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A POLYNOMIAL FORMULATION OF ADAPTIVE STRONG STABILITY PRESERVING MULTISTEP METHODS*

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Abstract. A new formulation of explicit multistep methods allows variable step-sizes by construction. This formulation can be used to construct time-adaptive strong stability preserving (SSP) multistep methods of any order for the solution of time-dependent PDEs. The new formulation is implemented in a MATLAB package, and some numerical examples are presented.

Key words. adaptive SSP multistep methods, variable step-sizes, strong stability preserving, TVD schemes

AMS subject classifications. 65L05, 65L06, 65L20

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1. Introduction.

Often, the numerical solution of partial differential equations (PDEs) requires the use of ordinary differential equation (ODE) methods as part of the general technique in order to solve systems of the form

$$u_t = Lu, \quad u(t_0) = u_0, \tag{1}$$

where L is a difference operator that arises from the semidiscretization of PDEs.

Special methods for time-dependent hyperbolic PDEs have been developed to ensure stability and avoid spurious oscillations of the numerical solutions during shocks. These are called *strong stability preserving* (SSP) methods and are a class of ODE solvers that can be one of two types: one-step or multistep methods. Such methods preserve essential solution properties, such as monotonicity, contractivity, positivity, and maximum principles.

Several thorough studies on SSP methods and their discretizations have been published by Gottlieb, Shu, and Tadmor [7], Higueras [9], Gottlieb, Ketcheson, and Shu [6], and, particularly on SSP multistep methods, by Lenferink [12] and Ruuth and Hundsdorfer [15]. While SSP one-step methods have order barriers, SSP multistep methods can have arbitrarily high order. Nevertheless, we know of only one study on variable step-size SSP multistep methods, which is by Hadjimichael et al. [8]. These authors developed adaptive explicit SSP multistep methods of orders 2 and 3, pointing out that methods of order "at least 3 seem to have a complicated structure." They suggest looking for a new formulation with a simple structure that may be used for higher order explicit SSP multistep methods.

The aim of this paper is to develop a methodology that allows for given SSP multistep methods to be formulated as variable step-size methods. While in section 2 we review existing theory for SSP methods, we do not revisit the proofs for optimality made in [8] but rather use those results whenever possible, and we present a general approach to making such methods adaptive. This approach is open to various step-size selection criteria and can be combined with conventional error control using a

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tolerance parameter, or a greedy step-size selection scheme employing the maximal step-size that locally fulfills the SSP condition, as in [8].

The order p of explicit k-step SSP multistep methods with nonnegative coefficients is less than the step number k. The most widely used variable step-size implementations of multistep methods are based on the Nordsieck representation [5], which does not have a straightforward extension to such lower order methods. Arévalo and Söderlind [2] introduced a formulation that constructs adaptive k-step methods that are identified by a fixed set of parameters. These *parametric* multistep methods are described in section 3. The computations are advanced by constructing and evaluating a polynomial at each step, where the step-size is chosen so as to control the local error. The main feature of this formulation is that the methods are intrinsically adaptive, and so require no extension to variable step-sizes. A complete technique was developed for explicit and implicit multistep methods of maximal order, i.e., for $p \geq k$. However, due to the specific order conditions associated with an SSP property for optimal methods with nonnegative coefficients, i.e., that $p < k$ should be allowed, the technique is not directly applicable in the SSP context. In section 4 we extend the original formulation to include explicit multistep methods with $p < k$. The new approach developed in this paper offers a straightforward construction of lower order explicit multistep methods, which are given a fully adaptive representation. Thus, each variable step-size k-step method of order p is completely identified by a set of $2k-p-1$ fixed parameters, where k and p can be chosen freely. As the formulation of these types of methods is not unique, in section 5 we design specific formulations that can describe adaptive versions of known fixed step-size SSP methods while keeping the formulations as simple as possible.

In section 6 we analyze formulations for optimal SSP methods. In general, these methods have several coefficients equal to zero. We propose a formulation that preserves each method's pattern of zero coefficients. These formulations are implemented in an adaptive ODE code, as explained in section 7, and numerical examples are given in section 8.

Because variable step-size methods have coefficients that vary from step to step as a function of the step-size ratios, it is important to study how the positivity of these coefficients is affected by each change of step-size. Although this topic is discussed for some particular examples, its general study is outside the scope of this paper. Instead, the focus here is on a methodology that permits an easy extension of explicit fixed step-size multistep formulas to variable step-size formulas. Such an extension has the property that it reverts to the original formula when the step-size is kept constant.

2. Linear multistep methods and strong stability preservation. We consider ODEs of the form

$$\dot{y} = F(y), \quad y(t_0) = y_0, \quad t \in [t_0, t_{\mathrm{f}}], \tag{2}$$

where $F : \mathcal{R}^m \to \mathcal{R}^m$. When an explicit linear multistep method with fixed step-size h is applied to this problem, a sequence of approximations $y_n \approx y(t_n)$ is computed from the difference equation

$$y_n = \sum_{i=1}^{k} (\alpha_i y_{n-i} + h\beta_i F(y_{n-i})), \tag{3}$$

where k is the step number and α_i and β_i are the coefficients of the method. The method is chosen to suit the properties of the vector field F. In particular, SSP methods, also known as total variation diminishing (TVD) methods [16] or contractivity preserving methods [12], were developed for the time integration of semidiscretizations of hyperbolic conservation laws.

The setting for SSP methods is summarized as follows. Consider the autonomous system (2), where, for a given norm, the vector field F is assumed to have the property

$$\|y + hF(y)\| \le \|y\| \quad \text{for all} \quad y \quad \text{and} \quad h \le h^*. \tag{4}$$

This implies $F(0) = 0$, which obviously holds for linear vector fields but also for many interesting nonlinear vector fields associated with PDEs. If F is linear, we denote it by L, and (4) can be expressed in terms of the logarithmic norm [4, 14, 17] as $\mu[L] \le 0$, where

$$\mu[L] = \lim_{h\to 0^+} \frac{\|I + hL\| - 1}{h}. \tag{5}$$

The condition $\mu[L] \le 0$ implies that $\|y(t)\|$ is a nonincreasing function of t, and thus $y = 0$ is a stable solution. For nonlinear vector fields satisfying $F(0) = 0$, by using the operator norm

$$\|F\| = \sup_{\|y\|\neq 0} \frac{\|F(y)\|}{\|y\|},$$

we can readily define the corresponding logarithmic norm $\mu[F]$ as in (5); this is a straightforward special application of the general extension of the logarithmic norm to nonlinear maps [17]. Thus (4) implies $\mu[F] \le 0$, and once again $\|y(t)\|$ is a nonincreasing function of t. Moreover, if $\mu[F] < 0$, then $\|y + hF(y)\| \le \|y\|$ in a nonempty interval, $0 < h < h^*$, since $\|y + hF(y)\|$ is a convex function of h.

