,\text{e-01}\Delta t f_n,\\
Y_3 &= Y_2 + 1.8943721061280203\,\text{e-01}\Delta t F_2,
\end{aligned}
$$

$$
\begin{aligned}
Y_4 &= 9.9253459073824102\,\text{e-}02 y_n + 9.0074654092617590\,\text{e-}01 Y_3 + 1.7063491218218491\,\text{e-}01 \Delta t F_3,\\
Y_5 &= 5.2632270935350933\,\text{e-}01 y_n + 4.7367729064649067\,\text{e-}01 Y_4 + 8.9732104670700696\,\text{e-}02 \Delta t F_4,\\
Y_6 &= Y_5 + 1.8943721061280203\,\text{e-}01 \Delta t F_5,\\
Y_7 &= 1.3130188311917806\,\text{e-}01 y_n + 2.4873462486305245\,\text{e-}02 \Delta t f_n + 2.3116942601563637\,\text{e-}06 Y_2\\
&\quad + 8.6869580518656186\,\text{e-}01 Y_6 + 1.6456331020558435\,\text{e-}01 \Delta t F_6,\\
Y_8 &= 1.8332627761890183\,\text{e-}01 Y_2 + 3.4728818664152943\,\text{e-}02 \Delta t F_2 + 5.9086889835505332\,\text{e-}03 Y_3\\
&\quad + 8.1076503339754757\,\text{e-}01 Y_7 + 1.5358906638922670\,\text{e-}01 \Delta t F_7,\\
Y_9 &= 1.3789243236016317\,\text{e-}02 Y_3 + 2.6121957750924324\,\text{e-}03 \Delta t F_3,\\
&\quad + 9.8621075676398373\,\text{e-}01 Y_8 + 1.8682501483770966\,\text{e-}01 \Delta t F_8,\\
y_{n+1} &= 4.9675940773150854\,\text{e-}04 y_{n-2} + 1.7898560493677686\,\text{e-}02 y_n + 2.0231601518094915\,\text{e-}04 Y_4\\
&\quad + 1.7826598991396123\,\text{e-}01 Y_3 + 3.3770211876430631\,\text{e-}02 \Delta t F_3\\
&\quad + 8.0313637416944861\,\text{e-}01 Y_9 + 1.5214391446434000\,\text{e-}01 \Delta t F_9.
\end{aligned}
$$

HB(2,10,4). Here $c(\text{HB(2,10,4)}) = 6.102$, $c_{\text{eff}}(\text{HB(2,10,4)}) = 0.610$, and

$$
\begin{aligned}
\sigma = [&0, 0.16199536174015935, 0.32587309121796598, 0.48975082069577258, 0.39110537738046303\\
&0.55498310685826957, 0.47054816607752142, 0.63442589555532791, 0.79830362503313468, 0.96218135451094122]^T.
\end{aligned}
$$

$$
\begin{aligned}
Y_2 &= 9.9838267569696360\,\text{e-}01 y_n + 1.6361268604319576\,\text{e-}01 \Delta t f_n + 1.6173243030364048\,\text{e-}03 y_{n-1},\\
Y_3 &= Y_2 + 1.6387772947780663\,\text{e-}01 \Delta t F_2,\\
Y_4 &= Y_3 + 1.6387772947780663\,\text{e-}01 \Delta t F_3,\\
Y_5 &= 4.0163969692480539\,\text{e-}01 y_n + 5.9836030307519472\,\text{e-}01 Y_4 + 9.8057927877615150\,\text{e-}02 \Delta t F_4,\\
Y_6 &= Y_5 + 1.6387772947780663\,\text{e-}01 \Delta t F_5,\\
Y_7 &= 4.3651141473686855\,\text{e-}01 y_n + 7.1534499538223190\,\text{e-}02 \Delta t f_n + 3.2677181024377802\,\text{e-}03 Y_3\\
&\quad + 1.2142963792919311\,\text{e-}02 Y_2 + 1.9899613355148157\,\text{e-}03 \Delta t F_2,\\
&\quad + 5.4807790336777440\,\text{e-}01 Y_6 + 8.9817762380867569\,\text{e-}02 \Delta t F_6,\\
Y_8 &= Y_7 + +1.6387772947780663\,\text{e-}01 \Delta t F_7,\\
Y_9 &= Y_8 + 1.6387772947780663\,\text{e-}01 \Delta t F_8,\\
Y_{10} &= Y_9 + 1.6387772947780663\,\text{e-}01 \Delta t F_9,\\
y_{n+1} &= 2.7123097803231889\,\text{e-}03 y_{n-1} + 6.9146647649389378\,\text{e-}03 Y_3 + 1.1331595617783755\,\text{e-}03 \Delta t F_3\\
&\quad + 2.1863321246897169\,\text{e-}01 Y_4 + 2.3225424910426631\,\text{e-}02 \Delta t F_4\\
&\quad + 7.7173981298576633\,\text{e-}01 Y_{10} + 1.2647096829973448\,\text{e-}01 \Delta t F_{10}.
\end{aligned}
$$

HB(3,10,4). Here $c(\text{HB(3,10,4)}) = 6.142$, $c_{\text{eff}}(\text{HB(3,10,4)}) = 0.614$, and

$\sigma = [0, 0.16282659661384036, 0.32565319322768072, 0.48847978984152113, 0.35907995652089209,$

$0.48552698907685793, 0.55293076340580660, 0.62414211119929675, 0.78175633090122820, 0.94458292751506845]^T.$

$$
\begin{aligned}
Y_2 &= y_n + 1.6282659661384036\,\text{e-01}\Delta t f_n,\\
Y_3 &= Y_2 + 1.6282659661384036\,\text{e-01}\Delta t F_2,\\
Y_4 &= Y_3 + 1.6282659661384036\,\text{e-01}\Delta t F_3,\\
Y_5 &= 4.4867735985957147\,\text{e-01}y_n + 5.5132264014042853\,\text{e-01}Y_4 + 8.9769989130223021\,\text{e-02}\Delta t F_4,\\
Y_6 &= 6.9705129853931833\,\text{e-02}y_n + 9.3029487014606804\,\text{e-01}Y_5 + 1.5147674755319884\,\text{e-01}\Delta t F_5,\\
Y_7 &= 1.9509480297883888\,\text{e-01}y_n + 3.1766622786092102\,\text{e-02}\Delta t f_n + 1.4397346095268116\,\text{e-03}Y_2,\\
&\quad + 8.0346546241163441\,\text{e-01}Y_6 + 1.3082554674125191\,\text{e-01}\Delta t F_6,\\
Y_8 &= 3.3918333816126425\,\text{e-02}Y_2 + 5.5228068580921580\,\text{e-03}\Delta t F_2 + 2.0092983397903494\,\text{e-01}Y_3,\\
&\quad + 7.6515183220483873\,\text{e-01}Y_7 + +1.2458706873075814\,\text{e-01}\Delta t F_7,\\
Y_9 &= 1.4299235887157244\,\text{e-02}Y_3 + 2.3282959136844139\,\text{e-03}\Delta t F_3 + 3.1633116249260595\,\text{e-03}Y_4,\\
&\quad + 9.8253745248791668\,\text{e-01}Y_8 + +1.5998322943424034\,\text{e-01}\Delta t F_8,\\
Y_{10} &= Y_9 + 1.6282659661384036\,\text{e-01}\Delta t F_9,\\
y_{n+1} &= 4.9225322847329942\,\text{e-04}y_{n-2} + 1.7871006145269043\,\text{e-04}y_n + 2.4021344291524174\,\text{e-03}Y_3\\
&\quad + 3.9113137370776901\,\text{e-04}\Delta t F_3 + 1.6901708746032448\,\text{e-01}Y_4 + 4.1446692144727487\,\text{e-04}\Delta t F_4\\
&\quad + 8.2790981482059733\,\text{e-01}Y_{10} + 1.3480573745043264\,\text{e-01}\Delta t F_{10}.
\end{aligned}
$$

A.3 Nine canonical HB$_{\text{RK4}}(k,8,p)$ methods considered in the thesis

HB(2,8,4). $c = 4.488$, $c_{\text{eff}} = 0.561$, and

$\sigma = [0, 0.22261252811822593, 0.32399579913749438, 0.54660832725572039, 0.76922085537394613,$
$0.54316218644572012, 0.70408011066418930, 0.86203294068817893]^T.$

$$
\begin{aligned}
Y_2 &= y_n + 2.2261252811822591\,\text{e-01}\Delta t f_n,\\
Y_3 &= 9.9155909424179067\,\text{e-02}y_{n-1} + 2.2073347674778324\,\text{e-02}\Delta t f_{n-1}\\
&\quad + 9.0084409057582082\,\text{e-01}Y_2 + 2.0053918044344757\,\text{e-01}\Delta t F_2,\\
Y_4 &= Y_3 + 2.2261252811822591\,\text{e-01}\Delta t F_3,\\
Y_5 &= 9.9999999999999978\,\text{e-01}Y_4 + 2.2261252811822588\,\text{e-01}\Delta t F_4,\\
Y_6 &= 5.8328007348206479\,\text{e-01}y_n + 1.2984545175882706\,\text{e-01}f_n + 4.1671992651793521\,\text{e-01}Y_5\\
&\quad + 9.2767076359398890\,\text{e-02}\Delta t F_5,
\end{aligned}
$$

$$
\begin{aligned}
Y_7 &= 1.9246504339345005\,\text{e-01}Y_2 + 4.2845129884199973\,\text{e-02}\Delta t F_2 + 8.0753495660654995\,\text{e-01}Y_6 \\
&\quad + 1.7976739823402593\,\text{e-01}\Delta t F_6, \\
Y_8 &= 1.3429709587574074\,\text{e-01}Y_2 + 2.9896216031834413\,\text{e-02}\Delta t F_2 + 8.6570290412425932\,\text{e-01}Y_7, \\
&\quad + 1.9271631208639151\,\text{e-01}\Delta t F_7, \\
y_{n+1} &= 3.7214624473466788\,\text{e-03}y_{n-1} + 2.1571407005371301\,\text{e-02}y_n + 8.3654211005038531\,\text{e-02}Y_2 \\
&\quad + 1.8622475399567143\,\text{e-02}\Delta t F_2 + 8.9105291954224342\,\text{e-01}Y_8 + 1.9835954310642495\,\text{e-01}\Delta t F_8.
\end{aligned}
$$

HB(2,8,5). $c = 3.579$, $c_{\text{eff}} = 0.447$, and

$$
\begin{aligned}
\sigma = [&0, 0.19404251163017916, 0.40401651468816963, 0.55883284598278449, 0.56369942258171279, \\
&0.52394260398583692, 0.71711922603985434, 0.88706348512404587]^T.
\end{aligned}
$$

$$
\begin{aligned}
Y_2 &= 9.1466922705235709\,\text{e-01}y_n + 8.5330772947642991\,\text{e-02}y_{n-1} + 2.5553414626387477\,\text{e-01}\Delta t f_n \\
&\quad + 2.3839138313947392\,\text{e-01}\Delta t f_{n-1}, \\
Y_3 &= 5.8121281984410744\,\text{e-02}y_{n-1} + 1.6237533451858632\,\text{e-02}f_{n-1} + 9.4187871801558920\,\text{e-01}Y_2 \\
&\quad + 2.6313575112596349\,\text{e-01}\Delta t F_2, \\
Y_4 &= 1.9712986864736182\,\text{e-01}y_n + 1.0159588081044613\,\text{e-02}\Delta t f_n + 8.0287013135263818\,\text{e-01}Y_3 \\
&\quad + 2.2430046568541404\,\text{e-01}\Delta t F_3, \\
Y_5 &= 4.9121434066055292\,\text{e-01}y_n + 1.3723216378206793\,\text{e-01}f_n + 5.0878565933944719\,\text{e-01}Y_4 \\
&\quad + 1.4214112079575425\,\text{e-01}\Delta t F_4, \\
Y_6 &= 5.6613523163124690\,\text{e-01}y_n + 1.5816305917604756\,\text{e-01}f_n + 4.3386476836875315\,\text{e-01}Y_5 \\
&\quad + 1.2121022540177456\,\text{e-01}\Delta t F_5, \\
Y_7 &= 9.1646079651557688\,\text{e-02}y_n + 2.4379466606891546\,\text{e-02}y_{n-1} + 2.5603466290936419\,\text{e-02}f_n \\
&\quad + 5.7845025808405991\,\text{e-03}f_{n-1} + 2.4695884662466314\,\text{e-01}Y_6 + 2.4695884662466314\,\text{e-01}\Delta t F_6, \\
Y_8 &= 1.1026153152324736\,\text{e-01}y_n + 8.5066501387831076\,\text{e-03}y_{n-1} + 3.0804126224230666\,\text{e-02}f_n \\
&\quad + 2.3765307900262215\,\text{e-03}f_{n-1} + 3.0113037742442610\,\text{e-02}Y_2 + 8.4127782627221176\,\text{e-03}\Delta t F_2 \\
&\quad + 8.5111878059552704\,\text{e-01}Y_7 + 2.3777984930084314\,\text{e-01}\Delta t F_7, \\
y_{n+1} &= 1.7950283215485924\,\text{e-01}Y_2 + 5.0148295810124532\,\text{e-02}\Delta t F_2 + 7.3789956884808536\,\text{e-02}Y_3 \\
&\quad + 2.0614942623764843\,\text{e-02}\Delta t F_3 + 1.7607159013164154\,\text{e-02}Y_6 + 4.9189698455916753\,\text{e-03}\Delta t F_6 \\
&\quad + 7.2910005194716787\,\text{e-01}Y_8 + 2.0369107629834105\,\text{e-01}\Delta t F_8.
\end{aligned}
$$

