Strong stability preserving explicit Runge–Kutta methods of maximal effective order

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Abstract

We apply the concept of effective order to strong stability preserving (SSP) explicit Runge–Kutta methods. Relative to classical Runge–Kutta methods, methods with an effective order of accuracy are designed to satisfy a relaxed set of order conditions, but yield higher order accuracy when composed with special starting and stopping methods. We show that this allows the construction of four-stage SSP methods with effective order four (such methods cannot have classical order four). However, we also prove that effective order five methods—like classical order five methods—require the use of non-positive weights and so cannot be SSP. By numerical optimization, we construct explicit SSP Runge–Kutta methods up to effective order four and establish the optimality of many of them. Numerical experiments demonstrate the validity of these methods in practice.

1 Introduction

Strong stability preserving time discretization methods were originally developed for the solution of nonlinear hyperbolic partial differential equations (PDEs). Solutions of such PDEs may contain discontinuities even when the initial conditions are smooth. Many numerical methods for their solution are based on a method-of-lines approach in which the problem is first discretized in space to yield a system of ODEs. The spatial discretization is often chosen to ensure the solution is total variation diminishing (TVD), in order to avoid the appearance of spurious oscillations near discontinuities, *when coupled with first-order forward Euler time integration.* Strong stability preserving (SSP) time discretizations (also known as TVD discretizations [11]) are high-order time discretizations that guarantee the TVD property (or other convex functional bounds), with a possibly different step-size restriction [9]. Section 2 reviews Runge–Kutta methods and the concept of strong stability preserving methods.

Explicit SSP Runge–Kutta methods cannot have order greater than four [24]. However, a Runge–Kutta method may achieve an effective order of accuracy higher than its classical order by the use of special starting and stopping procedures. The conditions for a method to have effective order q are in general less restrictive than the conditions for a method to have classical order q. Section 3 presents

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a brief overview of the algebraic representation of Runge–Kutta methods, following Butcher [4]. This includes the concept of effective order and a list of effective order conditions.

We examine the SSP properties of explicit Runge–Kutta methods whose effective order is greater than their classical order. Previous studies of SSP Runge–Kutta method have considered only the classical order of the methods. Three natural questions are:

- Can an SSP Runge–Kutta method have effective order of accuracy greater than four?
- If we only require methods to have *effective* order q, is it possible to achieve larger SSP coefficient compared to methods with *classical* order q?
- SSP Runge–Kutta methods of order four require at least five stages. Can SSP methods of effective order four have fewer stages?

We show in Section 4 that the answer to the first question is negative. We answer the second question by numerically solving the problem of optimizing the SSP coefficient over the class of methods with effective order q; see Section 5. Most of the methods we find are shown to be optimal, as they achieve a certain theoretical upper bound on the SSP coefficient that is obtained by considering only linear problems [20]. We answer the last question affirmatively by construction, also in Section 5.

The paper concludes with numerical experiments in Section 6 and conclusions in Section 7.

2 Strong stability preserving Runge–Kutta methods

Strong stability preserving (SSP) time-stepping methods were originally introduced for time integration of systems of hyperbolic conservation laws [26]

$$\boldsymbol{U}_t + \nabla \cdot \boldsymbol{f}(\boldsymbol{U}) = 0, \tag{2.1}$$

with appropriate initial and boundary conditions. A spatial discretization gives the system of ODEs

$$\boldsymbol{u}'(t) = \boldsymbol{F}(\boldsymbol{u}(t)), \tag{2.2}$$

where $\boldsymbol{u}$ is a vector of continuous-in-time grid values approximating the solution $\boldsymbol{U}$ at discrete grid points. Of course, (2.2) can arise in many ways and $\boldsymbol{F}$ need not necessarily represent a spatial discretization. Particularly, $\boldsymbol{F}$ may be time-dependent, but we can always make a transformation to an autonomous form. In any case, a time discretization then produces a sequence of solutions $\boldsymbol{u}^n \approx \boldsymbol{u}(t_n)$. This work studies explicit Runge–Kutta time discretizations. An explicit s-stage Runge–Kutta method takes the form

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + \Delta t \sum_{i}^{s} b_i \boldsymbol{F}(\boldsymbol{Y}_i),$$

where

$$\boldsymbol{Y}_i = \boldsymbol{u}^n + \Delta t \sum_{j}^{i-1} a_{ij} \boldsymbol{F}(\boldsymbol{Y}_j).$$

Such methods are characterized by the coefficient matrix $A = (a_{ij}) \in \mathbb{R}^{s\times s}$, the weight vector $\boldsymbol{b} = (b_i) \in \mathbb{R}^s$ and the abscissa $\boldsymbol{c} = (c_i) \in \mathbb{R}^s$, where $c_i = \sum_{j=1}^{i-1} a_{ij}$. The accuracy and stability of the method depend on the coefficients of the Butcher tableau $(A, \boldsymbol{b}, \boldsymbol{c})$ [4].

In some cases, the solutions of hyperbolic conservation laws satisfy a monotonicity property. For example, if (2.1) is scalar then solutions are monotonic in the total variation semi-norm [16]. For this reason, many popular spatial discretizations are designed such that, for a suitable class of problems, the

solution $\boldsymbol{u}$ in (2.2) computed with the forward Euler scheme is non-increasing (in time) in some norm, semi-norm, or convex functional; i.e.,

$$\|\boldsymbol{u} + \Delta t \boldsymbol{F}(\boldsymbol{u})\| \leq \|\boldsymbol{u}\|, \quad \text{for all } \boldsymbol{u} \text{ and for } 0 \leq \Delta t \leq \Delta t_{\text{FE}}. \tag{2.3}$$

Note that Δt_{FE} is a property of $\boldsymbol{F}$ (and is independent of $\boldsymbol{u}$). If this is the case, then an SSP method also generates a solution whose norm is non-increasing in time, under a modified time-step restriction.

Definition 2.1 (Strong Stability Preserving)**.** *A Runge–Kutta method is said to be* strong stability preserving *with* SSP coefficient $\mathcal{C} > 0$ *if, whenever the forward Euler condition* (2.3) *holds and*

$$0 \leq \Delta t \leq \mathcal{C} \Delta t_{\text{FE}},$$

the Runge–Kutta method generates a monotonic sequence of solution values $\boldsymbol{u}^n$ *satisfying*

$$\|\boldsymbol{u}^{n+1}\| \leq \|\boldsymbol{u}^n\|.$$

The SSP coefficient $\mathcal{C}$ is a property of the particular time-stepping method and quantifies the allowable time step size relative to that of the forward Euler method. Generally we want the SSP coefficient to be as large as possible for efficiency. To allow a fair comparison of explicit methods we different number of stages, we consider the *effective SSP coefficient*

$$\mathcal{C}_{\text{eff}} = \frac{\mathcal{C}}{s}.$$

Note that the use of the word *effective* here is unrelated to the concept of *effective order* introduced in Section 3.

2.1 Optimal SSP schemes

We say that an SSP Runge–Kutta method is optimal if it has the largest possible SSP coefficient for a given order and a given number of stages. The search for these optimal methods was originally based on expressing the Runge–Kutta method as combinations of forward Euler steps (the Shu–Osher form) and solving a non-linear optimization problem [11, 12, 23, 25, 27, 28]. However, the SSP coefficient is related to the *radius of absolute monotonicity* [21] and, for irreducible Runge–Kutta methods, the two are equivalent [7, 15]. This gives a simplified algebraic characterization of the SSP coefficient [8]; it is the maximum value of r such that the following conditions hold:

$$K(I + rA)^{-1} \geq 0 \tag{2.4a}$$

$$\boldsymbol{e}_{s+1} - rK(I + rA)^{-1}\boldsymbol{e}_s \geq 0, \tag{2.4b}$$

provided that $I + rA$ is invertible. Here

$$K = \begin{pmatrix} A \\ \boldsymbol{b}^{\mathsf{T}} \end{pmatrix},$$

while $\boldsymbol{e}_s$ denotes the vector of ones of length s and I is the $s \times s$ identity matrix. The inequalities are understood component-wise.

The optimization problem of finding optimal SSP Runge–Kutta methods can thus be written as follows:

$$\max_{A,\boldsymbol{b},r} r \quad \text{subject to} \quad (2.4) \text{ and } \Phi(K) = 0. \tag{2.5}$$

Here $\Phi(K)$ represents the order conditions.

