# On the relations between $\mathrm{B}_{2}$ VMs and Runge-Kutta collocation methods 

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#### Abstract

The principal aim of this paper is a rigorous analysis of the relations between Block Boundary Value Methods ( $\mathrm{B}_{2} \mathrm{VMs}$ ) with minimal blocksize defined over a suitable nonuniform finer mesh and well-known Runge-Kutta collocation methods. Moreover, a further aspect that will be briefly investigated is the construction of an extended finer mesh for building $\mathrm{B}_{2} \mathrm{VMs}$ with nonminimal blocksize. Some advantages that may arise from the use of the so-obtained methods will be also discussed.


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## 1. Introduction

In the nineties Boundary Value Methods (BVMs) were introduced for the numerical solution of differential problems, see [1] and the references therein. They are Linear Multistep Methods (LMMs) coupled with suitable boundary conditions. Many negative results concerning the stability properties of LMMs used as initial value methods have been overcome in this more general setting. This is the case of the second Dahlquist barrier which, without doubt, constitutes a severe restriction on the order of accuracy for methods well-suited for the solution of stiff differential equations. In this regard, the results concerning the stability properties of BVMs have been reported in [1] and in several papers among which we quote [2-7]. On the other hand, for the numerical solution of conservative problems, the BVM approach also turns out to be successful for overcoming the pessimistic conclusions reported in [8-10]. In particular, the results concerning the applicability of BVMs for the numerical solution of Hamiltonian systems are described in [11-13].

As previously mentioned, by construction a BVM approximates the solution of the initial value problem

$$
\left\{\begin{array}{l}
y^{\prime}(t)=f(t, y), \quad t \in\left[t_{0}, T\right] \\
y\left(t_{0}\right)=y_{0} \in \mathbb{R}
\end{array}\right.
$$

by means of a discrete boundary value one. It follows that if $\tau_{0} \equiv t_{0}<\tau_{1}<\cdots<\tau_{s} \equiv T$ is an assigned grid over [ $\left.t_{0}, T\right]$ and $\mathbf{y}=\left(y_{1}, y_{2}, \ldots, y_{s}\right)^{\mathrm{T}}$ is the corresponding numerical solution provided by a BVM, all the entries in $\mathbf{y}$ must be computed simultaneously. A refinement of the mesh thus determines an increase of the dimension of the system of algebraic equations which have to be solved all at once. This may represent a relevant drawback that becomes more marked in the case of an high nonlinearity of the function $f$ defining the continuous problem.

When the block version of BVMs ( $\mathrm{B}_{2} \mathrm{VMs}$ in the sequel), introduced in [14,15], is applied for solving problem (1), instead, two different meshes are used: a coarser mesh which subdivides $\left[t_{0}, T\right]$ into contiguous subintervals and a finer mesh defined over each of them and composed of a fixed number of points. A selected BVM is then applied for approximating the exact solution over each subinterval. Making use of the initial value $y_{0}$ of the continuous problem the numerical integration can

[^0]be therefore operated in a step-by-step fashion thus reducing, in general, the computational cost for solving the discrete problem with respect to that of BVMs. As a matter of fact, a number of algebraic systems of equations of fixed size has to be solved instead of a unique system of very large dimension. In the former case, the simplified Newton method or iterative procedures based on suitable nonlinear splittings may be conveniently used [16-19].

From a theoretical point of view, $\mathrm{B}_{2} \mathrm{VMs}$ are related to one-step methods and a suitable reformulation of the discrete problem they generate for (1) allows one to read them as Runge-Kutta (RK for short) methods. More precisely, as the number of nodes composing the finer mesh varies, a family of RK methods is derived from a particular BVM implemented in block form.
$\mathrm{B}_{2} \mathrm{VMs}$ have been used in the computational code GAMD designed for solving stiff ordinary and algebraic differential equations [19-21]. The code implements a variable stepsize, variable order block-Generalized Adams Method with a uniform finer mesh. In this case, the freedom of choosing the blocksize $s$ of the $\mathrm{B}_{2} \mathrm{VM}$ has been exploited for deriving the implemented order variation strategy. Another application of $\mathrm{B}_{2}$ VMs constructed over a uniform finer mesh can be found in [22]. Here we are interested in considering different distributions of the points composing the finer mesh. In particular our principal aim is the establishment of the existing connections between $\mathrm{B}_{2} \mathrm{VMs}$ and well-known RK collocation methods. As a matter of fact, even thought such relations have been mentioned in previous works like [22,23], a systematic analysis of them has never been reported.

The paper is organized as follows. In Section 2 we describe in some detail the construction of BVMs over an assigned nonuniform partition of the integration interval. In Section $3 \mathrm{~B}_{2} \mathrm{VMs}$ are introduced and their connections with RK schemes are discussed. In particular, we prove that $\mathrm{B}_{2} \mathrm{VMs}$ with minimal blocksize are equivalent to stiffly accurate RK collocation methods. The obtained results are then specialized in Section 4 where their relations with well-known RK schemes are put into evidence. Finally, in Section 5 a possible extension of the finer mesh for building $B_{2}$ VMs with larger blocksizes is proposed and an example aimed to compare the performances of $\mathrm{B}_{2} \mathrm{VMs}$ used with different blocksizes is reported.

## 2. Boundary value methods

Let us assume that the partition $\pi=\left\{\tau_{0} \equiv t_{0}<\tau_{1}<\tau_{2}<\cdots<\tau_{s} \equiv T\right\}$ of the integration interval [ $t_{0}, T$ ] has been assigned with

$$
\begin{equation*}
\tau_{n}=\tau_{n-1}+\hat{h}_{n}, \quad n=1,2, \ldots, s \tag{2}
\end{equation*}
$$

and let us denote by $y_{n}$ the numerical approximation of $y\left(\tau_{n}\right)$. As is well-known, the discrete problem generated by a $k$ step LMM is a difference equation of order $k$ so that its solution is uniquely determined once $k$ conditions are imposed for it. Obviously one of them, namely the initial value $y_{0}$, is inherited directly from the continuous problem. Concerning the remaining $k-1$ conditions, the BVM approach establishes splitting them into $k_{1}-1$ initial and $k_{2}=k-k_{1}$ final ones. The parameter $k_{1}$ depends on the particular formula and is chosen in order to ensure good stability properties of the method itself [1]. The discrete problem generated by a BVM is then given by

$$
\begin{equation*}
\sum_{j=-k_{1}}^{k_{2}} \alpha_{j+k_{1}}^{(n)} y_{n+j}-\hat{h}_{n} \sum_{j=-k_{1}}^{k_{2}} \beta_{j+k_{1}}^{(n)} f_{n+j}=0, \quad n=k_{1}, \ldots, s-k_{2} \tag{3}
\end{equation*}
$$

$$
\begin{equation*}
y_{0}, y_{1}, \ldots, y_{k_{1}-1}, y_{s-k_{2}+1}, \ldots, y_{s} \text { fixed, } \tag{4}
\end{equation*}
$$

with $f_{n+j}=f\left(\tau_{n+j}, y_{n+j}\right)$. Here, $\left\{\alpha_{j}^{(n)}\right\}_{j=0}^{k}$ and $\left\{\beta_{j}^{(n)}\right\}_{j=0}^{k}$ are the coefficients of the $n$-th LMM; their values depend on the distribution of the nodes on which such formula is constructed. In particular, in the case of a uniform mesh, $\alpha_{j}^{(n)}=\alpha_{j}^{\left(k_{1}\right)}$ and $\beta_{j}^{(n)}=\beta_{j}^{\left(k_{1}\right)}$ for each $j=0,1, \ldots, k$ and $n=k_{1}, \ldots, s-k_{2}$.
Usually, the boundary values in (4) are replaced with the following equations:

$$
\begin{align*}
& \sum_{j=-n}^{k-n} \alpha_{j+n}^{(n)} y_{n+j}-\hat{h}_{n} \sum_{j=-n}^{k-n} \beta_{j+n}^{(n)} f_{n+j}=0, \quad n=1, \ldots, k_{1}-1,  \tag{5}\\
& \sum_{j=-n}^{k-n} \alpha_{j+n}^{(n)} y_{s-k+j+n}-\hat{h}_{n} \sum_{j=-n}^{k-n} \beta_{j+n}^{(n)} f_{s-k+j+n}=0, \quad n=s-k_{2}+1, \ldots, s . \tag{6}
\end{align*}
$$