HB(2,8,6). $c = 1.924$, $c_{\text{eff}} = 0.240$, and

$$
\begin{aligned}
\sigma = [&0, 0.25483103267570167, 0.41250202581152862, 0.56015515567079699, 0.45054490021686211, \\
&0.60769759336536922, 0.77759075139631639, 1]^T.
\end{aligned}
$$

$$
\begin{aligned}
Y_2 &= 7.7208656328609560\,\text{e-01}y_n + 2.2791343671390432\,\text{e-01}y_{n-1} + 4.0125717863993610\,\text{e-01}\Delta t f_n \\
&\quad + 8.1487290749669899\,\text{e-02}\Delta t f_{n-1},
\end{aligned}
$$

$$
\begin{aligned}
Y_3 &= 4.6568479538393481\,\text{e-}01 y_n + 1.9271583925672603\,\text{e-}02 f_n + 1.6429215402831460\,\text{e-}02 y_{n-1} \\
&\quad + 8.5383439283674492\,\text{e-}03 f_{n-1} + 5.1788598921323370\,\text{e-}01 Y_2 + 2.6914789192083438\,\text{e-}01 \Delta t F_2, \\
Y_4 &= 4.7609765752621358\,\text{e-}01 y_n + 7.1769757816432536\,\text{e-}02 \Delta t f_n + 5.2390234247378653\,\text{e-}01 Y_3 \\
&\quad + 2.7227462025652238\,\text{e-}01 \Delta t F_3, \\
Y_5 &= 7.7739261842832785\,\text{e-}01 y_n + 2.8082795102820712\,\text{e-}01 f_n + 3.3977224643634799\,\text{e-}02 y_{n-1} \\
&\quad + 1.8863015692803745\,\text{e-}01 Y_4 + 9.8032018914058175\,\text{e-}02 \Delta t F_4, \\
Y_6 &= 4.4987183051494317\,\text{e-}01 y_n + 7.3935840789499330\,\text{e-}02 f_n + 5.5012816948505694\,\text{e-}01 Y_5 \\
&\quad + 2.8590431134874000\,\text{e-}01 \Delta t F_5, \\
Y_7 &= 3.9591547785500325\,\text{e-}01 y_n + 7.3424005123931130\,\text{e-}03 y_{n-1} + 1.1216458953291714\,\text{e-}01 f_n \\
&\quad + 5.9674212163260454\,\text{e-}01 Y_6 + 3.1012981119991551\,\text{e-}01 \Delta t F_6, \\
Y_8 &= 2.9222723151846319\,\text{e-}01 y_n + 8.1809457502216715\,\text{e-}02 f_n + 7.0777276848153969\,\text{e-}01 Y_7 \\
&\quad + 3.6783298363637484\,\text{e-}01 \Delta t F_7, \\
y_{n+1} &= 2.2187752112193082\,\text{e-}01 y_n + 4.2018330130825544\,\text{e-}02 \Delta t f_n + 8.6867035017904395\,\text{e-}04 y_{n-1} \\
&\quad + 1.5746135117867068\,\text{e-}02 Y_3 + 8.1833437496791894\,\text{e-}03 \Delta t F_3 + 1.6931964521599721\,\text{e-}01 Y_4 \\
&\quad + 8.7996251143812029\,\text{e-}02 \Delta t F_4 + 3.1163911912258085\,\text{e-}01 Y_6 + 1.6196038066087362\,\text{e-}03 \Delta t F_6 \\
&\quad + 7.3576606509672654\,\text{e-}02 Y_7 + 3.8238123736175217\,\text{e-}02 \Delta t F_7 + 2.0697230256177232\,\text{e-}01 Y_8 \\
&\quad + 1.0756452207778448\,\text{e-}01 \Delta t F_8.
\end{aligned}
$$

HB(3,8,7). $c = 1.828$, $c_{\text{eff}} = 0.229$, and
$\sigma = [0, 0.20718217223115340, 0.29097088331375731, 0.40039909153603215, 0.53852084630271446,$
$0.60106447416936848, 0.76632817862941627, 0.91524497754031431]^T.$

$$
\begin{aligned}
Y_2 &= 7.7524862524912430\,\text{e-}01 y_n + 2.0911304381847140\,\text{e-}01 y_{n-1} + 1.5638330932404368\,\text{e-}02 y_{n-2} \\
&\quad + 3.3320092038559879\,\text{e-}01 \Delta t f_n + 1.1437095752883478\,\text{e-}01 \Delta t f_{n-1}, \\
Y_3 &= 6.8633302066772672\,\text{e-}01 y_n + 5.4513662560166085\,\text{e-}02 f_n + 3.0502380464163606\,\text{e-}05 y_{n-2} \\
&\quad + 3.1363647695180913\,\text{e-}01 Y_2 + 1.7153833892871764\,\text{e-}01 \Delta t F_2, \\
Y_4 &= 6.0294956915719689\,\text{e-}01 y_n + 6.7968244478158968\,\text{e-}02 \Delta t f_n + 9.1441978160103528\,\text{e-}01 y_{n-2} \\
&\quad + 3.9695898886464298\,\text{e-}01 Y_3 + 2.1711022338491229\,\text{e-}01 \Delta t F_3, \\
Y_5 &= 5.1665264234610353\,\text{e-}01 y_n + 8.1337583516052664\,\text{e-}02 f_n + 2.4005033416819453\,\text{e-}04 y_{n-2} \\
&\quad + 4.8310730731972817\,\text{e-}01 Y_4 + 2.6422763648976022\,\text{e-}01 \Delta t F_4, \\
Y_6 &= 5.8556466015419750\,\text{e-}01 y_n + 2.3114273505665700\,\text{e-}01 f_n + 2.2872729253596902\,\text{e-}02 y_{n-1} \\
&\quad + 1.2509864991026416\,\text{e-}02 f_{n-1} + 1.7323979653098297\,\text{e-}02 y_{n-2} + 8.7135630305161908\,\text{e-}03 f_{n-2} \\
&\quad + 3.7423863093910736\,\text{e-}01 Y_5 + 2.0468369539846526\,\text{e-}01 \Delta t F_5, \\
Y_7 &= 3.4191713189186990\,\text{e-}01 y_n + 9.5095924661400266\,\text{e-}01 y_{n-1} + 7.5924392758473357\,\text{e-}03 y_{n-2} \\
&\quad + 1.8700598038223282\,\text{e-}01 f_n + 5.2011159906676104\,\text{e-}02 f_{n-1} + 5.5539450417088254\,\text{e-}01 Y_6 \\
&\quad + 3.0376393594757339\,\text{e-}01 \Delta t F_6,
\end{aligned}
$$

$$\begin{aligned}
Y_8 &= 1.1363326850737532\,\text{e-}01 y_n + 6.2149856790386038\,\text{e-}02 f_n + 7.6756748200085712\,\text{e-}02 y_{n-1} \\
&\quad + 4.1980847431326157\,\text{e-}03 f_{n-1} + 5.6551924741635156\,\text{e-}03 y_{n-2} + 2.8010880832937834\,\text{e-}01 Y_2 \\
&\quad + 1.5320092920029513\,\text{e-}01 \Delta t F_2 + 5.2384598248899694\,\text{e-}01 Y_7 + 2.8650898825282928\,\text{e-}01 \Delta t F_7, \\
y_{n+1} &= 2.2414616285513067\,\text{e-}01 y_n + 4.1420414228058998\,\text{e-}02 \Delta t f_n + 4.1615518198974411\,\text{e-}03 y_{n-1} \\
&\quad + 2.2760926710086657\,\text{e-}03 \Delta t f_{n-1} + 3.8645926596874401\,\text{e-}04 y_{n-2} + 1.2535638715240446\,\text{e-}01 Y_4 \\
&\quad + 6.8561624703917162\,\text{e-}02 \Delta t F_4 + 9.8291412642577472\,\text{e-}02 Y_5 + 5.3758879769127056\,\text{e-}02 \Delta t F_5 \\
&\quad + 2.0682681603894068\,\text{e-}01 Y_6 + 1.1312054265514121\,\text{e-}01 \Delta t F_6 + 3.4083121022508062\,\text{e-}01 Y_8 \\
&\quad + 1.8641205329588703\,\text{e-}01 \Delta t F_8.
\end{aligned}$$

HB(4,8,8). $c = 1.538$, $c_{\text{eff}} = 0.192$, and

$$\sigma = [0, 0.23368675485636115, 0.36350725513869420, 0.49031960833186361, 0.48947493167245792, 0.64507077479935448, 0.80327799918322207, 0.98003214772997627]^T.$$

$$\begin{aligned}
Y_2 &= 6.4546474847411439\,\text{e-}01 y_n + 3.1741107005251123\,\text{e-}01 y_{n-1} + 3.0324271794764990\,\text{e-}02 y_{n-2} \\
&\quad + 1.4682597489273576\,\text{e-}03 \Delta t f_{n-2} + 6.7999096786094055\,\text{e-}03 y_{n-3} + 4.4226664734388918\,\text{e-}03 \Delta t f_{n-3} \\
&\quad + 4.1981076775815634\,\text{e-}01 \Delta t f_n + 2.0644440355370802\,\text{e-}01 \Delta t f_{n-1}, \\
Y_3 &= 5.7204975600063535\,\text{e-}01 y_n + 9.1739031137173827\,\text{e-}02 f_n + 7.3128512482644112\,\text{e-}02 y_{n-1} \\
&\quad + 4.7562840639905124\,\text{e-}02 f_{n-1} + 4.8596839464650852\,\text{e-}03 y_{n-3} + 2.5158681521488639\,\text{e-}03 f_{n-3} \\
&\quad + 3.4996204757025545\,\text{e-}01 Y_2 + 2.2761558431192522\,\text{e-}01 \Delta t F_2, \\
Y_4 &= 6.0520113339487402\,\text{e-}01 y_n + 9.2518035631088485\,\text{e-}02 \Delta t f_n + 9.6852720995804862\,\text{e-}04 y_{n-2} \\
&\quad + 4.3088647601450072\,\text{e-}04 \Delta t f_{n-2} + 3.9383033939516798\,\text{e-}01 Y_3 + 2.5614755498079894\,\text{e-}01 \Delta t F_3, \\
Y_5 &= 6.3994776350311566\,\text{e-}01 y_n + 3.3777288893505930\,\text{e-}01 f_n + 1.0648899163235218\,\text{e-}01 y_{n-1} \\
&\quad + 6.9260521880789461\,\text{e-}02 f_{n-1} + 3.3870895944620866\,\text{e-}02 y_{n-2} + 2.2029656716006023\,\text{e-}02 f_{n-2} \\
&\quad + 3.8555830149051172\,\text{e-}03 y_{n-3} + 2.1583676590500595\,\text{e-}01 Y_4 + 1.4038039818475362\,\text{e-}01 \Delta t F_4, \\
Y_6 &= 5.2859357653495542\,\text{e-}01 y_n + 1.1401370030387713\,\text{e-}01 f_n + 2.3448581130923671\,\text{e-}03 y_{n-2} \\
&\quad + 1.0749109928639197\,\text{e-}03 f_{n-2} + 4.6906156535195265\,\text{e-}01 Y_5 + 3.0507800207797564\,\text{e-}01 \Delta t F_5, \\
Y_7 &= 3.8581660902762860\,\text{e-}01 y_n + 2.5093541859975410\,\text{e-}01 f_n + 1.0426883206501705\,\text{e-}01 y_{n-1} \\
&\quad + 6.7816528394372161\,\text{e-}02 f_{n-1} + 2.3620556837138790\,\text{e-}02 y_{n-2} + 7.8981101524640586\,\text{e-}03 f_{n-2} \\
&\quad + 4.2885933382164629\,\text{e-}04 y_{n-3} + 4.8586514273639381\,\text{e-}01 Y_6 + 3.1600706170442672\,\text{e-}01 \Delta t F_6, \\
Y_8 &= 2.3131427353780087\,\text{e-}01 y_n + 1.5044698102706502\,\text{e-}01 f_n + 8.3735751327340138\,\text{e-}02 y_{n-1} \\
&\quad + 5.4461796924834716\,\text{e-}02 f_{n-1} + 1.6120387745938696\,\text{e-}02 y_{n-2} + 4.2030300790358950\,\text{e-}03 \Delta t f_{n-2} \\
&\quad + 5.7883017581142207\,\text{e-}04 y_{n-3} + 3.7647159056082048\,\text{e-}04 \Delta t f_{n-3} + 1.4600830316254704\,\text{e-}01 Y_2 \\
&\quad + 1.4600830316254704\,\text{e-}01 Y_2 + 9.4963912428430206\,\text{e-}02 \Delta t F_2 + 5.2224245405056202\,\text{e-}01 Y_7 \\
&\quad + 3.3966689290029084\,\text{e-}01 \Delta t F_7, \\
y_{n+1} &= 3.0828674101059494\,\text{e-}01 y_n + 7.7119758745246639\,\text{e-}02 \Delta t f_n + 5.1247705886954958\,\text{e-}03 y_{n-1} \\
&\quad + 3.3331547238027517\,\text{e-}03 \Delta t f_{n-1} + 2.6875920819359363\,\text{e-}03 y_{n-2} + 1.7480119526367670\,\text{e-}03 \Delta t f_{n-2}
\end{aligned}$$

$$+ 2.7346332218247476\,\text{e-}04 y_{n-3} + 5.7261505381507337\,\text{e-}02 Y_3 + 3.7242927044469659\,\text{e-}02 \Delta t F_3$$
$$+ 4.4836843245315194\,\text{e-}01 Y_6 + 2.9161917256001402\,\text{e-}01 \Delta t F_6 + 1.7799749516192995\,\text{e-}01 Y_8$$
$$+ 1.1576970745437280\,\text{e-}01 \Delta t F_8.$$

