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Investigation of Efficient High-Order Implicit Runge-Kutta Methods Based on Generalized Summation-by-Parts Operators

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This paper summarizes several new developments in the theory of high-order implicit Runge-Kutta (RK) methods based on generalized summation-by-parts (GSBP) operators. The theory is applied to the construction of several known and novel Runge-Kutta schemes. This includes the well-known families of fully-implicit Radau IA/IIA and Lobatto IIIC Runge-Kutta methods. In addition, a novel family of GSBP-RK schemes based on Gauss quadrature rules is presented along with a few optimized diagonally-implicit GSBP-RK schemes. The novel schemes are all L-stable and algebraically stable. The stability and relative efficiency of the schemes is investigated with numerical simulation of the linear convection equation with both time-independent and time-dependent convection velocities. The numerical comparison includes a few popular non-GSBP Runge-Kutta time-marching methods for reference.

I. Introduction

Nordstrom and Lundquist[1] observed that finite-difference operators satisfying the classical summation-by-parts (SBP) property,[2] along with simultaneous approximation terms (SATs), can be used to construct high-order fully-implicit time-marching methods. With a dual-consistent choice of SAT coefficient,[3,4] this family of methods is L-stable and leads to superconvergence of linear functionals.[5] In addition, those based on diagonal-norm operators are B-stable.[5] Dual-consistency also enables each time step (SBP block) to be solved sequentially in time, rather than having to solve the global problem all at once. However, the stages (pointwise solution) within each time step are fully-coupled and must be solved simultaneously. Given the relatively large minimum number of stages in classical SBP time-marching methods, this approach is relatively inefficient.

A generalization of the classical SBP property[2] was presented in Del Rey Fernández *et al.*[6] The generalized SBP (GSBP) framework enables the construction of high-order SBP time-marching methods with significantly fewer stages. Boom and Zingg[7] showed that GSBP time-marching methods have similar accuracy and superconvergence characteristics and maintain the same stability properties as those based on classical SBP operators. Using a dual-consistent implementation, where each time step is solved sequentially in time, the GSBP framework yields the potential for constructing significantly more efficient SBP time-marching methods.

In a second paper, Boom and Zingg[8] showed that all dual-consistent SBP and GSBP time-marching methods are implicit Runge-Kutta schemes. The order of the GSBP operator corresponds to the minimum stage order. Likewise, the rate of superconvergence is related to the minimum global order of the equivalent Runge-Kutta scheme. These minimum guaranteed results can be superseded using the full and simplifying Runge-Kutta order conditions. Furthermore, the connection to Runge-Kutta schemes provides the tools required to construct nonlinearly stable dense-norm GSBP time-marching methods, as well as diagonally-implicit GSBP time-marching methods.

The objective of this paper is to summarize several recent developments in GSBP time-marching theory, and to present several known and novel GSBP time-marching methods. The stability and relative accuracy

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of these methods is investigated and compared with classical SBP and popular non-SBP implicit time-marching methods. This paper is organised as follows: Section II introduces GSBP time-marching methods for the discretization of initial value problems (IVPs). In addition, it presents the characterization of dual-consistent SBP and GSBP time-marching methods as Runge-Kutta schemes. The accuracy and stability properties of GSBP-RK methods is summarized in Section III. This theory is then applied to the construction and analysis of known and novel time-marching methods based on GSBP operators in Section IV. Finally, numerical simulation in Section V is used to demonstrate various aspects of the theory, and to compare the stability and efficiency of GSBP-RK time-marching methods. A summary concludes the paper in Section VI.

II. Implicit Runge-Kutta Methods Based on Generalized Summation-by-Parts Operators

II.A. Generalized summation-by-parts operators and simultaneous approximation terms

This paper considers discrete approximations of IVPs for nonlinear systems of ordinary differential equations (ODEs):

$$\mathcal{Y}' = \mathcal{F}(\mathcal{Y}, t), \quad \mathcal{Y}(t_0) = \mathcal{Y}_0, \quad \text{with} \quad 0 \le t \le T, \tag{1}$$

where $\mathcal{Y} \in \mathbb{C}^M$, $\mathcal{Y}' = \frac{d\mathcal{Y}}{dt}$, $\mathcal{F}(\mathcal{Y}, t) : \{\mathbb{C}^M, \mathbb{R}\} \to \mathbb{C}^M$, and $\mathcal{Y}_0$ is the vector of initial data. Applying a time-marching method, each time step is defined by a subdomain $[t_0, t_f] \subset [0, T]$. The motivation for time-marching methods which satisfy the SBP or GSBP property is the ability to construct discrete estimates of the solution which mimic the continuous case. This is done using the energy method. An estimate of the solution is constructed by taking the inner product of the solution and IVP. The inner products are then related to the initial condition through the use of integration-by-parts (IBP) in the continuous case and SBP or GSBP in the discrete case. The GSBP definition presented in Del Rey Fernández *et al.*[6] is:

$$\mathbf{u}^* H D \mathbf{v} + \mathbf{u}^* D^T H \mathbf{v} = \mathbf{u}^* \tilde{E} \mathbf{v} \approx \bar{\mathcal{U}} \mathcal{V} \big|_{t_0}^{t_f}, \tag{2}$$

where $\bar{\mathcal{U}}$ is the complex conjugate of the continuous function $\mathcal{U}$, $\mathbf{u}$ is the restriction of $\mathcal{U}$ onto the abscissa $\mathbf{t} = [t_1, \ldots, t_n]$, $\mathbf{u}^*$ is the conjugate transpose of $\mathbf{u}$. H is a symmetric positive definite (SPD) matrix which defines a discrete inner product and norm:

$$(\mathbf{u}, \mathbf{v})_H = \mathbf{u}^* H \mathbf{v}, \quad ||\mathbf{u}||_H^2 = \mathbf{u}^* H \mathbf{u}. \tag{3}$$

The norm is typically classified as diagonal or non-diagonal. We will refer to all non-diagonal norms as dense.[6] Finally, D is a linear first-derivative GSBP operator defined as:

Definition 1 Generalized summation-by-parts operator:[6] *A linear operator $D = H^{-1}\Theta$ is a GSBP approximation to the first derivative of order $\mathcal{O}(h_n^q)$ on the abscissa $\mathbf{t} = [t_1, \ldots, t_n]$, where all t_i are unique and $h_n = \frac{t_f - t_0}{n}$, if D satisfies:*

$$D\mathbf{t}^j = j\mathbf{t}^{j-1}, \quad j \in [0, q], \tag{4}$$

with $q \ge 1$, where $\mathbf{t}^j = [t_1^j, \ldots, t_n^j]^T$ forms a monomial with the convention that $\mathbf{t}^{-1} = \mathbf{0}$, and $(\Theta + \Theta^T) = \tilde{E}$ such that

$$(\mathbf{t}^i)^* \tilde{E} \mathbf{t}^j = (i + j) \int_{t_0}^{t_f} \tilde{t}^{i+j-1} d\tilde{t} = t_f^{i+j} - t_0^{i+j}, \quad i, j, \in [0, r], \tag{5}$$

with $r \ge q$.