This means that the method in (3), called the main method, is coupled with $k_{1}-1$ initial additional methods and $k_{2}$ final ones. Often, all these formulas are chosen so that they have the same order of accuracy. In particular, for each $n=k_{1}, k_{1}+1, \ldots, s-k_{2}$, the $n$-th formula has (at least) order $p$ if its coefficients satisfy

$$
\begin{equation*}
\sum_{j=-k_{1}}^{k_{2}}\left(\left(\xi_{j, n}\right)^{\ell} \alpha_{j+k_{1}}^{(n)}-\ell\left(\xi_{j, n}\right)^{\ell-1} \beta_{j+k_{1}}^{(n)}\right)=0, \quad \ell=0,1, \ldots, p \tag{7}
\end{equation*}
$$

with

$$
\begin{equation*}
\xi_{j, n} \equiv \frac{\tau_{n+j}-\tau_{n}}{\tau_{n}-\tau_{n-1}} \tag{8}
\end{equation*}
$$

Such order conditions are obtained by applying the Taylor series expansion of the exact solution at $\tau_{n}$ and the first two of them are called conditions of consistency. Similar relations must be satisfied by the coefficients of the additional methods. For later reference, the order conditions are now stated in matrix form. Let

$$
\begin{align*}
& \boldsymbol{\alpha}^{(n)}=\left(\begin{array}{c}
\alpha_{0}^{(n)} \\
\alpha_{1}^{(n)} \\
\vdots \\
\alpha_{k}^{(n)}
\end{array}\right), \quad \boldsymbol{\beta}^{(n)}=\left(\begin{array}{c}
\beta_{0}^{(n)} \\
\beta_{1}^{(n)} \\
\vdots \\
\beta_{k}^{(n)}
\end{array}\right), \quad L_{p}=\left(\begin{array}{ccc}
0 & & \\
1 & \ddots & \\
& \ddots & \ddots \\
\\
& & p
\end{array}\right),  \tag{9}\\
& V_{n, k, \mu}^{(p)}=\left(\begin{array}{ccc}
1 & \ldots & 1 \\
\xi_{-\mu, n} & \cdots & \xi_{k-\mu, n} \\
\vdots & & \vdots \\
\left(\xi_{-\mu, n}\right)^{p} & \ldots & \left(\xi_{k-\mu, n}\right)^{p}
\end{array}\right), \tag{10}
\end{align*}
$$

where

$$
\mu \equiv \mu\left(n, k_{1}, k, s\right)= \begin{cases}n & \text { if } n=1, \ldots, k_{1}-1  \tag{11}\\ k_{1} & \text { if } n=k_{1}, \ldots, s-k_{2} \\ n+k-s & \text { if } n=s-k_{2}+1, \ldots, s\end{cases}
$$

The relations (7), together with the corresponding ones for the additional methods, can be equivalently stated as

$$
\begin{equation*}
V_{n, k, \mu}^{(p)} \boldsymbol{\alpha}^{(n)}=L_{p} V_{n, k, \mu}^{(p)} \boldsymbol{\beta}^{(n)}, \quad n=1,2, \ldots, s \tag{12}
\end{equation*}
$$

We now briefly describe some families of BVMs which we shall consider in this paper; for further details on them refer to [1,6,7].
(i) Generalized Backward Differentiation Formulas (GBDFs)

The methods in this family are derived by fixing "a priori" the coefficient vectors $\boldsymbol{\beta}^{(n)}$ as, see (11),

$$
\begin{equation*}
\boldsymbol{\beta}^{(n)}=\mathbf{e}_{\mu+1}, \quad n=1,2, \ldots, s \tag{13}
\end{equation*}
$$

with $k_{1}=\left\lceil\frac{k+1}{2}\right\rceil$ and, hereafter, $\mathbf{e}_{l}$ the $l$-th unit basis vector in $\mathbb{R}^{k+1}, l=1,2, \ldots, k+1$. For each $n$, the corresponding coefficient vector $\boldsymbol{\alpha}^{(n)}$ is then selected in order to gain the maximum attainable order of accuracy, which results in being $p=k$.
(ii) Generalized Adams Methods (GAMs)

These are methods with coefficient vectors $\boldsymbol{\alpha}^{(n)}$ "a priori" fixed as, see (11),

$$
\boldsymbol{\alpha}^{(n)}=\mathbf{e}_{\mu+1}-\mathbf{e}_{\mu}, \quad n=1,2, \ldots, s
$$

with $k_{1}=\left\lceil\frac{k}{2}\right\rceil$. The first equation in (12) is therefore trivially satisfied and, consequently, the maximum attainable order is now $p=k+1$. When $k$ is odd, these schemes are also called Extended Trapezoidal Rules (ETRs).
(iii) Top Order Methods (TOMs)

The main formula of this family of BVMs is a $k$-step LMM without "a priori" restrictions on the choice of its coefficients. This permits one to construct methods having the highest possible order, which is given by $p=2 k$. The step-number $k$ is restricted to be odd and the number of initial conditions has been chosen as $k_{1}=\frac{k+1}{2}$ for stability reasons. Concerning the additional methods, they are usually taken to be equal to the ones used for the ( $2 k-1$ )-step ETR having order $2 k$.
(iv) BS methods (BSs)

They are a class of LMMs based on B-Splines with distinct nodes that can be interpreted as (spline) collocation methods. This means that for a $k$-step BS method, a $k+1$ degree spline function, continuous up to the $k$-th derivative can be associated with the numerical solution. They were originally introduced in $[24,25]$ and they resulted in being convergent only for $k \leq 2$. In recent papers [6,7] the authors proved that, when implemented as BVMs with $k_{1}=\left\lceil\frac{k}{2}\right\rceil$ and $k_{2}=k-k_{1}$ boundary conditions, these methods are convergent of order $p=k+1$ for each $k$ and that, when $k$ is odd, they satisfy very good stability properties. Concerning the additional methods (5)- (6), their coefficients are always derived by imposing the not-a-knot condition for the collocation spline over suitable knots near the extremes of the interval $\left[t_{0}, T\right]$. The so-obtained additional methods turn out to be of the same order of accuracy of the main formula.

## 3. $B_{2}$ VMs: definition and connections with RK schemes

When a $k$-step $\mathrm{B}_{2} \mathrm{VM}$ is applied for solving problem (1), the interval of integration is discretized by means of two different meshes. The first one, called a coarser mesh, subdivides [ $t_{0}, T$ ] into $m$ subintervals determined by the nodes

$$
\begin{equation*}
t_{r}=t_{r-1}+h_{r}, \quad r=1, \ldots, m, \quad t_{m} \equiv T \tag{14}
\end{equation*}
$$

Then, each subinterval $\left[t_{r-1}, t_{r}\right]$ is discretized by means of a finer mesh composed by a fixed number of nodes, say $s+1$, and an assigned distribution of such nodes, that is

$$
\begin{equation*}
t_{n, r}=t_{r-1}+c_{n} h_{r}, \quad n=0,1, \ldots, s \tag{15}
\end{equation*}
$$

with

$$
\begin{equation*}
c_{0}=0<c_{1}<\cdots<c_{s}=1 . \tag{16}
\end{equation*}
$$

In order to provide the numerical solution for the initial value problem (1), the integration begins by applying a selected $k$-step BVM on the first subinterval [ $t_{0}, t_{1}$ ], making use of the initial value $y_{0}$ provided by the continuous problem. An approximation of the solution at $t=t_{1}$ is thus obtained and this is used as the initial value for the computation of the numerical solution over the second subinterval $\left[t_{1}, t_{2}\right]$ through the same BVM. The integration proceeds in this way until the entire interval $\left[t_{0}, T\right]$ has been covered. This procedure defines a $\mathrm{B}_{2} \mathrm{VM}$.