Following [16, 19], we will numerically solve the optimization problem (2.5) to find optimal explicit SSP Runge–Kutta methods for various effective orders of accuracy. However, we first need to define the order conditions $\Phi(K)$ for these methods. This is discussed in the next section.

i	tree t_i	elementary weight	$\gamma(t_i)$	i	tree t_i	elementary weight	$\gamma(t_i)$
0	$\emptyset$	1	0	9		$\boldsymbol{b}^T\boldsymbol{c}^4$	5
1		$\boldsymbol{b}^T\boldsymbol{e}$	1	10		$\boldsymbol{b}^T C^2 A\boldsymbol{c}$	10
2		$\boldsymbol{b}^T\boldsymbol{c}$	2	11		$\boldsymbol{b}^T CA\boldsymbol{c}^2$	15
3		$\boldsymbol{b}^T\boldsymbol{c}^2$	3	12		$\boldsymbol{b}^T CA^2\boldsymbol{c}$	30
4		$\boldsymbol{b}^T A\boldsymbol{c}$	6	13		$\boldsymbol{b}^T(A\boldsymbol{c})^2$	20
5		$\boldsymbol{b}^T\boldsymbol{c}^3$	4	14		$\boldsymbol{b}^T A\boldsymbol{c}^3$	20
6		$\boldsymbol{b}^T CA\boldsymbol{c}$	8	15		$\boldsymbol{b}^T ACA\boldsymbol{c}$	40
7		$\boldsymbol{b}^T A\boldsymbol{c}^2$	12	16		$\boldsymbol{b}^T A^2\boldsymbol{c}^2$	60
8		$\boldsymbol{b}^T A^2\boldsymbol{c}$	24	17		$\boldsymbol{b}^T A^3\boldsymbol{c}$	120

Table 3.1: Elementary weights of trees up to order five for a Runge–Kutta method with Butcher tableau $(A, \boldsymbol{b}, \boldsymbol{c})$. Here C is a diagonal matrix with components $c_i = \sum_{j=1}^{i-1} a_{ij}$ and exponents of vectors represent component exponentiation. By convention $\alpha_0 = \alpha(t_0) = 1$, where t_0 denotes the empty tree.

3 The effective order of Runge–Kutta methods

The definition, construction, and application of methods with an effective order of accuracy relies on the use of starting and stopping methods. Specifically, we consider a *starting method* S, a *main method* M, and a *stopping method* S^{-1}. The successive use of these three methods results in a method $P = S^{-1}MS$, which denotes the application method S, followed by method M, followed by method S^{-1}. We want P to have order q, whereas M might have lower classical order $p < q$. We then say M has *effective order* q.

When the method P is used for n steps, $P^n = (S^{-1}MS)^n = (S^{-1}MS)\cdots(S^{-1}MS)(S^{-1}MS)$, it turns out that only M need be used repeatedly, as in $S^{-1}M^nS$, because SS^{-1} leaves the solution unchanged up to order q. The starting method introduces a perturbation to the solution, followed by n time steps of the main method M, and finally the stopping method is used to correct the solution. In Section 5.2, we propose alternative starting and stopping procedures which allow the overall procedure to be SSP.

The effective order of a Runge–Kutta method is defined in an abstract algebraic context introduced by Butcher [1] and developed further in [2,3,5,14] and others. We follow the book [4] in our description and derivation of the effective order conditions.

3.1 The algebraic representation of Runge–Kutta methods

In Butcher's algebraic theory of Runge–Kutta methods [4], methods are viewed as elements in an group G, consisting of real-valued functions on the set of rooted trees. A Runge–Kutta method corresponds to the map that takes each rooted tree t to the corresponding elementary weight $\Phi(t)$ of that Runge–Kutta method. Table 3.1 lists the elementary weights for trees of up to degree five; a general recursive formula can be found in [4, Definition 312A]. For a function $\alpha \in G$ we write the values of the elementary weights as $\alpha_i = \alpha(t_i)$ for tree t_i. A special element of the group $E \in G$ corresponds to the (hypothetical) method which takes one exact step of the solution. The values of $E(t)$ are denoted $1/\gamma(t)$, where $\gamma(t)$ denotes the density of tree t [4] and these are included in Table 3.1. Classical order conditions follow from comparing the elementary weights of a method with these values.

Let $\alpha, \beta \in G$ correspond to Runge–Kutta methods M_1 and M_2 respectively. The application of method M_1 followed by method M_2 corresponds to the multiplicative group operation $\alpha\beta$.[1] This is defined by

[1] We write M_2M_1 to mean the application of M_1 followed by the application of M_2 (following matrix and operator ordering convention) but when referring to products of elements of G we use the reverse ordering ($\alpha\beta$) to match the convention in [4].

q	Effective order conditions
1	$\alpha_1 = 1.$
2	$\alpha_2 = \frac{1}{2}.$
3	$\alpha_3 = \frac{1}{3} + 2\beta_2, \quad \alpha_4 = \frac{1}{6}.$
4	$\alpha_5 = \frac{1}{4} + 3\beta_2 + 3\beta_3, \quad \alpha_6 = \frac{1}{8} + \beta_2 + \beta_3 + \beta_4, \quad \alpha_7 = \frac{1}{12} + \beta_2 - \beta_3 + 2\beta_4, \quad \alpha_8 = \frac{1}{24}.$
5	$\alpha_9 = \frac{1}{5} + 4\beta_2 + 6\beta_3 + 4\beta_5, \quad \alpha_{10} = \frac{1}{10} + \frac{5}{3}\beta_2 - 2\beta_2^2 + \frac{5}{2}\beta_3 + \beta_4 + \beta_5 + 2\beta_6,$ $\alpha_{11} = \frac{1}{15} + \frac{4}{3}\beta_2 + \frac{1}{2}\beta_3 + 2\beta_4 + 2\beta_6 + \beta_7, \quad \alpha_{12} = \frac{1}{30} + \frac{1}{3}\beta_2 - 2\beta_2^2 + \frac{1}{2}\beta_3 + \frac{1}{2}\beta_4 + \beta_6 + \beta_8,$ $\alpha_{13} = \frac{1}{20} + \frac{2}{3}\beta_2 - \beta_2^2 + \beta_3 + \beta_4 + 2\beta_6, \quad \alpha_{14} = \frac{1}{20} + \beta_2 + 3\beta_4 - \beta_5 + 3\beta_7,$ $\alpha_{15} = \frac{1}{40} + \frac{1}{3}\beta_2 + \frac{3}{2}\beta_4 - \beta_6 + \beta_7 + \beta_8, \quad \alpha_{16} = \frac{1}{60} + \frac{1}{3}\beta_2 - \frac{1}{2}\beta_3 + \beta_4 - \beta_7 + 2\beta_8, \quad \alpha_{17} = \frac{1}{120}.$

Table 3.2: Effective order five conditions on α (main method M) in terms of order conditions on β (starting method S). See also [4, § 389]. Recall that α_i and β_i are the elementary weights associated with the index i in Table 3.1. We assume that $\beta_1 = 0$ (see Section 3.2.1).

partitioning the input tree and computing over the resulting forest [4, § 383]. It is expressed by

$$(\alpha\beta)(t) = \sum_{w \lhd t} \Big(\prod_{v \in t \setminus w} \alpha(v)\beta(w) \Big), \tag{3.1}$$

where $w \lhd t$ indicates a subtree of t which includes the root of t and $w \setminus t$ indicates the forest induced by removing w from t [4]. Multiplicity in choosing w must also be accounted for.

Two Runge–Kutta methods M_1 and M_2, are equivalent up to order p if their corresponding elements in G, α and β, satisfy $\alpha(t) = \beta(t)$, for every tree t with $r(t) \leq p$, where $r(t)$ denotes the order of the tree (number of vertices). We denote this equivalence relation by

$$M_1 \underset{p}{\simeq} M_2,$$

In this sense, methods have inverses: the product of α^{-1} and α must match the identity method up to order p. Note that inverse methods up to order p are not unique and inverse methods of explicit methods need not be implicit. We can then define the effective order of accuracy of a method M with starting method S and stopping method S^{-1}.

Definition 3.1. *[4, § 389] Suppose M is a Runge–Kutta method with corresponding $\alpha \in G$. Then the method M is of effective order q if there exists a method S (with corresponding $\beta \in G$) such that*

$$(\beta\alpha\beta^{-1})(t) = E(t), \text{ for every tree with } r(t) \leq q, \tag{3.2}$$

where β^{-1} is an inverse of β up to order q. Recall that E represents one exact step of the solution.

3.2 Effective order conditions

For the main method M to have effective order q its coefficients, and those of the starting and stopping methods, must satisfy a set of algebraic conditions. These *effective order conditions* can be found by rewriting (3.2) as $(\beta\alpha)(t) = (E\beta)(t)$ and applying the product operation (3.1). For trees up to order five these are tabulated in Table 3.2 (and also in [4, § 389]). In general, the effective order conditions allow more degrees of freedom on methods than the classical order conditions. Note that these conditions match the classical order conditions up to second order.