The existence of GSBP operators and their relationship to a quadrature rule of order $\mathcal{O}(h_n^\tau)$ is presented in Del Rey Fernández *et al.*[6] Sharper bounds on some of these results are presented in Boom.[9] The classical SBP definition differs in that $\tilde{E}$ must be equal to $\mathbf{diag}(-1, 0, \ldots, 0, 1)$, and therefore $\mathbf{u}^* \tilde{E} \mathbf{v}$ is strictly equal $\bar{\mathcal{U}} \mathcal{V} \big|_{t_0}^{t_f}$.

IVPs require a means to impose the initial condition. In addition, it is often most efficient to use multiple time steps, necessitating a means to couple the solution between time-steps. A natural approach when using GSBP operators is to use SATs.[1,5,7–9] The SAT technique requires an approximation of the solution at the beginning and end of each time step $\tilde{y}_{t_0} \approx \mathcal{Y}(t_0)$ and $\tilde{y}_{t_f} \approx \mathcal{Y}(t_f)$. In general, these values may be projected from the stage solution values, similar to early work presented in Refs. 10–13. The projection operator χ is defined by

$$\chi_{t_0}^T \mathbf{t}^j = {t_0}^j \quad \text{and} \quad \chi_{t_f}^T \mathbf{t}^j = {t_f}^j, \quad j \in [0, q \leq r \leq n-1]. \tag{6}$$

Following References 6–9, the fully-discrete form of (1) using a single time step can then be written as

$$(D \otimes I_M)\mathbf{y}_{\mathrm{d}} = \mathbf{F}_{\mathrm{d}} - \sigma(H^{-1}\chi_{t_0} \otimes I_M)((\chi_{t_0}^T \otimes I_M)\mathbf{y}_{\mathrm{d}} - (I_n \otimes \mathcal{Y}_0)), \tag{7}$$

with

$$\mathbf{y}_{\mathrm{d}} = \begin{bmatrix} y_{\mathrm{d},1} \\ \vdots \\ y_{\mathrm{d},n} \end{bmatrix}, \quad \mathbf{F}_{\mathrm{d}} = \begin{bmatrix} \mathcal{F}(y_{\mathrm{d},1}, t_1) \\ \vdots \\ \mathcal{F}(y_{\mathrm{d},n}, t_n) \end{bmatrix}, \quad y_{\mathrm{d},i} = \begin{bmatrix} y_{\mathrm{d},k,1} \\ \vdots \\ y_{\mathrm{d},k,M} \end{bmatrix}, \tag{8}$$

where σ is the SAT penalty parameter. A natural choice of SAT penalty parameter is $\sigma = -1$, which renders the discretization dual-consistent.[3–5,7] In addition, when using multiple time steps, this choice of SAT penalty parameter decouples the solution within each time step from the solution in subsequent time steps. This enables each time step to be solved sequentially in time like a Runge-Kutta method.

To ensure the compatibility of the SBP and GSBP operators with the SAT implementation, the following condition is imposed:[6]

Condition 1

$$\tilde{E} = \Theta + \Theta^T = \chi_{t_f}\chi_{t_f}^T - \chi_{t_0}\chi_{t_0}^T. \tag{9}$$

Furthermore, to guarantee a unique solution for linear IVPs, a second condition is imposed:[1,5]

Condition 2 *For $\sigma \leq -1/2$, all eigenvalues of $\Theta - \sigma\chi_{t_0}\chi_{t_0}^T$ must have strictly positive real parts.*

II.B. Runge-Kutta Characterization

Boom and Zingg[8] showed that all dual-consistent SBP and GSBP time-marching methods are implicit Runge-Kutta schemes. Consider the i^{th} time step of a dual-consistent SBP or GSBP time-marching method ($\sigma = -1$) applied to (1) with $M = 1$:

$$D\mathbf{y}_{\mathrm{d}}^{[i]} = H^{-1}\Theta\mathbf{y}_{\mathrm{d}}^{[i]} = \mathbf{f}_{\mathrm{d}}^{[i]} - H^{-1}\chi_{t_0^{[i]}}\left(\chi_{t_0^{[i]}}^T\mathbf{y}_{\mathrm{d}}^{[i]} - \chi_{t_f^{[i-1]}}^T\mathbf{y}_{\mathrm{d}}^{[i-1]}\right). \tag{10}$$

The simplification to a scalar IVP ($M = 1$) is done without any loss of generality. Rearranging for the stage solution values and simplifying gives

$$\mathbf{y}_{\mathrm{d}}^{[i]} = \left(\Theta + \chi_{t_0^{[i]}}\chi_{t_0^{[i]}}^T\right)^{-1} H\mathbf{f}_{\mathrm{d}}^{[i]} + \mathbb{1}\tilde{y}^{[i-1]}, \tag{11}$$

where $\tilde{y}^{[i-1]} = \chi_{t_f^{[i-1]}}^T\mathbf{y}_{\mathrm{d}}^{[i-1]}$ and $\mathbb{1} = [1, \ldots, 1]^T$. Projecting (11) to the end of the time step yields

$$\tilde{y}^{[i]} = \chi_{t_f^{[i]}}^T\left(\Theta + \chi_{t_0^{[i]}}\chi_{t_0^{[i]}}^T\right)^{-1} H\mathbf{f}_{\mathrm{d}}^{[i]} + \tilde{y}^{[i-1]}, \tag{12}$$

where $\tilde{y}^{[i]} = \chi_{t_f^{[i]}}^T\mathbf{y}_{\mathrm{d}}^{[i]}$. These two equations ((11) and (12)) describe a Runge-Kutta method with n internal stage approximations:

$$y_k = \tilde{y}^{[i-1]} + h_N\sum_{j=1}^{n} A_{kj}\mathcal{F}(y_{\mathrm{d},j}, t^{[i-1]} + c_j h) \quad \text{for } k = 1, \ldots, n, \tag{13}$$

and solution update

$$\tilde{y}^{[i]} = \tilde{y}^{[i-1]} + h_N\sum_{j=1}^{n} b_j\mathcal{F}(y_{\mathrm{d},j}, t^{[i-1]} + c_j h). \tag{14}$$

The matrices A_{kj} and b_j define the coefficients of the Runge-Kutta method with abscissa $\mathbf{c}$, and step size $h_N = t_f - t_0$. Formally, the coefficient matrices of the equivalent Runge-Kutta scheme defined in terms of the components of a GSBP-SAT discretization are:

$$\begin{aligned} A &= \tfrac{1}{h_N}\left(\Theta + \chi_{t_0}\chi_{t_0}^T\right)^{-1} H, \\ b^T = \chi_{t_f}^T A &= \tfrac{1}{h_N}\chi_{t_f}^T\left(\Theta + \chi_{t_0}\chi_{t_0}^T\right)^{-1} H, \end{aligned} \tag{15}$$

with abscissa

$$\mathbf{c} = \frac{\mathbf{t} - \mathbb{1}t_0^{[i]}}{h_N}. \tag{16}$$

The additional factors of h_N^{-1} in (15) remove the step size implicitly defined in the norm H. Similarly, the form of the GSBP-RK abscissa (16) rescales and translates the interval from $[t_0, t_f]$ to $[0, 1]$.