HB(5,8,9). $c = 1.223$, $c_{\text{eff}} = 0.153$, and

$$\sigma = [0, 0.17739162674285275, 0.25102007867404336, 0.34856844954048155, 0.47370737396576351,$$
$$0.60374397005041947, 0.76821571470950301, 0.89165832852894700]^T.$$

$$\begin{aligned}
Y_2 &= 7.7610069368656864\,\text{e-}01 y_n + 1.8107401575144788\,\text{e-}01 y_{n-1} + 1.9024372448481035\,\text{e-}02 y_{n-2} \\
&\quad + 1.5558034905201492\,\text{e-}02 \Delta t f_{n-2} + 2.0838855725201940\,\text{e-}02 y_{n-3} + 1.7041910088499954\,\text{e-}02 \Delta t f_{n-3} \\
&\quad + 2.9620623883005234\,\text{e-}03 y_{n-4} + 2.9019785117900954\,\text{e-}01 \Delta t f_n + 1.4808140794735961\,\text{e-}01 \Delta t f_{n-1}, \\
Y_3 &= 8.0482908790541208\,\text{e-}01 y_n + 5.7130047310679548\,\text{e-}02 f_n + 1.0012940917179889\,\text{e-}04 y_{n-2} \\
&\quad + 8.1885320903523663\,\text{e-}05 f_{n-2} + 2.9916274905106115\,\text{e-}05 y_{n-3} + 2.4465377266357034\,\text{e-}05 f_{n-3} \\
&\quad + 5.6765757317956030\,\text{e-}06 y_{n-4} + 1.9503518983477430\,\text{e-}01 Y_2 + 1.5949878501428907\,\text{e-}01 \Delta t F_2, \\
Y_4 &= 7.4495822577025694\,\text{e-}01 y_n + 7.7149536543122954\,\text{e-}02 \Delta t f_n + 3.4309578761870633\,\text{e-}04 y_{n-2} \\
&\quad + 2.8058198787133586\,\text{e-}04 \Delta t f_{n-2} + 9.4432466438276220\,\text{e-}05 y_{n-3} + 7.7226390148197287\,\text{e-}05 \Delta t f_{n-3}, \\
&\quad + 1.8592122219145097\,\text{e-}05 y_{n-4} + 2.5458565385346676\,\text{e-}01 Y_3 + 2.0819885122318751\,\text{e-}01 \Delta t F_3, \\
Y_5 &= 6.7807771190788235\,\text{e-}01 y_n + 1.0185385671585835\,\text{e-}02 f_n + 1.0531479263431690\,\text{e-}03 y_{n-2} \\
&\quad + 8.6125901092185062\,\text{e-}04 f_{n-2} + 2.6050777566247521\,\text{e-}04 y_{n-3} + 2.1304193227970674\,\text{e-}04 f_{n-3} \\
&\quad + 5.4027415207471699\,\text{e-}05 y_{n-4} + 3.2055460497490490\,\text{e-}01 Y_4 + 2.6214792349804306\,\text{e-}01 \Delta t F_4, \\
Y_6 &= 6.2093551763480770\,\text{e-}01 y_n + 1.8254892961717523\,\text{e-}01 f_n + 1.6017166879650935\,\text{e-}02 y_{n-1} \\
&\quad + 1.3098757505451713\,\text{e-}02 f_{n-1} + 1.5265894870645863\,\text{e-}02 y_{n-2} + 1.2484371082401208\,\text{e-}02 f_{n-2} \\
&\quad + 1.4611718964131484\,\text{e-}03 y_{n-4} + 7.3216474248262203\,\text{e-}04 f_{n-4} + 3.8038745228299600\,\text{e-}06 y_{n-5} \\
&\quad + 3.4632024871848238\,\text{e-}01 Y_5 + 2.8321893573790141\,\text{e-}01 \Delta t F_5, \\
Y_7 &= 5.4218005281447990\,\text{e-}01 y_n + 2.0905915335856534\,\text{e-}01 f_n + 1.8095364251024124\,\text{e-}02 y_{n-1} \\
&\quad + 1.4798296732371005\,\text{e-}02 f_{n-1} + 2.0529310217713724\,\text{e-}02 y_{n-2} + 1.6788765348861815\,\text{e-}02 f_{n-2} \\
&\quad + 1.8619126310112206\,\text{e-}03 y_{n-4} + 9.1553825352006467\,\text{e-}04 f_{n-4} + 4.1733336008577054\,\text{e-}01 Y_6 \\
&\quad + 3.4129309657401619\,\text{e-}01 \Delta t F_6, \\
Y_8 &= 1.4642860095330767\,\text{e-}01 y_n + 1.1974856416003735\,\text{e-}01 f_n + 1.6464068932915202\,\text{e-}01 y_{n-1} \\
&\quad + 1.3464231728726073\,\text{e-}01 f_{n-1} + 1.7019074547371504\,\text{e-}02 y_{n-2} + 1.3918112493817223\,\text{e-}02 \Delta t f_{n-2}, \\
&\quad + 1.7419530907733821\,\text{e-}02 y_{n-3} + 1.4245603665964805\,\text{e-}02 \Delta t f_{n-3} + 2.8371231190407816\,\text{e-}03 y_{n-4} \\
&\quad + 2.1731622111534517\,\text{e-}04 \Delta t f_{n-4} + 3.1392257091847781\,\text{e-}01 Y_3 + 2.5672427982087054\,\text{e-}01 \Delta t F_3, \\
&\quad + 3.3773241022491457\,\text{e-}01 Y_7 + 2.7619584515212864\,\text{e-}01 \Delta t F_7, \\
y_{n+1} &= 2.8927892326225457\,\text{e-}01 y_n + 2.3657083026739503\,\text{e-}01 \Delta t f_n + 1.1765397636180749\,\text{e-}01 y_{n-1} \\
&\quad + 9.6216822706229069\,\text{e-}02 \Delta t f_{n-1} + 2.7056138680600039\,\text{e-}02 y_{n-2} + 2.2126372427404797\,\text{e-}02 \Delta t f_{n-2} \\
&\quad + 1.0960339384603930\,\text{e-}02 y_{n-3} + 8.9633097323081213\,\text{e-}03 \Delta t f_{n-3} + 3.2641193827615050\,\text{e-}03 y_{n-4}
\end{aligned}$$

$$+ 8.6357934909297757\,\text{e-}04\Delta t f_{n-4} + 7.6539234279753426\,\text{e-}02 Y_5 + 6.2593396011697860\,\text{e-}02\Delta t F_5$$
$$+ 2.0249334675863637\,\text{e-}01 Y_6 + 1.6559802776535187\,\text{e-}01\Delta t F_6 + 2.7275392188958186\,\text{e-}01 Y_8$$
$$+ 2.2305676829973772\,\text{e-}01\Delta t F_8.$$

HB(6,8,10). $c = 1.129$, $c_{\text{eff}} = 0.141$, and

$$\sigma = [0, 0.20493520858591369, 0.28755191075293396, 0.39537633148833934, 0.52910482203627929, 0.63011206358460470, 0.77167306977743766, 0.95822498755651653]^T.$$

$$\begin{aligned}
Y_2 = {} & 6.5934278485397058\,\text{e-}01 y_n + 2.7129766867160660\,\text{e-}01 y_{n-1} + 2.2561117768429083\,\text{e-}02 y_{n-2} \\
& + 1.9976182479924671\,\text{e-}02\Delta t f_{n-2} + 4.2673939424285171\,\text{e-}02 y_{n-3} + 3.7784581855676763\,\text{e-}02\Delta t f_{n-3} \\
& + 4.1244892817086038\,\text{e-}03 y_{n-5} + 1.9681574312971303\,\text{e-}03\Delta t f_{n-5} + 3.7005665994801734\,\text{e-}01\Delta t f_n \\
& + 2.4021379576086102\,\text{e-}01\Delta t f_{n-1}, \\
Y_3 = {} & 7.9690582929904408\,\text{e-}01 y_n + 6.6852878927958645\,\text{e-}02 f_n + 2.0887639667393782\,\text{e-}04 y_{n-2} \\
& + 1.8494442777771281\,\text{e-}04 f_{n-2} + 7.0545127182818079\,\text{e-}05 y_{n-3} + 6.2462434181584023\,\text{e-}05 f_{n-3} \\
& + 1.0815679273108855\,\text{e-}05 y_{n-5} + 5.7093373688202266\,\text{e-}06 f_{n-5} + 2.0280393349782605\,\text{e-}01 Y_2 \\
& + 1.7956771578348829\,\text{e-}01\Delta t F_2, \\
Y_4 = {} & 7.3795086539303412\,\text{e-}01 y_n + 9.0478602498241009\,\text{e-}02\Delta t f_n + 6.9641442224658602\,\text{e-}04 y_{n-2} \\
& + 6.1662288736050370\,\text{e-}04\Delta t f_{n-2} + 2.1061519949752520\,\text{e-}04 y_{n-3} + 1.8648400763617229\,\text{e-}04\Delta t f_{n-3}, \\
& + 3.4481428340611811\,\text{e-}05 y_{n-5} + 1.8434707565897658\,\text{e-}05\Delta t f_{n-5} + 2.6110762355688122\,\text{e-}01 Y_3 \\
& + 2.3119127290628558\,\text{e-}01\Delta t F_3, \\
Y_5 = {} & 6.7611439061096146\,\text{e-}01 y_n + 1.2409283293381215\,\text{e-}01 f_n + 3.4808081657280833\,\text{e-}03 y_{n-2} \\
& + 2.8291463082360819\,\text{e-}03 f_{n-2} + 2.5522768119857651\,\text{e-}04 y_{n-4} + 1.1730195521995916\,\text{e-}04 f_{n-4} \\
& + 3.2014957354211188\,\text{e-}01 Y_4 + 2.8346850398062506\,\text{e-}01\Delta t F_4, \\
Y_6 = {} & 4.3912480999809772\,\text{e-}01 y_n + 3.8881217792583872\,\text{e-}01 f_n + 2.0149381583842649\,\text{e-}01 y_{n-1} \\
& + 1.7840770457735203\,\text{e-}01 f_{n-1} + 4.9854282896529156\,\text{e-}02 y_{n-2} + 4.4142238995820711\,\text{e-}02 f_{n-2} \\
& + 2.1724739244445894\,\text{e-}02 y_{n-3} + 1.9235631848131148\,\text{e-}02 f_{n-3} + 7.8964242346278544\,\text{e-}03 y_{n-4} \\
& + 2.7595589213657667\,\text{e-}03 f_{n-4} + 1.8992722707143276\,\text{e-}04 y_{n-5} + 2.7971600056080148\,\text{e-}01 Y_5 \\
& + 2.4766759905736477\,\text{e-}01\Delta t F_5, \\
Y_7 = {} & 4.3813909501758574\,\text{e-}01 y_n + 3.5829211253408377\,\text{e-}01 f_n + 1.3205222132099081\,\text{e-}01 y_{n-1} \\
& + 1.1692236603980932\,\text{e-}01 f_{n-1} + 5.8588248325692510\,\text{e-}02 y_{n-2} + 5.1875512186321381\,\text{e-}02 f_{n-2} \\
& + 5.2885025645609688\,\text{e-}03 y_{n-3} + 4.6825735036520521\,\text{e-}03 f_{n-3} + 8.7700950069937479\,\text{e-}03 y_{n-4} \\
& + 7.7652632296055764\,\text{e-}03 f_{n-4} + 1.3785863145923214\,\text{e-}03 y_{n-5} + 3.5578325144958400\,\text{e-}01 Y_6 \\
& + 3.1501946079122317\,\text{e-}01\Delta t F_6, \\
Y_8 = {} & 3.1840343066112459\,\text{e-}01 y_n + 2.8192242505028797\,\text{e-}01 f_n + 1.3021156069844683\,\text{e-}01 y_{n-1} \\
& + 1.1529259871812977\,\text{e-}01 f_{n-1} + 3.4600985434197332\,\text{e-}02 y_{n-2} + 3.0636584858661858\,\text{e-}02\Delta t f_{n-2}, \\
& + 1.7474572346572272\,\text{e-}02 y_{n-3} + 1.5472426922138219\,\text{e-}02\Delta t f_{n-3} + 4.0817513115598489\,\text{e-}03 y_{n-4}
\end{aligned}$$

$$
\begin{aligned}
&+ 3.7954488095818866\,\text{e-}04\Delta t f_{n-4} + 2.8788271497124708\,\text{e-}04 y_{n-5} + 2.5489861389443879\,\text{e-}04\Delta t f_{n-5}\\
&+ 6.4039737828785984\,\text{e-}02 Y_2 + 5.6702398434554102\,\text{e-}02\Delta t F_2 + 4.3090007900434185\,\text{e-}01 Y_7\\
&+ 3.8152979374319551\,\text{e-}01\Delta t F_7,\\
y_{n+1} = {}& 4.2210499879829200\,\text{e-}01 y_n + 1.0470152640211661\,\text{e-}01\Delta t f_n + 1.2276097197837371\,\text{e-}03 y_{n-1}\\
&+ 1.0869565962217109\,\text{e-}03\Delta t f_{n-1} + 4.3342452063532613\,\text{e-}03 y_{n-2} + 3.8376499800913989\,\text{e-}03\Delta t f_{n-2}\\
&+ 4.6636785685590012\,\text{e-}04 y_{n-4} + 3.8350618707223751\,\text{e-}04\Delta t f_{n-4} + 5.8155782931149167\,\text{e-}05 y_{n-5}\\
&+ 6.7885924613408699\,\text{e-}02 Y_4 + 6.0107909183184344\,\text{e-}02\Delta t F_4 + 3.4732819124494774\,\text{e-}01 Y_6\\
&+ 3.0753313731823845\,\text{e-}01\Delta t F_6 + 1.5659450677742751\,\text{e-}01 Y_8 + 1.3865272433961967\,\text{e-}01\Delta t F_8.
\end{aligned}
$$