Remark 3.2. *The effective order conditions of the main method for the "tall" trees $t_1, t_2, t_4, t_8, t_{17}, \ldots$ match the classical order conditions and these are precisely the order conditions for linear problems. This follows from inductive application of the product operation (3.1) on the tall trees. Therefore, methods of effective order q have classical order at least q for linear problems.*

q	p	Order conditions for main method M	Order conditions for starting method S
3	2	$\alpha_1 = 1,\ \alpha_2 = \frac{1}{2},\ \alpha_4 = \frac{1}{6}.$	$\beta_1 = 0,\ \beta_2 = -\frac{1}{6} + \frac{1}{2}\alpha_3.$
4	2	$\alpha_1 = 1,\ \alpha_2 = \frac{1}{2},\ \alpha_4 = \frac{1}{6},$ $\frac{1}{4} - \alpha_3 + \alpha_5 - 2\alpha_6 + \alpha_7 = 0,\ \alpha_8 = \frac{1}{24}.$	$\beta_1 = 0,\ \beta_2 = -\frac{1}{6} + \frac{1}{2}\alpha_3,$ $\beta_3 = \frac{1}{12} - \frac{1}{2}\alpha_3 + \frac{1}{3}\alpha_5,\ \beta_4 = -\frac{1}{24} - \frac{1}{3}\alpha_5 + \alpha_6.$
4	3	$\alpha_1 = 1,\ \alpha_2 = \frac{1}{2},\ \alpha_3 = \frac{1}{3},\ \alpha_4 = \frac{1}{6},$ $\frac{1}{12} - \alpha_5 + 2\alpha_6 - \alpha_7 = 0,\ \alpha_8 = \frac{1}{24}.$	$\beta_1 = 0,\ \beta_2 = 0,\ \beta_3 = -\frac{1}{12} + \frac{1}{3}\alpha_5,$ $\beta_4 = -\frac{1}{24} - \frac{1}{3}\alpha_5 + \alpha_6.$
5	2	$\alpha_1 = 1,\ \alpha_2 = \frac{1}{2},\ \alpha_4 = \frac{1}{6},\ \alpha_8 = \frac{1}{24},\ \alpha_{17} = \frac{1}{120},$ $\frac{1}{4} - \alpha_3 + \alpha_5 - 2\alpha_6 + \alpha_7 = 0,$ $\frac{1}{4}\alpha_9 - \alpha_{10} + \alpha_{13} = \beta_2^2,\quad \beta_2 = -\frac{1}{6} + \frac{1}{2}\alpha_3,$ $\frac{3}{10} - \frac{3}{2}\alpha_3 + \alpha_5 + \frac{1}{2}\alpha_9 - 3\alpha_{10} + 3\alpha_{11} - \alpha_{14} = 6\beta_2^2,$ $\frac{1}{15} - \frac{1}{2}\alpha_3 + \alpha_6 + \frac{1}{2}\alpha_9 - 2\alpha_{10} + \alpha_{11} + \alpha_{12} - \alpha_{15} = 2\beta_2^2,$ $\frac{19}{60} - \alpha_3 + \alpha_5 - 2\alpha_6 + \alpha_{11} - 2\alpha_{12} + \alpha_{16} = 4\beta_2^2.$	$\beta_1 = 0,\ \beta_2 = -\frac{1}{6} + \frac{1}{2}\alpha_3,$ $\beta_3 = \frac{1}{12} - \frac{1}{2}\alpha_3 + \frac{1}{3}\alpha_5,\ \beta_4 = -\frac{1}{24} - \frac{1}{3}\alpha_5 + \alpha_6$ $\beta_5 = -\frac{1}{120} + \frac{1}{4}\alpha_3 - \frac{1}{2}\alpha_5 + \frac{1}{4}\alpha_9,$ $\beta_6 = \frac{7}{720} + \beta_2^2 + \frac{1}{12}\alpha_3 - \frac{1}{2}\alpha_6 - \frac{1}{8}\alpha_9 + \frac{1}{2}\alpha_{10},$ $\beta_7 = \frac{8}{45} - 2\beta_2^2 - \frac{7}{12}\alpha_3 + \frac{1}{2}\alpha_5 - \alpha_6 + \frac{1}{4}\alpha_9 - \alpha_{10} + \alpha_{11},$ $\beta_8 = -\frac{1}{120} + \beta_2^2 + \frac{1}{8}\alpha_9 - \frac{1}{2}\alpha_{10} + \alpha_{12}.$
5	3	$\alpha_1 = 1,\ \alpha_2 = \frac{1}{2},\ \alpha_3 = \frac{1}{3},\ \alpha_4 = \frac{1}{6},\ \alpha_8 = \frac{1}{24},$ $\alpha_{17} = \frac{1}{120},\ \frac{1}{12} - \alpha_5 + 2\alpha_6 - \alpha_7 = 0,$ $\frac{1}{4}\alpha_9 - \alpha_{10} + \alpha_{13} = 0,$ $\frac{1}{5} - \alpha_5 - \frac{1}{2}\alpha_9 + 3\alpha_{10} - 3\alpha_{11} + \alpha_{14} = 0,$ $\frac{1}{10} - \alpha_6 - \frac{1}{2}\alpha_9 + 2\alpha_{10} - \alpha_{11} - \alpha_{12} + \alpha_{15} = 0,$ $\frac{1}{60} - \alpha_5 + 2\alpha_6 - \alpha_{11} + 2\alpha_{12} - \alpha_{16} = 0.$	$\beta_1 = 0,\ \beta_2 = 0,\ \beta_3 = -\frac{1}{12} + \frac{1}{3}\alpha_5$ $\beta_4 = -\frac{1}{24} - \frac{1}{3}\alpha_5 + \alpha_6,$ $\beta_5 = \frac{3}{40} - \frac{1}{2}\alpha_5 + \frac{1}{4}\alpha_9,$ $\beta_6 = \frac{3}{80} - \frac{1}{2}\alpha_6 - \frac{1}{8}\alpha_9 + \frac{1}{2}\alpha_{10},$ $\beta_7 = -\frac{1}{60} + \frac{1}{2}\alpha_5 - \alpha_6 + \frac{1}{4}\alpha_9 - \alpha_{10} + \alpha_{11},$ $\beta_8 = -\frac{1}{120} + \frac{1}{8}\alpha_9 - \frac{1}{2}\alpha_{10} + \alpha_{12}.$
5	4	$\alpha_1 = 1,\ \alpha_2 = \frac{1}{2},\ \alpha_3 = \frac{1}{3},\ \alpha_4 = \frac{1}{6},\ \alpha_5 = \frac{1}{4},$ $\alpha_6 = \frac{1}{8},\ \alpha_7 = \frac{1}{12},\ \alpha_8 = \frac{1}{24},\ \alpha_{17} = \frac{1}{120},$ $\frac{1}{4}\alpha_9 - \alpha_{10} + \alpha_{13} = 0,$ $\frac{1}{20} + \frac{1}{2}\alpha_9 - 3\alpha_{10} + 3\alpha_{11} - \alpha_{14} = 0,$ $\frac{1}{40} + \frac{1}{2}\alpha_9 - 2\alpha_{10} + \alpha_{11} + \alpha_{12} - \alpha_{15} = 0,$ $\frac{1}{60} - \alpha_{11} + 2\alpha_{12} - \alpha_{16} = 0.$	$\beta_1 = 0,\ \beta_2 = 0,$ $\beta_3 = 0,\ \beta_4 = 0,$ $\beta_5 = -\frac{1}{20} + \frac{1}{4}\alpha_9,$ $\beta_6 = -\frac{1}{40} - \frac{1}{8}\alpha_9 + \frac{1}{2}\alpha_{10},$ $\beta_7 = -\frac{1}{60} + \frac{1}{4}\alpha_9 - \alpha_{10} + \alpha_{11},$ $\beta_8 = -\frac{1}{120} + \frac{1}{8}\alpha_9 - \frac{1}{2}\alpha_{10} + \alpha_{12}.$

Table 3.3: Effective order q, classical order p conditions on α and β for the main and starting methods, M and S respectively.

3.2.1 Order conditions of the main and starting methods

As recommended in [4], we consider the β_i as free parameters when determining the α_i. The relationship in Table 3.2 between the α_i and β_i is mostly linear (although there are a few β_2^2 terms). It is thus straightforward to (mostly) isolate the equations for α_i and determine the β_i as linear combination of the α_i. This separation provides maximal degrees of freedom and minimizes the number of constraints when constructing the method M. The resulting effective order conditions for the main method M are given in Table 3.3 (up to effective order five). For a specified classical and effective order, these are the equality constraints $\Phi(K)$ in the optimization problem (2.5) for method M.

Constructing the main method M then determines the α values and we obtain a set of order conditions on β (for that particular choice of M). These are given in the right-half of Table 3.3. We can also find the order conditions of S^{-1} in terms of the β_i (see [4, Table 386(III)]). We note that increasing the classical order of the main method results in setting more of the β_i to zero.

Tables 3.2 and 3.3 both assume that $\beta_1 = 0$ (i.e., the starting and stopping methods perturb the solution but do not advance the solution in time). This assumption is without loss of generality following [4, Lemma 389A], the proof of which shows that we can always find starting procedures with $\beta_1 = 0$ for

which the main method has effective order q, whenever this holds for a starting method with $\beta_1 \neq 0$.

4 Explicit SSP Runge–Kutta methods have effective order at most four

The classical order of any explicit SSP Runge–Kutta method cannot be greater than four [24]. It turns out that the effective order of any explicit SSP Runge–Kutta method also cannot be greater than four, although the proof of this result is more involved. We begin by recalling a well-known result.

Lemma 4.1. *(see [21, Theorem 4.2], [24, Lemma 4.2]) Any irreducible Runge–Kutta method with positive SSP coefficient $\mathcal{C} > 0$ must have positive weights $\boldsymbol{b} > \boldsymbol{0}$.*

The main result of this section is

Theorem 4.2. *Any explicit Runge–Kutta method with positive weights $\boldsymbol{b} > \boldsymbol{0}$ has effective order at most four.*

The proof of Theorem 4.2 is deferred to the end of this section.