The objective is to find methods that reproduce this behavior. A numerical method whose solution is nonincreasing for all vector fields F satisfying (4) for stepsizes $0 < h \le c\,h^*$ is said to be SSP. Obviously, the explicit Euler method is SSP with $c = 1$.

Whether the vector field F satisfies $\mu[F] < 0$ depends on the choice of norm, but the choice is not restricted to specific norms, such as inner product norms. A standard objective is to construct semidiscretizations of hyperbolic conservation laws so that the total variation of discrete solutions does not increase in time [16], where the *total variation* in space is defined as

$$\|u\|_{TV} = \sum_{j=1}^{m} |u_{j+1} - u_j|, \quad u \in \mathcal{R}^m.$$

This is easily seen to be a seminorm (referred to as the TV norm). If a semidiscretization satisfies $\mu[F] < 0$ with respect to the TV norm, and the time stepping method is SSP, the resulting method will overcome deficiencies that may occur in other methods, such as numerically induced oscillations in space, which are not present in the exact solutions of conservation laws. Thus the SSP method will produce a TVD scheme for time steps $h \le c\,h^*$.

To investigate linear multistep methods reducing total variation, further definitions are needed.

DEFINITION 2.1 ([6]). *Let problem* (2) *satisfy condition* (4). *A k-step method given by formula* (3) *is an SSP method if there is a constant c such that the method applied to problem* (2) *with $0 < h \le c\,h^*$ produces a sequence $\{y_i\}$ satisfying*

$$\|y_n\| \le \max\{\|y_{n-1}\|, \|y_{n-2}\|, \ldots, \|y_{n-k}\|\}. \tag{6}$$

The maximal value of c is called the SSP constant of the method and is denoted by C.

Remark 2.2 ([6]). Consider an explicit method defined by formula (3) with $\alpha_i \geq 0$, $\beta_i \geq 0$ for all i, and let $\gamma = \min_i\{\frac{\alpha_i}{\beta_i} | \beta_i \neq 0\}$. If $\gamma > 0$, the method is SSP with $C = \gamma$.

Although there are implicit multistep methods with larger SSP constants, the added cost of solving the implicit system of equations usually makes explicit methods computationally more efficient [6]. For example, the trapezoidal method, of order 2, has SSP constant $C = 2$, while the optimal explicit 3-step SSP method of order 2 has $C = 0.5$. Thus, this last method may require four times as many steps per unit time. However, the cost of solving the implicit system is often far beyond the cost of the extra steps.

It is known that for $k \geq 2$ there is no explicit k-step SSP method of order $p = k$ with all $\beta_i \geq 0$ [6]. Therefore, we will explore methods of order $p < k$. For brevity, we will refer to a k-step, order p method as a (k, p) method.

Remark 2.3 ([12]). The SSP constant of an explicit (k, p) method with $p > 1$, $\alpha_i \geq 0, \beta_i \geq 0$ satisfies

$$C \leq \frac{k-p}{k-1}.$$

Thus, increasing the number of steps allows for larger upper bounds on the SSP constant.

3. Parametric multistep methods. A new formulation for linear multistep methods where each k-step method of maximal order is represented by a fixed set of parameters was introduced by Arévalo and Söderlind [2]. This formulation supports variable step-sizes by construction and has a simple structure, but it is valid only for maximal order, i.e., when $p \geq k$. Thus an extension to SSP methods is needed.

The parametric formula of a k-step method is defined as a linear combination of state values, y_{n-i}, where $i = 1, \ldots, k$, and their corresponding vector field values, $y'_{n-i} = F(y_{n-i})$. The vectors y_{n-i} represent the approximation of the solution $y(t)$ to the initial value problem (2) at a sample of times $t_{n-k}, \ldots, t_{n-1}$ with $h_{n-i} = t_{n+1-i} - t_{n-i}$. Let Π_p denote the space of polynomials of degree p. A k-step method in parametric form approximates the solution $y(t)$ for $t > t_{n-1}$ by constructing a polynomial $P_n \in \Pi_p$ and defining

$$y_n = P_n(t_n). \tag{7}$$

The formulation of parametric multistep methods makes use of the state and derivative *slacks*, defined as follows.

DEFINITION 3.1 ([2]). *Let the sequences* $\{y_{n-i}\}_{i=0}^k$ *and* $\{y'_{n-i}\}_{i=0}^k$ *be given for a fixed* n. *Further, let* $P_n \in \Pi_p$ *with* $p \leq k+1$. *The state slack* s_{n-i} *and the derivative slack* s'_{n-i} *at* t_{n-i} *are defined by*

$$s_{n-i} = P_n(t_{n-i}) - y_{n-i}, \qquad s'_{n-i} = \dot{P}_n(t_{n-i}) - y'_{n-i}, \qquad i = 0, \ldots, k. \tag{8}$$

Further, in [2] it was demonstrated that every explicit k-step method of order p can be defined by $y_n = P_n(t_n)$, with the polynomial $P_n \in \Pi_k$ satisfying the conditions

$$\begin{cases} s_{n-1} = 0, \\ s'_{n-1} = 0, \\ s_{n-i}\cos\theta_{i-1} + h_{n-i}s'_{n-i}\sin\theta_{i-1} = 0; \quad i = 2, \ldots, k, \end{cases} \tag{9}$$

where $\theta_i \in (-\frac{\pi}{2}, \frac{\pi}{2}]$ are the *method parameters*. The first two conditions are called *structural conditions* and specify the explicitness of the method. The additional linear combinations of state and derivative slacks are called *slack balance conditions* and specify the particular method. Arévalo et al. [3] showed that the following parametric equivalence holds between the coefficients of a classical, constant step-size, multistep formula of maximal order and the method parameters:

$$\tan\theta_{i-1} = \frac{\beta_i}{\alpha_i} \quad \text{for } i = 2, \dots, k. \tag{10}$$

Note that for a variable step-size method the parameters θ_{i-1} are constants, even though the coefficients α_i, β_i vary from step to step. Thus, with (9), a variable step-size k-step method is defined in terms of constants $\theta_1, \dots, \theta_{k-1}$.

We need to consider a modified framework for SSP multistep methods. Our goal is to construct a general parametric formulation for explicit multistep methods that, while similar to (9), also covers SSP methods for which $p < k$. For this general formulation of explicit SSP multistep methods we will also prove an equivalence similar to (10), which will be seen to be essential to SSP methods.