III. Properties of Implicit Runge-Kutta Methods Based on Generalized Summation-by-Parts Operators

This section reviews common properties of implicit Runge-Kutta methods and how they relate to the conditions imposed on SBP and GSBP time-marching methods. It further explores concepts which are not imposed by the GSBP theory and how they can be exploited to generate more favourable GSBP time-marching methods in terms of accuracy, stability, and efficiency.

III.A. Stage-order conditions

It is common to discuss the accuracy of SBP and GSBP spatial operators with respect to the pointwise error. In the context of IVPs, it is more common to discuss the accuracy of the solution projected to the end of each time step. However, the accuracy of the internal stages can impact of the convergence of the solution at the end of each time step for stiff IVPs.[14,15] This phenomenon is known as order reduction. For Runge-Kutta methods, the accuracy of the internal stage approximations is called stage order. A Runge-Kutta method is said to have stage order $\mathcal{O}(h_N^{\hat{q}})$ if:

$$\mathbf{c}^i = iA\mathbf{c}^{i-1}, \text{ for } i \in [1, \hat{q}], \tag{17}$$

Boom and Zingg[8] showed that the minimum stage order of GSBP-RK time-marching methods is equivalent to the order of accuracy of the GSBP operator. Therefore, by definition all Runge-Kutta time-marching methods based on GSBP operators of order q also have stage order $\hat{q} \geq q$.

III.B. Order conditions

We now consider the global order of accuracy of GSBP-RK time-marching methods, the accuracy of the solution projected to the end of each time step. This does not address the rate of order reduction exhibited by IVPs with a stiff source term or singular perturbation problems.

To begin, consider what has been shown for linear IVPs through the theory of superconvergence. Hicken and Zingg[3,4] developed the theory of superconvergent functionals for classical SBP-SAT discretizations of linear problems. The theory implies that the stage value coincident with the end of each time step is superconvergent. Boom and Zingg[7] extended this theory for GSBP time-marching methods, proving that when the solution is projected to the end of each time step, it remains superconvergent. The rate of superconvergence is restricted by $2q + 1$ and by the accuracy ρ with which the norm H approximates the L_2 inner product. For diagonal norms, this is simply the order of the associated quadrature rule of order $\tau \geq 2q$. In the case of dense norms it is more complex;[6,9] however ρ is always greater than or equal to the order q of the GSBP operator itself.

These results were extended in Boom and Zingg[8] for general nonlinear IVPs by examining the simplifying order conditions for Runge-Kutta schemes derived in Butcher.[16] For diagonal-norm GSBP time-marching methods, the global order for nonlinear problems was shown to be consistent with to the superconvergence theory, *i.e.* $\min(2q + 1, \tau)$. For the dense-norm GSBP time-marching methods, it was only shown that the methods are guaranteed to converge with a minimum order of $\min(\rho, q + 1)$ for nonlinear problems. These are minimum guaranteed order results based on the definition of the GSBP operators and their relation to the SATs.

Boom and Zingg[8] also observed that the simplifying Runge-Kutta order conditions, as well as the full Runge-Kutta order conditions,[17,18] can be used to construct higher-order GSBP-RK methods relative to their stage order. The order of these methods supersede the guaranteed minimum order discussed above. This can be used for constructing high-order diagonally-implicit time-marching methods which are limited to stage-order one. An example of this is given in Section IV.

III.C. Stability

Lundquist and Nordström showed that classical SBP time-marching methods are unconditionally stable for linear problems. This includes A-stability and L-stability. In addition, they showed that classical SBP time-marching methods associated with a diagonal-norm are unconditionally stable for nonlinear problems. This includes both B-stability[a] and energy-stability. The latter is a stability definition introduced in Lundquist and Nordström,[5] and similar in nature to the definition of monotonic schemes in Burrage and Butcher.[20]

In Boom and Zingg[7] these results were extended for GSBP time-marching methods. With the connection to Runge-Kutta schemes, Boom and Zingg[8] observed that these results imply that all SBP and GSBP time-marching methods are AN-stable and algebraically stable.[15,18,19] This is a result of the equivalent Runge-Kutta methods being non-confluent,[15] *i.e.* all c_i are unique.

IV. Examples of Implicit Runge-Kutta Methods Based on Generalized Summation-by-Parts Operators

This section reviews some known and novel Runge-Kutta schemes which are based on GSBP operators.

IV.A. Lobatto IIIC Runge-Kutta methods

Many spatial and temporal discretizations are based on the Gauss-Lobatto family of quadrature rules. For example, Gassner[21] considered diagonal-norm GSBP operators based on these quadrature rules. Applying the GSBP operators of Gassner as dual-consistent SBP time-marching methods leads to the family of Lobatto IIIC discontinuous-collocation Runge-Kutta methods. For example, consider the four-stage diagonal-norm GSBP operator based on Gauss-Lobatto points in the interval $[-1, 1]$:

$$\mathbf{t} = \begin{bmatrix} -1 & -\frac{1}{5}\sqrt{5} & \frac{1}{5}\sqrt{5} & 1 \end{bmatrix}^T. \tag{18}$$

The corresponding norm, whose entries are the Gauss-Lobatto quadrature weights, and resulting GSBP operator are:

$$H = \begin{bmatrix} \frac{1}{6} & & & \\ & \frac{5}{6} & & \\ & & \frac{5}{6} & \\ & & & \frac{1}{6} \end{bmatrix}, \quad D = \begin{bmatrix} -3 & -\frac{5\sqrt{5}}{\sqrt{5}-5} & -\frac{5\sqrt{5}}{\sqrt{5}+5} & \frac{1}{2} \\ \frac{\sqrt{5}}{\sqrt{5}-5} & 0 & \frac{\sqrt{5}}{2} & -\frac{5\sqrt{5}}{\sqrt{5}+5} \\ \frac{\sqrt{5}}{\sqrt{5}+5} & \frac{-\sqrt{5}}{2} & 0 & -\frac{5\sqrt{5}}{\sqrt{5}-5} \\ -\frac{1}{2} & \frac{5\sqrt{5}}{\sqrt{5}+5} & \frac{5\sqrt{5}}{\sqrt{5}-5} & 3 \end{bmatrix}, \tag{19}$$

with exact projection operators $\chi_{-1} = [1, 0, \ldots, 0]^T$ and $\chi_1 = [0, \ldots, 0, 1]^T$. Applying the Runge-Kutta characterization, the coefficients of the equivalent Runge-Kutta scheme are

$$A = \begin{bmatrix} \frac{1}{12} & -\frac{-\sqrt{5}}{12} & \frac{-\sqrt{5}}{12} & -\frac{1}{12} \\ \frac{1}{12} & \frac{1}{4} & \frac{10-7\sqrt{5}}{60} & \frac{\sqrt{5}}{60} \\ \frac{1}{12} & \frac{10+7\sqrt{5}}{60} & \frac{1}{4} & -\frac{\sqrt{5}}{60} \\ \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \end{bmatrix}, \tag{20}$$

[a] B-stability is sometimes referred to as BN-stability when the distinction between autonomous and non-autonomous ODEs is made (Compare Definitions 2.9.2 and 2.9.3 of Jackiewicz[19] and Definition 12.2 in Hairer and Wanner[15]).

and

$$b = \begin{bmatrix} \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \end{bmatrix}, \tag{21}$$

with abscissa:

$$\mathbf{c} = \begin{bmatrix} 0 & \frac{1}{2} - \frac{1}{10}\sqrt{5} & \frac{1}{2} + \frac{1}{10}\sqrt{5} & 1 \end{bmatrix}^T. \tag{22}$$

This is the four-stage Lobatto IIIC discontinuous-collocation Runge-Kutta scheme.[22–26] Likewise, using the approach of Gassner[21] or that of Carpenter and Gottlieb[27] on Radau quadrature points leads to the families of Radau IA and IIA discontinuous-collocation Runge-Kutta schemes.