Corollary 4.3. *Let M denote an irreducible explicit Runge–Kutta method with $\mathcal{C} > 0$. Then M has effective order at most four.*

Proof. The proof follows immediately from Lemma 4.1 and Theorem 4.2. □

Remark 4.4. *It is worth noting here an additional result that follows directly from what we have proved. Using Theorem 4.2 and [6, Theorem 4.1], it follows that any irreducible explicit Runge–Kutta method with positive radius of circle contractivity has effective order at most four.*

The proof of Theorem 4.2 makes use of the following lemma.

Lemma 4.5. *Let $\boldsymbol{b}, \boldsymbol{v} \in \mathbb{R}^n$ be given such that*

$$b_i > 0 \text{ for all } i, \tag{4.1a}$$

$$\sum_{i=1}^{n} b_i = 1, \tag{4.1b}$$

$$\sum_{i=1}^{n} b_i v_i^2 = \left(\sum_{i=1}^{n} b_i v_i \right)^2. \tag{4.1c}$$

Then all v_i are equal but at most one; in other words, there exists $\mu \in \mathbb{R}$ and an integer k such that $v_i = \mu$ for all $i \neq k$.

Proof. First observe that in the case that $v_i = 0$ for all i, the stated result holds. Otherwise, let k be an integer between 1 and n such that $v_k \neq 0$. Then by collecting terms in powers of v_k, (4.1c) can be written as

$$b_k(1 - b_k)v_k^2 - 2b_k v_k \sum_{i \neq k} b_i v_i + \sum_{i \neq k} b_i v_i^2 - \left(\sum_{i \neq k} b_i v_i \right)^2 = 0.$$

This is a quadratic equation in v_k whose roots are real if and only if

$$4b_k^2 \left(\sum_{i \neq k} b_i v_i \right)^2 - 4b_k(1 - b_k) \left(\sum_{i \neq k} b_i v_i^2 - \left(\sum_{i \neq k} b_i v_i \right)^2 \right) \geq 0.$$

Expanding and canceling terms yields

$$(1-b_k)\sum_{i\neq k} b_i v_i^2 - \left(\sum_{i\neq k} b_i v_i\right)^2 \leq 0.$$

By (4.1b), $1-b_k = \sum_{j\neq k} b_j$, so we have

$$\sum_{j\neq k} b_j \sum_{i\neq k} b_i v_i^2 - \sum_{j\neq k} b_j v_j \sum_{i\neq k} b_i v_i \leq 0.$$

Noting that the terms corresponding to $i=j$ in the two double sums cancel and this gives

$$\sum_{j\neq k} b_j \sum_{i\neq k,j} b_i v_i (v_i - v_j) \leq 0.$$

Adding the left hand side to itself, but with i, j reversed, yields

$$\sum_{j\neq k} b_j \sum_{i\neq k,j} b_i v_i (v_i - v_j) - \sum_{i\neq k} b_i \sum_{j\neq k,i} b_j v_j (v_i - v_j) \leq 0.$$

This simplifies to

$$\sum_{j\neq k} \sum_{i\neq k,j} b_j b_i (v_i - v_j)^2 \leq 0.$$

Together with (4.1a), this implies that $v_i = v_j$ for all $i, j \neq k$. □

We can now prove Theorem 4.2:

Proof of Theorem 4.2. Any method of effective order five must have classical order at least two (see [4] or Table 3.3). Thus it is sufficient to show that any method with all positive weights cannot satisfy the conditions of effective order five and classical order two.

Let $(A, \boldsymbol{b}, \boldsymbol{c})$ denote the coefficients of an explicit Runge–Kutta method with effective order at least five, classical order at least two, and positive weights $\boldsymbol{b} > \boldsymbol{0}$. The effective order five and classical order two conditions (see Table 3.3) include the following:

$$\boldsymbol{b}^T \boldsymbol{e} = 1, \tag{4.2a}$$

$$\boldsymbol{b}^T A \boldsymbol{c} = \frac{1}{6}, \tag{4.2b}$$

$$\frac{1}{2}\boldsymbol{b}^T \boldsymbol{c}^2 - \frac{1}{6} = \beta_2, \tag{4.2c}$$

$$\frac{1}{4}\boldsymbol{b}^T \boldsymbol{c}^4 - \boldsymbol{b}^T C^2 A \boldsymbol{c} + \boldsymbol{b}^T (A\boldsymbol{c})^2 = \beta_2^2, \tag{4.2d}$$

where the powers on vectors are understood component-wise. Define

$$\boldsymbol{v} = \frac{1}{2}\boldsymbol{c}^2 - A\boldsymbol{c}$$

and

$$\boldsymbol{w} = \boldsymbol{v}^2 - \beta_2 \boldsymbol{v}. \tag{4.3}$$

Then substituting (4.2b) in (4.2c) gives

$$\beta_2 = \boldsymbol{b}^T \boldsymbol{v}. \tag{4.4}$$

Also, (4.2d) can be expressed as

$$\beta_2^2 = \boldsymbol{b}^T \boldsymbol{v}^2. \tag{4.5}$$

Multiplying (4.4) by β_2 and subtracting from (4.5) gives

$$\boldsymbol{b}^T \boldsymbol{w} = 0. \tag{4.6}$$

We divide the analysis into three cases.

Case 1: $\beta_2 = 0$**.** First consider the case that $\beta_2 = 0$. Then $\boldsymbol{b}^T\boldsymbol{v}^2 = 0$, but $\boldsymbol{v} \neq \boldsymbol{0}$ because explicit methods cannot have stage order two [24]. This implies that $b_j \leq 0$ for some j, which is a contradiction. So far we have proven the result for classical order $p \geq 3$ and the proof is similar to the result mentioned in [24]. The remainder of our proof deals with classical order two, where $\beta_2 \neq 0$.

Case 2: $\boldsymbol{w} = \boldsymbol{0}, \beta_2 \neq 0$**.** By the definition of $\boldsymbol{w}$ in (4.3), we have $v_i^2 - \beta_2 v_i = 0$ for all $i \in \{1, \ldots, s\}$, so for each i either $v_i = 0$ or $v_i = \beta_2$. Let the set $J = \{i : v_i = \beta_2\}$. Note that $v_1 = 0$ because the first row of matrix A is identically zero. Since $\beta_2 \neq 0$ and $\boldsymbol{v} \neq \boldsymbol{0}$, the set J is not empty. Then (4.4) yields

$$\beta_2 = \sum_{i=1}^{s} b_i v_i = \sum_{i \in J} b_i \beta_2 = \beta_2 \sum_{i \in J} b_i,$$

which implies $\sum_{i \in J} b_i = 1$, but this contradicts (4.2a)

Case 3: $\boldsymbol{w} \neq \boldsymbol{0}, \beta_2 \neq 0$**.** Since $\boldsymbol{b} > \boldsymbol{0}$, (4.6) implies that $\boldsymbol{w}$ contains both positive and negative elements. Furthermore, $v_1 = 0$ for any explicit method, thus $w_1 = 0$. Then, we can choose $i, j \in \{2, \ldots, s\}$ such that $w_i < 0 < w_j$. By (4.3) $v_i \neq 0$, $v_j \neq 0$, and $v_i \neq v_j$. Application of Lemma 4.5 reveals that all v_k for $k \in \{1, 2, \ldots, s\}$ must be equal except for one, which is a contradiction since $v_1 = 0$.

□

5 Optimal explicit SSP Runge–Kutta schemes with maximal effective order

In this section, we use the SSP theory and Butcher's theory of effective order (Sections 2 and 3) to find optimal explicit SSP Runge–Kutta schemes with prescribed effective order and classical order. According to Corollary 4.3, there are no explicit SSPRK methods of effective order five, and therefore we need only consider methods with effective order up to four.

Recall from Section 3 that the methods with an effective order of accuracy involve a main method M as well as starting and stopping methods S and S^{-1}. In Section 5.2 we introduce a novel approach to construction of starting and stopping methods in order to allow them to be SSP.

We denote by ESSPRK(s, q, p) an s-stage explicit SSP Runge–Kutta method of effective order q and classical order p. Also we write SSPRK(s, q) for an s-stage explicit SSP Runge–Kutta method of order q.

5.1 The main method

Our search is carried out in two steps, first searching for optimal main methods M and then for possible corresponding methods S and S^{-1}. For a given number of stages, effective order, and classical order, our aim is thus to find an optimal main method, meaning one with the largest possible SSP coefficient $\mathcal{C}$.

To find a method ESSPRK(s, q, p) with Butcher tableau $(A, \boldsymbol{b}, \boldsymbol{c})$, we consider the optimization problem (2.5) with $\Phi(K)$ representing the conditions for effective order q and classical order p (as per Table 3.3). The methods are found through numerical search, using MATLAB's optimization toolbox. Specifically, we use `fmincon` with a sequential quadratic programming approach [16, 19]. This process does not guarantee a global minimizer, so many searches from random initial guesses are performed to help ensure the method with the largest possible SSP coefficient is found.