4. Parametric formulations of explicit SSP multistep methods. Our approach to finding an adaptive formulation for SSP methods is based on obtaining a general formulation for all explicit k-step methods of a fixed order $p \le k-1$.

As a method of order p is defined by polynomials of degree p, the $p+1$ coefficients of $P_n \in \Pi_p$ must be uniquely determined by $p+1$ interpolation conditions. For an explicit (k,p) SSP method we can construct these conditions as $p+1$ slack conditions. Consider each pair of coefficients (α_i, β_i) in (3), where either $\alpha_i = \beta_i = 0$ or $\alpha_i \ne 0$. Note that for SSP methods, if $\beta_i = 0$, the value of γ in Remark 2.2 is not influenced by the value of α_i. We call a pair (α_i, β_i) with $\alpha_i \ne 0$ a *nonzero pair*. It is these pairs that determine the value of γ.

For a pair of coefficients satisfying $(\alpha_i, \beta_i) = (0,0)$, the interpolation conditions that define P_n cannot include s_{n-i} or s'_{n-i}, because these slacks contain y_{n-i} and y'_{n-i}. On the other hand, if $\alpha_i \ne 0$, the slack s_{n-i}, the only one that contains the term y_{n-i}, must be present in the interpolation conditions. The derivative slack s'_{n-i} may or may not be present, depending on the value of β_i. Thus, to construct the polynomial of a (k,p) SSP method we can select one of the following alternatives acting at each $t = t_{n-i}$ for each $i \in \{1, \dots, k\}$ corresponding to a nonzero pair:

$$\begin{aligned} &1.\ s_{n-i} + h_{n-i}\tau_i s'_{n-i} = 0, \\ &2.\ \begin{cases} s_{n-i} = 0, \\ s'_{n-i} = 0. \end{cases} \end{aligned} \tag{11}$$

The way in which these conditions are chosen for particular methods will be discussed in sections 5 and 6.

Much of the literature on SSP methods has focused on finding the (k,p) method with largest SSP constant. Using standard optimization techniques, Lenferink [12] obtained all optimal explicit SSP multistep methods up to $k = 20$ steps and order $p = 7$. Ketcheson [11] constructed an algorithm for computing the coefficients of optimal explicit SSP methods given the number of steps and the order required and presented a table of optimal SSP constants up to $k = 50$ steps and order $p = 15$.

Table 1 shows the SSP constants of optimal explicit SSP multistep methods up to $k = 7$ steps and order $p = 5$. Note that the optimal SSP constant for a fixed order

TABLE 1
SSP constants of optimal explicit multistep methods up to $k = 7$ steps and order $p = 5$. No optimal methods of order 1 can be found for $k > 1$ nor of order $p = 3$ for $k \geq 7$.

k \ p	1	2	3	4	5
1	1.0				
2	-				
3	-	0.5			
4	-	0.667	0.333		
5	-	0.75	0.5	0.021	
6	-	0.8	0.583	0.165	
7	-	0.833	-	0.282	0.038

increases as the number of steps increases, so it can pay off to construct methods of a larger number of steps without increasing the order of accuracy, as long as the number of nonzero coefficients of the method remains low. This is of particular interest if the methods are adaptive and the pattern of zero coefficients of the fixed step-size formula is to be preserved in its variable step-size extension.

Remark 4.1 ([12]). There is no optimal order 1 SSP method for $k > 1$. The supremum of the SSP constants for explicit $(k, 1)$ SSP methods with $k > 1$ is obtained when $\alpha_i = \beta_i = 0$ for $i = 2, \ldots, k$, but in that case the method reduces to the one-step method. Also, there is no optimal $(k, 3)$ SSP method for $k > 6$, and in fact, the same phenomenon occurs after some value of k for all odd values of p.

Optimal SSP multistep methods were originally defined for constant step-sizes. In this context, a k-step SSP method satisfies the discrete monotonicity property (6). For adaptive multistep methods with formula

$$y_n = \sum_{i=1}^{k} (\alpha_{i,n} y_{n-i} + h_{n-1}\beta_{i,n} F(y_{n-i})), \tag{12}$$

Hadjimichael et al. [8] propose the use of an alternative monotonicity condition,

$$\|y + hF(y)\| \leq \|y\| \quad \text{for all} \quad y \quad \text{and} \quad h \leq h^*(y). \tag{13}$$

In this case, if $\alpha_{i,n}, \beta_{i,n} \geq 0$ and

$$h_{n-1} \leq C_n \min_{0 \leq j \leq k-1} h^*(y_{n-k-j}), \quad \text{where} \quad C_n = \min_i \left\{ \frac{\alpha_{i,n}}{\beta_{i,n}} \;\middle|\; \beta_{i,n} \neq 0 \right\} > 0, \tag{14}$$

the solution given by (12) will satisfy the discrete monotonicity property (6).

For constant step-sizes, the coefficients of the multistep formula remain constant, and it is clear that $C_n = C$. In fact, if the step-sizes are slowly varying, the variable coefficients are slowly varying too, and C_n will remain close to C as long as the patterns of nonzero coefficients of the variable step-size formula and the constant step-size formula are the same.

The step ratios are defined as $\Omega_j = \frac{1}{h_{n-1}} \sum_{i=0}^{j-1} h_{n-k+i}$. The following is an extension of Remark 2.3 for the variable step-size case.

Remark 4.2 ([8]). The SSP coefficient of an explicit (k, p) method with $p > 1$, $\alpha_i \geq 0, \beta_i \geq 0$ requires that $\Omega_k > p$ and satisfies

$$C_n \leq \frac{\Omega_k - p}{\Omega_k - 1}.$$

TABLE 2
Possible sets of slack conditions to construct optimal k-step SSP methods of order 2.

Structure	Order: $p = 2$
$\mathcal{A}$	$\begin{cases} s_{n-1} = 0 \\ s'_{n-1} = 0 \\ s_{n-k} + h_{n-k}\,\tau_k\, s'_{n-k} = 0 \end{cases}$
$\mathcal{B}$	$\begin{cases} s_{n-1} + h_{n-1}\,\tau_1\, s'_{n-1} = 0 \\ s_{n-k} = 0 \\ s'_{n-k} = 0 \end{cases}$
$\mathcal{C}$	$\begin{cases} s_{n-1} + h_{n-1}\,\tau_1\, s'_{n-1} = 0 \\ s_{n-i} + h_{n-i}\,\tau_i\, s'_{n-i} = 0 \\ s_{n-k} + h_{n-k}\,\tau_k\, s'_{n-k} = 0 \end{cases}$ $i \in \{2, 3, \ldots, k-1\}$

There are many different possible sets of slack conditions that may define SSP methods of various orders. In the example below we look for a parametric formulation of optimal explicit k-step SSP methods of order 2 with $k \geq 3$. We restrict our choices by only considering formulations that include s_{n-1} and s'_{n-1}, that is, the last computed values.