Remark 1. In the sequel, when a GBDF is the selected method used to construct a $B_{2} V M$, we shall refer to the latter as a block-GBDF. Similarly, this will be done for the methods in the other families of BVMs.

Remark 2. It is important to note that the blocksize $s$ must be greater than a minimum value, say $\bar{s}$, which depends on the BVM used and on the corresponding additional methods; in particular, for each $k, \bar{s}=k$ for all $k$-step $\mathrm{B}_{2} \mathrm{VMs}$ based on the methods introduced in the previous section, with the only exception of the $k$-step block-TOM for which $\bar{s}=2 k-1$. In fact in the former case, both the main and the additional formulas have the same stepnumber, i.e. $k$. For the $k$-step block-TOM, instead, the additional methods are $(2 k-1)$-step LMMs for preserving the order $2 k$ of accuracy of the scheme. In any case, one verifies that $\bar{s}=\max (k, p-1)$, where $p$ is the order of the used BVM.

For each subinterval of integration, the finer mesh (15) plays the role of the mesh $\pi$ given in (2). In particular, the two meshes coincide when $m=r=1$ (see (14)) by letting $\tau_{n}=t_{n, 1}$ and $\hat{h}_{n}=\left(c_{n}-c_{n-1}\right)\left(T-t_{0}\right)$. Therefore, in the new notation, for each $n=1,2, \ldots, s, j=-\mu, \ldots, k-\mu$, with $\mu$ defined in (11), the values of $\xi_{j, n}$ are given by, see (8),

$$
\begin{equation*}
\xi_{j, n}=\frac{t_{n+j, r}-t_{n, r}}{t_{n, r}-t_{n-1, r}}=\frac{c_{n+j}-c_{n}}{c_{n}-c_{n-1}}, \quad r=1,2, \ldots, m \tag{17}
\end{equation*}
$$

In the previous expression we have not introduced the index $r$ on $\xi_{j, n}$ since the ratios do not depend on it. By virtue of this property the coefficients of the method are invariant with respect to the subinterval of integration since the order conditions are invariant too (see (12)). Therefore, the discrete problem composed of the Eqs. (3) and (5)-(6), for the generic subinterval [ $t_{r-1}, t_{r}$ ], becomes

$$
\sum_{j=-\mu}^{k-\mu} \alpha_{j+\mu}^{(n)} y_{n+j, r}-h_{r} \phi_{n} \sum_{j=-\mu}^{k-\mu} \beta_{j+\mu}^{(n)} f_{n+j, r}=0, \quad n=1,2, \ldots, s
$$

where $y_{n+j, r} \approx y\left(t_{n+j, r}\right), f_{n+j, r}=f\left(t_{n+j, r}, y_{n+j, r}\right), \phi_{n}=c_{n}-c_{n-1}$, and $\mu$ is defined in (11). By denoting with

$$
Y_{r}=\left(y_{1, r}, y_{2, r}, \ldots, y_{s, r}\right)^{\mathrm{T}}, \quad F_{r}=\left(f_{1, r}, f_{2, r}, \ldots, f_{s, r}\right)^{\mathrm{T}},
$$

such a discrete problem can be stated in matrix form as

$$
\begin{equation*}
A Y_{r}-h_{r} B F_{r}+\mathbf{a} y_{0, r}-h_{r} \mathbf{b} f_{0, r}=\mathbf{0} . \tag{18}
\end{equation*}
$$

Here $\mathbf{0}=(0,0, \ldots, 0)^{\mathrm{T}} \in \mathbb{R}^{s},[\mathbf{a} \mid A] \in \mathbb{R}^{s \times(s+1)}$ is given by

$$
[\mathbf{a} \mid A]=\left(\begin{array}{l|llllll}
\alpha_{0}^{(1)} & \alpha_{1}^{(1)} & \cdots & \alpha_{k}^{(1)} & & &  \tag{19}\\
\vdots & \vdots & & \vdots & & & \\
\alpha_{0}^{\left(k_{1}\right)} & \alpha_{1}^{\left(k_{1}\right)} & \cdots & \alpha_{k}^{\left(k_{1}\right)} & & & \\
& \ddots & & & \ddots & & \\
& & \ddots & & & \ddots & \\
& & & \alpha_{0}^{\left(s-k_{2}\right)} & \alpha_{1}^{\left(s-k_{2}\right)} & \cdots & \alpha_{k}^{\left(s-k_{2}\right)} \\
& & & \vdots & \vdots & & \vdots \\
& & & \alpha_{0}^{(s)} & \alpha_{1}^{(s)} & \cdots & \alpha_{k}^{(s)}
\end{array}\right) \equiv \hat{A}
$$

and, by denoting with $\tilde{\beta}_{j}^{(n)} \equiv \phi_{n} \beta_{j}^{(n)}$, the matrix $[\mathbf{b} \mid B] \equiv \hat{B}$ is similarly defined via the formal substitution $\tilde{\beta}_{j}^{(n)} \leftrightarrow \alpha_{j}^{(n)}$.

Remark 3. The coefficient matrices $\hat{A}$ and $\hat{B}$ for a block-TOM have a slightly different structure due to the additional methods used that are $(2 k-1)$-step LMMs.

From a theoretical point of view, a $\mathrm{B}_{2} \mathrm{VM}$ can be read as a one-step method. In fact, for each subinterval $\left[t_{r-1}, t_{r}\right]$, the only information inherited from the past consists of $y_{0, r} \approx y\left(t_{0, r}\right)=y\left(t_{r-1}\right)$. Moreover, in the case of a uniform finer mesh, for each family of $\mathrm{B}_{2} \mathrm{VM}$ considered here, the coefficient matrix $A$ in (19) turns out to be nonsingular independently of the blocksize. Hereafter we shall assume that such nonsingularity holds true even for the matrix $A$ corresponding to the assigned distribution of the finer mesh (15)-(16). This seems a reasonable assumption since, otherwise, the method does not provide a unique solution for the simple equation $y^{\prime}=0$. Under such a hypothesis, it is possible to relate $\mathrm{B}_{2} \mathrm{VMs}$ to RK methods, whose stages play a role similar to the internal steps. In fact, the consistency conditions imply that (see (7) with $\ell=0$ )

$$
A \mathbf{e}+\mathbf{a}=\mathbf{0} \Leftrightarrow-A^{-1} \mathbf{a}=\mathbf{e},
$$

being $\mathbf{e}=(1,1, \ldots, 1)^{\mathrm{T}} \in \mathbb{R}^{s}$. Therefore the discrete problem (18), generated by a $\mathrm{B}_{2} \mathrm{VM}$ for the $r$-th subinterval of integration, can be stated in the equivalent form

$$
\begin{equation*}
Y_{r}=\mathbf{e} y_{0, r}+h_{r} A^{-1} \hat{B}\binom{f_{0, r}}{F_{r}} \tag{20}
\end{equation*}
$$

so that such a method coincides with the RK scheme, used over the coarser mesh, defined by the following Butcher tableau

$$
\begin{array}{c|c}
c_{0} &  \tag{21}\\
\vdots & \mathcal{A} \\
c_{s} & \\
\hline & \mathbf{e}_{s+1}^{\mathrm{T}} \not{A}
\end{array}
$$

where $\mathbf{e}_{s+1}=(0, \ldots, 0,1)^{\mathrm{T}} \in \mathbb{R}^{s+1}$ and

$$
\mathcal{A}=\binom{\mathbf{0}^{\mathrm{T}}}{A^{-1} \hat{B}} \equiv\left(\begin{array}{cccc}
0 & 0 & \cdots & 0  \tag{22}\\
a_{10} & a_{11} & \cdots & a_{1 s} \\
\vdots & \vdots & & \vdots \\
a_{s 0} & a_{s 1} & \cdots & a_{s s}
\end{array}\right) .
$$

Remark 4. In general this is an $(s+1)$-stage RK method having the last stage which coincides with the new approximation (stiffly accurate method). However, the tableau corresponding to a block-GBDF has all zero entries in the first row and column since $\mathbf{b}=\mathbf{0}$ (see (13), (19) and the subsequent sentence). The first stage, corresponding to $c_{0}=0$, can be therefore removed from the scheme. This is because the remaining stages do not depend on the value of $f_{0, r}$ and the new approximation coincides with the last stage. The RK method equivalent to a block-GBDF with blocksize $s$ is therefore more properly an $s$ stage method.