5.1.1 Optimal SSP coefficients

Useful bounds on the optimal SSP coefficient can be obtained by considering an important relaxation. In the relaxed problem, the method is required to be accurate and strong stability preserving only for linear, constant-coefficient initial value problems. This leads to a reduced set of order conditions and a

q	p	stages s										
		1	2	3	4	5	6	7	8	9	10	11
3	2	–	–	**0.33**	**0.50**	**0.53**	**0.59**	**0.61**	**0.64**	**0.67**	**0.68**	**0.69**
4	2	–	–	–	0.22	0.39	**0.44**	**0.50**	**0.54**	**0.57**	**0.60**	**0.62**
4	3	–	–	–	0.19	0.37	0.43	**0.50**	**0.54**	**0.57**	**0.60**	**0.62**

Table 5.1: Effective SSP coefficients $\mathcal{C}_{\text{eff}} = \mathcal{C}/s$ of the best known ESSPRK(s, q, p) methods. Entries in bold achieve the bound $\mathcal{C}^{\text{lin}}_{s,q}$ given by the linear SSP coefficient and are therefore optimal. If no positive $\mathcal{C}$ can be found, we use "–" to indicate non-existence. The optimal fourth-order linear SSP coefficients are $\mathcal{C}^{\text{lin}}_{4,4} = 0.25$, $\mathcal{C}^{\text{lin}}_{5,4} = 0.40$ and $\mathcal{C}^{\text{lin}}_{6,4} = 0.44$.

relaxed absolute monotonicity condition [16, 17, 20]. We denote the maximal SSP coefficient for linear problems (maximized over all methods with order q and s stages) by $\mathcal{C}^{\text{lin}}_{s,q}$.

Let $\mathcal{C}_{s,q}$ denote the maximal SSP coefficient (relevant to non-linear problems) over all methods of s stages with order q. Let $\mathcal{C}_{s,q,p}$ denote the object of our study, i.e. the maximal SSP coefficient (relevant to non-linear problems) over all methods of s stages with effective order q and classical order p. From Remark 3.2 and the fact that the ESSPRK(s, q, p) methods form a super class of the SSPRK(s, q) methods, we have

$$\mathcal{C}_{s,q} \leq \mathcal{C}_{s,q,p} \leq \mathcal{C}^{\text{lin}}_{s,q}. \tag{5.1}$$

The effective SSP coefficients for methods with up to eleven stages are shown in Table 5.1. Recall from Section 4 that $q = 5$ implies a zero SSP coefficient and from Section 3 that for $q = 1, 2$, the class of explicit Runge–Kutta methods with effective order q is the simply the class of explicit Runge–Kutta methods with order q. Therefore we consider only methods of effective order $q = 3$ and $q = 4$. Exact optimal values of $\mathcal{C}^{\text{lin}}_{s,q}$ are known for many classes of methods; for example see [16, 17, 20]. Those results and (5.1) allow us to determine the optimal value of $\mathcal{C}_{s,q,p}$ *a priori* for the cases $q = 3$ (for any s) and for $q = 4, s = 10$, since in those cases we have $\mathcal{C}_{s,q} = \mathcal{C}^{\text{lin}}_{s,q}$.

5.1.2 Effective order three methods

Since $\mathcal{C}_{s,q} = \mathcal{C}^{\text{lin}}_{s,q}$ for $q = 3$, the optimal effective order three methods have SSP coefficients equal to the corresponding optimal classical order three methods. In the cases of three and four stages, we are able to determine exact coefficients for families of optimal methods of effective order three.

Theorem 5.1. *A family of optimal three-stage, effective order three SSP Runge–Kutta methods of classical order two, with SSP coefficient $\mathcal{C} = 1$, is given by*

$$\begin{aligned}
\boldsymbol{Y}_1 &= \boldsymbol{u}^n, \\
\boldsymbol{Y}_2 &= \boldsymbol{u}^n + \Delta t \boldsymbol{F}(\boldsymbol{Y}_1), \\
\boldsymbol{Y}_3 &= \boldsymbol{u}^n + \gamma \Delta t \boldsymbol{F}(\boldsymbol{Y}_1) + \gamma \Delta t \boldsymbol{F}(\boldsymbol{Y}_2), \\
\boldsymbol{u}^{n+1} &= \boldsymbol{u}^n + \frac{5\gamma - 1}{6\gamma} \Delta t \boldsymbol{F}(\boldsymbol{Y}_1) + \frac{1}{6} \Delta t \boldsymbol{F}(\boldsymbol{Y}_2) + \frac{1}{6\gamma} \Delta t \boldsymbol{F}(\boldsymbol{Y}_3),
\end{aligned}$$

where $1/4 \leq \gamma \leq 1$ is a free parameter.

Theorem 5.2. *A family of optimal four-stage, effective order three SSP Runge–Kutta methods of classical*

order two, with SSP coefficient $\mathcal{C} = 2$ is given by

$$\begin{aligned}
\boldsymbol{Y}_1 &= \boldsymbol{u}^n, \\
\boldsymbol{Y}_2 &= \boldsymbol{u}^n + \frac{1}{2}\Delta t \boldsymbol{F}(\boldsymbol{Y}_1), \\
\boldsymbol{Y}_3 &= \boldsymbol{u}^n + \frac{1}{2}\Delta t \boldsymbol{F}(\boldsymbol{Y}_1) + \frac{1}{2}\Delta t \boldsymbol{F}(\boldsymbol{Y}_2), \\
\boldsymbol{Y}_4 &= \boldsymbol{u}^n + \gamma \Delta t \boldsymbol{F}(\boldsymbol{Y}_1) + \gamma \Delta t \boldsymbol{F}(\boldsymbol{Y}_2) + + \gamma \Delta t \boldsymbol{F}(\boldsymbol{Y}_3), \\
\boldsymbol{u}^{n+1} &= \boldsymbol{u}^n + \frac{8\gamma - 1}{12\gamma}\Delta t \boldsymbol{F}(\boldsymbol{Y}_1) + \frac{1}{6}\Delta t \boldsymbol{F}(\boldsymbol{Y}_2) + \frac{1}{6}\Delta t \boldsymbol{F}(\boldsymbol{Y}_3) + \frac{1}{12\gamma}\Delta t \boldsymbol{F}(\boldsymbol{Y}_4),
\end{aligned}$$

where $1/6 \le \gamma \le 1/2$ is a free parameter.

Proof. In either theorem, feasibility can be verified by direct calculation of the conditions in problem (2.5). Optimality follows because $\mathcal{C} = \mathcal{C}^{\text{lin}}_{s,q}$. □

Theorem 5.1 gives a *family* of three-stage methods. The particular value of $\gamma = 1/4$ corresponds to the classical Shu–Osher SSPRK$(3, 3)$ method [11]. Similarly, in Theorem 5.2 the particular value of $\gamma = 1/6$ corresponds to the usual SSPRK$(4, 3)$ method. It seems possible that for each number of stages, the ESSPRK$(s, 3, 2)$ methods may form a family in which an optimal SSPRK$(s, 3)$ method is a particular member.

5.1.3 Effective order four methods

The ESSPRK$(s, 4, p)$ methods can have classical order $p = 2$ or 3. In either case, for stages $7 \le s \le 11$ the methods found are optimal because the SSP coefficient attains the upper bound of $\mathcal{C}^{\text{lin}}_{s,q}$. For fewer stages, the new methods still have SSP coefficients up to 30% larger than that of explicit SSPRK(s, q) methods. In the particular case of four-stage methods we have the following:

Remark 5.3. *In contrast with the non-existence of an SSPRK(4, 4) method [11, 24], we are able to find ESSPRK(4, 4, 2) and ESSPRK(4, 4, 3) methods. The coefficients of these methods are found in Tables 5.3 and 5.4.*

Additionally, we find two families of methods with effective order four, for which $\mathcal{C}_{\text{eff}}$ asymptotically approaches unity. The families consist of second order methods with $s = n^2 + 1$ stages and SSP coefficient $\mathcal{C} = n^2 - n$. They are optimal since $\mathcal{C} = \mathcal{C}^{\text{lin}}_{4,2}$ [20, Theorem 5.2(c)]. It is convenient to express the coefficients in the modified Shu–Osher form [9]

$$\begin{aligned}
\boldsymbol{Y}_i &= v_i \boldsymbol{u}^n + \sum_{j=1}^{i-1} (\alpha_{ij} \boldsymbol{Y}_j + \Delta t \beta_{ij} \boldsymbol{F}(\boldsymbol{Y}_j)), \ 1 \le i \le s+1 \\
\boldsymbol{u}^{n+1} &= \boldsymbol{Y}_{s+1},
\end{aligned}$$

because of the sparsity of the matrices $\alpha, \beta \in \mathbb{R}^{(s+1)\times s}$ and vector $\boldsymbol{v} \in \mathbb{R}^s$. For $n \ge 3$ the non-zero elements are given by

$$\begin{aligned}
v_1 = 0, \qquad v_{n^2+2} &= \frac{2}{(n^2+1)\big((n-1)^2+1\big)}, \\
\alpha_{n^2-2n+4,(n-2)^2} &= \frac{n^2 - 1 \pm \sqrt{n^3 - 3n^2 + n + 1}}{4n^2 - 6n + 2}, \\
\alpha_{n^2+2,n^2+1} &= \frac{n(n-1)^2}{(2n-1)(n^2+1)(1 - \alpha_{n^2-2n+4,(n-2)^2})}, \\
\alpha_{n^2+2,n^2-2n+2} &= 1 - v_{n^2+2,1} - \alpha_{n^2+2,n^2+1}, \\
\alpha_{i+1,i} &= \begin{cases} 1 - \alpha_{i+1,(n-2)^2}, & i = n^2 - 2n + 3 \\ 1, & \text{otherwise}, \end{cases}
\end{aligned}$$