HB(8,8,11). Here $c = 1.014$, $c_{\text{eff}} = 0.127$, and

$$
\begin{aligned}
\sigma = [&0, 0.15268988968167027, 0.21725324947576041, 0.28998857391287741, 0.39819129640841544,\\
&0.53457208078593688, 0.68259864745713894, 0.84979736116107674]^T.
\end{aligned}
$$

$$
\begin{aligned}
Y_2 = {}& 8.1103704590185588\,\text{e-}01 y_n + 2.4324163373012761\,\text{e-}01\Delta t f_n + 1.4208568406076721\,\text{e-}01 y_{n-1}\\
&+ 1.4007611169626422\,\text{e-}01\Delta t f_{n-1} + 1.5066264171139909\,\text{e-}02 y_{n-2} + 1.4853176214286525\,\text{e-}02\Delta t f_{n-2}\\
&+ 2.8099548818331672\,\text{e-}02 y_{n-3} + 2.7702126114323208\,\text{e-}02\Delta t f_{n-3} + 2.4287954904775805\,\text{e-}03 y_{n-5}\\
&+ 2.3944441036439445\,\text{e-}03\Delta t f_{n-5} + 1.0382748777756081\,\text{e-}03 y_{n-6} + 1.0235901576721863\,\text{e-}03\Delta t f_{n-6}\\
&+ 2.4438667965197313\,\text{e-}04 y_{n-7},\\
Y_3 = {}& 8.5511450738191930\,\text{e-}01 y_n + 5.2639045593528763\,\text{e-}02 f_n + 9.3925044979080267\,\text{e-}05 y_{n-2}\\
&+ 9.2596627017957431\,\text{e-}05 f_{n-2} + 3.2067262659279082\,\text{e-}05 y_{n-3} + 3.1613723055544038\,\text{e-}05 f_{n-3}\\
&+ 5.6716673029924927\,\text{e-}06 y_{n-5} + 5.5914507354467365\,\text{e-}06 f_{n-5} + 1.4153869199331039\,\text{e-}06 y_{n-6}\\
&+ 1.3953685594756185\,\text{e-}06 f_{n-6} + 1.4475198995218319\,\text{e-}01 Y_2 + 1.4270470700008570\,\text{e-}01\Delta t F_2,\\
Y_4 = {}& 8.2352428913866937\,\text{e-}01 y_n + 8.8833394040492286\,\text{e-}02\Delta t f_n + 2.5814485463276876\,\text{e-}03 y_{n-1},\\
&+ 2.5449381287343999\,\text{e-}03\Delta t f_{n-1} + 2.6320601231020584\,\text{e-}03 y_{n-2} + 2.5948338865528918\,\text{e-}03\Delta t f_{n-2},\\
&+ 3.6670179053706922\,\text{e-}04 y_{n-4} + 3.6151538636730151\,\text{e-}04\Delta t f_{n-4} + 9.1716730787826345\,\text{e-}05 y_{n-5},\\
&+ 9.0419545861898491\,\text{e-}05\Delta t f_{n-5} + 2.1055466132365234\,\text{e-}05 y_{n-7} + 1.1435609446183388\,\text{e-}05\Delta t f_{n-7}\\
&+ 1.7078272820444360\,\text{e-}01 Y_3 + 1.6836728253021724\,\text{e-}01\Delta t F_3,\\
Y_5 = {}& 7.6032116269499905\,\text{e-}01 y_n + 9.5881297974883095\,\text{e-}02 f_n + 9.6180598693505965\,\text{e-}04 y_{n-2}\\
&+ 9.4820279570481864\,\text{e-}04 f_{n-2} + 2.6578471794413635\,\text{e-}04 y_{n-3} + 2.6202562266568923\,\text{e-}04 f_{n-3}\\
&+ 5.6173647859647601\,\text{e-}05 y_{n-5} + 5.5379162397595059\,\text{e-}05 f_{n-5} + 1.2155568501817746\,\text{e-}05 y_{n-6}\\
&+ 1.1983647630988639\,\text{e-}05 f_{n-6} + 3.9299384314209267\,\text{e-}06 y_{n-7}\\
&+ 2.3837898744532887\,\text{e-}01 Y_4 + 2.3500750193209827\,\text{e-}01\Delta t F_4,\\
Y_6 = {}& 6.9983466985186893\,\text{e-}01 y_n + 1.2956442460318052\,\text{e-}01 f_n + 2.8967198527552257\,\text{e-}03 y_{n-2}\\
&+ 2.8557504320688007\,\text{e-}03 f_{n-2} + 6.7508210352595736\,\text{e-}04 y_{n-3} + 6.6553415822813205\,\text{e-}04 f_{n-3}\\
&+ 1.6643027134335468\,\text{e-}04 y_{n-5} + 1.6407638413705952\,\text{e-}04 f_{n-5} + 3.1802892674455783\,\text{e-}05 y_{n-6}\\
&+ 3.1353092156885634\,\text{e-}05 f_{n-6} + 1.1055821875271658\,\text{e-}05 y_{n-7}
\end{aligned}
$$

$$
\begin{aligned}
&\quad + 2.9638423920595686\,\text{e-}01 Y_5 + 2.9219236315370234\,\text{e-}01 \Delta t F_5,\\
Y_7 &= 6.0574881606740139\,\text{e-}01 y_n + 2.3297431473474603\,\text{e-}01 f_n + 3.3753836873017876\,\text{e-}02 y_{n-1}\\
&\quad + 3.3276443402842873\,\text{e-}02 f_{n-1} + 2.7993139590496700\,\text{e-}02 y_{n-2} + 2.7597221873039132\,\text{e-}02 f_{n-2}\\
&\quad + 5.3489846227695956\,\text{e-}03 y_{n-4} + 4.3913218505049869\,\text{e-}03 f_{n-4} + 2.3824913067828989\,\text{e-}04 y_{n-6}\\
&\quad + 6.0472984562104276\,\text{e-}05 f_{n-6} + 2.5154238491232192\,\text{e-}05 y_{n-7} + 2.4798472441638635\,\text{e-}05 f_{n-7}\\
&\quad + 3.2689181947714496\,\text{e-}01 Y_6 + 3.2226846300780199\,\text{e-}01 \Delta t F_6,\\
Y_8 &= 3.8965567608777574\,\text{e-}01 y_n + 3.8414462630458424\,\text{e-}01 f_n + 1.5375660107791925\,\text{e-}01 y_{n-1}\\
&\quad + 1.5158196245455205\,\text{e-}01 f_{n-1} + 6.4127244057980148\,\text{e-}02 y_{n-2} + 6.3220267832173022\,\text{e-}02 \Delta t f_{n-2},\\
&\quad + 1.2244580326318902\,\text{e-}02 y_{n-3} + 1.2071400527091672\,\text{e-}02 \Delta t f_{n-3} + 1.3095278699834218\,\text{e-}02 y_{n-4},\\
&\quad + 1.2910067146998279\,\text{e-}02 \Delta t f_{n-4} + 1.9449899420479685\,\text{e-}03 y_{n-6} + 1.6901811414378354\,\text{e-}03 \Delta t f_{n-6},\\
&\quad + 2.6584451991244312\,\text{e-}04 y_{n-7} + 3.6490978528821150\,\text{e-}01 Y_7 + 3.5974872613647962\,\text{e-}01 \Delta t F_7,\\
y_{n+1} &= 1.7329798410746522\,\text{e-}01 y_n + 1.7084696420360562\,\text{e-}01 \Delta t f_n + 1.8707063834335549\,\text{e-}01 y_{n-1}\\
&\quad + 1.5607925894041397\,\text{e-}01 \Delta t f_{n-1} + 1.6136705664081385\,\text{e-}02 y_{n-2} + 1.5908478042340208\,\text{e-}02 \Delta t f_{n-2}\\
&\quad + 2.5055945296315552\,\text{e-}02 y_{n-3} + 2.4701569445104252\,\text{e-}02 \Delta t f_{n-3} + 3.3438361249250393\,\text{e-}03 y_{n-5}\\
&\quad + 3.2965429671907086\,\text{e-}03 \Delta t f_{n-5} + 4.0917492363145604\,\text{e-}04 y_{n-6} + 4.0338780563844469\,\text{e-}04 \Delta t f_{n-6}\\
&\quad + 3.6232928533262959\,\text{e-}04 y_{n-7} + 1.2710361897120864\,\text{e-}04 \Delta t f_{n-7} + 2.6100514217537768\,\text{e-}01 Y_4\\
&\quad + 2.5731364627150821\,\text{e-}01 \Delta t F_4 + 3.3331824407951544\,\text{e-}01 Y_8 + 3.2860399622045328\,\text{e-}01 \Delta t F_8.
\end{aligned}
$$

HB(8,8,12). Here $c = 0.725$, $c_{\text{eff}} = 0.091$, and

$$
\begin{aligned}
\sigma = [&0, 0.1.7212403254650316, 0.24425675249794856, 0.34035459582662780, 0.45417142083423701,\\
&0.60344726903342638, 0.76962419428759421, 0.89834625032999504]^T.
\end{aligned}
$$

$$
\begin{aligned}
Y_2 &= 7.2166103628541844\,\text{e-}01 y_n + 2.9897481594889874\,\text{e-}01 \Delta t f_n + 1.7182396066394406\,\text{e-}01 y_{n-1}\\
&\quad + 2.3686652409203576\,\text{e-}01 \Delta t f_{n-1} + 3.0492336407939545\,\text{e-}02 y_{n-2} + 4.2034962460909459\,\text{e-}02 \Delta t f_{n-2}\\
&\quad + 5.7326702973902084\,\text{e-}02 y_{n-3} + 7.9027260334443905\,\text{e-}02 \Delta t f_{n-3} + 1.2816087284349817\,\text{e-}02 y_{n-5}\\
&\quad + 1.7667512934597937\,\text{e-}02 \Delta t f_{n-5} + 2.7218711957034138\,\text{e-}02 y_{n-6} + 3.7522134087774545\,\text{e-}03 \Delta t f_{n-6}\\
&\quad + 3.1580051887426901\,\text{e-}03 y_{n-7} + 1.1071856855378482\,\text{e-}03 \Delta t f_{n-7},\\
Y_3 &= 8.8230568173627133\,\text{e-}01 y_n + 6.2570762540582803\,\text{e-}02 f_n + 1.6354825764457442\,\text{e-}04 y_{n-2}\\
&\quad + 2.2545812097385896\,\text{e-}04 f_{n-2} + 7.6970681542182055\,\text{e-}05 y_{n-3} + 1.0610730728963756\,\text{e-}04 f_{n-3}\\
&\quad + 2.9037647634409629\,\text{e-}05 y_{n-5} + 4.0029613078377147\,\text{e-}05 f_{n-5} + 2.9177568410225919\,\text{e-}06 y_{n-6}\\
&\quad + 4.0222499726361334\,\text{e-}06 f_{n-6} + 6.2588277221591309\,\text{e-}06 y_{n-7} + 2.5435364972131703\,\text{e-}06 f_{n-7}\\
&\quad + 1.1741558509234430\,\text{e-}01 Y_2 + 1.6186230027284165\,\text{e-}01 \Delta t F_2,\\
Y_4 &= 8.4312853626751461\,\text{e-}01 y_n + 8.8726925375650995\,\text{e-}02 \Delta t f_n + 5.9591987710203216\,\text{e-}04 y_{n-2}\\
&\quad + 8.2150050191533868\,\text{e-}04 \Delta t f_{n-2} + 2.5560559777943544\,\text{e-}04 y_{n-3} + 3.5236301881607464\,\text{e-}04 \Delta t f_{n-3},\\
&\quad + 1.1778804485958780\,\text{e-}04 y_{n-5} + 1.3533550547256473\,\text{e-}04 \Delta t f_{n-5} + 1.6144699424334645\,\text{e-}05 y_{n-7},\\
&\quad + 7.4860357153000911\,\text{e-}06 \Delta t f_{n-7} + 1.5588600551332013\,\text{e-}01 Y_3 + 2.1489538559030735\,\text{e-}01 \Delta t F_3,
\end{aligned}
$$