### 3.1. Accuracy and stability properties

Clearly, the described reformulation of a $\mathrm{B}_{2} \mathrm{VM}$ as a RK scheme has not affected the accuracy and stability properties of the method. For this reason, in the sequel we shall refer to the original formulation (18) of the discrete problem for the discussion of such properties. As usual for one-step methods, they are studied by considering only the first application of it, i.e., the one corresponding to $r=1$. Moreover, without loss of generality, in the sequel we shall assume for simplicity the coarser mesh (14) to be composed by equally spaced nodes, that is $h_{r}=h$ for each $r=1,2, \ldots, m$.

Concerning the accuracy properties, they are studied by considering the asymptotical behavior of the local error with respect to the stepsize $h$. From the derivation of a $\mathrm{B}_{2} \mathrm{VM}$ of order $p$, it follows that the residual obtained when the continuous solution (assumed to be suitably regular) is inserted into (18) (local truncation error) is given by

$$
\begin{equation*}
A \hat{Y}_{1}-h B \hat{F}_{1}+\mathbf{a} y\left(t_{0,1}\right)-h \mathbf{b} f\left(t_{0,1}, y\left(t_{0,1}\right)\right)=h^{p+1} \mathbf{v} y^{(p+1)}\left(t_{0,1}\right)+O\left(h^{p+2}\right) \equiv \boldsymbol{\tau}_{1}, \tag{23}
\end{equation*}
$$

where $\hat{Y}_{1}=\left(y\left(t_{1,1}\right), \ldots, y\left(t_{s, 1}\right)\right)^{\mathrm{T}}, \hat{F}_{1}=\left(f\left(t_{1,1}, y\left(t_{1,1}\right)\right), \ldots, f\left(t_{s, 1}, y\left(t_{s, 1}\right)\right)\right)^{\mathrm{T}}$ and $\mathbf{v}$ is the vector of the principal error coefficients of the composite scheme. By subtracting (18) from (23), both premultiplied by $A^{-1}$, and considering that $y_{0,1}=y\left(t_{0,1}\right)$, one obtains

$$
\left(\hat{Y}_{1}-Y_{1}\right)-h A^{-1} B\left(\hat{F}_{1}-F_{1}\right)=A^{-1} \boldsymbol{\tau}_{1} .
$$

Consequently, since $\hat{F}_{1}-F_{1}=J\left(\hat{Y}_{1}-Y_{1}\right)$, being

$$
J=\operatorname{diag}\left(\frac{\partial f}{\partial y}\left(t_{1,1}, \zeta_{1,1}\right), \ldots, \frac{\partial f}{\partial y}\left(t_{s, 1}, \zeta_{s, 1}\right)\right)
$$

if $h$ is sufficiently small a first order approximation of the local error is given by

$$
\hat{Y}_{1}-Y_{1}=\left(I-h A^{-1} B J\right)^{-1} A^{-1} \boldsymbol{\tau}_{1}=h^{p+1}\left(A^{-1} \mathbf{v}\right) y^{(p+1)}\left(t_{0,1}\right)+O\left(h^{p+2}\right)
$$

A very important consideration must be made at this point regarding the role played by the components of the solution vector $Y_{1}$. In fact, the $\mathrm{B}_{2} \mathrm{VM}$ approach establishes to consider all of them as belonging to the numerical solution; the RK approach for a stiffly accurate method, instead, considers only the last entry of $Y_{1}$ as part of the numerical solution. This implies that the definition of order of convergence is different for the two approaches. In particular, with the former one the order of convergence coincides with that of the LMMs associated with each row of the coefficient matrices (i.e. the socalled stage order in the RK literature). With the RK approach, instead, the order of convergence is defined on the base of the asymptotical behavior, with respect to $h$, of $\mathbf{e}_{s}^{T}\left(\hat{Y}_{1}-Y_{1}\right)$, where $\mathbf{e}_{s}$ is the last unit vector in $\mathbb{R}^{s+1}$. Consequently, a higher order of convergence (superconvergence) of the method may occur in this case. As an example, if $\mathbf{e}_{s}^{\mathrm{T}}\left(A^{-1} \mathbf{v}\right)=0$ then the RK formula is considered to have at least order $p+1$. However, in the sequel, we will adopt the $\mathrm{B}_{2} \mathrm{VM}$ approach. Therefore, when speaking about the order of a RK method derived from a $\mathrm{B}_{2} \mathrm{VM}$, we will refer to the stage order. We observe that by using this approach the order reduction phenomenon cannot occur [26].

On the other side, the analysis of the stability properties of the method takes into account only the last entry of $Y_{1}$ in both of the approaches. As it is well-known, such analysis is done by considering the behavior of the numerical solution provided by the method applied for solving the classical test equation

$$
y^{\prime}=\lambda y, \quad \operatorname{Re}(\lambda)<0
$$

In this case, the resulting discrete problem (18) for the first subinterval of integration reduces to

$$
\begin{equation*}
(A-q B) Y_{1}=-(\mathbf{a}-q \mathbf{b}) y_{0,1}, \quad q=h \lambda \tag{24}
\end{equation*}
$$

Then, obviously, the last entry in $Y_{1}$ is given by

$$
y_{s, 1}=-\mathbf{e}_{s}^{\mathrm{T}}(A-q B)^{-1}(\mathbf{a}-q \mathbf{b}) y_{0,1} \equiv R(q) y_{0,1} .
$$

The usual property of $A$-stability is equivalent to require that the so-called stability function $R(q)$ of the method verifies

$$
q \in \mathbb{C}^{-} \Rightarrow|R(q)|<1
$$

In particular, the method is perfectly $A$-stable when also the converse holds true. The weaker notion of $A(\vartheta)$-stability requires that

$$
|R(q)| \leq 1, \quad \forall q \in \mathbb{C}^{-}:|\arg (q)-\pi| \leq \vartheta
$$

Moreover, a $\mathrm{B}_{2} \mathrm{VM}$ is said to be $L$-stable $(L(\vartheta)$-stable) if it is $A$-stable $(A(\vartheta)$-stable) and, in addition, $|R(q)| \rightarrow 0$ as $|q| \rightarrow \infty$. The latter property is highly desirable when the method is applied for solving stiff problems. On the other hand, when a conservative one, like an Hamiltonian system, is to be integrated, the use of symmetric and perfectly $A$-stable schemes is more appropriate. In particular, a $\mathrm{B}_{2} \mathrm{VM}$ is symmetric if it is constructed over a symmetric finer mesh, i.e., $c_{j}=1-c_{s-j}, j=$ $0,1, \ldots, s$, and its coefficient matrices, see (19) and the subsequent sentence, satisfy

$$
P_{s} \hat{A} P_{s+1}=-\hat{A}, \quad P_{s} \hat{B} P_{s+1}=\hat{B},
$$

where, for any integer $m, P_{m}$ denotes the antiidentity matrix of size $m$, i.e. the matrix with 1 's in the main antidiagonal and 0 's elsewhere. It is known that this is the case of $B_{2}$ VMs based on the ETR, BS and TOM methods constructed over a symmetric finer mesh, [1,7]. When the previous property holds true, the numerical solution, provided by the method starting from $y_{0,1}$ with stepsize $h$, coincides with the one provided by the same method starting from $y_{s, 1}$ with stepsize $-h$ in the reverse order. In particular, this implies that the stiffly accurate RK method corresponding to a symmetric $\mathrm{B}_{2} \mathrm{VM}$ is symmetric (or time-reversible) as well.