$\rho(t) = (\beta\alpha)(t)$	$\tau(t) = (\alpha\beta^{-1})(t)$
$\rho_1 = \alpha_1$	$\tau_1 = \alpha_1$
$\rho_2 = \alpha_2 + \beta_2$	$\tau_2 = \alpha_2 - \beta_2$
$\rho_3 = \alpha_3 + \beta_3$	$\tau_3 = \alpha_3 - 2\alpha_1\beta_2 - \beta_3$
$\rho_4 = \alpha_4 + \alpha_1\beta_2 + \beta_4$	$\tau_4 = \alpha_4 - \alpha_1\beta_2 - \beta_4$
$\rho_5 = \alpha_5 + \beta_5$	$\tau_5 = \alpha_5 - 3\alpha_1^2\beta_2 - 3\alpha_1\beta_3 - \beta_5$
$\rho_6 = \alpha_6 + \alpha_2\beta_2 + \beta_6$	$\tau_6 = \alpha_6 - (\alpha_1^2 + \alpha_2 - \beta_2)\beta_2 - \alpha_1\beta_3 - \alpha_1\beta_4 - \beta_6$
$\rho_7 = \alpha_7 + \alpha_1\beta_3 + \beta_7$	$\tau_7 = \alpha_7 - 2\alpha_1\beta_4 - \alpha_1^2\beta_2 - \beta_7$
$\rho_8 = \alpha_8 + \alpha_1\beta_4 + \alpha_2\beta_2 + \beta_8$	$\tau_8 = \alpha_8 - \alpha_1\beta_4 - \alpha_2\beta_2 + \beta_2^2 - \beta_8$

Table 5.2: Order conditions on ρ and τ up to effective order four for starting and stopping methods R and T, respectively. The upper block represents the effective order three conditions. As in Table 3.2 and Table 3.3 we assume $\beta_1 = 0$.

where $1 \le i \le n^2$ and

$$\beta_{i,j} = \frac{\alpha_{i,j}}{n^2 - n}, \quad 1 \le i \le n^2 + 2, \;\; 1 \le j \le n^2 + 1.$$

In [9, § 6.2.2], a similar pattern was found for SSPRK$(s, 3)$ methods.

5.2 Starting and stopping methods

Having constructed an ESSPRK(s, q, p) scheme that can be used as the main method M, we want to find perturbation methods S and S^{-1} such that the Runge–Kutta scheme $S^{-1}MS$ attains classical order q, equal to the effective order of method M. We also want the resulting overall process to be SSP. However at least one of the S and S^{-1} methods is not SSP: if $\beta_1 = 0$ then $\sum_i b_i = 0$ implies the presence of at least one negative weight and thus neither scheme can be SSP. Even if we consider methods with $\beta_1 \neq 0$, one of S or S^{-1} must step backwards and thus that method cannot be SSP (unless we consider the downwind operator [10, 18, 25]).

In order to overcome this problem and achieve "bona fide" SSPRK methods with an effective order of accuracy, we need to choose different starting and stopping methods. We consider methods R and T which each take a positive step such that $R \underset{q}{\simeq} MS$ and $T \underset{q}{\simeq} S^{-1}M$. That is, the order conditions of R and T must match those of MS and $S^{-1}M$, respectively, up to order q. This gives a new $TM^{n-2}R$ scheme which is equivalent up to order q to the $S^{-1}M^nS$ scheme and attains classical order q. Each starting and stopping procedures now take a positive step forward in time.

To derive order conditions for the R and T methods, consider their corresponding functions in group G to be ρ and τ respectively. Then the equivalence is expressed as

$$\rho(t) = (\beta\alpha)(t) \text{ and } \tau(t) = (\alpha\beta^{-1})(t), \quad \text{for all trees } t \text{ with } r(t) \le q. \tag{5.2}$$

Rewriting the second condition in (5.2) as $(\tau\beta)(t) = \alpha(t)$, the order conditions for the starting and stopping methods can be determined by (3.1) and are given in Table 5.2. These conditions could be constructed more generally but here we have assumed $\beta_1 = 0$ (see Section 3.2.1); this will be sufficient for constructing SSP starting and stopping conditions.

5.2.1 Optimizing the starting and stopping methods

It turns out that the order conditions from (5.2) do not contradict the SSP requirements. We can thus find methods R and T using the optimization procedure described in Section 2.1 with the order conditions given by Table 5.2 for $\Phi(K)$ in (2.5).

The values of α_i are determined by the main method M. Also note that for effective order q, the algebraic expressions on β up to order $q-1$ are already found by the optimization procedure of the main

0				
0.730429885783319	0.730429885783319			
0.644964638145795	0.251830917810810	0.393133720334985		
1.000000000000000	0.141062771617064	0.220213358584678	0.638723869798257	
	0.384422161080494	0.261154113377550	0.127250689937518	0.227173035604438

(a) Main method M, ESSPRK$(4,4,2)$

0					
0.545722177514735	0.545722177514735				
0.842931687441527	0.366499989048164	0.476431698393363			
0.574760809487828	0.135697968350722	0.176400587890242	0.262662253246864		
0.980872743236632	0.103648417776838	0.134737771331049	0.200625899485633	0.541860654643112	
	0.233699169638954	0.294263351266422	0.065226988215286	0.176168374199685	0.230642116679654

(b) Starting method R

0				
0.509877496215340	0.509877496215340			
0.435774135529007	0.182230305923759	0.253543829605247		
0.933203341300203	0.148498121305090	0.206610981494095	0.578094238501017	
	0.307865440399752	0.171863794704750	0.233603236964822	0.286667527930676

(c) Stopping method T

Table 5.3: ESSPRK(4,4,2): an effective order four SSPRK method with four stages and classical order two with its associated starting and stopping methods.

method (see Table 3.3). However, the values of the order q elementary weights on β are not known; these are β_3 and β_4 for effective order three and β_5, β_6, β_7 and β_8 for effective order four. From Table 5.2, we see that both the R and T methods depend on these parameters. Our approach is to optimize for both methods at once: we solve a modified version of the optimization problem (2.5) where we simultaneously maximize both SSP coefficients subject to the constraints given in (5.2) and conditions on β given by Table 3.3. The unknown elementary weights on β are used as free parameters. In practice, we maximize the objective function $\min(r_1, r_2)$, where r_1 and r_2 are the radii of absolute monotonicity of the methods R and T.

We were able to construct starting and stopping schemes for each main method, with an SSP coefficient at least as large as that of the main method. This allows the usage of a uniform time-step $\Delta t \leq \mathcal{C}\Delta t_{\text{FE}}$, where $\mathcal{C}$ is the SSP coefficient of the main method. The additional computational cost of the starting and stopping methods is minimal: for methods R and T associated with an s-stage main method, at most $s+1$ and s stages, respectively, appear to be required. Tables 5.3 and 5.4 show the coefficients of the schemes where the main method is ESSPRK$(4,4,2)$ and ESSPRK$(4,4,3)$, respectively.

It is important to note that in practice, if accurate values are needed at any time other than the final time, the computation must invoke the stopping method to obtain them. Furthermore, changing step-size would require first applying the stopping method with the old step-size and then applying the starting method with the new step-size.

6 Numerical experiments

Having constructed strong stability preserving $TM^{n-2}R$ schemes in the previous section, we now numerically verify their properties. Specifically, we use a convergence study to show that the procedure attains order of accuracy q, the effective order of M. We also demonstrate on Burgers' equation that the SSP coefficient accurately measures the maximal time-step for which the methods are strong stability preserving.

0				
0.601245068769724	0.601245068769724			
0.436888719886063	0.139346829159954	0.297541890726109		
0.747760163757110	0.060555450075478	0.129301708677891	0.557903005003740	
	0.220532078662434	0.180572397883936	0.181420582644840	0.417474940808790

(a) Main method M, ESSPRK$(4,4,3)$

0					
0.438463764036947	0.438463764036947				
0.639336395725557	0.213665532574654	0.425670863150903			
0.434353425654020	0.061345094040860	0.122213530726218	0.250794800886942		
0.843416464962307	0.039559973266996	0.078812561688700	0.161731525131914	0.563312404874697	
	0.154373542967849	0.307547588471376	0.054439037790856	0.189611674483496	0.294028156286422

(b) Starting method R

0				
0.556337718891090	0.556337718891090			
0.428870688216872	0.166867537553458	0.262003150663414		
0.815008947642716	0.104422177204659	0.163956032598547	0.546630737839510	
	0.203508169408374	0.096469758967330	0.321630956102914	0.378391115521382

(c) Stopping method T

Table 5.4: ESSPRK(4,4,3): an effective order four SSPRK method with four stages and classical order three with its associated starting and stopping methods.