$$
\begin{aligned}
Y_5 = {} & 7.9642457262950050\,\text{e-}01 y_n + 1.4409041503285133\,\text{e-}01 f_n + 5.1660441506838160\,\text{e-}03 y_{n-1} \\
& + 7.1216081654160400\,\text{e-}03 f_{n-1} + 7.7807141267142842\,\text{e-}03 y_{n-2} + 1.0726040204329599\,\text{e-}02 f_{n-2} \\
& + 2.3759365866667559\,\text{e-}03 y_{n-4} + 3.2753280658425971\,\text{e-}03 f_{n-4} + 2.3440300821086580\,\text{e-}05 y_{n-5} \\
& + 3.2313436133750819\,\text{e-}05 f_{n-5} + 5.3763191003535675\,\text{e-}04 y_{n-6} + 4.3743238670981973\,\text{e-}04 f_{n-6} \\
& + 6.4232479795509141\,\text{e-}05 y_{n-7} + 1.8762742781578270\,\text{e-}01 Y_4 + 2.5865226525638890\,\text{e-}01 \Delta t F_4, \\
Y_6 = {} & 7.4764957307865498\,\text{e-}01 y_n + 1.7701607714521619\,\text{e-}01 f_n + 3.3218501253453204\,\text{e-}04 y_{n-1} \\
& + 4.5793094845726591\,\text{e-}04 f_{n-1} + 9.0107500421638519\,\text{e-}03 y_{n-2} + 1.2421696215721046\,\text{e-}02 f_{n-2} \\
& + 1.7416175013016521\,\text{e-}03 y_{n-4} + 2.4008926475511355\,\text{e-}03 f_{n-4} + 4.3039648929302639\,\text{e-}04 y_{n-5} \\
& + 5.9331958131056471\,\text{e-}04 f_{n-5} + 4.4731057590959722\,\text{e-}04 y_{n-6} + 1.5076426237399762\,\text{e-}04 f_{n-6} \\
& + 2.4038816730014245\,\text{e-}01 Y_5 + 3.3138515374234367\,\text{e-}01 \Delta t F_5, \\
Y_7 = {} & 6.1745548221487967\,\text{e-}01 y_n + 3.1312805025999069\,\text{e-}01 f_n + 4.2412176225693266\,\text{e-}02 y_{n-1} \\
& + 5.8466960736675185\,\text{e-}02 f_{n-1} + 4.9944968347668012\,\text{e-}02 y_{n-2} + 6.8851230076908382\,\text{e-}02 f_{n-2} \\
& + 1.0145303110375972\,\text{e-}04 y_{n-3} + 1.3985725124302436\,\text{e-}04 f_{n-3} + 1.5993482674454652\,\text{e-}02 y_{n-4} \\
& + 2.2047685518281849\,\text{e-}02 f_{n-4} + 3.5923397458610504\,\text{e-}03 y_{n-6} + 2.9894235900082373\,\text{e-}03 f_{n-6} \\
& + 4.4453715536715897\,\text{e-}04 y_{n-7} + 2.7005556060497254\,\text{e-}01 Y_6 + 3.7228289759502070\,\text{e-}01 \Delta t F_6, \\
Y_8 = {} & 2.4196889423575463\,\text{e-}01 y_n + 3.3356425200855944\,\text{e-}01 f_n + 2.2016436475752582\,\text{e-}01 y_{n-1} \\
& + 3.0350579516113685\,\text{e-}01 f_{n-1} + 6.4245402901202134\,\text{e-}02 y_{n-2} + 8.8564977872107875\,\text{e-}02 f_{n-2} \\
& + 5.9217191572622209\,\text{e-}02 y_{n-3} + 8.1633378023060463\,\text{e-}02 \Delta t f_{n-3} + 1.1547451078126639\,\text{e-}02 y_{n-4} \\
& + 1.5918644806170210\,\text{e-}02 \Delta t f_{n-4} + 1.4359310727332320\,\text{e-}02 y_{n-5} + 1.9794911065941997\,\text{e-}02 \Delta t f_{n-5}, \\
& + 8.1253686364574258\,\text{e-}03 y_{n-6} + 1.9506757245185613\,\text{e-}03 \Delta t f_{n-6} + 2.1207276385246167\,\text{e-}05 y_{n-7} \\
& + 2.9235118451593681\,\text{e-}05 \Delta t f_{n-7} + 1.6418249474769908\,\text{e-}01 Y_4 + 2.2633244337619918\,\text{e-}01 \Delta t F_4, \\
& + 2.1616831406689457\,\text{e-}01 Y_7 + 2.9799707196835323\,\text{e-}01 \Delta t F_7, \\
y_{n+1} = {} & 5.5292046391219385\,\text{e-}01 y_n + 1.0671296270883678\,\text{e-}01 \Delta t f_n + 2.7461390628635146\,\text{e-}04 y_{n-1} \\
& + 3.7856676797598521\,\text{e-}04 \Delta t f_{n-1} + 2.7296960735284474\,\text{e-}03 y_{n-2} + 3.7630003304890587\,\text{e-}03 \Delta t f_{n-2} \\
& + 6.8313005651956388\,\text{e-}04 y_{n-4} + 9.4172338575675574\,\text{e-}04 \Delta t f_{n-4} + 5.1195289480250074\,\text{e-}05 y_{n-5} \\
& + 7.0574850109464491\,\text{e-}05 \Delta t f_{n-5} + 1.6190146908812175\,\text{e-}04 y_{n-6} + 1.1100475610122682\,\text{e-}04 \Delta t f_{n-6} \\
& + 1.4327702870586996\,\text{e-}05 y_{n-7} + 2.0868116163691602\,\text{e-}01 Y_5 + 2.8767571885448334\,\text{e-}01 \Delta t F_5 \\
& + 6.2831970742143431\,\text{e-}02 Y_6 + 8.6616502460049746\,\text{e-}02 \Delta t F_6 \\
& + 1.7165153921097320\,\text{e-}01 Y_8 + 2.3662883389978145\,\text{e-}01 \Delta t F_8.
\end{aligned}
$$

A.4 Eight canonical HB$_{\mathbf{RK5}}(k, 8, p)$ methods considered in the thesis

HB(2,8,5). $c(\mathrm{HB}(2,8,5)) = 3.579$, $c_{\mathrm{eff}}(\mathrm{HB}(2,8,5)) = 0.447$, and
$\sigma = [0, 0.19404251163017974, 0.40401651468815830, 0.55883284598288607, 0.56369942258165218,$
$0.52394260398583981, 0.71711922603984812, 0.88706348512405175]^T$.

$$
\begin{aligned}
Y_2 &= 8.5330772947640868\,\text{e-}02 y_{n-1} + 9.1466922705235909\,\text{e-}01 y_n \\
&\quad + 2.3839138313946667\,\text{e-}02 \Delta t f_{n-1} + 2.5553414626387394\,\text{e-}01 \Delta t f_n, \\
Y_3 &= 5.8121281984419446\,\text{e-}02 y_{n-1} + 1.6237533451860981\,\text{e-}02 \Delta t f_{n-1} \\
&\quad + 9.4187871801558054\,\text{e-}01 Y_2 + 2.6313575112595966\,\text{e-}01 \Delta t F_2, \\
Y_4 &= 1.9712986864712356\,\text{e-}01 y_n + 1.0159588080993598\,\text{e-}02 \Delta t f_n \\
&\quad + 8.0287013135287633\,\text{e-}01 Y_3 + 2.2430046568547937\,\text{e-}01 \Delta t F_3, \\
Y_5 &= 4.9121434066075126\,\text{e-}01 y_n + 1.3723216378212261\,\text{e-}01 \Delta t f_n \\
&\quad + 5.0878565933924869\,\text{e-}01 Y_4 + 1.4214112079569804\,\text{e-}01 \Delta t F_4, \\
Y_6 &= 5.6613523163119228\,\text{e-}01 y_n + 1.5816305917603155\,\text{e-}01 \Delta t f_n \\
&\quad + 4.3386476836880766\,\text{e-}01 Y_5 + 1.2121022540178913\,\text{e-}01 \Delta t F_5, \\
Y_7 &= 2.4379466606894672\,\text{e-}02 y_{n-1} + 9.1646079651563017\,\text{e-}02 y_n + 5.7845025808415593\,\text{e-}03 \Delta t f_{n-1} \\
&\quad + 2.5603466290937710\,\text{e-}02 \Delta t f_n + 8.8397445374154238\,\text{e-}01 Y_6 + 2.4695884662465947\,\text{e-}01 \Delta t F_6, \\
Y_8 &= 8.5066501387783613\,\text{e-}03 y_{n-1} + 1.1026153152332141\,\text{e-}01 y_n + 2.3765307900248875\,\text{e-}03 \Delta t f_{n-1} \\
&\quad + 3.0804126224251160\,\text{e-}02 \Delta t f_n + 3.0113037742332344\,\text{e-}02 Y_2 + 8.4127782626912673\,\text{e-}03 \Delta t F_2 \\
&\quad + 8.5111878059556789\,\text{e-}01 Y_7 + 2.3777984930085327\,\text{e-}01 \Delta t F_7, \\
y_{n+1} &= 1.7950283215483376\,\text{e-}01 Y_2 + 5.0148295810117142\,\text{e-}02 \Delta t F_2 + 7.3789956884862590\,\text{e-}02 Y_3 \\
&\quad + 2.0614942623779831\,\text{e-}02 \Delta t F_3 + 1.7607159013146464\,\text{e-}02 Y_6 + 4.9189698455867070\,\text{e-}03 \Delta t F_6 \\
&\quad + 7.2910005194715732\,\text{e-}01 Y_8 + 2.0369107629833699\,\text{e-}01 \Delta t F_8.
\end{aligned}
$$

HB(2,8,6). $c(\mathrm{HB}(2,8,6)) = 1.928$, $c_{\mathrm{eff}}(\mathrm{HB}(2,8,6)) = 0.241$, and
$\sigma = [0, 0.25363940776759103, 0.41769862843541011, 0.55858629218273137,$
$0.44857413336445040, 0.60876081294741335, 0.77828368655151881, 1.0]^T$.

$$
\begin{aligned}
Y_2 &= 2.2466032447218601\,\text{e-}01 y_{n-1} + 7.7533967552781402\,\text{e-}01 y_n \\
&\quad + 8.0163687649745852\,\text{e-}02 \Delta t f_{n-1} + 3.9813604459003121\,\text{e-}01 \Delta t f_n, \\
Y_3 &= 1.5727894480995694\,\text{e-}02 y_{n-1} + 4.4955319448393410\,\text{e-}01 y_n + 8.1555750585504752\,\text{e-}03 \Delta t f_{n-1} \\
&\quad + 1.2370905625165185\,\text{e-}02 \Delta t f_n + 5.3471891103507030\,\text{e-}01 Y_2 + 2.7727425431562364\,\text{e-}01 \Delta t F_2,
\end{aligned}
$$

$$
\begin{aligned}
Y_4 &= 4.8652494932663776\,\text{e-01}y_n + 7.7850048923667162\,\text{e-02}\Delta t f_n \\
&\quad + 5.1347505067336219\,\text{e-01}Y_3 + 2.6625841885699791\,\text{e-01}\Delta t F_3, \\
Y_5 &= 3.3099298116698636\,\text{e-02}y_{n-1} + 7.7828210986359747\,\text{e-01}y_n + 2.7850699521087263\,\text{e-01}\Delta t f_n \\
&\quad + 1.8861859201970396\,\text{e-01}Y_4 + 9.7806676317262586\,\text{e-02}\Delta t F_4, \\
Y_6 &= 4.4391622919228768\,\text{e-01}y_n + 7.0963184319293438\,\text{e-02}\Delta t f_n \\
&\quad + 5.5608377080771221\,\text{e-01}Y_5 + 2.8835283306001480\,\text{e-01}\Delta t F_5, \\
Y_7 &= 7.5572930600594206\,\text{e-03}y_{n-1} + 3.9542431237669295\,\text{e-01}y_n + 1.1282041854170644\,\text{e-01}\Delta t f_n \\
&\quad + 5.9701839456324768\,\text{e-01}Y_6 + 3.0957915785098955\,\text{e-01}\Delta t F_6, \\
Y_8 &= 2.9222138699529565\,\text{e-01}y_n + 8.2134460325541475\,\text{e-02}\Delta t f_n \\
&\quad + 7.0777861300470457\,\text{e-01}Y_7 + 3.6701299148283639\,\text{e-01}\Delta t F_7, \\
y_{n+1} &= 8.5291473379695698\,\text{e-04}y_{n-1} + 2.2105846504903937\,\text{e-01}y_n + 4.1781207986124481\,\text{e-02}\Delta t f_n \\
&\quad + 1.6086912766711807\,\text{e-02}Y_3 + 8.3417411458222290\,\text{e-03}\Delta t F_3 + 1.7061295802146498\,\text{e-01}Y_4 \\
&\quad + 8.8469997480380536\,\text{e-02}\Delta t F_4 + 3.1027955846040262\,\text{e-01}Y_6 + 1.6089300644885274\,\text{e-01}\Delta t F_6 \\
&\quad + 7.4043943063124507\,\text{e-02}Y_7 + 3.8394899966554236\,\text{e-02}\Delta t F_7 \\
&\quad + 2.0706524790545994\,\text{e-01}Y_8 + 1.0737204355935072\,\text{e-01}\Delta t F_8.
\end{aligned}
$$