IV.B. Gauss GSBP-RK time-marching methods

The generalized framework cannot be used in the same way to construct the well-known Gauss collocation Runge-Kutta methods of Butcher[16] and Kuntzmann.[28] The methods of Butcher and Kuntzmann are of order $2n$, where n is the number of stages; however GSBP-RK schemes are limited to order $2q+1$[7,8] with $q \leq n-1$. Therefore, the maximum order of a GSBP-RK scheme is $2n-1$. However, GSBP-RK schemes are by definition L-stable, while the above methods of Butcher and Kuntzmann are not. Consider the four-stage GSBP operator based on Gauss quadrature points in the interval $[-1,1]$, shown here to sixteen decimal places:

$$\mathbf{t} = \begin{bmatrix} -0.8611363115940526 & -0.3399810435848563 & 0.3399810435848563 & 0.8611363115940526 \end{bmatrix}^T. \tag{23}$$

The corresponding norm, whose entries are the Gauss quadrature weights, and resulting GSBP operator are:

$$H = \begin{bmatrix} 0.3478548451374539 & & & \\ & 0.6521451548625461 & & \\ & & 0.6521451548625461 & \\ & & & 0.3478548451374539 \end{bmatrix}, \tag{24}$$

$$D = \begin{bmatrix} -3.3320002363522817 & 4.8601544156851962 & -2.1087823484951789 & 0.5806281691622644 \\ -0.7575576147992339 & -0.3844143922232086 & 1.4706702312807167 & -0.3286982242582743 \\ 0.3286982242582743 & -1.4706702312807167 & 0.3844143922232086 & 0.7575576147992339 \\ -0.5806281691622644 & 2.1087823484951789 & -4.8601544156851962 & 3.3320002363522817 \end{bmatrix}, \tag{25}$$

with projection operators

$$\chi_{-1} = \begin{bmatrix} 1.5267881254572668 & -0.8136324494869273 & 0.4007615203116504 & -0.1139171962819899 \end{bmatrix}^T \tag{26}$$

and

$$\chi_{1} = \begin{bmatrix} -0.1139171962819899 & 0.4007615203116504 & -0.8136324494869273 & 1.5267881254572668 \end{bmatrix}^T \tag{27}$$

Applying the Runge-Kutta characterization, the coefficients of the equivalent Runge-Kutta scheme are

$$A = \begin{bmatrix} 0.0950400941860569 & -0.0470608105772507 & 0.0330840931816566 & -0.0116315325874891 \\ 0.1772065313616314 & 0.1906741915282288 & -0.0555183314150631 & 0.0176470867327749 \\ 0.1781035081124255 & 0.3263151032211517 & 0.1906741915282288 & -0.0251022810693778 \\ 0.1694061893528291 & 0.3339017452341202 & 0.3322201270240200 & 0.0950400941860569 \end{bmatrix}, \tag{28}$$

and

$$b = \begin{bmatrix} 0.0869637112843635 & 0.1630362887156365 & 0.1630362887156365 & 0.0869637112843635 \end{bmatrix}, \tag{29}$$

with abscissa:

$$\mathbf{c} = \begin{bmatrix} 0.0694318442029737 & 0.3300094782075719 & 0.6699905217924281 & 0.9305681557970263 \end{bmatrix}^T. \tag{30}$$

Note that the abscissa and solution update are equivalent to the methods of Butcher and Kuntzmann. Only the A coefficient matrix for the stages is different. The method based on the GSBP operator, which to our knowledge has not been presented previously, is seventh order accurate with stage order three. This is one order lower than the corresponding method of Butcher and Kuntzmann for both stage order and global order; however the GSBP-RK scheme is L-stable.

IV.C. Diagonally-implicit GSBP-RK methods

To demonstrate the application of the extended theory, diagonally-implicit Runge-Kutta schemes are constructed which are based on GSBP operators. Diagonally-implicit methods are often more efficient than fully-implicit schemes, especially in terms of memory usage, and are therefore of particular interest. For these examples, coefficients of the GSBP operator are first constrained such that the resulting Runge-Kutta scheme is diagonally-implicit and satisfies the minimal requirements of Definition 1. The former is done by using the fact that the inverse of a lower triangular matrix is also lower triangular. Therefore, decomposing Θ into symmetric $\Theta_S = \frac{1}{2}\tilde{E}$ and anti-symmetric components Θ_A (See Ref. 6), the coefficients of Θ_A are chosen such that $H^{-1}(\Theta + \chi_{t_0^{[i]}}\chi_{t_0^{[i]}}^T)$, the inverse of the coefficient matrix A, is lower triangular. The remaining coefficients in the GSBP operator and corresponding Runge-Kutta scheme, including the abscissa and weights of the associated quadrature, are solved for using the full-order conditions of Runge-Kutta schemes.

The first example is a novel three-stage third-order GSBP scheme. Several coefficients are determined by solving the full order conditions. The remaining free coefficients are chosen to minimize the L_2-norm of the fourth-order conditions.[29] The abscissa of the GSBP operator to sixteen decimal places is:

$$\mathbf{t} = \begin{bmatrix} 0.0585104413419415 & 0.8064574322792799 & 0.2834542075672883 \end{bmatrix}^T, \tag{31}$$

which is already chosen to be for the domain $[0, 1]$. The norm is determined to be:

$$H = \begin{bmatrix} 0.1008717264855379 & & \\ & 0.4574278841698629 & \\ & & 0.4417003893445992 \end{bmatrix}, \tag{32}$$

which are the weights of the associated quadrature rule, and the GSBP derivative operator is:

$$D_1 = \begin{bmatrix} -12.3737796851209214 & -3.4099304182988046 & 15.7837101034197260 \\ -1.6186577488308495 & 1.2158491567586837 & 0.4028085920721658 \\ -0.9626808228023090 & 1.4979849320764039 & -0.5353041092740949 \end{bmatrix}, \tag{33}$$

with projection operators:

$$\chi_0 = \begin{bmatrix} 1.7239953104443755 & 0.1995165337199744 & -0.9235118441643498 \end{bmatrix}^T, \tag{34}$$

and

$$\chi_1 = \begin{bmatrix} -0.6898048930346554 & 1.0733748002069487 & 0.6164300928277068 \end{bmatrix}^T. \tag{35}$$

It is interesting to note that the abscissa is not ordered, $t_i \not> t_{i-1}$. This is not uncommon for time-marching methods, though it is often chosen for GSBP operators.[6] This additional flexibility enables a third-order method that is diagonally-implicit to be constructed with only three stages. The equivalent diagonally-implicit Runge-Kutta scheme has the following coefficient matrices:

$$A = \begin{bmatrix} 0.0585104413426586 & & \\ 0.0389225469556698 & 0.7675348853239251 & \\ 0.1613387070350185 & -0.5944302919004032 & 0.7165457925008468 \end{bmatrix}, \tag{36}$$

and

$$b = \begin{bmatrix} 0.1008717264855379 & 0.4574278841698629 & 0.4417003893445992 \end{bmatrix}, \tag{37}$$

with $\mathbf{c} = \mathbf{t}$. Note that even though the GSBP derivative operator is dense, the resulting Runge-Kutta scheme is diagonally-implicit. In addition, since the norm associated with the GSBP operator is diagonal, the scheme is by definition L-stable, Algebraically-stable and energy-stable.

