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A Charge Oriented Mixed Multirate Method for a special Class of Index-1 Network Equations in Chip Design [★]

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Abstract

Multirate methods make use of latency that occurs in electrical circuits to simulate more efficiently the transient behaviour of networks: different stepsizes are used for subcircuits according to the different levels of activity. As modelling is usually done by applying modified nodal analysis (MNA), the network equations are given by coupled systems of stiff differential-algebraic equations. Following the idea of mixed multirate for ordinary differential equations, a ROW-based 2-level multirate method is developed for index-1 DAEs arising in circuit simulation. To obtain order conditions, P-series are generalised to MDA-series for partitioned DAE systems.

Key words: Circuit simulation, partitioned systems, differential-algebraic equations, mixed multirate ROW schemes, P-series theory, MDA-series theory
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1 Introduction

In full chip design it has to be verified whether the network design coincides with the functional demands. To do so, modified nodal analysis (MNA) is commonly used in industrial applications to generate automatically network model equations from designer's drafts: Kirchhoff's current and voltage laws, together with characteristic equations for each basic element based on a charge oriented description of MOS-transistors, lead to stiff differential-algebraic equations (DAEs) of the following form:

$$\begin{aligned} A \cdot \dot{z} &= f(x) \\ 0 &= z - q(x) \end{aligned} \quad \text{on } t \in [t_0, t_{\text{end}}], \quad x(t_0) = x_0, \quad (1)$$

with $x \in \mathbb{R}^n$ denoting the n unknown node potentials and $f(x) \in \mathbb{R}^n$ the currents produced by static elements. The incidence matrix $A \in \{-1, 0, 1\}^{n \times m}$ describes the network's topology related to charge storing elements (capacitances) and associates charge flow $\dot{z} = dq(x)/dt$ caused by these elements to the static currents $f(x)$ at each node.

Electrical networks often consist of subcircuits which show largely differing levels of activity, i. e. the inner signals of some parts are characterized by a high level of activity while others tend to change quite slowly. In terms of the mathematical model the network equations comprise of systems running on different time scales. The basic idea of *Multirate methods* is to prevent parts to be integrated more often than necessary to guarantee given error tolerances. Therefor latency is exploited to reduce computational costs.

To take advantage of the multirate feature, the network model equations have to be split in an appropriate way. Since dynamic network elements are said to react slowly or fast we can suppose that two or more nodes connected by such an element have the same level of activity at each time, i. e. regarding the whole network there is no coupling between the latent and active part through capacities. Thus the network equations (1) can be split into an active (subindex a) and latent (subindex l) part that are linked only by the static currents f_l and f_a via the coupling node potentials x_a and x_l :

$$\begin{aligned} A_l \cdot \dot{z}_l &= f_l(x_l, x_a) & A_a \cdot \dot{z}_a &= f_a(x_l, x_a) \\ 0 &= z_l - q_l(x_l) & 0 &= z_a - q_a(x_a) \end{aligned} \quad (2)$$

In the following we will assume that both networks are regular, i. e. they fulfill the following special index 1 conditions:

$$\begin{aligned} A_l \cdot \partial q_l / \partial x_l &\text{ is smooth and regular along the solution } x_l(t), \\ A_a \cdot \partial q_a / \partial x_a &\text{ is smooth and regular along the solution } x_a(t). \end{aligned} \quad (3)$$

We will show in this paper how the multirate idea for ordinary differential equations can be transferred to differential-algebraic equations of type (2–3).

The paper is organised as follows: Starting from multirate schemes for ODE systems recapitulated in Section 2, a mixed multirate method for the coupled system (2) of index-1 DAEs is introduced in Section 3. Its order conditions are derived by generalising P-series to MDA-series theory in Section 4. Details for MDAE23, an implementation of an embedded scheme with order 3(2), conclude this paper.

2 Multirate schemes for ODE systems

Before we state and investigate a multirate method for the coupled system (2) that treats both parts with different stepsizes, we take a closer look at multirate schemes for coupled ODEs:

$$\dot{y}_L = f_L(y_L, y_A), \quad y_L(t_0) = y_{L,0} \quad (4a)$$

$$\dot{y}_A = f_A(y_L, y_A), \quad y_A(t_0) = y_{A,0} \quad (4b)$$

Since we have to deal with stiff models, we concentrate on multirate methods based on implicit Runge-Kutta (IRK) and Rosenbrock-Wanner (ROW) schemes.