Example 4.3. The parametric formulation of an explicit $(k, 2)$ method in the interval $[t_{n-1}, t_n]$ is given by a second degree polynomial. In order to find the corresponding polynomial coefficients three equations in terms of slack conditions are needed. To render a k-step method, slack conditions for $t = t_{n-k}$ must be part of the formulation. There are many different possible sets of slack conditions that may define k-step methods of order 2.

Table 2 shows some possible different formulations for an optimal $(k, 2)$ SSP method categorized in one of three different structures. The first two only include slack conditions for the points at $t = t_{n-k}$ and $t = t_{n-1}$, and the third also includes one of the intermediate points. Here we will analyze what type of method is described by structure $\mathcal{B}$. The polynomial of the optimal method must be of the form

$$P(t) = A\frac{(t - t_n)^2}{h_{n-1}^2} + y'_{n-1}\frac{t - t_n}{h_{n-1}} + y_{n-1} \tag{15}$$

and satisfy the conditions given in Table 2. Using this, together with (7), we get that the nonzero coefficients of the multistep formula are

$$\alpha_{1,n} = \frac{\Omega_k^2}{\Omega_k^2 + 2(\tau_1 - 1)\Omega_k - 2\tau_1 + 1}, \tag{16}$$

$$\alpha_{k,n} = \frac{2(\tau_1 - 1)\Omega_k - 2\tau_1 + 1}{\Omega_k^2 + 2(\tau_1 - 1)\Omega_k - 2\tau_1 + 1}, \tag{17}$$

$$\beta_{1,n} = \frac{\tau_1\Omega_k^2}{\Omega_k^2 + 2(\tau_1 - 1)\Omega_k - 2\tau_1 + 1}, \tag{18}$$

$$\beta_{k,n} = \frac{\Omega_k((\tau_1 - 1)\Omega_k - 2\tau_1 + 1)}{\Omega_k^2 + 2(\tau_1 - 1)\Omega_k - 2\tau_1 + 1}. \tag{19}$$

The SSP coefficient is then given by

$$\gamma_n(k) = \min\left\{\frac{1}{\tau_1}, \frac{2(\tau_1 - 1)\Omega_k - 2\tau_1 + 1}{\Omega_k^2 + 2(\tau_1 - 1)\Omega_k - 2\tau_1 + 1}\right\} \tag{20}$$

as long as the coefficients remain nonnegative. As the parameter τ_1 is independent of the step number n, we can consider the constant step-size case, i.e., when $\Omega_j = j$. Then

$$\gamma(k) = \min\left\{\frac{1}{\tau_1}, \frac{2(\tau_1-1)k-2\tau_1+1}{k((\tau_1-1)k-2\tau_1+1)}\right\}, \tag{21}$$

and bearing in mind the positivity of the coefficients, we get that for each fixed value of k the value of τ_1 that maximizes $\gamma > 0$ is $\tau_1 = (k-1)/(k-2)$ and the constant of the optimal SSP k-step method of order 2 is

$$C(k) = \frac{k-2}{k-1}. \tag{22}$$

Nevertheless, we observe that the coefficient $\beta_{k,n}$, which agrees with the constant step-size coefficient $\beta_k = 0$ when the step-size is kept constant, does not remain zero in the variable step-size extension, and it even becomes negative if $\Omega_k < k$. The implication is that the method would not be SSP if, after $k-1$ constant step-sizes, the step-size is allowed to increase. Thus, this formulation is ill-fitted for SSP methods. ∎

In the next section we derive a formulation for explicit (k,p) methods with $p < k$, where the pattern of zero coefficients of the fixed step-size formula is retained in the variable step-size extension.

5. A formulation for explicit multistep methods of lower orders.

We have suggested possible parametric formulations for explicit $(k,2)$ SSP methods using different combinations of slack conditions. In order to formulate a general explicit (k,p) method with $p < k$, we need $p+1$ interpolation conditions. There must be at least one slack present for each nonzero pair (α_i, β_i), but having one slack condition for each point at t_{n-i}, $i = 1, \ldots, k$, might result in an overdetermined system. Therefore, we consider using linear combinations of the slack conditions. In the classical formulation of explicit multistep methods, a k-step, order p method is defined by its coefficients $\alpha_1, \ldots, \alpha_k$ (α_0 is normalized to 1) and $\beta_1, \ldots, \beta_k$, and $p+1$ order conditions. We are looking for a parametric formulation of (k,p) methods that includes methods that can be obtained by fixing $2k-p-1$ parameters, so that there is a one-to-one correspondence between the classical coefficients of a method and its parameters in the polynomial formulation. Here we do not assume that the methods are SSP.

We add one more alternative to the set of conditions given in (11), combining one or more balance slacks with the condition at the farthest point, $t = t_{n-k}$. The slack s_{n-k} must be present in the formulation to guarantee the prescribed number of steps. Thus, to p interpolation conditions for $i \in \{1, \ldots, k-1\}$ chosen from (11), add one condition,

$$\sum \left(\lambda_i s_{n-i} + h_{n-i}\tau_i s'_{n-i}\right) + s_{n-k} + h_{n-k}\tau_k s'_{n-k} = 0, \tag{23}$$

so that each slack s_{n-i}, s'_{n-i} appears at most once in the formulation. The constants λ_i and τ_i in (11) and (23) are the *method parameters* of this formulation, where the constants τ_i correspond to $\tan\theta_i$ in (9). As these parameters do not depend on the step-sizes, we can use a fixed step-size formulation of the method to calculate their values. The following theorem gives the formulas that allow us to calculate these parameters for a set of given method coefficients.

Procedure 1: Formulation of explicit methods of order $p < k$.
To define the method polynomial $P_n \in \Pi_p$, use the following rules to set up the interpolation conditions:

- If $(\alpha_i, \beta_i) = (0, 0)$, do not include either s_{n-i} or s'_{n-i}.
- If $\alpha_i = 0, \beta_i \neq 0$, include only $s'_{n-i} = 0$.
- For each $\alpha_i \neq 0$ and $\beta_i \neq 0$, include one of the following:

$$\begin{cases} s_{n-i} = 0, \\ s'_{n-i} = 0, \end{cases} \tag{24}$$

$$\text{or} \quad s_{n-i} + h_{n-i}\tau_i s'_{n-i} = 0, \tag{25}$$

$$\text{or} \quad \sum \left(\lambda_i s_{n-i} + h_{n-i}\tau_i s'_{n-i}\right) + s_{n-k} + h_{n-k}\tau_k s'_{n-k} = 0, \tag{26}$$

so that the total number of conditions adds up to $p + 1$.