HB(3,8,7). $c(\text{HB3,7}) = 1.985$, $c_{\text{eff}}(\text{HB3,7}) = 0.248$, and

$$
\begin{aligned}
\sigma = [&0, 0.23238423077254125, 0.43157605300450452, 0.51665386361543786, 0.51477152933306880, \\
&0.61128565004088331, 0.80299254893179406, 0.97139112591737997]^T.
\end{aligned}
$$

$$
\begin{aligned}
Y_2 &= 1.4925968280605849\,\text{e-02}y_{n-2} + 2.3495988386171324\,\text{e-01}y_{n-1} + 7.5011414785768094\,\text{e-01}y_n \\
&\quad + 7.5011414785768094\,\text{e-01}y_n + 9.8749233646170027\,\text{e-04}\Delta t f_{n-2} \\
&\quad + 1.1835567846327205\,\text{e-01}\Delta t f_{n-1} + 3.7785288039573245\,\text{e-01}\Delta t f_n, \\
Y_3 &= 1.2535802855249516\,\text{e-03}y_{n-2} + 6.0712465229408402\,\text{e-02}y_{n-1} + 3.0740500785919228\,\text{e-01}y_n \\
&\quad + 3.0582518578506329\,\text{e-02}\Delta t f_{n-1} + 6.3062894662587432\,\text{e-01}Y_2 + 3.1766493756190683\,\text{e-01}\Delta t F_2, \\
Y_4 &= 1.7052069812097479\,\text{e-03}y_{n-2} + 5.7947192464619834\,\text{e-01}y_n + 1.2833789695649112\,\text{e-01}\Delta t f_n \\
&\quad + 4.1882286837258076\,\text{e-01}Y_3 + 2.1097246018109728\,\text{e-01}\Delta t F_3, \\
Y_5 &= 4.8131554327040214\,\text{e-03}y_{n-2} + 6.8105088341897568\,\text{e-01}y_n + 4.0624591870494882\,\text{e-04}\Delta t f_{n-2} \\
&\quad + 2.0345321607400946\,\text{e-01}\Delta t f_n + 3.1413596114831965\,\text{e-01}Y_4 + 1.5823882017793225\,\text{e-01}\Delta t F_4 \\
Y_6 &= 1.5200956268346024\,\text{e-02}y_{n-2} + 8.6164082778426798\,\text{e-02}y_{n-1} + 4.3396462911064942\,\text{e-01}y_n \\
&\quad + 6.5324392705808148\,\text{e-03}\Delta t f_{n-2} + 4.3403189977776466\,\text{e-02}\Delta t f_{n-1} + 2.1859977653752233\,\text{e-01}\Delta t f_n \\
&\quad + 4.9399853608364526\,\text{e-02}Y_2 + 2.4884048688266474\,\text{e-02}\Delta t F_2 \\
&\quad + 4.1527047823421243\,\text{e-01}Y_5 + 2.0918302473329856\,\text{e-01}\Delta t F_5, \\
Y_7 &= 3.4119928157359449\,\text{e-03}y_{n-2} + 8.4215417390459360\,\text{e-02}y_{n-1} + 2.5130064617084391\,\text{e-01}y_n \\
&\quad + 4.2421594267478636\,\text{e-02}\Delta t f_{n-1} + 1.2658696449354065\,\text{e-01}\Delta t f_n + 3.1882440663148194\,\text{e-02}Y_2
\end{aligned}
$$

$$
\begin{aligned}
&+ 1.6060051757485608\,\text{e-}02\Delta t F_2 + 6.2918950295979903\,\text{e-}01 Y_6 + 3.1693985067086861\,\text{e-}01\Delta t F_6,\\
Y_8 &= 4.5802256267512779\,\text{e-}03 y_{n-2} + 6.8014280255773163\,\text{e-}03 y_{n-1} + 3.5211663048013697\,\text{e-}01 y_n\\
&+ 3.4260641231843789\,\text{e-}03\Delta t f_{n-1} + 1.5219759482972633\,\text{e-}01\Delta t f_n\\
&+ 6.3650171586752868\,\text{e-}01 Y_7 + 3.2062321101961477\,\text{e-}01\Delta t F_7,\\
y_{n+1} &= 7.4154625332934973\,\text{e-}04 y_{n-2} + 6.7706372245015384\,\text{e-}03 y_{n-1} + 2.0258451448699699\,\text{e-}01 y_n\\
&+ 2.2909414626356983\,\text{e-}04\Delta t f_{n-2} + 3.4105539599526419\,\text{e-}03\Delta t f_{n-1} + 4.3547572463320666\,\text{e-}02\Delta t f_n\\
&+ 7.3590775403134828\,\text{e-}02 Y_3 + 3.7069673377105303\,\text{e-}02\Delta t F_3 + 5.0524412028802479\,\text{e-}02 Y_4\\
&+ 2.5450519324168110\,\text{e-}02\Delta t F_4 + 1.2745500705109852\,\text{e-}01 Y_5 + 6.4202550602009439\,\text{e-}02\Delta t F_5\\
&+ 1.3592702168921109\,\text{e-}01 Y_6 + 6.8470134599602564\,\text{e-}02\Delta t F_6 + 2.0360650705769195\,\text{e-}01 Y_7\\
&+ 1.0256213054877544\,\text{e-}01\Delta t F_7 + 1.9879957880523283\,\text{e-}01 Y_8 + 1.0014075016122419\,\text{e-}01\Delta t F_8.
\end{aligned}
$$

HB(3,8,8). $c(\text{HB3,8}) = 1.2768075760100959$, $c_{\text{eff}}(\text{HB3,8}) = 0.142$, and

$$
\begin{aligned}
\sigma = [&0, 0.25296754862842130, 0.49225600819417081, 0.38258434445584055, 0.52068124026466622,\\
&0.66409362807151318, 0.82737810802943035, 0.99952769821951859]^T.
\end{aligned}
$$

$$
\begin{aligned}
Y_2 &= 8.0431323301685648\,\text{e-}02 y_{n-2} + 3.2481755805462698\,\text{e-}01 y_{n-1} + 5.9475111864368724\,\text{e-}01 y_n\\
&+ 4.6581108212267103\,\text{e-}01\Delta t f_n + 1.8438464137399815\,\text{e-}02\Delta t f_{n-2} + 2.5439820702634880\,\text{e-}01\Delta t f_{n-1},\\
Y_3 &= 2.4171274094767832\,\text{e-}02 y_{n-2} + 1.6721827271891193\,\text{e-}01 y_{n-1} + 2.8639801559108519\,\text{e-}01 y_n\\
&+ 1.3096591519409165\,\text{e-}01\Delta t f_{n-1} + 3.5749571242699091\,\text{e-}02\Delta t f_n\\
&+ 5.2221243759523517\,\text{e-}01 Y_2 + 4.0899854246408857\,\text{e-}01\Delta t F_2,\\
Y_4 &= 1.6800381323275146\,\text{e-}02 y_{n-2} + 8.6844142788677892\,\text{e-}01 y_n + 9.2813613590216702\,\text{e-}03\Delta t f_{n-2}\\
&+ 2.6053433474971283\,\text{e-}01\Delta t f_n + 1.1475819078994613\,\text{e-}01 Y_3 + 8.9879002087812424\,\text{e-}02\Delta t F_3\\
Y_5 &= 9.1006378797032876\,\text{e-}03 y_{n-2} + 1.0279733503699048\,\text{e-}01 y_{n-1} + 5.4917319650357377\,\text{e-}01 y_n\\
&+ 6.0407197050953022\,\text{e-}02\Delta t f_{n-1} + 1.8615358628248924\,\text{e-}01\Delta t f_n\\
&+ 3.3892883057973244\,\text{e-}01 Y_4 + 2.6545020326308943\,\text{e-}01\Delta t F_4,\\
Y_6 &= 1.5646584710065064\,\text{e-}04 y_{n-2} + 4.4496943168820677\,\text{e-}02 y_{n-1} + 5.6844782633522883\,\text{e-}01 y_n\\
&+ 1.9228056514734587\,\text{e-}01\Delta t f_n + 1.2254457918364704\,\text{e-}04\Delta t f_{n-2} + 1.2029047152794712\,\text{e-}02\Delta t f_{n-1}\\
&+ 3.8689876464884976\,\text{e-}01 Y_5 + 3.0302041742098068\,\text{e-}01\Delta t F_5,\\
Y_7 &= 3.8029033753200900\,\text{e-}04 y_{n-2} + 9.8568707329330651\,\text{e-}02 y_{n-1} + 4.6604816598757948\,\text{e-}01 y_n\\
&+ 2.9944054323220566\,\text{e-}02\Delta t f_{n-1} + 2.6718504127925830\,\text{e-}01\Delta t f_n\\
&+ 4.3500283634555797\,\text{e-}01 Y_6 + 3.4069568862122601\,\text{e-}01\Delta t F_6,\\
Y_8 &= 4.0244510078320417\,\text{e-}02 y_{n-1} + 2.8757414798790559\,\text{e-}01 y_n + 1.2228665877155598\,\text{e-}02\Delta t f_{n-1}\\
&+ 1.2228665877155598\,\text{e-}02\Delta t f_{n-1} + 7.6434139892082836\,\text{e-}02\Delta t f_n + 2.2891887418237039\,\text{e-}01 Y_2\\
&+ 1.7929003436658830\,\text{e-}01\Delta t F_2 + 4.4326246775140354\,\text{e-}01 Y_7 + 3.4716465979670741\,\text{e-}01\Delta t F_7,\\
y_{n+1} &= 4.6991204294326554\,\text{e-}04 y_{n-2} + 2.5355314573089469\,\text{e-}02 y_{n-1} + 3.7576148261446241\,\text{e-}01 y_n
\end{aligned}
$$

$$
\begin{aligned}
&+ 8.0519039451696986\,\text{e-}03\Delta t f_{n-1} + 1.2273329474329865\,\text{e-}01\Delta t f_n + 9.8829402744482122\,\text{e-}03Y_3\\
&+ 7.7403521565336227\,\text{e-}03\Delta t F_3 + 3.7697941785698019\,\text{e-}02Y_4 + 2.9525155155720927\,\text{e-}02\Delta t F_4\\
&+ 4.2640032452885113\,\text{e-}01Y_6 + 3.3395817235147696\,\text{e-}01\Delta t F_6\\
&+ 1.2443208418050744\,\text{e-}01Y_8 + 9.7455628019803939\,\text{e-}02\Delta t F_8.
\end{aligned}
$$

HB(4,8,9). $c(\text{HB(4,8,9)}) = 1.1072614332708535$, $c_{\text{eff}}(\text{HB(4,8,9)}) = 0.138$, and

$$
\begin{aligned}
\sigma = [&0, 0.25155135020798175, 0.33714858504761824, 0.42083600219067197, 0.52197758259043459,\\
&0.61235929113974452, 0.80010716066276477, 0.92838294990938930]^T.
\end{aligned}
$$

$$
\begin{aligned}
Y_2 &= 2.4878773640400584\,\text{e-}03y_{n-3} + 1.0886557083497138\,\text{e-}01y_{n-2} + 3.5232127968034910\,\text{e-}01y_{n-1}\\
&\quad + 2.4257986119599170\,\text{e-}02\Delta t f_{n-2} + 5.3632527212063930\,\text{e-}01y_n + 2.2468743959507928\,\text{e-}03\Delta t f_{n-3}\\
&\quad + 3.1819159332551755\,\text{e-}01\Delta t f_{n-1} + 4.8437094980932627\,\text{e-}01\Delta t f_n,\\
Y_3 &= 2.9653728741651749\,\text{e-}04y_{n-3} + 1.7322332295411080\,\text{e-}03y_{n-2} + 7.3993714823404610\,\text{e-}04y_{n-1}\\
&\quad + 6.6825875624355879\,\text{e-}04\Delta t f_{n-1} + 7.8294205493188451\,\text{e-}01y_n + 1.5644302036458392\,\text{e-}03\Delta t f_{n-2}\\
&\quad + 9.2574322636738746\,\text{e-}02\Delta t f_n + 2.1428923740292397\,\text{e-}01Y_2 + 1.9353084191681177\,\text{e-}01\Delta t F_2,\\
Y_4 &= 1.3328822642268510\,\text{e-}03y_{n-3} + 7.5405609181160536\,\text{e-}03y_{n-2} + 5.4406075373148559\,\text{e-}03y_{n-1}\\
&\quad + 7.5518365192625836\,\text{e-}01y_n + 6.8100998477308248\,\text{e-}03\Delta t f_{n-2} + 4.9135708820303506\,\text{e-}03\Delta t f_{n-1}\\
&\quad + 1.4774585638289806\,\text{e-}01\Delta t f_n + 2.3050229735408373\,\text{e-}01Y_3 + 2.0817332784108561\,\text{e-}01\Delta t F_3,\\
Y_5 &= 6.6563925837921211\,\text{e-}04y_{n-3} + 3.7212264758549655\,\text{e-}02y_{n-2} + 9.3714259258191338\,\text{e-}02y_{n-1}\\
&\quad + 6.0780006835904099\,\text{e-}01y_n + 1.2768430013380214\,\text{e-}02\Delta t f_{n-2} + 8.4636072784869912\,\text{e-}02\Delta t f_{n-1}\\
&\quad + 2.4967320077254984\,\text{e-}01\Delta t f_n + 2.6060776836583893\,\text{e-}01Y_4 + 2.3536245419115054\,\text{e-}01\Delta t F_4,\\
Y_6 &= 5.4494044120533287\,\text{e-}03y_{n-3} + 3.4995199298042602\,\text{e-}02y_{n-2} + 4.2704083918843797\,\text{e-}02y_{n-1}\\
&\quad + 4.2704083918843797\,\text{e-}02y_{n-1} + 6.4181541863574953\,\text{e-}01y_n + 2.8464632091918449\,\text{e-}02\Delta t f_{n-2}\\
&\quad + 3.8567300039247104\,\text{e-}02\Delta t f_{n-1} + 2.8241457003403286\,\text{e-}01\Delta t f_n\\
&\quad + 2.7503589373531079\,\text{e-}01Y_5 + 2.4839291378807801\,\text{e-}01\Delta t F_5,\\
Y_7 &= 2.5011934342737919\,\text{e-}03y_{n-3} + 5.5906845523761711\,\text{e-}02y_{n-2} + 1.9404609815047866\,\text{e-}01y_{n-1}\\
&\quad + 3.3859835585876863\,\text{e-}01y_n + 2.2589005262156191\,\text{e-}03\Delta t f_{n-3} + 1.0409742223035454\,\text{e-}02\Delta t f_{n-2}\\
&\quad + 1.7524867417920084\,\text{e-}01\Delta t f_{n-1} + 3.0579802175403870\,\text{e-}01\Delta t f_n\\
&\quad + 4.0894750703271721\,\text{e-}01Y_6 + 3.6933238596117729\,\text{e-}01\Delta t F_6,\\
Y_8 &= 4.0142804521193960\,\text{e-}03y_{n-3} + 6.0909105818209096\,\text{e-}02y_{n-2} + 1.3352939198048103\,\text{e-}01y_{n-1}\\
&\quad + 3.2178057775983659\,\text{e-}01y_n + 3.0406855944862508\,\text{e-}02\Delta t f_{n-2} + 1.2059427698663250\,\text{e-}01\Delta t f_{n-1}\\
&\quad + 2.9060939728506185\,\text{e-}01\Delta t f_n + 5.1061882695041964\,\text{e-}02Y_2 + 4.6115471162221387\,\text{e-}02\Delta t F_2\\
&\quad + 4.8386497105927491\,\text{e-}03Y_3 + 4.3699252635390397\,\text{e-}03\Delta t F_3 + 1.1772456578284952\,\text{e-}01Y_5\\
&\quad + 1.0632047883677373\,\text{e-}01\Delta t F_5 + 3.0614154580086955\,\text{e-}01Y_7 + 2.7648533273350501\,\text{e-}01\Delta t F_7,\\
y_{n+1} &= 1.4180351748984421\,\text{e-}03y_{n-3} + 4.2143433044927181\,\text{e-}03y_{n-2} + 7.3643693912603114\,\text{e-}03y_{n-1}\\
&\quad + 4.1454707028866394\,\text{e-}01y_n + 3.7401714145701638\,\text{e-}04\Delta t f_{n-3} + 3.8060959931057389\,\text{e-}03\Delta t f_{n-2}
\end{aligned}
$$

$$+ 6.6509761561061032\,\text{e-}03\Delta t f_{n-1} + 1.0109547389376111\,\text{e-}01\Delta t f_n + 3.2294689720816705\,\text{e-}01 Y_5$$
$$+ 2.9166273429589340\,\text{e-}01\Delta t F_5 + 7.0881911533472647\,\text{e-}02 Y_7 + 6.4015515580712751\,\text{e-}02\Delta t F_7$$
$$+ 1.7862737309904494\,\text{e-}01 Y_8 + 1.6132357520245166\,\text{e-}01\Delta t F_8.$$