## 3.2. $\mathrm{B}_{2} \mathrm{VMs}$ with minimal blocksize and RK collocation schemes

As is well-known, the numerical approximation provided by a (polynomial) collocation method for (1) coincides with the values of a polynomial of degree $\eta$ which collocates the differential equation at $\eta$ assigned points. In particular, an $(s+1)$ stage stiffly accurate RK scheme verifying the so-called simplifying assumption

$$
\begin{equation*}
C(\eta): \sum_{j=0}^{s} a_{n j} c_{j}^{\ell-1}=\frac{c_{n}^{\ell}}{\ell}, \quad n=0,1, \ldots, s, \ell=1,2, \ldots, \eta, \tag{25}
\end{equation*}
$$

is a collocation method if and only if $\eta=s+1$, as proved in [27, Theorem 7.8]. It is worth noting that for an ( $s+1$ )-stage stiffly accurate RK collocation scheme the condition $C(s+1)$ uniquely determines the coefficients of the method once the abscissae $c_{j}$ have been assigned. In order to discuss the existing relations between RK collocation methods and $\mathrm{B}_{2} \mathrm{VM}$ with minimal blocksize, we need to move our notation towards the more standard one used in the RK framework. This is done with the following lemma.

Lemma 1. The order conditions (12) for the coefficients of $a \mathrm{~B}_{2} \mathrm{VM}$ with a finer mesh as in (15) can be reformulated as

$$
\begin{equation*}
W_{n, k, \mu}^{(p)} \boldsymbol{\alpha}^{(n)}=L_{p} W_{n, k, \mu}^{(p)} \tilde{\boldsymbol{\beta}}^{(n)}, \quad n=1, \ldots, s, \tag{26}
\end{equation*}
$$

where

$$
\begin{equation*}
\tilde{\boldsymbol{\beta}}^{(n)} \equiv\left(\tilde{\beta}_{0}^{(n)}, \ldots, \tilde{\beta}_{k}^{(n)}\right)^{\mathrm{T}}=\phi_{n} \boldsymbol{\beta}^{(n)}, \quad \text { with } \phi_{n}=c_{n}-c_{n-1} \tag{27}
\end{equation*}
$$

$L_{p}$ and $\mu$ are defined in (9) and (11), respectively, and

$$
W_{n, k, \mu}^{(p)}=\left(\begin{array}{ccc}
\left(c_{n-\mu}\right)^{0} & \ldots & \left(c_{n-\mu+k}\right)^{0}  \tag{28}\\
\vdots & & \vdots \\
\left(c_{n-\mu}\right)^{p} & \ldots & \left(c_{n-\mu+k}\right)^{p}
\end{array}\right) .
$$

Proof. Let $\Phi_{n}=\operatorname{diag}\left(1, \phi_{n}, \ldots, \phi_{n}^{p}\right)$ and $P^{c_{n}}$ be the generalized Pascal matrix, namely the lower triangular matrix with non-zero entries given by

$$
\left(P^{c_{n}}\right)_{i j}=\binom{i-1}{j-1} c_{n}^{i-j}, \quad 1 \leq j \leq i \leq p+1
$$

It is known that $P^{c_{n}}=e^{c_{n} L_{p}}$ (see, for example, [28]) from which one plainly deduces that $P^{c_{n}}$ and $L_{p}$ commute. Moreover

$$
\begin{equation*}
W_{n, k, \mu}^{(p)}=P^{c_{n}}\left(\Phi_{n} V_{n, k, \mu}^{(p)}\right) \tag{29}
\end{equation*}
$$

In fact, by denoting with $\mathbf{v}(t)=\left(1, t, \ldots, t^{p}\right)^{\mathrm{T}}$, from (28) we obtain that for each $j=1,2, \ldots, k+1$, the $j$-th column of $W_{n, k, \mu}^{(p)}$ is equal to $\mathbf{v}\left(c_{n-\mu+j-1}\right)$ and from (10) and (17) we get that the same column of $\Phi_{n} V_{n, k, \mu}^{(p)}$ is equal to $\mathbf{v}\left(c_{n-\mu+j-1}-c_{n}\right)$. Then, (29) is a consequence of the fact that $\mathbf{v}(t)=P^{c_{n}} \mathbf{v}\left(t-c_{n}\right)$ [28].
From the previous arguments the statement (26) follows by multiplying from the left both sides of (12) by $P^{c_{n}} \Phi_{n}$. In fact, due to (29) the left-hand side becomes

$$
P^{c_{n}} \Phi_{n} V_{n, k, \mu}^{(p)} \boldsymbol{\alpha}^{(n)}=W_{n, k, \mu}^{(p)} \boldsymbol{\alpha}^{(n)}
$$

Concerning the right-hand side in (12), by considering that $\Phi_{n} L_{p}=\phi_{n} L_{p} \Phi_{n}$, as one easily verifies, and by taking into account (27), from (29) one obtains

$$
\begin{aligned}
P^{c_{n}} \Phi_{n} L_{p} V_{n, k, \mu}^{(p)} \boldsymbol{\beta}^{(n)} & =\phi_{n} P^{c_{n}} L_{p} \Phi_{n} V_{n, k, \mu}^{(p)} \boldsymbol{\beta}^{(n)} \\
& =L_{p} P^{c_{n}} \Phi_{n} V_{n, k, \mu}^{(p)} \tilde{\boldsymbol{\beta}}^{(n)}=L_{p} W_{n, k, \mu}^{(p)} \tilde{\boldsymbol{\beta}}^{(n)} .
\end{aligned}
$$

We are now in the position to prove the following main result.
Theorem 1. $A \mathrm{~B}_{2} \mathrm{VM}$ based on a $k$-step $B V M$ of order $p$ with minimal blocksize $\bar{s}=\max (k, p-1)$ and nonsingular coefficient matrix $A$ is equivalent to a $R K$ collocation method.
Proof. In order to prove the statement we need to show that (25) holds true with $\eta=\bar{s}$ for the RK methods derived from the block-GBDFs and $\eta=\bar{s}+1$ in all the other cases (see Remark 4). We observe that the RK method (20) has been obtained by multiplying from the left both sides of (18) by $A^{-1}$. This implies that the corresponding local truncation error is given by $A^{-1} \boldsymbol{\tau}_{1}=h^{p+1}\left(A^{-1} \mathbf{v}\right) y^{(p+1)}\left(t_{0,1}\right)+O\left(h^{p+2}\right)$. Therefore, for each $n=1,2, \ldots, \bar{s}$, the $n$-th equation in (20)-(22) can be interpreted as the one generated by a $\bar{s}$-step LMM of order $p$ with

$$
\boldsymbol{\alpha}^{(n)}=\mathbf{e}_{n+1}-\mathbf{e}_{1} \in \mathbb{R}^{\bar{s}+1}, \quad \tilde{\boldsymbol{\beta}}^{(n)}=\left(a_{n 0}, a_{n 1}, \ldots, a_{n \bar{s}}\right)^{\mathrm{T}}
$$