To extend a fixed step-size method with given coefficients $\alpha_1, \dots, \alpha_k, \beta_1, \dots, \beta_k$, in a way that preserves the pattern of zero coefficients, we observe the rules listed in Procedure 1.

There is some freedom in choosing the interpolation conditions, but the following theorem gives formulas for the method coefficients once the choice has been made.

THEOREM 5.1. *For a* (k, p) *method defined by* $p + 1$ *slack conditions chosen according to Procedure* 1, *the method parameters can be defined as follows:*

$$\tau_i = \frac{\beta_i}{\alpha_i} \quad \textit{when } (25) \textit{ is used,}$$

$$\tau_i = \frac{\beta_i}{\alpha_k}, \quad \lambda_i = \frac{\alpha_i}{\alpha_k}, \quad \textit{when } (26) \textit{ is used.}$$

Proof. Consider the constant step-size formulation of a method defined as prescribed in Procedure 1.

As the method is of order p, and P_n is of degree p, formula (3) is satisfied exactly when y_{n-i} and y'_{n-i} are replaced by $P_n(t_{n-i})$ and $\dot{P}_n(t_{n-i})$, respectively. Inserting the polynomial into the formula, we obtain

$$P_n(t_n) = \sum_{i=1}^{k} (\alpha_i P_n(t_{n-i}) + h\beta_i \dot{P}_n(t_{n-i})), \tag{27}$$

and subtracting (27) from (3), we get

$$P_n(t_n) - y_n = \sum \left(\alpha_i s_{n-i} + h\beta_i s'_{n-i}\right) + \sum \left(\alpha_i s_{n-i} + h\beta_i s'_{n-i}\right) + \alpha_k s_{n-k} + h\beta_k s'_{n-k}, \tag{28}$$

where the first sum corresponds to the indexes involved in (25) and the second sum to those involved in (26). From (25) we get that each term in the first sum satisfies

$$s_{n-i} + h\frac{\beta_i}{\alpha_i} s'_{n-i} = 0, \tag{29}$$

and from (26) we have that

$$\sum \left(\frac{\alpha_i}{\alpha_k} s_{n-i} + h\frac{\beta_i}{\alpha_k} s'_{n-i}\right) + s_{n-k} + h\frac{\beta_k}{\alpha_k} s'_{n-k} = 0. \tag{30}$$

Thus we conclude that $y_n = P_n(t_n)$. ∎

Theorem 5.1 states the relation between the set of method coefficients in the classical formulation, α_i and β_i, and the parameters in the polynomial formulation, τ_i and λ_j. Thus, given the coefficients in formula (3), one can obtain the method parameters from Theorem 5.1. It is important to note that the method parameters do not vary with the step-sizes, so that this relation, obtained for the constant coefficients of a fixed step-size method, gives the method parameters for the equivalent variable step-size method in the new formulation.

Example 5.2. To construct the variable step-size extension of the 6-step, order 3 formula with coefficients $\alpha_1 = 1/4, \alpha_2 = 0, \alpha_3 = 1/2, \alpha_4 = 1/8, \alpha_5 = 1/8, \beta_1 = 1/16, \beta_2 = 565/96, \beta_3 = -253/48, \beta_4 = 199/96, \beta_5 = 1/8$, we set up the following system of four equations to calculate the coefficients of the method polynomial $P_n \in \Pi_3$ according to Procedure 1:

$$
\begin{aligned}
&s_{n-1} + \tau_1 h s'_{n-1} = 0,\\
&s'_{n-2} = 0,\\
&s_{n-3} + \tau_3 h(\Omega_3 - \Omega_2) s'_{n-3} = 0,\\
&\lambda_4 s_{n-4} + \tau_4 h(\Omega_2 - \Omega_1) s'_{n-4} + s_{n-5} + \tau_5 h \Omega_1 s'_{n-5} = 0.
\end{aligned}
$$

From Theorem 5.1 we have that $\tau_1 = 1/4, \tau_3 = -253/24, \tau_4 = 199/12, \tau_5 = 1, \lambda_4 = 1$. The variable step-size method will advance the solution by setting $y_n = P_n(t_n)$.

In particular, for SSP methods, for which $\alpha_i = 0 \Rightarrow \beta_i = 0$, we have a similar procedure for constructing the interpolation conditions that define the method polynomial. Note that by construction the pattern of zero coefficients of the fixed step-size formula is preserved by the variable step-size extension. It is also clear that if the constant coefficients are positive, the variable step-size coefficients will remain positive for some change in the step-sizes, which in some cases may have to be quite small. This would require limiting the allowed step-size ratios in the method implementation, but as will be seen in the next section, precise bounds of the step-size ratios may be difficult to calculate.

Procedure 2: Formulation of explicit formulas for SSP methods.

- If $(\alpha_i, \beta_i) = (0, 0)$, do not include either s_{n-i} or s'_{n-i}.
- If $\alpha_i \neq 0, \beta_i = 0$, include only $s_{n-i} = 0$.
- For each $\alpha_i \neq 0$ and $\beta_i \neq 0$, include one of the following:

$$
\left\{ \begin{array}{l} s_{n-i} = 0, \\ s'_{n-i} = 0, \end{array} \right. \tag{31}
$$

$$
\text{or} \quad s_{n-i} + h_{n-i}\tau_i s'_{n-i} = 0, \tag{32}
$$

$$
\text{or} \quad \sum \left(\lambda_i s_{n-i} + h_{n-i}\tau_i s'_{n-i}\right) + s_{n-k} + h_{n-k}\tau_k s'_{n-k} = 0, \tag{33}
$$

so that the total number of conditions adds up to $p + 1$.

COROLLARY 5.3. *The method parameters of a method constructed using Procedure 2 are*

$$
\begin{aligned}
\hat{\tau}_i &= \frac{\beta_i}{\alpha_i} \quad \textit{when (32) is used,}\\
\tau_i &= \frac{\beta_i}{\alpha_k}, \quad \lambda_i = \frac{\alpha_i}{\alpha_k} \quad \textit{when (33) is used.}
\end{aligned}
$$

Let $\gamma = \min_i\{\frac{1}{\hat{\tau}_i}, \frac{\lambda_i}{\tau_i} | \hat{\tau}_i \neq 0, \tau_i \neq 0\}$. *If* $\gamma > 0$, *the SSP constant is* $C = \gamma$.