6.1 Convergence study

We consider the van der Pol system [13]

$$\begin{aligned} u_1'(t) &= u_2(t), \\ u_2'(t) &= \mu\big(1 - u_1^2(t)\big)u_2(t) - u_1(t), \end{aligned} \tag{6.1}$$

over the time interval $t \in [0, 50]$ with $\mu = 2$ and initial values $u_1(0) = 2$ and $u_2(0) = 1$. The reference solution for the convergence study is calculated by MATLAB's `ode45` solver with relative and absolute tolerances set to 10^{-13}.

We solve the initial value problem (6.1) using SSP $TM^{n-2}R$ schemes. The solution is computed using $n = 100 \cdot 2^k$ time steps for $k = 2, \ldots, 7$. The error at $t = 50$ with respect to time-step is shown in Figure 6.1 on a logarithmic scale. The convergence study is performed for $TM^{n-2}R$ schemes with various number of stages s and the results show that the schemes attain an order of accuracy equal to the effective order of their main method M. It is important in doing this sort of convergence study that the effective order of accuracy can only be obtained after the stopping method is applied. Intermediate steps will typically only be order p accurate (the classical order of the main method). Finally, we note that the methods with more stages generally exhibit smaller errors (for a given step size).

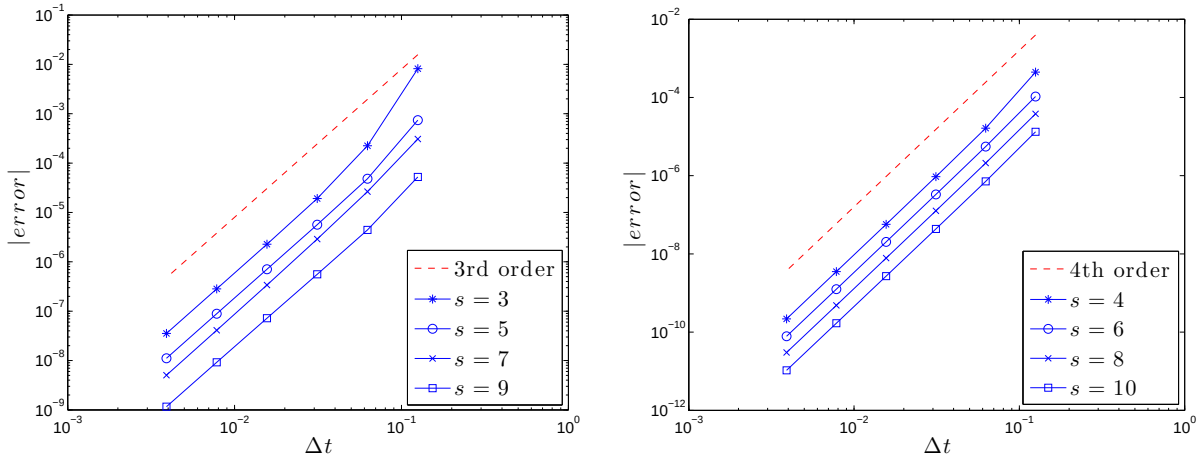
6.2 Burgers' equation

The inviscid Burgers' equation consists of the scalar hyperbolic conservation law

$$U_t + f(U)_x = 0, \tag{6.2}$$

with flux function $f(U) = \frac{1}{2}U^2$. We consider initial data $U(0, x) = \frac{1}{2} - \frac{1}{4}\sin \pi x$, on a periodic domain $x \in [0, 2)$. The solution advances to the right where it eventually exhibits a shock. We perform a semi-discretization using an upwind approximation to obtain the system of ODEs

$$\frac{\mathrm{d}}{\mathrm{d}t}u_i = -\frac{f(u_i) - f(u_{i-1})}{\Delta x}.$$



(a) ESSPRK$(s, 3, 2)$ (b) ESSPRK$(s, 4, 2)$

Figure 6.1: Convergence study of $TM^{n-2}R$ Runge–Kutta schemes when (a) M is an ESSPRK$(s, 3, 2)$ method and (b) M is an ESSPRK$(s, 4, 2)$ method.

This spatial discretization is total-variation-diminishing (TVD) when coupled with the forward Euler method under the restriction [22]

$$\Delta t \leq \Delta t_{\text{FE}} = \Delta x / \|U(0, x)\|_\infty.$$

Recall that a time discretization with SSP coefficient $\mathcal{C}$ will give a TVD solution for $\Delta t \leq \mathcal{C}\Delta t_{\text{FE}}$.

Burgers' equation was solved using an SSP $TM^{n-2}R$ scheme with time-step restriction $\Delta t \leq \sigma \Delta t_{\text{FE}}$, where σ indicates the size of the time step. We integrate to roughly time $t_{\text{f}} = 1.62$ with 200 points in space. Figure 6.2 shows that if σ is chosen less than the SSP coefficient of the main method, then no oscillations are observed. If this stability limit is violated, then oscillations may appear.

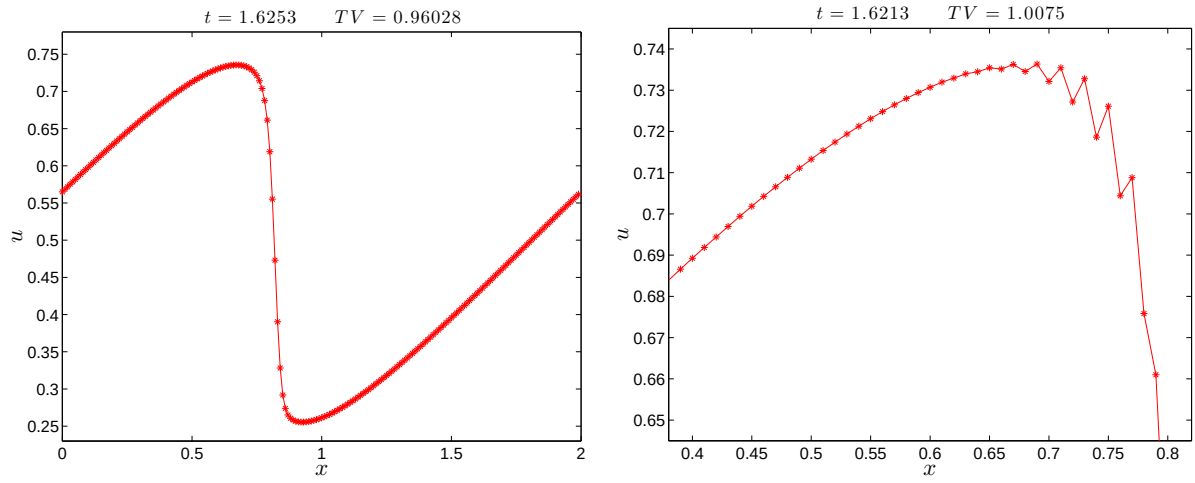
We measure these oscillations by computing the total variation of the numerical solution. When M is an ESSPRK$(4, 4, 2)$ method, it turns out that $\sigma = 1.57$ is the largest value of σ for which the total variation is monotonically decreasing during the calculation. This is 79% larger than the value of the SSP coefficient $\mathcal{C} = 0.88$.

We also consider Burgers' equation with a discontinuous square wave initial condition

$$U(0, x) = \begin{cases} 1, & 0.5 \leq x \leq 1.5 \\ 0, & \text{otherwise.} \end{cases} \tag{6.3}$$

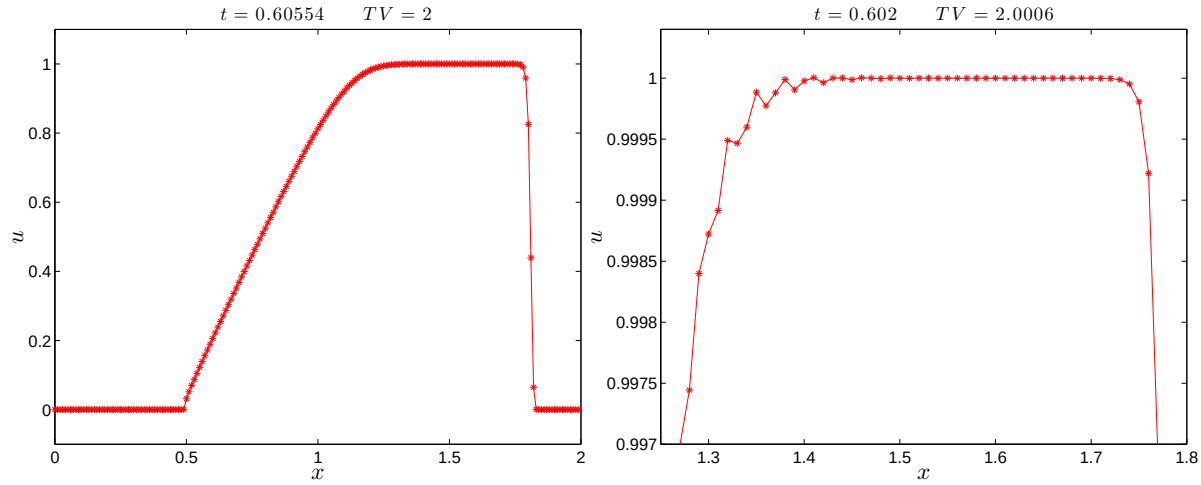
The solution consists of a rarefaction (i.e., an expansion fan) and a moving shock. Again we use 200 points in space and we compute the solution until roughly time $t_{\text{f}} = 0.6$. Figure 6.3 shows the result of solving the discontinuous problem using an SSP $TM^{n-2}R$ scheme, where M is an ESSPRK$(5, 4, 2)$ method with SSP coefficient $\mathcal{C} = 1.95$. In this case, $\sigma = 1.98$ appears to be the largest value for which the total variation is monotonically decreasing during the calculation. This is 2% larger than the value of the SSP coefficient. Figure 6.3b shows part of the solution exhibiting oscillations when σ is larger than the SSP coefficient. For various schemes, Table 6.1 shows the maximum observed values of σ for which the numerical solution is total variation decreasing for the entire computation. With the exception of the four-stage effective order four methods, we note good agreement between the SSP coefficient predicted by the theory and the maximum time-step for which the numerical solution is TVD.