The main idea of such onestep multirate schemes is to integrate the latent part in one macrostep with stepsize h_l , i. e. get an approximation $y_{L,1}$ to the exact solution $y_L(t_0 + h_l)$ and to compute approximations $y_{A,1}, \dots, y_{A,r}$ to the active part on the grid $\{t_0, t_1, \dots, t_r = t_0 + h_l\}$ with $t_\mu - t_{\mu-1} = h_{a,\mu}$ ($\mu = 1, \dots, r$), i. e. perform r microsteps with stepsizes $h_{a,1}, \dots, h_{a,r}$ (see Fig. 1). Note that r usually changes from macrostep to macrostep.

In its most general way this procedure can be defined as follows:

$$y_{L,1} = y_{L,0} + \sum_{i=1}^{s_L} b_i^L \cdot k_i^L,$$

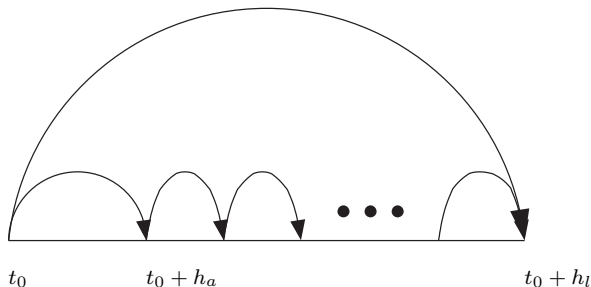


Fig. 1. macro- and microsteps

$$\begin{aligned}
y_{A,\mu} &= y_{A,\mu-1} + \sum_{i=1}^{s_A} b_i^A \cdot k_i^{A,\mu} \quad (\mu = 1, \dots, r), \\
k_i^L &= \Phi_L(h_l; y_{L,0}, Y_i^A, k_1^L, \dots, k_{s_L}^L) \quad (i = 1, \dots, s_L), \\
k_i^{A,\mu} &= \Phi_A(h_{a,\mu}; y_{A,\mu-1}, Y_i^{L,\mu}, k_1^{A,\mu}, \dots, k_{s_A}^{A,\mu}) \quad (i = 1, \dots, s_A),
\end{aligned}$$

where Φ_* denotes an s_* stage IRK or ROW scheme with coefficients $\alpha^*, \beta^*, \gamma^*$ as usual ($* \in \{L, A\}$).

As the subsystems depend on each other, we cannot use methods for latent and active part individually. Hence the crucial point in doing multirate is to handle the couplings in an appropriate way, i. e. to get sufficiently accurate values of one part to compute the other one:

$$Y_i^A \approx y_A(t_0 + \alpha_i^L h_l) \quad (i = 1, \dots, s_L), \quad (5a)$$

$$Y_i^{L,\mu} \approx y_L(t_0 + \sum_{\nu=1}^{\mu-1} h_{a,\nu} + \alpha_i^A h_{a,\mu}) \quad (i = 1, \dots, s_A; \mu = 1, \dots, r). \quad (5b)$$

As this produces additional computational costs, multirate only makes sense if the overhead is surpassed by the gain achieved using bigger stepsizes for the latent part. This leads to some “natural” conditions:

- the latent part is much larger than the active one ($\sim n_A \ll n_L$),
- there is a wide difference in the level of activity ($\sim h_a \ll h_l$),
- the coupling is weak ($\sim \|\partial f_L / \partial y_A\| \ll \|\partial f_L / \partial y_L\|$, accordingly for f_A).

Remark 1 *If the different parts interdepend to a great extend, we cannot expect multirate potential in terms of wide differing stepsizes anyway and the whole system will rather be computed using a “singlerate”-method [2].*

Now we have a look at some strategies for the couplings (5a,5b):

(1) *Extrapolation/Interpolation [2]*

Following a “slowest first”-strategy the macrostep is performed first. The coupling values Y_i^A are obtained by extrapolation. Then the r later microsteps are done with $Y_i^{L,\mu}$ given by interpolation of the latent part. Due to the extra- and interpolation this is a kind of multistep method.