Proof. The proof follows from Remark 2.2. Note that $\alpha_k \neq 0$ because for $\alpha_k = 0$ either the method is not a k-step method (if $\beta_k = 0$), or the value of γ is zero (if $\beta_k \neq 0$). ∎

6. Alternative formulations of optimal SSP methods. The method parameters of an optimal k-step SSP formula of order p, represented here by SSPkp, can be calculated using Theorem 5.1, thus effectively converting a fixed step-size method to variable step-size. Its coefficients, α_i, β_i, $i = 1, \dots, k$, can be obtained using Ketcheson's algorithm [11]. Alternatively, given the method parameters λ_j and τ_j obtained with Procedure 2, the coefficients of an SSPkp method, α_i and β_i, can be determined by solving the system consisting of the parametric relations in Corollary 5.3 together with the $p + 1$ order conditions. Note that λ_j and τ_j depend only on the fixed step-size method coefficients α_i, β_i. It is clear that the variable step-size formulas are not SSP methods without the appropriate restriction to the step-size ratios. In this paper the emphasis is on the construction of the adaptive formulas, but further attention must be given to the step-size ratio restrictions and the SSP coefficients.

Example 6.1. Consider the optimal SSP32 method with constant coefficients $\alpha_1 = \frac{3}{4}, \alpha_2 = 0, \alpha_3 = \frac{1}{4}, \beta_1 = \frac{3}{2}$, and $\beta_2 = \beta_3 = 0$. This method has $\tau_1 = 2,\ \tau_2 = 0,\ \tau_3 = 0$, and in this case there is no parameter λ, as $k = p + 1$.

We can express the adaptive method by a variable step-size formula

$$y_n = \sum_{i=1}^{3} \left(\alpha_{i,n}(\Omega_1, \Omega_2) y_{n-i} + h_{n-1} \beta_{i,n}(\Omega_1, \Omega_2) y'_{n-i} \right). \tag{34}$$

If we use Procedure 2 to construct the optimal SSP32 method, the equations that must be solved to advance the solution are

$$\begin{cases} s_{n-1} = 0, \\ s'_{n-1} = 0, \\ s_{n-3} = 0, \end{cases} \tag{35}$$

and solving this system and evaluating the method polynomial at $t = t_n$ yields

$$\begin{aligned}
\alpha_{1,n}(\Omega_1, \Omega_2) &= \frac{\Omega_2^2 - 1}{\Omega_2^2}, \\
\alpha_{2,n}(\Omega_1, \Omega_2) &= 0, \\
\alpha_{3,n}(\Omega_1, \Omega_2) &= \frac{1}{\Omega_2^2}, \\
\beta_{1,n}(\Omega_1, \Omega_2) &= \frac{\Omega_2 + 1}{\Omega_2^2}, \\
\beta_{2,n}(\Omega_1, \Omega_2) &= 0, \\
\beta_{3,n}(\Omega_1, \Omega_2) &= 0.
\end{aligned}$$

When all step-sizes are set equal, then $\Omega_1 = 1$ and $\Omega_2 = 2$, and the coefficients coincide with the fixed step-size SSP32 method. Note that the pattern of zero coefficients is preserved. Also, as long as $\Omega_2 > 1$, the variable coefficients remain positive. This result coincides with that of Hadjimichael et al. [8].

Consider the pairs of constant step-size coefficients (α_i, β_i) of an explicit SSP method given by (3). As was discussed previously, each nonzero pair must have $\alpha_i \neq 0$. As we can determine from Table 3 in [11], optimal SSP methods with $(k,p) \neq (6,3), k \leq 50$, satisfy the following conditions:

1. $\alpha_1 \neq 0$, $\beta_1 \neq 0$, $\alpha_k \neq 0$.
2. If p is even, $\beta_k = 0$, and there are p pairs of nonzero coefficients.
3. If p is odd, $\beta_k \neq 0$, and there are $p-1$ pairs of nonzero coefficients.

The single exception to this rule, the optimal $(6,3)$ method, has p pairs of nonzero coefficients. An optimal method can be constructed by choosing $p+1$ slack conditions that depend only on the points corresponding to nonzero coefficients, to preserve the pattern of zeros of the constant step-size method. This simplified strategy is described in Procedure 3.

Procedure 3: Formulation of optimal SSP methods.

- Take structural conditions at the point $t = t_{n-1}$.
- Take slack balance conditions at the intermediate points $t = t_{n-j}$ with $\alpha_j \neq 0$, $1 < j < k$. The method parameters are $\tau_j = \beta_j/\alpha_j$.
- Add the state slack $s_{n-k} = 0$. If p is odd, also add the derivative slack $s'_{n-k} = 0$. (For the $(6,3)$ method, take a slack balance condition at t_{n-6}.)

Example 6.2. The optimal explicit $(k,3)$ SSP methods with $k = 4, 5$ are constructed as

$$\begin{cases} s_{n-1} = 0, \\ s'_{n-1} = 0, \\ s_{n-k} = 0, \\ s'_{n-k} = 0. \end{cases} \tag{36}$$

The nonzero variable coefficients of the multistep formula can be derived from (36) as

$$\alpha_{1,n} = \frac{(\Omega_k - 3)\Omega_k^2}{(\Omega_k - 1)^3}, \tag{37}$$

$$\alpha_{k,n} = \frac{3\Omega_k - 1}{(\Omega_k - 1)^3}, \tag{38}$$

$$\beta_{1,n} = \frac{\Omega_k^2}{(\Omega_k - 1)^2}, \tag{39}$$

$$\beta_{k,n} = \frac{\Omega_k}{(\Omega_k - 1)^2}. \tag{40}$$

The SSP coefficient is given by

$$\gamma_k = \min\left\{ \frac{\Omega_k - 3}{\Omega_k - 1}, \frac{3\Omega_k - 1}{(\Omega_k - 1)\Omega_k} \right\} \tag{41}$$

when the coefficients are positive and $\gamma_k > 0$, that is, when $\Omega_k > 3$. It can be easily shown that $\gamma_k = \frac{\Omega_k - 3}{\Omega_k - 1}$ if $3 < \Omega_k \leq 5.828$, while $\gamma_k = \frac{3\Omega_k - 1}{(\Omega_k - 1)\Omega_k}$ if $\Omega_k \geq 5.828$, but from Remark 4.2 we know that $C_n \leq \frac{\Omega_k - 3}{\Omega_k - 1}$, so the method is not optimal if $\Omega_k \geq 5.828$. These results agree with those of Hadjimichael et al. [8].