Consequently, such two coefficient vectors satisfy the order conditions (26). However, on minimal blocksize (11) and (28) reduce to

$$
\mu=\mu\left(n, k_{1}, \bar{s}, \bar{s}\right)=n, \quad W_{n, \bar{s}, n}^{(p)}=\left(\begin{array}{cccc}
1 & 1 & \ldots & 1 \\
c_{0} & c_{1} & \ldots & c_{\bar{s}} \\
\vdots & \vdots & & \vdots \\
c_{0}^{p} & c_{1}^{p} & \ldots & c_{\bar{s}}^{p}
\end{array}\right) \equiv W^{(p)}
$$

and then the order conditions (26) now become

$$
L_{p} W^{(p)}\left(\begin{array}{c}
a_{n 0} \\
a_{n 1} \\
\vdots \\
a_{n \bar{s}}
\end{array}\right)=W^{(p)}\left(\mathbf{e}_{n+1}-\mathbf{e}_{1}\right)
$$

Since the first one of the previous equations is trivially satisfied (see (9)), some linear algebra on the remaining order conditions allows one to rewrite them as

$$
G_{p} W^{(p-1)}\left(\begin{array}{c}
a_{n 0} \\
\vdots \\
a_{n \overline{5}}
\end{array}\right)=W^{(p-1)} D\left(\mathbf{e}_{n+1}-\mathbf{e}_{1}\right),
$$

where $G_{p}=\operatorname{diag}(1, \ldots, p)$ and $D=\operatorname{diag}\left(c_{0}, \ldots, c_{\bar{s}}\right)$. By considering that $c_{0}=0$, see (16), one gets $D \mathbf{e}_{1}=\mathbf{0} \in \mathbb{R}^{\bar{s}+1}$. Therefore,

$$
W^{(p-1)}\left(\begin{array}{c}
a_{n 0} \\
\vdots \\
a_{n \bar{s}}
\end{array}\right)=G_{p}^{-1}\left(\begin{array}{c}
c_{n} \\
\vdots \\
c_{n}^{p}
\end{array}\right), \quad n=1,2, \ldots, \bar{s} .
$$

It is easy to see that such equations are essentially the conditions (25), with $\eta=p$, recast in matrix form. In fact, they also hold true when $n=0$ since $c_{0}=0$ and all the entries in the first row of $\mathcal{A}$ in (22) are zero. We recall that $p=k$ for the block-GBDFs and $p>k$ in all the other cases and that $\bar{s}=\max (k, p-1)$. It follows that $p=\bar{s}$ in the former case and $p=\bar{s}+1$ in the latter ones. This completes the proof.

In the following section we shall analyze the question of the distribution of the points in the finer mesh which, as we have seen, uniquely characterizes a stiffly accurate RK collocation method. This will allow us to put into evidence the equivalences between the classes of $\mathrm{B}_{2} \mathrm{VMs}$ with minimal blocksize already defined and some classes of known and (so far) unknown RK collocation methods.

## 4. Possible choices for the finer mesh

The simplest choice for the finer mesh certainly consists of a set of equally spaced nodes. With such a choice the obtained $B_{2}$ VMs are not always pre-stable, that is they do not always have the corresponding matrix pencils $A-q B$ contained in $\mathbb{C}^{+}$. In particular, the property of pre-stability is always satisfied by the "lower" order formulae, it is satisfied by the "medium" order formulae when the blocksize is sufficiently large and it disappears for the "higher" order ones. The exact ranges of the orders corresponding to the three previous cases depend on the family of BVMs, as reported in [1, Table 11.2]. The absence of pre-stability is due to the effect of the additional methods on the whole composite scheme and it represents a drawback since a non pre-stable method cannot be $A$-stable (see (24)). In order to overcome this problem, in [1] a second distribution of the finer mesh was proposed. It is characterized by the introduction of a suitable number of auxiliary nodes with a geometric progression distribution near the extremes of the subintervals. This choice of the finer mesh was successful since almost all the corresponding $B_{2} \mathrm{VMs}$ turned out to be $A$-stable independently of the blocksize.

In this paper we consider other choices for the finer mesh and in the remaining part of this section we will introduce them for a $\mathrm{B}_{2} \mathrm{VM}$ with minimal blocksize $\bar{s}$. They are derived from the abscissae of the following Gauss type quadrature formulae: Legendre-Gauss-Radau (LGR), Chebyshev-Gauss-Radau (CGR), Legendre-Gauss-Lobatto (LGL), Chebyshev-GaussLobatto (CGL). More precisely, by denoting with $\mathcal{L}_{\bar{s}}(\cdot)$ and $\mathcal{T}_{\bar{s}}(\cdot)$ the Legendre polynomial of degree $\bar{s}$ and the Chebyschev polynomial of the first kind having the same degree, respectively, such abscissae are the roots of the polynomials $\mathcal{P}_{\bar{s}}(c)$ listed below:

- LGR: $\mathscr{P}_{\bar{s}}(c)=\mathscr{L}_{\bar{s}-1}(c)+\mathscr{L}_{\bar{s}}(c)$,
- CGR: $\mathscr{P}_{\bar{s}}(c)=\mathcal{T}_{\bar{s}-1}(c)+\mathcal{T}_{\bar{s}}(c)$,
- LGL: $\mathcal{P}_{\bar{s}}(c)=\left(1-c^{2}\right) \mathscr{L}_{\bar{s}}^{\prime}(c)$,
- CGL : $\mathcal{P}_{\mathcal{S}}(c)=\left(1-c^{2}\right) \mathcal{T}_{\bar{s}}^{\prime}(c)$.

It is well-known that the Lobatto type formulae are symmetric and closed, namely their abscissae include both the extremes of the interval $[-1,1]$. The Radau type formulae, instead, are not symmetric and semi-closed since only the left extreme of such interval is included. In any case, the nodes of the finer mesh for a $\mathrm{B}_{2} \mathrm{VM}$ with minimal blocksize $\bar{s}$ are selected as follows

$$
\begin{equation*}
c_{j}=\frac{1-\hat{c}_{j}}{2}, \tag{30}
\end{equation*}
$$

with

$$
\mathcal{P}_{\bar{s}}\left(\hat{c}_{j}\right)=0, \quad \hat{c}_{\ell}>\hat{c}_{\ell+1}>\cdots>\hat{c}_{\bar{s}}, j=\ell, \ldots, \bar{s},
$$

and $\ell=0,1$ for the nodes derived from a Lobatto and a Radau type formula, respectively. We observe, in fact, that $\mathscr{P}_{\bar{s}}$ is a polynomial of degree $\bar{s}+1$ in the former case (see LGL and CGL) and of degree $\bar{s}$ in the latter one (see LGR and CGR). Obviously, the abscissae $c_{j}$ defined in (30) are contained in the interval $[0,1]$. We must underline the fact that in the literature, see for example [29,30], the finer meshes (30) corresponding to the abscissae of an LGR quadrature formulae are always called Radau-right since they include the right extreme of the interval $[0,1]$ and not the left one. However, for later convenience, in the Radau case we formally include the node $c_{0}=0$ since the $B_{2} \mathrm{VMs}$ always require it. In the sequel we will refer to the above described finer meshes by using the acronym for the corresponding quadrature formula name.