As a second example, a four-stage fourth-order diagonally-implicit GSBP scheme is constructed. This goes beyond the order guaranteed by the GSBP theory alone. After restricting to the coefficients of the GSBP operator to satisfy Defintion 1, the full Runge-Kutta order conditions are applied. It is theoretically possible to derive a similar method using the simplifying order conditions; however the scheme described below does not satisfy the fourth-order simplifying conditions. The abscissa to sixteen decimal places is:

$$\mathbf{t} = \begin{bmatrix} 0.5975501145870646 & 0.1236947892666459 & 0.9813648784844768 & 0.2188347157850838 \end{bmatrix}, \tag{38}$$

already chosen to be for the domain $[0, 1]$. The corresponding norm is:

$$H = \begin{bmatrix} 0.5263633266867775 & & & \\ & 0.3002573924935185 & & \\ & & 0.1447678514141155 & \\ & & & 0.0286114294055885 \end{bmatrix}, \tag{39}$$

which defines the weights of the associated quadrature rule, and the GSBP derivative operator is:

$$D = \begin{bmatrix} 0.1993658318073258 & -1.654157580888287 & 1.006020084619771 & 0.4487716644611903 \\ -1.648792506689303 & -1.212963928918776 & 1.978966716941006 & 0.8827897186670728 \\ 3.217338082860363 & -1.615712813301921 & -0.4880781006041668 & -1.113547168954275 \\ 1.271022350640990 & -0.6382938457303877 & 0.6005231745715582 & -1.233251679482160 \end{bmatrix}, \tag{40}$$

with projection operators:

$$\chi_0 = \begin{bmatrix} 0.8808689243587871 & 0.9884420520048577 & -0.6011474168414327 & -0.2681635595222120 \end{bmatrix}, \tag{41}$$

and

$$\chi_1 = \begin{bmatrix} 0.9.928785357819795 & -0.4986129934126102 & 0.4691078563418350 & 0.03662660128879568 \end{bmatrix}. \tag{42}$$

Applying the Runge-Kutta characterization of these operators yields the Runge-Kutta coefficient matrices:

$$A = \begin{bmatrix} 0.5975501145870646 & & & \\ -0.3662683378362842 & 0.4899631271029300 & & \\ -0.9122346095222909 & 1.395636663278596 & 0.4979628247281717 & \\ 4.870201094711127 & -3.007233691002447 & -2.425297972138512 & 0.7811652842149162 \end{bmatrix}, \tag{43}$$

and

$$b^T = \begin{bmatrix} 0.5263633266867775 & 0.3002573924935185 & 0.1447678514141155 & 0.02861142940558849 \end{bmatrix}, \tag{44}$$

with abscissa $\mathbf{c} = \mathbf{t}$. Again, since this Runge-Kutta scheme is constructed from a diagonal-norm GSBP operator, it is L-stable, algebraically-stable and energy-stable. It is also interesting to note that fourth-order is the highest order possible for diagonally-implicit Runge-Kutta schemes which are algebraically-stable.[30] Therefore, to construct a diagonally-implicit GSBP scheme of order greater than four, it must not be algebraically stable, and therefore cannot be based on a diagonal-norm GSBP operator.

V. Numerical Simulation

This section examines the efficiency of various fully-implicit time-marching methods based on classical SBP and GSBP operators. We solve the linear convection equation with unit wave speed and periodic boundary conditions:

$$\begin{aligned} \frac{\partial \mathcal{U}}{\partial t} &= -\frac{\partial \mathcal{U}}{\partial x}, \quad x \in [0, 2], \\ \mathcal{U}(t = 0, x) &= \sin(2\pi x), \\ \mathcal{U}(t, x = 0) &= \mathcal{U}(t, x = 2), \end{aligned} \tag{45}$$

The spatial derivative is discretized with a 100-block GSBP-SAT discretization, where each block is a 5-node operator associated with Legendre-Gauss quadrature.[6] This leads to an IVP of the form:

$$\frac{d\mathcal{Y}}{dt} = \mathcal{A}\mathcal{Y}, \quad \mathcal{Y}_0 = \sin(2\pi \mathbf{x}), \tag{46}$$

where $\mathcal{A}$ is a 500×500 matrix associated with the spatial discretization. The exact solution of this IVP is $\mathcal{Y} = e^{\mathcal{A}t}\mathcal{Y}_0$. Applying a Runge-Kutta time-marching method leads to a linear system equations, which is stored in Matlab's sparse format. Reverse Cuthill-McKee reordering is applied to the linear system and solved using the backslash operator. The solutions were computed using MATLAB 2013a on a 6-core intel Core i7-3930K processor at 3.2GHz with 32GB of RAM.

A summary of the GSBP and non-GSBP time-marching methods investigated is presented in Table 1 along with their associated properties and abbreviations used hereafter. Note that the Radau IIA schemes have stage order n, one higher than the associated GSBP operator, which is limited to $n - 1$. All methods were implemented as Runge-Kutta schemes.

Classical SBP Methods

Quadrature	Norm	Label	$\hat{q}$	p	L/B-stable
Gregory type	Diag.[1,2,5]	FD	$\frac{n}{4}$	$\frac{n}{2}$	Y / Y
	Block[1,5,31]	FDB	$\frac{n}{2}-1$	$\frac{n}{2}$	Y / N

GSBP Methods

Quadrature	Norm	Label	$\hat{q}$	p	L/B-stable
Newton-Cotes	Diag.[6,7]	NC	$\lceil \frac{n}{2} \rceil$	$2\lceil \frac{n}{2} \rceil$	Y / Y
	Dense[7,27]	NCD	$n-1$	$2\lceil \frac{n}{2} \rceil$	Y / N
Lobatto	Diag.*†[7,21,23–25]	LGL	$n-1$	$2n-2$	Y / Y
	Dense[7,27]	LGLD	$n-1$	$2n-2$	Y / N
Radau IA	Diag.*†[6,7,24,25]	LGRI	$n-1$	$2n-1$	Y / Y
Radau IIA	Diag.*†[9,24,25]	LGRII	n	$2n-1$	Y / Y
Gauss	Diag.†[6,7]	LG	$n-1$	$2n-1$	Y / Y

non-SBP Methods

Quadrature	Norm	Label	$\hat{q}$	p	L/B-stable
Gauss	$*$[16,28]	GRK	n	$2n$	N / Y
ESDIRK5	$*$[9]	ESDIRK5	2	5	Y / N