Methods with higher order and a larger number of steps depend, in general, on several step-size ratios; their variable step-size coefficients are high degree rational functions of these step-size ratios and are therefore difficult to study in terms of their SSP coefficients.

Example 6.3. The optimal explicit $(8,5)$ SSP method has nonzero coefficients $\alpha_1 = 1360/4363$, $\alpha_4 = 233/2112$, $\alpha_5 = 2323/10831$, $\alpha_8 = 896/2465$, $\beta_1 = 275/128$, $\beta_4 = 1044/1373$, $\beta_5 = 6661/4506$, and $\beta_8 = 1781/5144$. Thus, we construct the method as

$$\begin{cases} s_{n-1} = 0, \\ s'_{n-1} = 0, \\ s_{n-4} + h_{n-4}\tau_4 s'_{n-4} = 0, \\ s_{n-5} + h_{n-5}\tau_5 s'_{n-5} = 0, \\ s_{n-8} = 0, \\ s'_{n-8} = 0. \end{cases} \tag{42}$$

For this method we calculate $\tau_4 = \beta_4/\alpha_4 = 2433/353$, $\tau_5 = \beta_5/\alpha_5 = 2433/353$. The variable step-size formula preserves the pattern of zeros, and the positivity of the coefficients is also preserved as long as the step-sizes vary smoothly. Exact calculations of the bounds on the step-size ratios to secure positivity are difficult to perform. Equally difficult is the calculation of the SSP coefficient, but as it varies continuously with the step-size ratios, a slowly varying step-size sequence will produce an SSP coefficient that is close to the constant step-size SSP constant for the method, $C = 353/2433$. Although sharp bounds are hard to obtain, we found that positivity of the variable step-size coefficients for this method can be ensured for the extreme case when step-sizes are assumed to increase at a constant rate of 3.5% or decrease at the constant rate of 5.5%.

In the implementation of these methods, the variable coefficients of the adaptive method are not explicitly calculated. To advance the solution at each step, (42) is solved for the method polynomial, and the new solution is obtained by evaluating the polynomial at $t = t_n$. A new step-size h_{n-1} is selected at each step. This can be done in different ways. To use the greedy step-size selection of Hadjimichael et al. [8], a complicated stability analysis of the acceptable step-sizes is needed. As that approach means that each particular method must be analyzed and that these calculations can be difficult, and because the error cannot be monitored, we take an alternative approach. Given an error tolerance, we use controllers based on digital filter theory [1] to adapt the step-size to the error tolerance. By a continuity argument, the method coefficients remain positive when the step-size varies slowly.

7. Implementation. We implemented our formulation in the adaptive multistep solver MODES [3]. This ODE MATLAB toolbox, including the SSP module, is freely available for download [1]. The original package contains the explicit $p = k$ methods and the implicit $p = k$ and $p = k + 1$ methods. The user can choose fixed or variable step-sizes and has a choice of several step-size controllers designed both for general and for more specific needs. For each class of methods with k steps and order p there is a function that computes the coefficients of the method polynomial of degree p by solving the derived parametric formulation for that class. For instance, a 2-step explicit multistep method of order 2 is characterized by a second degree polynomial P_n,

$$P_n(t) = c_2(t - t_{n-1})^2 + c_1(t - t_{n-1}) + c_0,$$

satisfying the slack conditions in (9),

$$\begin{cases} s_{n-1} = 0, \\ s'_{n-1} = 0, \\ s_{n-2}\cos\theta_1 + h_{n-2}s'_{n-2}\sin\theta_1 = 0, \end{cases} \tag{43}$$

where these three conditions, together with the parameter value θ_1, uniquely determine the polynomial coefficients. Then the solution at time t_n is obtained as $P_n(t_n) = c_2h_{n-1}^2 + c_1h_{n-1} + c_0$.

The implementation in MODES was made by adding a function `polElow` which, given the method parameters λ and τ, computes the solution at t_n by solving the system for the coefficients of P_n, and then evaluates $y_n = P_n(t_n)$. We also have the option of calling some optimal (k, p) SSP methods for $p \leq 5$ by name, without giving their parameters explicitly. The step-size controllers in MODES provide an estimate of the local error at each step. By monitoring the error estimation, the controllers increase or decrease the step-size when the error estimate is below or above the specified tolerance, and in particular they reduce the step-size when a numerical instability is detected. This is particularly important for explicit SSP integrators that cannot operate with step-sizes above their stability limit. Using an adaptive implementation of these methods eliminates the need to calculate the SSP constant for each particular method, although care must be taken to set appropriate bounds for step-size changes. These bounds will be conservative, and the method will be costlier than when the greedy step-size selection is used, but on the other hand, the error will be monitored, keeping it below a given tolerance. Our implementation retains MODES's step-size controllers and its mechanism for calculating the starting values of the multistep methods, which are provided by Runge–Kutta methods. Because the MODES platform allows the user to set upper and lower limits on the step-size ratios, it is particularly suited for maintaining these ratios bounded, as required by SSP methods.

8. Numerical results. In this section we investigate the performance of the parametric SSP methods as implemented in MODES.

Problem 8.1. We consider the inviscid Burgers equation with periodic boundary conditions

$$\begin{aligned} &u_t + uu_x = 0, \\ &u(x,0) = g(x), \quad x \in [0,1], \end{aligned} \tag{44}$$

using the smooth initial function

$$g(x) = \frac{1}{2} + \sin(2\pi x). \tag{45}$$

Furthermore, the model is semidiscretized with the fifth order weighted essentially nonoscillatory (WENO) scheme [13, 10]. WENO is one of the spatial discretizations that are often combined with an SSP time integrator to preserve contractivity properties.

The step-size controllers in MODES are designed to obtain a smooth step-size sequence. The small change in step-sizes is crucial to guarantee the positivity of time-dependent SSP multistep coefficients. However, the implementation of an efficient controller that keeps the step-sizes near the SSP coefficient is beyond the scope of this paper.