In Table 1 we list the equivalences between some $\mathrm{B}_{2} \mathrm{VMs}$ with minimal blocksize and RK methods together with their stability properties. In particular, by numerical inspection, we found the block-GBDFs constructed over the CGR nodes to be

Table 1
Equivalences between $\mathrm{B}_{2} \mathrm{VMs}$ on minimal blocksize and RK collocation methods and their stability properties

| Nodes | $\mathrm{B}_{2}$ VM | RK method | Stability |
| :--- | :--- | :--- | :--- |
| LGR | GBDF | Radau IIa | L-stable |
| LGL | GBDF | Unknown | L $(\vartheta)$-stable |
| LGL | GAM, BS, TOM | Lobatto IIIa | Perfectly A-stable |
| CGR | GBDF | Unknown | L $\vartheta)$-stable |
| CGL | GBDF | Unknown except for the method of order 4 in [33] | L $(\vartheta)$-stable |
| CGL | GAM, BS, TOM | Methods in $[23,34]$ | Perfectly A-stable |

Table 2
Values of $\vartheta$ for the $L(\vartheta)$-stable $k$-step block-GBDFs

| $k$ | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| LGL | $89.722^{\circ}$ | $89.242^{\circ}$ | $88.819^{\circ}$ | $88.450^{\circ}$ | $88.295^{\circ}$ | $88.180^{\circ}$ |  |
| CGL | $89.890^{\circ}$ | $89.747^{\circ}$ | $89.700^{\circ}$ | $89.764^{\circ}$ | $89.936^{\circ}$ | $89.999^{\circ}$ | $88.146^{\circ}$ |

$\mathrm{L}(\vartheta)$-stable methods with $\vartheta \geq 89.999^{\circ}$, at least for $k \leq 9$. The numerically computed values of $\vartheta$ for the remaining $\mathrm{L}(\vartheta)$ stable methods are listed in Table 2. It is worth mentioning that the block-GBDFs, in their original formulation, constructed over the CGL nodes, are known in the literature as Chebyschev Spectral Collocation methods [22,31] and that, recently, on the same set of nodes another family of RK methods has been introduced in [32].

Remark 5. We observe that by using the LGR and CGR finer meshes we have constructed only block-GBDFs. This is because, as already observed, the associated equivalent RK methods do have the first stage, corresponding to $c_{0}=0$, inactive and such a node has been introduced only a posteriori.

## 5. Finer mesh for $B_{2}$ VMs with nonminimal blocksize

In this section we propose a possible extension of the finer meshes just described for building $\mathrm{B}_{2} \mathrm{VM}$ s with nonminimal blocksize. The main idea consists in the introduction of a suitable number of equidistant nodes in the middle of the subintervals. This seems a reasonable choice by virtue of the good stability properties of the main formula of the BVMs considered in this paper when defined over a uniform mesh [2-6]. Let $\left\{c_{n}\right\}_{n=0, \ldots, \bar{s}}$ be the starting abscissae of the finer mesh and let

$$
c_{v}-c_{v-1}=\max _{n=1, \ldots, \bar{s}}\left(c_{n}-c_{n-1}\right)
$$

The abscissae of the finer mesh $\left\{\bar{c}_{n}\right\}_{n=0, \ldots, s}$ for the corresponding $\mathrm{B}_{2} \mathrm{VM}$ with blocksize $s \geq \bar{s}$ are given by

$$
\bar{c}_{n}= \begin{cases}c_{n}, & n=0,1, \ldots, v-1 \\ \bar{c}_{n-1}+\left(c_{v}-c_{v-1}\right), & n=v, \ldots, s-\bar{s}+v \\ \bar{c}_{n-1}+\left(c_{n-s+\bar{s}}-c_{n-s+\bar{s}-1}\right), & n=s-\bar{s}+v+1, \ldots, s\end{cases}
$$

The proposed extension is represented graphically in Fig. 1. In the left plots the differences among two consecutive nodes for the finer meshes of type LGR and LGL, when $\bar{s}=7$, have been reported. In the right ones, we have plotted the same differences for the corresponding extended finer meshes with doubled blocksize $s=14$. The graphics corresponding to the extension of the CGR and CGL meshes are very similar with respect to the ones here reported. We observe that, even though this is not strictly necessary, a rescaling of the extended finer mesh may be operated if one prefers to have the nodes contained in the interval $[0,1]$.

Remark 6. It is important to underline the fact that from each $B_{2} V M$ constructed over the extended finer mesh a whole family of RK methods can be derived by simply varying the blocksize and by using the reformulation of the discrete problem described in Section 3 (see (18) and (20)).

The order of convergence of the so-obtained $\mathrm{B}_{2}$ VMs does not depend on the used blocksize. This is because, by construction, the asymptotic behavior, with respect to the stepsize, of the local error is preserved when the blocksize is increased.

Concerning stability, we found that a few additional nodes are sufficient for getting $L$-stable methods, when starting from methods that were only $L(\vartheta)$-stable on the minimal blocksize (see Table 3). As an example, in Fig. 2 we plot the boundary loci of the 6-step block-GBDFs based on the (extended) LGL nodes, for increasing values of the blocksize.

On the other hand, we have numerically verified that good stability properties of a $\mathrm{B}_{2} \mathrm{VM}$ are always preserved when the blocksize is increased. In particular, the proposed extension of the LGL and CGL finer meshes do not destroy the original symmetry of the nodes. Therefore, in view of what stated at the end of Section 3, the block-ETR, block-BS, and block-TOM methods constructed over the extended (symmetric) mesh turn out to be symmetric and perfectly $A$-stable schemes. This


Fig. 1. The finer mesh for a $\mathrm{B}_{2} \mathrm{VM}$ with nonminimal blocksize.


Fig. 2. Boundary loci for the 6-step block-GBDFs based on LGL nodes with different blocksizes and their details near the imaginary axis.

Table 3
Minimum blocksize for getting L-stable block-GBDFs

| $k$ | 3 | 4 | 5 | 6 | 7 | 8 |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| LGL | 4 | 7 | 7 | 9 | 9 | 11 | 8 |
| CGR | 3 | 4 | 6 | 7 | 8 | 11 |  |
| CGL | 4 | 6 | 6 | 7 | 8 | 10 |  |

means that the introduction of extra points for increasing the blocksize of symmetric $\mathrm{B}_{2} \mathrm{VMs}$ does not lead to an improvement of the accuracy and stability properties of such schemes. Nevertheless, a possible advantage that may arise from the use of symmetric $\mathrm{B}_{2}$ VMs with nonminimal blocksize is presented in the next example.


Fig. 3. Numerical results for the block-BS method of order 4 constructed by using the LGL finer mesh and its extension.
Example 1. Let us consider the Lotka-Volterra problem in logarithmic scale

$$
\left\{\begin{array}{l}
p^{\prime}(t)=8\left(1-e^{q}\right)  \tag{31}\\
q^{\prime}(t)=\left(e^{p}-1\right),
\end{array}\right.
$$

with $t \in[0,150000]$ and initial value $p(0)=\log 4, q(0)=0$. This is a non-reversible Hamiltonian system with Hamiltonian given by

$$
H(p, q)=\mathrm{e}^{p}-p+8\left(\mathrm{e}^{q}-q\right)
$$

It is known that when a non-reversible Hamiltonian system is solved by applying a symmetric RK scheme, like a Lobatto IIIa method, the long-time behavior of the numerical Hamiltonian should present a drift, [35]. For problem (31), however, such phenomenon appears to be significantly reduced if the blocksize of the equivalent $\mathrm{B}_{2} \mathrm{VM}$ is increased. In particular, the numerical experiments we have conducted suggest that this happens by using, with nonminimal blocksize, the block-ETR and the block-BS methods of orders 4 and 6 and the block-TOM of order 6 . All the methods have been constructed over the described extension of the LGL and CGL finer meshes, while a uniform coarser mesh has been always used for discretizing the interval of integration. Moreover, in order to keep constant the total number of mesh points, the stepsize $h$, representing the time-interval covered by one application of the block method, has been varied with the blocksize. This means, for example, that when the blocksize has been doubled the stepsize has been doubled as well. The discrete problems generated by the methods have been solved by means of the simplified Newton method with a tolerance for the residual in the iteration of the order of the machine precision.

In Fig. 3 we report the error in the Hamiltonian when problem (31) is solved by means of the block-BS method of order 4 with minimal blocksize $s=3$ and blocksize $s=15$ constructed over the extension of the LGL finer mesh; we recall that in the former case the method is equivalent to the 4 -stage Lobatto IIIa scheme (see Table 1 ). In order to put into evidence that the loss of superconvergence is not so important for this application, we plot only the values corresponding to the right end of each subinterval. As a matter of fact, they are the only values the users of RK methods consider as numerical solution. As one can see, a linear drift in the numerical Hamiltonian provided by the method with minimal blocksize is clearly present. In particular, we have verified that its slope is proportional to $h^{8}$. This result is in perfect agreement with the analysis reported in [35]. On the other hand, no drift in the numerical Hamiltonian seems to be present when the method with larger blocksize is used or, at least, its slope is no longer appreciable.