Table 1. Summary of SBP operators, their associated abbreviations and general properties. Notes: 1) the general properties of diagonal-norm NC operators only hold for the case of positive quadrature weights; 2) FD and FDB methods were implemented with their minimum number of stages; 3) the value for q given for FD applies only to $q \geq 2$. The * denotes existing methods in the Runge-Kutta literature, and the † denotes a method discussed in Section IV

V.A. Efficiency Comparisons

For the study of efficiency, the temporal domain is chosen to be $t \in [0, 2]$ and the SAT penalty values are chosen such that both the temporal and spatial discretizations are dual-consistent. Two error measures are used. The first is the stage error:

$$e_{\text{stage}} = \left|\left|\mathbf{e}\right|\right|_B, \tag{47}$$

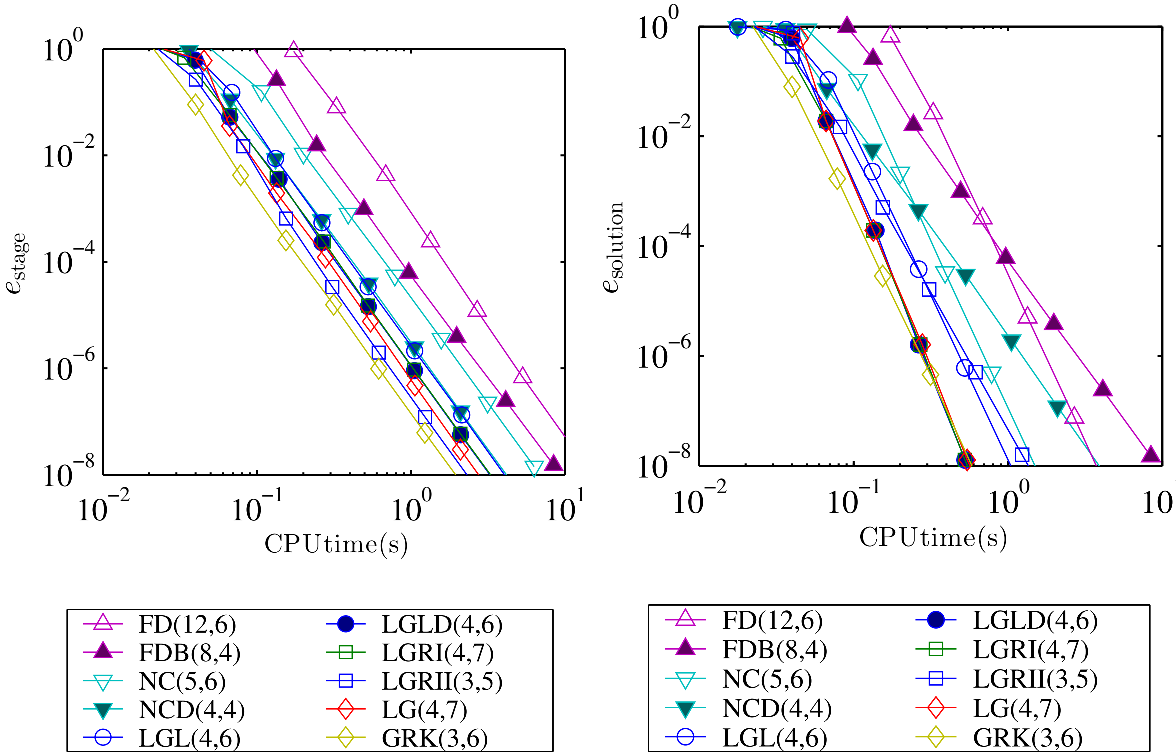
where B is a block diagonal matrix. For SBP and GSBP time-marching methods, the blocks are formed by the norm associated with method. For non-SBP Runge-Kutta methods, the diagonal of each block is populated with the entries of the b coefficient matrix. The vector $\mathbf{e}$ contains the error in the numerical solution at the abscissa locations, integrated in space using the norm of the spatial discretization H_s:

$$\mathbf{e}_{(j-1)n+k} = ||\mathbf{y}_{\text{d},(j-1)n+k} - \mathcal{Y}((j+c_k)h)||_{H_s}, \tag{48}$$

where the subscripts $j = 1, \ldots, N$ and $k = 1, \ldots, n$ are the step and stage indices, respectively. By comparing with the exact solution of the IVP, we isolate the temporal error from the spatial error. The second error measure used is the solution error at the end of the final time step, integrated in space:

$$e_{\text{solution}} = \left|\left|\tilde{y}_{\text{d},N} - \mathcal{Y}(T)\right|\right|_{H_s}. \tag{49}$$

Figure 1 shows the convergence of the stage and solution error with respect to CPU time in seconds for constant stage order, $\hat{q} = 3$. The stage error, e_{stage}, converges at the same rate for the various methods, as expected. Furthermore, the hierarchy in efficiency with respect to stage error negatively correlates with the



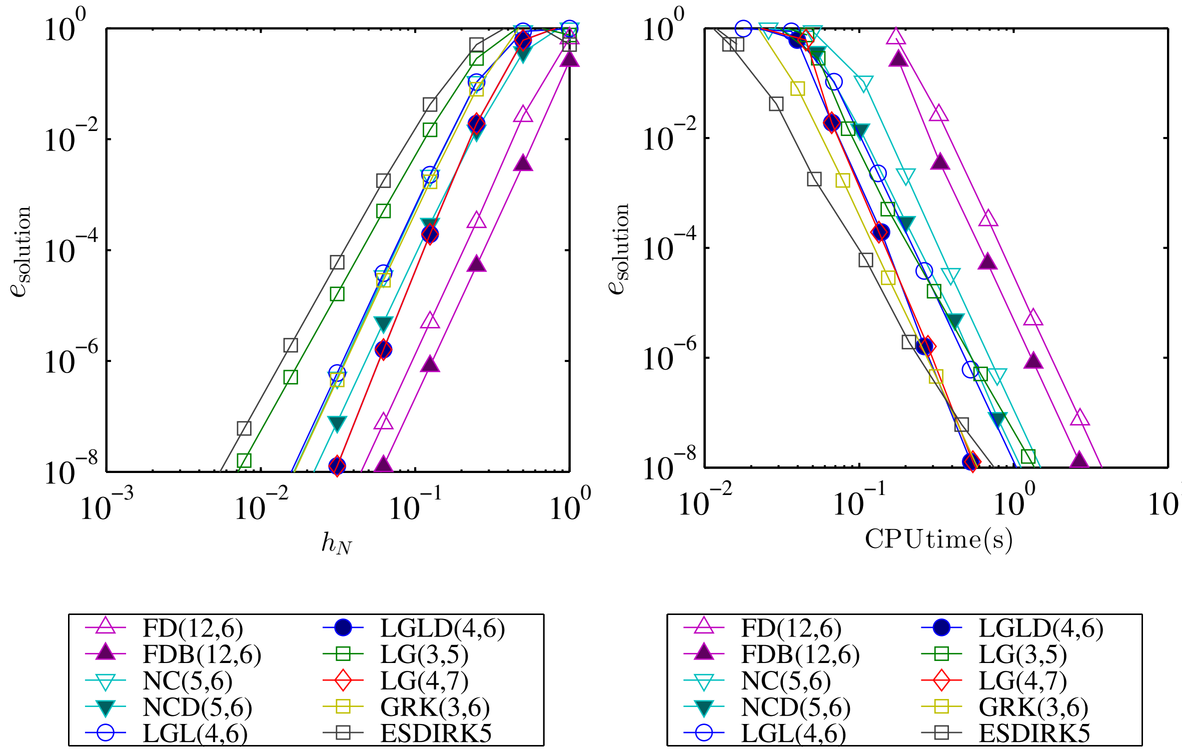
a) e_{stage} ($\hat{q} = 3$) b) e_{solution} ($\hat{q} = 3$)