HB(5,8,10). $c(\text{HB}(5,8,10)) = 0.97102752134084724$, $c_{\text{eff}}(\text{HB}(5,8,10)) = 0.121$, and

$$\sigma = [0, 0.24958883339246415, 0.42701272438250404, 0.49116336919436759, 0.46622895557249333,$$
$$0.63668736986589192, 0.83859323108451345, 0.96251481297888763]^T.$$

$$Y_2 = 4.9957599570804399\,\text{e-}03 y_{n-4} + 2.3867703762249295\,\text{e-}02 y_{n-3} + 1.1623750837352728\,\text{e-}01 y_{n-2}$$
$$+ 3.7062934480738507\,\text{e-}01 y_{n-1} + 4.8426968309975776\,\text{e-}01 y_n + 2.4579842731225043\,\text{e-}02\Delta t f_{n-3}$$
$$+ 3.9292914311878618\,\text{e-}02\Delta t f_{n-2} + 3.8168778604297438\,\text{e-}01\Delta t f_{n-1} + 4.9871880297589527\,\text{e-}01\Delta t f_n,$$
$$Y_3 = 4.2990452823252409\,\text{e-}03 y_{n-4} + 2.1276230373848806\,\text{e-}02 y_{n-3} + 4.0613421411792097\,\text{e-}03 y_{n-2}$$
$$+ 1.2082207981330481\,\text{e-}01 y_{n-1} + 5.3367948991826664\,\text{e-}01 y_n + 2.1911047736803007\,\text{e-}02\Delta t f_{n-3}$$
$$+ 4.1825201159809509\,\text{e-}03\Delta t f_{n-2} + 1.2442703956162555\,\text{e-}01\Delta t f_{n-1} + 8.2340013262737599\,\text{e-}02\Delta t f_n$$
$$+ 3.1586181247107531\,\text{e-}01 Y_2 + 3.2528615876398259\,\text{e-}01\Delta t F_2,$$
$$Y_4 = 6.3243190428049459\,\text{e-}04 y_{n-4} + 7.9640499357823604\,\text{e-}03 y_{n-3} + 3.1417925777444164\,\text{e-}02 y_{n-2}$$
$$+ 3.1417925777444164\,\text{e-}02 y_{n-2} + 2.5976334121008310\,\text{e-}01\Delta t f_n + 3.8146737214488240\,\text{e-}02 y_{n-1}$$
$$+ 3.8146737214488240\,\text{e-}02 y_{n-1} + 7.2517275923146729\,\text{e-}01 y_n + 6.5130172974623617\,\text{e-}04\Delta t f_{n-4}$$
$$+ 3.2355340180328360\,\text{e-}02\Delta t f_{n-2} + 3.9284918682647808\,\text{e-}02\Delta t f_{n-1}$$
$$+ 1.9666609593653750\,\text{e-}01 Y_3 + 2.0253400816587602\,\text{e-}01\Delta t F_3,$$
$$Y_5 = 2.6760347853459865\,\text{e-}03 y_{n-4} + 1.0863175574600597\,\text{e-}02 y_{n-3} + 5.4893345712409669\,\text{e-}02 y_{n-2}$$
$$+ 5.6531194539790150\,\text{e-}02\Delta t f_{n-2} + 6.0754767616767714\,\text{e-}02 y_{n-1} + 7.4123068994465302\,\text{e-}01 y_n$$
$$+ 1.8293072867059388\,\text{e-}03\Delta t f_{n-4} + 6.2567503270014688\,\text{e-}02\Delta t f_{n-1} + 3.6204183555279384\,\text{e-}01\Delta t f_n$$
$$+ 1.2958198636622298\,\text{e-}01 Y_4 + 1.3344831481942879\,\text{e-}01\Delta t F_4,$$
$$Y_6 = 2.0754355220173968\,\text{e-}03 y_{n-4} + 9.9730401759130158\,\text{e-}03 y_{n-3} + 3.8849179501725811\,\text{e-}03 y_{n-2}$$
$$+ 1.0270605061885065\,\text{e-}02\Delta t f_{n-3} + 5.0219517181393135\,\text{e-}02 y_{n-1} + 5.9613180834611079\,\text{e-}01 y_n$$
$$+ 4.0008319690136816\,\text{e-}03\Delta t f_{n-2} + 5.1717913321393104\,\text{e-}02\Delta t f_{n-1} + 1.6166392506298297\,\text{e-}01\Delta t f_n$$
$$+ 3.3771528082439317\,\text{e-}01 Y_5 + 3.4779166748853590\,\text{e-}01\Delta t F_5$$
$$Y_7 = 1.9608993238511814\,\text{e-}03 y_{n-4} + 8.9390249470190468\,\text{e-}03 y_{n-3} + 7.0820993991796144\,\text{e-}03 y_{n-2}$$
$$+ 3.6077646240821409\,\text{e-}02 y_{n-1} + 5.4667596049004419\,\text{e-}01 y_n + 9.1573341892354047\,\text{e-}03\Delta t f_{n-3}$$
$$+ 7.2934074920968945\,\text{e-}03\Delta t f_{n-2} + 3.7154092389681648\,\text{e-}02\Delta t f_{n-1} + 2.0450714080792248\,\text{e-}01\Delta t f_n$$
$$+ 3.9926436959908462\,\text{e-}01 Y_6 + 4.1117719202001485\,\text{e-}01\Delta t F_6,$$
$$Y_8 = 4.6616480075610230\,\text{e-}04 y_{n-4} + 2.8134173558822913\,\text{e-}02 y_{n-3} + 6.2852012068878693\,\text{e-}02 y_{n-2}$$
$$+ 1.4929250845196435\,\text{e-}01 y_{n-1} + 2.3329704249840494\,\text{e-}01 y_n + 4.8007372655349252\,\text{e-}04\Delta t f_{n-4}$$
$$+ 7.0903473726891715\,\text{e-}03\Delta t f_{n-3} + 6.4727323054746433\,\text{e-}02\Delta t f_{n-2} + 1.5374693834198766\,\text{e-}01\Delta t f_{n-1}$$
$$+ 2.4025790965868354\,\text{e-}01\Delta t f_n + 1.6378732074427735\,\text{e-}01 Y_2 + 1.6867423131129278\,\text{e-}01\Delta t F_2$$

$$+\,7.7259260620153106\,\text{e-02}Y_5 + 7.9564439649938395\,\text{e-02}\Delta t F_5$$
$$+\,2.8491151725674269\,\text{e-01}Y_7 + 2.9341240180640965\,\text{e-01}\Delta t F_7,$$
$$y_{n+1} = 7.0185277566430079\,\text{e-05}y_{n-4} + 5.1010981648964508\,\text{e-03}y_{n-3} + 1.0945795978915027\,\text{e-02}y_{n-2}$$
$$+\,2.1181421753514090\,\text{e-02}y_{n-1} + 4.5233021109160843\,\text{e-01}y_n + 1.6679706370347812\,\text{e-03}\Delta t f_{n-3}$$
$$+\,1.1272384910162456\,\text{e-02}\Delta t f_{n-2} + 2.1813410318448703\,\text{e-02}\Delta t f_{n-1} + 1.4536539995598871\,\text{e-01}\Delta t f_n$$
$$+\,1.4182112368892130\,\text{e-01}Y_4 + 1.4605263040648636\,\text{e-01}\Delta t F_4 + 1.9507160863566964\,\text{e-01}Y_6$$
$$+\,1.9507160863566964\,\text{e-01}Y_6 + 2.0089194626152740\,\text{e-01}\Delta t F_6 + 6.3701297148469727\,\text{e-02}Y_7$$
$$+\,6.5601948192475057\,\text{e-02}\Delta t F_7 + 1.0977725826043891\,\text{e-01}Y_8 + 1.1305267445854937\,\text{e-01}\Delta t F_8.$$

HB(7,8,11). $c(\text{HB(7,8,11)}) = 1.0785142576992566$, $c_{\text{eff}}(\text{HB(7,8,11)}) = 0.135$, and
$$\sigma = [0, 0.23852412645835103, 0.34289387913490704, 0.46930408292864162, 0.52758167512889376,$$
$$0.61814438712197051, 0.78984785222720000, 0.96683498505714671]^T.$$

$$Y_2 = 2.5946770415249232\,\text{e-04}y_{n-6} + 7.2545656889022826\,\text{e-03}y_{n-5} + 6.5530317423295140\,\text{e-02}y_{n-3}$$
$$+\,3.4428205021721510\,\text{e-02}y_{n-2} + 3.8264506557453076\,\text{e-01}y_{n-1} + 5.0988237858739793\,\text{e-01}y_n$$
$$+\,4.2117465668472572\,\text{e-03}\Delta t f_{n-5} + 6.0759806331246724\,\text{e-02}\Delta t f_{n-3} + 3.1921882141053542\,\text{e-02}\Delta t f_{n-2}$$
$$+\,3.5478906546011674\,\text{e-01}\Delta t f_{n-1} + 4.7276368851637224\,\text{e-01}\Delta t f_n,$$
$$Y_3 = 2.6734751055294141\,\text{e-05}y_{n-6} + 1.9743959979604529\,\text{e-04}y_{n-5} + 3.0849794661314076\,\text{e-03}y_{n-3}$$
$$+\,1.6542139395870611\,\text{e-02}y_{n-1} + 7.4751313789655527\,\text{e-01}y_n + 2.4788500350775258\,\text{e-05}\Delta t f_{n-6}$$
$$+\,6.2838397890436484\,\text{e-05}\Delta t f_{n-5} + 2.8603974811723370\,\text{e-03}\Delta t f_{n-3} + 1.5337895885733754\,\text{e-02}\Delta t f_{n-1}$$
$$+\,8.0363406978795196\,\text{e-02}\Delta t f_n + 2.3263556889059139\,\text{e-01}Y_2 + 2.1570004033777157\,\text{e-01}\Delta t F_2,$$
$$Y_4 = 2.4120309661236624\,\text{e-05}y_{n-6} + 4.7291316019706497\,\text{e-04}y_{n-3} + 4.8327392388944823\,\text{e-04}y_{n-2}$$
$$+\,7.0993109585855541\,\text{e-01}y_n + 1.6570301770652821\,\text{e-05}\Delta t f_{n-6} + 4.3848577505679626\,\text{e-04}\Delta t f_{n-3}$$
$$+\,4.4809229033317870\,\text{e-04}\Delta t f_{n-2} + 1.0376086291231772\,\text{e-01}\Delta t f_n$$
$$+\,2.8908859674769694\,\text{e-01}Y_3 + 2.6804337048301613\,\text{e-01}\Delta t F_3$$
$$Y_5 = 4.7899190522712981\,\text{e-04}y_{n-6} + 2.1572285347400129\,\text{e-03}y_{n-5} + 4.8753461944363551\,\text{e-03}y_{n-4}$$
$$+\,7.8131877588771166\,\text{e-03}y_{n-3} + 4.7596642918370527\,\text{e-02}y_{n-2} + 1.0099681717571710\,\text{e-01}y_{n-1}$$
$$+\,6.2434200822503372\,\text{e-01}y_n + 2.0001854582265112\,\text{e-03}\Delta t f_{n-5} + 4.5204281349388005\,\text{e-03}\Delta t f_{n-4}$$
$$+\,7.2443991380740941\,\text{e-03}\Delta t f_{n-3} + 4.4131677053492267\,\text{e-02}\Delta t f_{n-2} + 9.3644396867936477\,\text{e-02}\Delta t f_{n-1}$$
$$+\,3.3313595990211958\,\text{e-01}\Delta t f_n + 2.1173977728759796\,\text{e-01}Y_4 + 1.9632543174653289\,\text{e-01}\Delta t F_4$$
$$Y_6 = 7.8814982890040256\,\text{e-04}y_{n-6} + 3.4325376384250952\,\text{e-03}y_{n-5} + 3.2843942705524801\,\text{e-03}y_{n-4}$$
$$+\,2.4335969039436908\,\text{e-02}y_{n-3} + 4.2838443864996689\,\text{e-02}y_{n-2} + 2.2529137459966309\,\text{e-01}y_{n-1}$$
$$+\,4.4470760557371170\,\text{e-01}y_n + 9.7632618142431179\,\text{e-05}\Delta t f_{n-6} + 3.1826539277724207\,\text{e-03}\Delta t f_{n-5}$$
$$+\,3.0452951800182247\,\text{e-03}\Delta t f_{n-4} + 2.2564346150927735\,\text{e-02}\Delta t f_{n-3} + 3.9719867919393033\,\text{e-02}\Delta t f_{n-2}$$
$$+\,1.8476893133231126\,\text{e-01}\Delta t f_{n-1} + 4.1233354348266610\,\text{e-01}\Delta t f_n$$
$$+\,2.5532152518431356\,\text{e-01}Y_5 + 2.3673449225324000\,\text{e-01}\Delta t F_5,$$