For completeness, in Fig. 4 we report the corresponding results obtained by using the block-TOM method of order 6 with minimal blocksize $s=5$ and blocksize $s=25$ constructed over the CGL finer mesh and its extension. The same comments previously made also apply in this case.

## 6. Conclusions

The construction of RK collocation methods via $\mathrm{B}_{2} \mathrm{VMs}$ (with minimal blocksize) has been analyzed in detail. The analysis has permitted many classical known RK methods to be rederived, along with some "apparently" unknown ones. The analysis has also permitted such methods to be generalized by introducing extra points in order to extend the blocksize. This additional flexibility has either led to improve the stability properties of some $\mathrm{L}(\vartheta)$-stable methods or to reduce the drift in


Fig. 4. Numerical results for the block-TOM method of order 6 constructed by using the CGL finer mesh and its extension.
the approximation of a non-reversible Hamiltonian problem. By virtue of these results, a deeper study of the so-obtained $\mathrm{B}_{2}$ VMs with nonminimal blocksize seems to be an interesting topic for future investigations.

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## References

[1] L. Brugnano, D. Trigiante, Solving Differential Problems by Multistep Initial and Boundary Value Methods, Gordon and Breach Science Publishers, Amsterdam, 1998.
[2] L. Aceto, R. Pandolfi, Theoretical analysis of the stability for Extended Trapezoidal Rules (submitted for publication).
[3] L. Aceto, R. Pandolfi, D. Trigiante, One parameter family of linear difference equations and the stability problem for the numerical solution of ODEs, Adv. Differential Equations, Art. 19276 (2006) 1-14.
[4] L. Aceto, R. Pandolfi, D. Trigiante, Stability analysis of linear multistep methods via polynomial type variation, JNAIAM 2 (1-2) (2007) 1-9.
[5] L. Aceto, D. Trigiante, On the A-stable methods in the GBDF class, Nonlinear Anal. RWA 3 (2002) 9-23.
[6] F. Mazzia, A. Sestini, D. Trigiante, B-spline linear multistep methods and their continuous extensions, SIAM J. Numer. Anal. 44 (5) (2006) $1954-1973$.
[7] F. Mazzia, A. Sestini, D. Trigiante, BS linear multistep methods on non-uniform meshes, JNAIAM 1 (2006) 131-144.
[8] B. Cano, J.M. Sanz-Serna, Error growth in the numerical integration of periodic orbits by multistep methods, with application to reversible systems, IMA J. Numer. Anal. 18 (1998) 57-75.
[9] T. Eirola, J.M. Sanz-Serna, Conservation of integrals and symplectic structure in the integration of differential equations by linear multistep methods, Numer. Math. 61 (1992) 281-290.
[10] Yu.B. Suris, The canonicity of mappings generated by Runge-Kutta type methods when integrating the systems $\ddot{x}=-\partial U / \partial x$, U.S.S.R. Comput. Maths. Math. Phys. 29 (1) (1989) 138-144.
[11] L. Aceto, D. Trigiante, Symmetric schemes, time reversal symmetry and conservative methods for Hamiltonian systems, J. Comput. Appl. Math. 107 (1999) 257-274.
[12] L. Brugnano, Essentially symplectic boundary value methods for linear Hamiltonian systems, J. Comput. Math. 15 (3) (1997) $233-252$.
[13] F. Iavernaro, F. Mazzia, D. Trigiante, Multistep methods for conservative problems, Mediterr. J. Math. 2 (1) (2005) 53-69.
[14] L. Brugnano, D. Trigiante, Block boundary value methods for linear hamiltonian systems, Appl. Numer. Math. 81 (1997) 49-68.
[15] L. Brugnano, D. Trigiante, On the potentiality of sequential and parallel codes based on extended trapezoidal rules (ETRs), in: Time Integration (Amsterdam, 1996), Appl. Numer. Math. 25 (2-3) (1997) 169-184 (special issue).
[16] L. Brugnano, C. Magherini, Blended implementation of block implicit methods for ODEs, Appl. Numer. Math. 42 (1-3) (2002) 29-45.
[17] L. Brugnano, C. Magherini, Recent advances in linear analysis of convergence for splittings for solving ODE problems, Appl. Numer. Math. 59 (2009) 542-557.
[18] J.C. Butcher, On the implementation of implicit Runge-Kutta methods, BIT 16 (3) (1976) 237-240.
[19] F. Iavernaro, F. Mazzia, Solving ordinary differential equations by generalized Adams methods: Properties and implementation techniques, Appl. Numer. Math. 28 (1998) 107-126.
[20] F. Iavernaro, F. Mazzia, Block-boundary value methods for the solution of ordinary differential equations, SIAM J. Sci. Comput. 21 (1999) $323-339$.
[21] F. Mazzia, C. Magherini, Test Set for Initial Value Problem Solvers. Department of Mathematics, University of Bari, February 2008. Available at: http://www.dm.uniba.it/~testset.
[22] J. van Lent, Multigrid methods for time-dependent partial differential equations, Ph.D. Thesis, Katholieke Universiteit, Leuven, 2006.
[23] J. Vigo-Aguiar, H. Ramos, A family of A-stable Runge-Kutta collocation methods of higher order for initial-value problems, IMA J. Numer. Anal. 27 (2007) 798-817.
[24] F.R. Loscalzo, T.D. Talbot, Spline function approximation for solutions of ordinary differential equations, SIAM J. Numer. Anal. 4 (1967) $433-445$.
[25] F.R. Loscalzo, An introduction to the application of spline functions to initial value problems, in: T.N.E. Greville (Ed.), Theory and Applications of Spline Functions, Academic Press, New York, 1969, pp. 37-64.
[26] A. Prothero, A. Robinson, On the stability and accuracy of one-step methods for solving stiff systems of ordinary differential equations, Math. Comp. 28 (1974) 145-162.
[27] E. Hairer, S.P. Nørsett, G. Wanner, Solving ordinary differential equations I, nonstiff problems, 2nd ed., in: Springer Series in Computational Mathematics, vol. 8, Springer-Verlag, Berlin, 1993.
[28] L. Aceto, D. Trigiante, The matrices of Pascal and other greats, Amer. Math. Monthly 108 (2001) 232-245.
[29] J.C. Butcher, Integration processes based on Radau quadrature formulas, Math. Comput. 18 (1964) 233-244.
[30] E. Hairer, G. Wanner, Solving ordinary differential equations II, stiff and differential-algebraic problems, 2nd ed., in: Springer Series in Computational Mathematics, vol. 14, Springer-Verlag, Berlin, 1996.
[31] K. Wright, Chebyschev collocation methods of ordinary differential equations, Comput. J. 6 (1964) 358-365.
[32] J. Vigo-Aguiar, J. Martín-Vaquero, H. Ramos, Exponential fitting BDF-Runge-Kutta algorithms, Comput. Phys. Comm. 178 (1) (2008) 15-34.
[33] J. Vigo-Aguiar, H. Ramos, A fourth-order Runge-Kutta method based on BDF-type Chebyshev approximations, J. Comput. Appl. Math. 204 (1) (2007) 124-136.
[34] J. Vigo-Aguiar, H. Ramos, A new eight-order A-stable method for solving differential systems arising in chemical reactions, J. Math. Chem. 40 (1) (2006) 71-83.
[35] E. Faou, E. Hairer, T. Pham, Energy conservation with non-symplectic methods: Examples and counter-examples, BIT 44 (2004) 699-709.


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