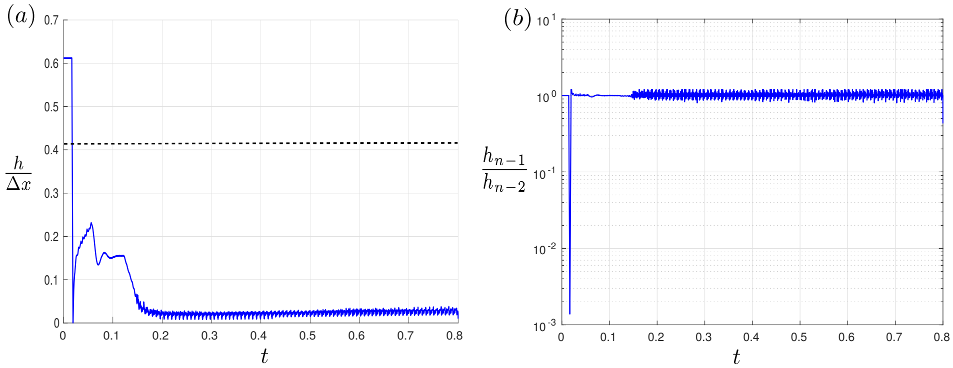

FIG. 1. *The adaptive optimal* $(8,5)$ *SSP method as described in Example* 6.3 *was used to solve the Burgers equation with an error tolerance of* 10^{-6}, $0.8h_{n-2} < h_{n-1} < 1.2h_{n-2}$, *and* 256 *spatial discretization points. The plot shows* (a) *the ratio* $\frac{h}{\Delta x}$ *for the optimal* $(8,5)$ *SSP method, and* (b) *the step-size ratios* $\frac{h_{n-1}}{h_{n-2}}$.

The problem was solved using the optimal (8,5) SSP formula described in section 6. Figure 1 shows (a) the ratio $\frac{h}{\Delta x}$, and (b) the step-size ratio, $\frac{h_{n-1}}{h_{n-2}}$, versus the simulation time. The implemented error controllers in MODES keep the step-sizes below the SSP bound (dashed line) during the shock formation, and so we observed no oscillations in the solution. Furthermore, the step-size ratios, $\frac{h_{n-1}}{h_{n-2}}$, remain close to the vicinity of 1. This indicates that step-size change is small at every step. However, a noticeable change in the step-size ratio in Figure 1(b) occurs when the step-size is controlled immediately after initialization. This suggests that the choice of initial step-size can be refined.

Problem 8.2. Another interesting test problem is the scalar ODE,

$$u'(t) = \sin(10t)u(1-u), \qquad u(0) = u_0, \tag{46}$$

with several different initial values $u_0 \in [0,1]$. The exact solution of (46),

$$u(t) = \frac{u_0}{u_0 + (1-u_0)\exp(\frac{\cos(10t)-1}{10})},$$

remains bounded in $[0,1]$ for any $u_0 \in [0,1]$ and $t > 0$. This property should be preserved for SSP numerical schemes applied to (46).

We solve (46) with two multistep methods of order 3, Adams–Bashforth (non-SSP) and the optimal (4,3) SSP method, utilizing the same step-size controller and the same tolerance. Figure 2 shows that the non-SSP method violates the bounds, while the solution remains bounded when the SSP method is applied. Note that the smooth step-size changes guarantee the positivity of the SSP multistep coefficients (37), where $\frac{h_{n-i}}{h_{n-i-1}} \in [1-\epsilon, 1+\epsilon]$ with $\epsilon = 0.1$ and $i = 1, \dots, 4$. Figure 3 shows the small step-size changes and their corresponding ratios that are seen to vary in the interval $[0.9, 1.1]$.

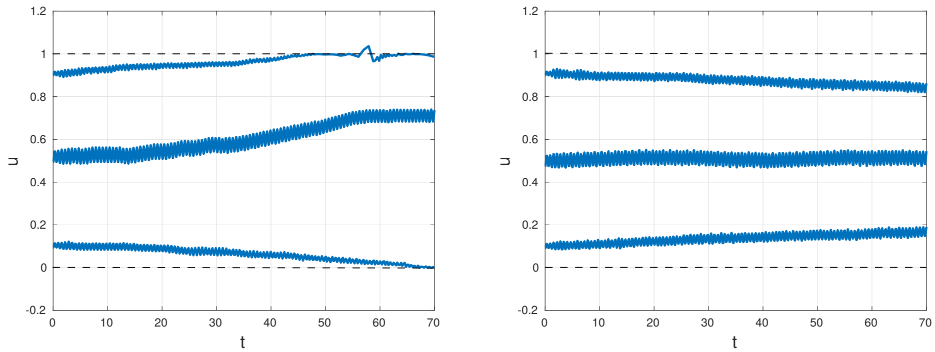

Fig. 2. *The solutions of* (46) *with three different initial values are obtained by the* 3*-step Adams–Bashforth method (left plot) and the* 4*-step optimal SSP method (right plot), both of order* 3*.*

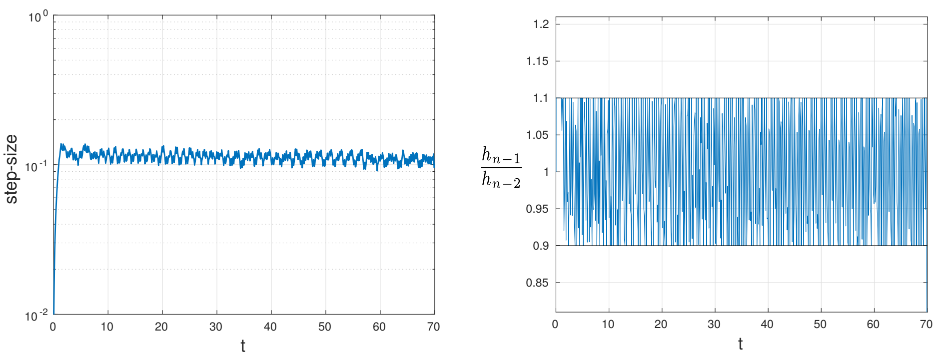

Fig. 3. *The step-size changes versus time for the optimal* $(4, 3)$ *SSP method (left plot) and the step-size ratios* $\frac{h_{n-1}}{h_{n-2}}$ *over the simulation time (right plot).*

9. Conclusion. The parametric formulation presented in this paper gives a simple structure to explicit SSP multistep methods of higher orders. With an addendum to the multistep ODE solver MODES, we have implemented adaptive explicit multistep methods of any order and any number of steps. For SSP methods, the available step-size controllers in MODES keep the step-sizes under the stability limit, in particular during the shock formation. We have proved an equivalence relation between the coefficients of the classical method formulas and the parameters that define an explicit k-step, order p method, with $p < k$.

Although we have observed that with the available controllers, SSP methods take steps within the stability bound, it is best to keep the ratio $\frac{h_n}{\Delta x}$ near or at the step-size limit $C_n h^*$ in order to take larger step-sizes. It would be useful to construct a specific controller that keeps the step-sizes as large as possible while requiring the method to satisfy the non-increasing condition.

The methodology employed in this paper is also suited to the development of adaptive implicit SSP methods. It is possible that adaptivity makes up for some of the additional computations required to solve the nonlinear systems.

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