$$
\begin{aligned}
Y_7 &= 9.1712252605348574\,\text{e-}04 y_{n-6} + 5.3106154915326864\,\text{e-}04 y_{n-5} + 1.4484312100184759\,\text{e-}03 y_{n-4} \\
&\quad + 2.3538759575491459\,\text{e-}02 y_{n-3} + 2.3163417208184062\,\text{e-}01 y_{n-1} + 3.6154680047434185\,\text{e-}01 y_n \\
&\quad + 5.1703537307344551\,\text{e-}04 \Delta t f_{n-6} + 4.9240104649720339\,\text{e-}04 \Delta t f_{n-5} + 1.3429875402002991\,\text{e-}03 \Delta t f_{n-4} \\
&\quad + 2.1825172367869829\,\text{e-}02 \Delta t f_{n-3} + 1.5882145148623342\,\text{e-}01 \Delta t f_{n-1} + 3.3522672314560986\,\text{e-}01 \Delta t f_n \\
&\quad + 3.8038365258310114\,\text{e-}01 Y_6 + 3.5269228002099440\,\text{e-}01 \Delta t F_6, \\
Y_8 &= 5.6492834785037982\,\text{e-}04 y_{n-6} + 2.0605118288583172\,\text{e-}03 y_{n-5} + 8.6879528615987963\,\text{e-}03 y_{n-4} \\
&\quad + 7.3422737165952628\,\text{e-}02 y_{n-2} + 9.3129218889008436\,\text{e-}02 y_{n-1} + 3.9748106289317864\,\text{e-}01 y_n \\
&\quad + 1.9105095868216996\,\text{e-}03 \Delta t f_{n-5} + 8.0554826230414336\,\text{e-}03 \Delta t f_{n-4} + 6.8077669480774303\,\text{e-}02 \Delta t f_{n-2} \\
&\quad + 8.6349548208734403\,\text{e-}02 \Delta t f_{n-1} + 3.6854502391197458\,\text{e-}01 \Delta t f_n + 5.0902778233268466\,\text{e-}03 Y_3 \\
&\quad + 4.7197130561683030\,\text{e-}03 \Delta t F_3 + 1.7389388365218951\,\text{e-}02 Y_5 + 1.6123466371520123\,\text{e-}02 \Delta t F_5 \\
&\quad + 4.0217392182500655\,\text{e-}01 Y_7 + 3.7289624958963929\,\text{e-}01 \Delta t F_7, \\
y_{n+1} &= 2.2576177061003726\,\text{e-}04 y_{n-6} + 6.7444921834467451\,\text{e-}04 y_{n-5} + 1.1735565895738690\,\text{e-}03 y_{n-4} \\
&\quad + 5.1736483759398724\,\text{e-}03 y_{n-3} + 1.2365374169134628\,\text{e-}02 y_{n-2} + 3.9657298353392281\,\text{e-}02 y_{n-1} \\
&\quad + 3.9653506378660275\,\text{e-}01 y_n + 5.6884514696624723\,\text{e-}05 \Delta t f_{n-6} + 6.2535030346603420\,\text{e-}04 \Delta t f_{n-5} \\
&\quad + 1.0881233893721177\,\text{e-}03 \Delta t f_{n-4} + 4.7970143547073473\,\text{e-}03 \Delta t f_{n-3} + 1.1465193047621908\,\text{e-}02 \Delta t f_{n-2} \\
&\quad + 3.6770305139953899\,\text{e-}02 \Delta t f_{n-1} + 1.5087275769598654\,\text{e-}01 \Delta t f_n + 3.9805481703267479\,\text{e-}03 Y_3 \\
&\quad + 3.6907700959079234\,\text{e-}03 \Delta t F_3 + 1.1860718640120570\,\text{e-}01 Y_4 + 1.0997275701688432\,\text{e-}01 \Delta t F_4 \\
&\quad + 1.8458049359935838\,\text{e-}01 Y_6 + 1.7114330411645667\,\text{e-}01 \Delta t F_6 + 1.1986532649283420\,\text{e-}01 Y_7 \\
&\quad + 1.1113930635329497\,\text{e-}01 \Delta t F_7 + 1.1716129307267698\,\text{e-}01 Y_8 + 1.0863212260411988\,\text{e-}01 \Delta t F_8.
\end{aligned}
$$

HB(7,8,12). $c(\text{HB(7,8,12)}) = 0.80110266354476745$, $c_{\text{eff}}(\text{HB(7,8,12)}) = 0.100$, and
$\sigma = [0, 0.24542753056807640, 0.34247100086335447, 0.43468829444860235, 0.55682843622863765,$
$0.61757295256705613, 0.79533083970127050, 0.93847995276937568]^T$.

$$
\begin{aligned}
Y_2 &= 5.2894477499746727\,\text{e-}03 y_{n-6} + 2.1033888944116286\,\text{e-}02 y_{n-5} + 1.0405200285779162\,\text{e-}01 y_{n-3} \\
&\quad + 4.6594593839432506\,\text{e-}02 y_{n-2} + 4.1064936993795986\,\text{e-}01 y_{n-1} + 4.1238069667072497\,\text{e-}01 y_n \\
&\quad + 6.0812233983290444\,\text{e-}04 \Delta t f_{n-6} + 2.2556675934975120\,\text{e-}02 \Delta t f_{n-5} + 1.2988597790621942\,\text{e-}01 \Delta t f_{n-3} \\
&\quad + 5.8163074422014384\,\text{e-}02 \Delta t f_{n-2} + 4.7234802415197297\,\text{e-}01 \Delta t f_{n-1} + 5.1476635322369069\,\text{e-}01 \Delta t f_n, \\
Y_3 &= 1.4740901019083411\,\text{e-}05 y_{n-6} + 6.7958735918013935\,\text{e-}05 y_{n-5} + 2.2555349086398474\,\text{e-}04 y_{n-3} \\
&\quad + 2.2555349086398474\,\text{e-}04 y_{n-3} + 4.6433041313443876\,\text{e-}04 y_{n-2} + 8.2695038374036622\,\text{e-}01 y_n \\
&\quad + 8.2695038374036622\,\text{e-}01 y_n + 7.5815159706814524\,\text{e-}05 \Delta t f_{n-5} + 2.8155378970530151\,\text{e-}04 \Delta t f_{n-3} \\
&\quad + 5.7961411722174706\,\text{e-}04 \Delta t f_{n-2} + 8.6236170149706567\,\text{e-}02 \Delta t f_n \\
&\quad + 1.7227703271869996\,\text{e-}01 Y_2 + 2.1504988131783029\,\text{e-}01 \Delta t F_2, \\
Y_4 &= 4.8260898815269079\,\text{e-}04 y_{n-6} + 4.3860019573741344\,\text{e-}03 y_{n-4} + 1.5449344199948227\,\text{e-}02 y_{n-2} \\
&\quad + 1.3165148793506732\,\text{e-}02 y_{n-1} + 7.8692734342040382\,\text{e-}01 y_n + 2.2363834772940651\,\text{e-}04 \Delta t f_{n-6} \\
&\quad + 4.4349055649211249\,\text{e-}03 \Delta t f_{n-4} + 1.9285099030364097\,\text{e-}02 \Delta t f_{n-2} + 1.6433784822598614\,\text{e-}02 \Delta t f_{n-1}
\end{aligned}
$$

$$
\begin{aligned}
&+ 1.7313220206249497\,\text{e-01}\Delta t f_n + 1.7958955264061419\,\text{e-01}Y_3 + 2.2417794973487604\,\text{e-01}\Delta t F_3\\
Y_5 &= 6.2745706888749721\,\text{e-05}y_{n-6} + 3.8965049836753624\,\text{e-03}y_{n-5} + 6.0323150991997317\,\text{e-03}y_{n-4}\\
&+ 1.0940482673652451\,\text{e-02}y_{n-3} + 2.6856703628222976\,\text{e-02}y_{n-2} + 5.8187490878337481\,\text{e-02}y_{n-1}\\
&+ 6.7051537269623074\,\text{e-01}y_n + 1.3450925858784642\,\text{e-03}\Delta t f_{n-5} + 7.5300150326641120\,\text{e-03}\Delta t f_{n-4}\\
&+ 1.3656779800534582\,\text{e-02}\Delta t f_{n-3} + 3.3524671493894008\,\text{e-02}\Delta t f_{n-2} + 7.2634249673899975\,\text{e-02}\Delta t f_{n-1}\\
&+ 2.4069082974226652\,\text{e-01}\Delta t f_n + 2.2350838433379089\,\text{e-01}Y_4 + 2.7900092523072823\,\text{e-01}\Delta t F_4,\\
Y_6 &= 5.3488530364275257\,\text{e-03}y_{n-6} + 4.3155134278030057\,\text{e-03}y_{n-5} + 2.4854662278709198\,\text{e-02}y_{n-4}\\
&+ 1.2925006051124819\,\text{e-02}y_{n-3} + 9.6157928560609049\,\text{e-02}y_{n-2} + 1.9305966285193615\,\text{e-01}y_{n-1}\\
&+ 4.8777687074532394\,\text{e-01}y_n + 2.0397556000102059\,\text{e-03}\Delta t f_{n-6} + 5.3869667699113759\,\text{e-03}\Delta t f_{n-5}\\
&+ 3.1025564399863342\,\text{e-02}\Delta t f_{n-4} + 1.6134019569893465\,\text{e-02}\Delta t f_{n-3} + 1.2003196710784730\,\text{e-01}\Delta t f_{n-2}\\
&+ 2.0287495934054137\,\text{e-01}\Delta t f_{n-1} + 5.0041213700781562\,\text{e-01}\Delta t f_n\\
&+ 1.7556150304806620\,\text{e-01}Y_5 + 2.1914981816591528\,\text{e-01}\Delta t F_5,\\
Y_7 &= 2.5613108121858982\,\text{e-03}y_{n-6} + 1.5982290879185158\,\text{e-02}y_{n-5} + 7.2142987723427324\,\text{e-02}y_{n-3}\\
&+ 3.9285071921962803\,\text{e-02}y_{n-2} + 2.4182328466779504\,\text{e-01}y_{n-1} + 3.2498587812919472\,\text{e-01}y_n\\
&+ 1.5040726354864437\,\text{e-02}\Delta t f_{n-5} + 9.0054609735292085\,\text{e-02}\Delta t f_{n-3} + 4.9038748352342044\,\text{e-02}\Delta t f_{n-2}\\
&+ 3.0186303912380291\,\text{e-01}\Delta t f_{n-1} + 4.0567319635560278\,\text{e-01}\Delta t f_n\\
&+ 3.0321917586624875\,\text{e-01}Y_6 + 3.7850226901574163\,\text{e-01}\Delta t F_6,\\
Y_8 &= 2.0735199012525212\,\text{e-04}y_{n-6} + 5.0022035374880352\,\text{e-03}y_{n-5} + 1.5667340447800264\,\text{e-02}y_{n-4}\\
&+ 7.9801165393548930\,\text{e-03}y_{n-3} + 1.1063281213334106\,\text{e-01}y_{n-2} + 1.7450809743309664\,\text{e-01}y_{n-1}\\
&+ 3.0027653932076498\,\text{e-01}y_n + 2.5883323019827541\,\text{e-04}\Delta t f_{n-6} + 1.9557219268842841\,\text{e-02}\Delta t f_{n-4}\\
&+ 9.9614155619494639\,\text{e-03}\Delta t f_{n-3} + 8.8630390452963226\,\text{e-02}\Delta t f_{n-2} + 2.1783487357403455\,\text{e-01}\Delta t f_{n-1}\\
&+ 3.7482903625869290\,\text{e-01}\Delta t f_n + 2.8350515421833086\,\text{e-02}Y_2 + 3.5389366072490651\,\text{e-02}\Delta t F_2\\
&+ 1.0158505836477495\,\text{e-01}Y_4 + 1.2680654176741249\,\text{e-01}\Delta t F_4\\
&+ 2.5578996481141669\,\text{e-01}Y_7 + 3.1929735906704115\,\text{e-01}\Delta t F_7,\\
y_{n+1} &= 2.5128359766961306\,\text{e-05}y_{n-6} + 1.7477652684814446\,\text{e-03}y_{n-5} + 2.8778138364805922\,\text{e-03}y_{n-4}\\
&+ 4.4169173225911251\,\text{e-03}y_{n-3} + 1.3666656018618394\,\text{e-02}y_{n-2} + 2.2366835384318023\,\text{e-02}y_{n-1}\\
&+ 5.1023862948181853\,\text{e-01}y_n + 5.7765647910606489\,\text{e-04}\Delta t f_{n-5} + 3.5923159008693379\,\text{e-03}\Delta t f_{n-4}\\
&+ 5.5135471689065456\,\text{e-03}\Delta t f_{n-3} + 1.7059805990601567\,\text{e-02}\Delta t f_{n-2} + 2.7920061188350664\,\text{e-02}\Delta t f_{n-1}\\
&+ 1.6854818130239199\,\text{e-01}\Delta t f_n + 8.4165792064117679\,\text{e-04}Y_2 + 1.0506242944155972\,\text{e-03}\Delta t F_2\\
&+ 2.7706659771574976\,\text{e-01}Y_5 + 3.4585654289272832\,\text{e-01}\Delta t F_5 + 4.1206074567182407\,\text{e-02}Y_7\\
&+ 5.1436696496365751\,\text{e-02}\Delta t F_7 + 1.2554592412435736\,\text{e-01}Y_8 + 1.5671639833131271\,\text{e-01}\Delta t F_8.
\end{aligned}
$$

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