We also note the necessity of our modified starting and stopping methods in the $RM^{n-2}T$ approach: in this example if we use the original approach of S and S^{-1}, the solution exhibits oscillations immediately following the application of the starting perturbation method S.



(a) $\sigma = 0.88$ (b) $\sigma = 1.60$

Figure 6.2: Solution of Burgers' equation at the final time with continuous initial data, using a $TM^{n-2}R$ scheme, where M is the optimal ESSPRK$(4, 4, 2)$. The SSP coefficient is $\mathcal{C} = 0.88$. Figure 6.2b shows a zoom in the region of space where oscillations appear. Here TV denotes the TV-norm of the solution at the final time: a value greater than 1 (the TV-norm of the initial condition) indicates a violation of the TVD condition.



(a) $\sigma = 1.95$ (b) $\sigma = 2.15$

Figure 6.3: Solution of Burgers' equation at the final time with discontinuous initial data, using a $TM^{n-2}R$ scheme, where M is ESSPRK$(5, 4, 2)$ method. The SSP coefficient is $\mathcal{C} = 1.95$. Figure 6.3b shows a zoom in the region of space where oscillations appear. Here TV denotes the TV-norm of the solution at the final time: a value greater than 2 indicates a violation of the TVD condition.

q	p	stages s								
		3	4	5	6	7	8	9	10	11
3	2	1.04(4%)	2.00(0%)	2.65(0%)	3.52(0%)	4.29(0%)	5.11(0%)	6.00(0%)	6.79(0%)	7.63(0%)
4	2	–	1.07(22%)	1.98(2%)	2.69(2%)	3.56(1%)	4.33(1%)	5.16(1%)	6.05(1%)	6.84(1%)
4	3	–	1.05(35%)	1.89(3%)	2.63(2%)	3.53(1%)	4.31(1%)	5.16(1%)	6.04(1%)	6.85(1%)

Table 6.1: Maximum observed coefficients exhibiting the TVD property on the Burgers' equation example with discontinuous data (6.3). The numbers in parenthesis indicate the increase relative to the corresponding SSP coefficients.

7 Conclusions

We use the theory of strong stability preserving time discretizations with Butcher's algebraic interpretation of order to construct explicit SSP Runge–Kutta schemes with an effective order of accuracy. These methods, when accompanied by starting and stopping methods, attain an order of accuracy higher than their (classical) order. We propose a new choice of starting and stopping methods to allow the overall procedure to be SSP. We prove that explicit Runge–Kutta methods with strictly positive weights have at most effective order four. This extends the barrier already known in the case of classical order explicit SSPRK methods.

SSP Runge–Kutta methods of effective order three and four are constructed by numerical optimization. Most of the methods found are optimal because they achieve the upper bound on the SSP coefficient known from linear problems. Also, despite the non-existence of four-stage, order four explicit SSPRK methods, we find effective order four methods with four stages (of classical order two and three). We perform numerical tests which confirm the accuracy and SSP properties of the new methods.

The ideas here are applied to explicit Runge–Kutta methods, but they could also be applied to other classes of methods including implicit Runge–Kutta methods, general linear methods, and Rosenbrock methods.

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References

[1] Butcher, J. C. The effective order of Runge-Kutta methods. In *Conf. on Numerical Solution of Differential Equations (Dundee, 1969)*. Springer, 1969, pp. 133–139.

[2] Butcher, J. C. An algebraic theory of integration methods. *Math. Comp. 26*, 117 (1972), 79–106.

[3] Butcher, J. C. Order and effective order. *Appl. Numer. Math. 28*, 2-4 (1998), 179–191. Eighth Conference on the Numerical Treatment of Differential Equations (Alexisbad, 1997).

[4] Butcher, J. C. *Numerical methods for ordinary differential equations*, second ed. Wiley, 2008.

[5] Butcher, J. C., and Sanz-Serna, J. M. The number of conditions for a Runge-Kutta method to have effective order *p*. *Appl. Numer. Math. 22*, 1-3 (1996), 103–111.

[6] Dahlquist, G., and Jeltsch, R. Reducibility and contractivity of Runge-Kutta methods revisited. *BIT 46*, 3 (2006), 567–587.

[7] Ferracina, L., and Spijker, M. N. Stepsize restrictions for the total-variation-diminishing property in general Runge-Kutta methods. *SIAM J. Numer. Anal. 42*, 3 (2004), 1073–1093.

[8] Ferracina, L., and Spijker, M. N. An extension and analysis of the Shu-Osher representation of Runge-Kutta methods. *Math. Comp. 74*, 249 (2005), 201–219.

[9] Gottlieb, S., Ketcheson, D. I., and Shu, C.-W. *Strong Stability Preserving Runge-Kutta And Multistep Time Discretizations*. World Scientific, Jan. 2011.

[10] Gottlieb, S., and Ruuth, S. J. Optimal strong-stability-preserving time-stepping schemes with fast downwind spatial discretizations. *J. Sci. Comput. 27*, 1-3 (2006), 289–303.

[11] Gottlieb, S., and Shu, C.-W. Total variation diminishing Runge-Kutta schemes. *Math. Comp. 67*, 221 (1998), 73–85.

[12] Gottlieb, S., Shu, C.-W., and Tadmor, E. Strong stability-preserving high-order time discretization methods. *SIAM Rev. 43*, 1 (2001), 89–112.

[13] Hairer, E., Nørsett, S. P., and Wanner, G. *Solving ordinary differential equations I: Nonstiff problems*, vol. 8 of *Springer Series in Computational Mathematics*. Springer-Verlag, 1987.

[14] Hairer, E., and Wanner, G. On the Butcher group and general multi-value methods. *Computing 13*, 1 (1974), 1–15.

[15] Higueras, I. On strong stability preserving time discretization methods. *J. Sci. Comput. 21*, 2 (2004), 193–223.

[16] Ketcheson, D. I. Highly efficient strong stability-preserving Runge-Kutta methods with low-storage implementations. *SIAM J. Sci. Comput. 30*, 4 (2008), 2113–2136.

[17] Ketcheson, D. I. Computation of optimal monotonicity preserving general linear methods. *Math. Comp. 78*, 267 (2009), 1497–1513.

[18] Ketcheson, D. I. Step sizes for strong stability preservation with downwind-biased operators. *SIAM J. Numer. Anal. 49*, 4 (2011), 1649–1660.

[19] Ketcheson, D. I., Macdonald, C. B., and Gottlieb, S. Optimal implicit strong stability preserving Runge-Kutta methods. *Appl. Numer. Math. 59*, 2 (2009), 373–392.

[20] Kraaijevanger, J. F. B. M. Absolute monotonicity of polynomials occurring in the numerical solution of initial value problems. *Numer. Math. 48*, 3 (1986), 303–322.

[21] Kraaijevanger, J. F. B. M. Contractivity of Runge-Kutta methods. *BIT 31*, 3 (1991), 482–528.

[22] Laney, C. B. *Computational gasdynamics*. Cambridge University Press, 1998.

[23] Ruuth, S. J. Global optimization of explicit strong-stability-preserving Runge-Kutta methods. *Math. Comp. 75*, 253 (2006), 183–207.

[24] Ruuth, S. J., and Spiteri, R. J. Two barriers on strong-stability-preserving time discretization methods. In *Proceedings of the Fifth International Conference on Spectral and High Order Methods (ICOSAHOM-01) (Uppsala)* (2002), vol. 17, pp. 211–220.

[25] Ruuth, S. J., and Spiteri, R. J. High-order strong-stability-preserving Runge-Kutta methods with downwind-biased spatial discretizations. *SIAM J. Numer. Anal. 42*, 3 (2004), 974–996.

[26] Shu, C.-W., and Osher, S. Efficient implementation of essentially nonoscillatory shock-capturing schemes. *J. Comput. Phys. 77*, 2 (1988), 439–471.

[27] Spiteri, R. J., and Ruuth, S. J. A new class of optimal high-order strong-stability-preserving time discretization methods. *SIAM J. Numer. Anal. 40*, 2 (2002), 469–491.

[28] Spiteri, R. J., and Ruuth, S. J. Non-linear evolution using optimal fourth-order strong-stability-preserving Runge-Kutta methods. *Math. Comput. Simulation 62*, 1-2 (2003), 125–135.