Figure 1. Linear Convection Equation: Convergence of the stage and solution error, e_{stage} and e_{solution} respectively, with respect to CPU time (s) for constant stage order. The numerical suffix in the legend indicates the number of stages in each time step n and the order p.

number of stages in each method. Thus, the classical SBP time-marching methods, FD and FDB, are the least efficient due the their relatively large number of stages. Of those with four stages, the novel GSBP time-marching method LG is the most efficient method with respect to stage error. This scheme is more efficient than the well-known LGRI scheme, which has the same properties; however, it is not as efficient as the three-stage GRK or LGRII methods.

Considering the solution error, e_{solution}, the hierarchy of efficiency remains negatively correlated with the number of stages in each method of a given order p. The higher than expected convergence rate for the dense-norm LGL time-marching method ($p = \rho + 1$) is only seen for linear problems (compare with Ref. 7). As expected, the GSBP time-marching methods are more efficient than those based on classical SBP operators. This is especially true for those with a nonuniform abscissa or an abscissa which does not include 0 or 1. The most efficient method overall is GRK. It is one order lower than the GSBP time-marching methods LG and LGRI, but also has one fewer stages. This method is not L-stable. Eventually, the LG and LGRI become more efficient than the GRK method below an error of about 10^{-7}.

Another perspective can be obtained by comparing methods of constant order p. Figure 2 shows the convergence of the solution error with respect to step size $h_N = t_f - t_0$ and CPU time in seconds for constant order, $p = 6$. This also includes the exclusively odd order GSBP time-marching methods based on Gauss quadrature of orders $p = 5$ and $p = 7$, as well as the fifth-order ESDIRK5 reference scheme. The error of classical SBP time-marching methods relative to time step size h_N is significantly smaller than the GSBP time-marching methods. This however does not account for the higher number of stages. Therefore, the GSBP time-marching methods are nevertheless more efficient, as shown in Figure 2 b). Apart from LGLD, which achieves higher than expected convergence, the well-known GRK scheme is the most efficient sixth-order scheme. As discussed above, the LG scheme of one order higher eventually becomes more efficient. It is also L-stable, which the GRK scheme is not.



a) e_{stage} b) e_{solution}

Figure 2. Linear Convection Equation: Convergence of the solution error, e_{solution}, with respect to step size h_N and CPU time (s). The numerical suffix in the legend indicates the number of stages in each time step n and the order p.

V.B. Diagonally-implicit methods

While diagonally-implicit methods typically require a greater number of stages to achieve the same order of accuracy, each stage can be solved sequentially. Thus, each time step requires the solution to multiple smaller systems of equations in place of one larger system. The higher efficiency is realized from the nonlinear scaling of computational work required in solving a system of equations.

For lower orders this effect is minimized as fully-implicit time-marching methods only require one or two coupled stages. For example, the three-stage third-order diagonally-implicit GSBP time-marching method developed in Section IV requires approximately the same computational effort as the two-stage third-order LG, LGRI, and LGRII schemes. Furthermore, the fully-implicit schemes have a much lower truncation error coefficient and are therefore more efficient.

As the order increases, so does the number of stages required by fully-implicit schemes. Thus, diagonally-implicit scheme have the potential to be more efficient. As an example, consider the ESDIRK5 scheme presented in Figure 2. It has the largest error as a function of step size h_N, but is the most efficient scheme considered above an error of about 10^{-7}. This highlights the potential advantage of considering higher-order diagonally-implicit GSBP time-marching methods in the future.

V.C. Stability

A method is said to be AN-stable if $\mathcal{Y}' = \lambda(t)\mathcal{Y}$ with $\lambda(t) \leq 0$ for $t \in [0, T]$ implies that $||\tilde{y}_{\text{d},T}|| \leq ||\mathcal{Y}_0||$. This is a simple extension of classical linear A-stability; however it has been shown to be more closely related to nonlinear stability definitions like B-stability.[15, 18, 19] Furthermore, the criteria for AN, B, BN, and algebraic stability are equivalent for non-confluent Runge-Kutta schemes.[15] Therefore in this paper, following Nordström and Lundquist,[5] a nonlinear transformation of the temporal domain is used to investigate AN-stability and demonstrate the value of nonlinear stability.

The transformation used in the present paper is:

$$\tau = \lfloor t \rfloor + \sin^2\left(\frac{\pi(t - \lfloor t \rfloor)}{2}\right), \tag{50}$$

where $\lfloor \rfloor$ is the floor operator. With this transformation, the PDE becomes:

$$\frac{\partial \mathcal{Y}}{\partial \tau} = -\frac{\partial t}{\partial \tau}\frac{\partial \mathcal{Y}}{\partial x}, \quad x \in [0, 2], \tag{51}$$

$$\mathcal{Y}(\tau = 0, x) = \sin(2\pi x), \tag{52}$$

$$\mathcal{Y}(\tau, x = 0) = \mathcal{Y}(\tau, x = 2). \tag{53}$$

This is equivalent to introducing a time-dependent convection velocity. Applying the same spatial discretization as before, the resulting IVP has the form:

$$\frac{d\mathcal{Y}}{d\tau} = \lambda(\tau)\mathcal{A}\mathcal{Y}, \quad \mathcal{Y}_0 = \sin(2\pi \mathbf{x}), \tag{54}$$

where $\lambda(\tau) = \frac{\partial t}{\partial \tau}$. The stability function, or iteration matrix, of a Runge-Kutta method applied to this IVP is:

$$M_{AN} = I_M + h_N b^T \Lambda(\tau) \otimes \mathcal{A}(I_{Mn} - h_N A\Lambda(\tau) \otimes \mathcal{A})\mathbb{1}_n \otimes I_M. \tag{55}$$

where $\Lambda(\tau)$ is a diagonal matrix which contains the projection of $\lambda(\tau)$ onto the abscissa of the time-marching method. The method is stable if eigenvalues remain within the unit disk and any eigenvalue of the unit disk is simple. In addition, consider the following measure of the solution:

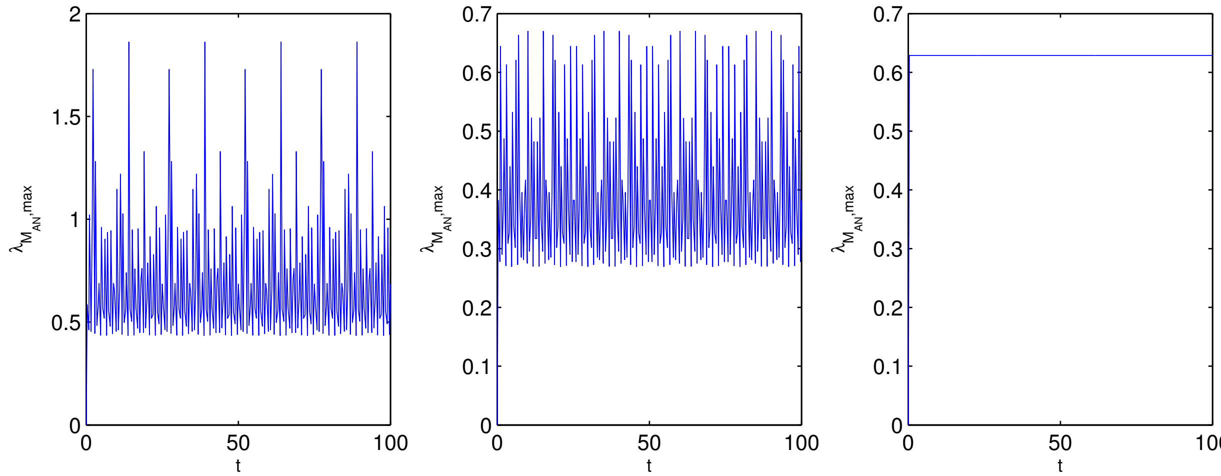
$$E = \left|\left|\tilde{y}_{\mathrm{d},j}\right|\right|_{H_s}, \tag{56}$$

at time step j. This serves to highlight the instability, though it is not as rigorous an approach as studying the eigenvalues of the stability matrix.

For this comparison consider the five-stage sixth-order diagonal and dense-norm GSBP time-marching methods based on Newton-Cotes quadrature. The former is by definition algebraically stable, and hence AN-stable, while the latter method is not. Both methods are L-stable. For these simulations, the temporal domain is $\tau \in [0, 100]$, and the time step size chosen is $h_N = 0.390625$. Three cases are chosen for this comparison:

1. The dense-norm Newton-Cotes GSBP time-marching method applied to the IVP with the transformed temporal coordinate;
2. The diagonal-norm Newton-Cotes GSBP time-marching method applied to the IVP with the transformed temporal coordinate; and
3. The dense-norm Newton-Cotes GSBP time-marching method applied to the IVP without the transformed temporal coordinate. This case only requires A-stability.

Figure 3 shows the evolution of the magnitude of the largest eigenvalue of the stability matrix. Plots a) and b) of this Figure show large variation due to the temporal transformation. However, only for the dense-norm GSBP time-marching method, which is not AN-stable, do the eigenvalues leave the unit disk. Interestingly, in this case the eigenvalues lie within the unit disk for the majority of the time steps; however, the time steps which are unstable are sufficient to increase the measure of the solution (Figure 4 a)). For the diagonal-norm GSBP time-marching method, the eigenvalues all remain within the unit disk as predicted. The measure of the solution (Figure 4 b)) decrease rapidly towards zero. Finally, in the third case the temporal transformation is removed and $\lambda(\tau)$ becomes constant. The requirement for stability is reduced to A-stability. Given that all GSBP time-marching methods are L-stable, even the dense-norm GSBP time-marching method is stable for this case.

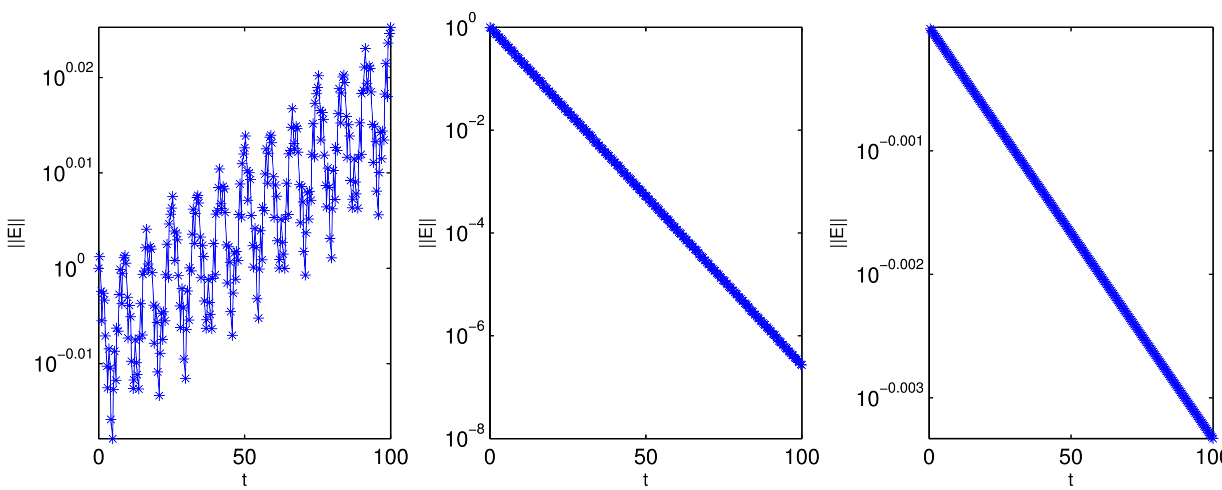


a) M_{AN}: Dense-norm NC with temporal transformation

b) M_{AN}: Diagonal-norm NC with temporal transformation

c) M_{AN}: Dense-norm NC without temporal transformation

Figure 3. Linear Convection Equation: The time evolution of the maximum magnitude of the eigenvalues of the stability matrix (55)**.**



a) Energy: Dense-norm NC with temporal transformation

b) Energy: Diagonal-norm NC with temporal transformation

c) Energy: Dense-norm NC without temporal transformation

Figure 4. Linear Convection Equation: The time evolution of the solution measure (56)**.**

VI. Conclusions

This paper presents a summary of recent developments in the theory of GSBP time-marching methods and their characterization as Runge-Kutta schemes. This theory is then applied to the construction of some known and novel time-marching methods. This includes the well-known Lobatto IIIC and Radau IA/IIA discontinuous collocation Runge-Kutta schemes, a novel GSBP-RK scheme based on Gauss quadrature points, and some novel diagonally-implicit and algebraically stable GSBP-RK schemes. Numerical simulation of the linear convection equation with time-independent and time-dependent convection velocities is presented to demonstrate the theory and to evaluate the stability and relative efficiency of GSBP time-marching methods. In comparison with classical SBP time-marching methods, the GSBP based schemes are more efficient. The novel Gauss based GSBP time-marching method retains the same properties as the Radau IA scheme, and is slightly more efficient with respect to stage error. The global error however is comparable. Comparison with the non-SBP Gauss collocation methods is difficult as their orders do not match. For the same number of stages, the non-SBP method is one order higher and more efficient; however, it is not L-stable. When the SBP method is one order higher, the efficiency is comparable. Inclusion of a fifth-order ESDIRK scheme highlights the potential benefit of constructing higher-order GSBP time-marching methods in the future which are diagonally-implicit.

Acknowledgments

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