(2) *Generalised multirate [7]*

The intention of generalised multirate is to preserve the one-step character of the underlying methods. Thus the couplings Y_i^A and $Y_i^{L,\mu}$ are determined in RK-like manner as internal stage evaluations using the increments $k_i^L, k_i^{A,\mu}$ and additional weights δ^L and δ^A as we will see later on. Generalised multirate uses equidistant microstepsizes during one macrostep, i. e. $h_{a,1} = \dots = h_{a,r}$ and the rejection of one microstep leads to the rejection of the corresponding macrostep and all microsteps.

(3) *Mixed multirate [1]*

This ansatz builds up on generalised multirate and yields an adaptive stepsize control for both macro- and microsteps. To relax the fixed micro step character the incremental formulation of generalised multirate is used only for the first step in each component, i.e. for $Y_i^{L,1}$ and Y_i^A (the so-called *compound step*). To compute the *later microsteps* dense output formulae are employed to get $Y_i^{L,2}, \dots, Y_i^{L,r}$. In other words, the compound step yields $y_{L,1}$ and $y_{A,1}$, where the coupling of active to latent and vice versa is done in the way of generalised multirate, and the later microsteps produce $y_{A,2}, \dots, y_{A,r}$, where there is only a coupling latent to active, given by dense output formulae for the latent part. Thus a rejection of one of the later microsteps does not influence the latent part.

3 A mixed multirate scheme for coupled index-1 DAE systems

In order to set up a multirate method for the split network equations (2) according to mixed multirate for ODEs and based on ROW schemes we linearly transform the network equations to index-1 Hessenberg form:

$$\begin{aligned} \dot{y}_l &= w_l(x_l, x_a) & \dot{y}_a &= w_a(x_l, x_a) \\ 0 &= y_l - g_l(x_l), & 0 &= y_a - g_a(x_a) \\ 0 &= \tilde{y}_l - \tilde{g}_l(x_l) & 0 &= \tilde{y}_a - \tilde{g}_a(x_a) \end{aligned} \tag{6}$$

with $x_\lambda, y_\lambda \in \mathbb{R}^{n_\lambda}$ and $\tilde{y}_\lambda \in \mathbb{R}^{m_\lambda - n_\lambda}$ for $\lambda \in \{l, a\}$, accordingly for the functions $w_\lambda, g_\lambda, \tilde{g}_\lambda$.

This can be seen as follows: because of the index-1 assumption (3) the matrix A_λ has full rank, i.e.

$$A_\lambda = S_\lambda \cdot \left(I_{n_\lambda} \middle| 0_{n_\lambda \times (m_\lambda - n_\lambda)} \right) \cdot T_\lambda$$

with $S_\lambda \in \mathbb{R}^{n_\lambda \times n_\lambda}, T_\lambda \in \mathbb{R}^{m_\lambda \times m_\lambda}$ regular holds. Equation (6) follows now by multiplying the first line of the latent part of (2) with S_λ^{-1} , the second one with T_λ and setting $(y_\lambda, \tilde{y}_\lambda)^t := T_\lambda \cdot z_\lambda$, $(g_\lambda, \tilde{g}_\lambda)^t := T_\lambda \cdot q_\lambda$ and $w_\lambda := S_\lambda^{-1} \cdot f_\lambda$.

Furthermore the first two lines of (6) solely define index 1 systems with respect to x_l and x_a respectively because $\partial g_\lambda / \partial x_\lambda = (I_{n_\lambda} \middle| 0_{n_\lambda \times (m_\lambda - n_\lambda)}) \cdot T_\lambda \cdot \partial q_\lambda / \partial x_\lambda = S_\lambda^{-1} \cdot A_\lambda \cdot \partial q_\lambda / \partial x_\lambda$ is regular according to assumption (3).

Thus we can omit the third line for the moment in order to define a method (we keep in mind that $\tilde{y}_\lambda = \tilde{g}_l(x_l)$) and concentrate on the remainder:

$$\begin{aligned} \dot{y}_l &= w_l(x_l, x_a) & \dot{y}_a &= w_a(x_l, x_a) \\ 0 &= y_l - g_l(x_l) & 0 &= y_a - g_a(x_a) \end{aligned} \quad (7)$$

3.1 Compound step

Without loss of generality, we will derive the compound step for the latent part only. Applying a generalised multirate ROW scheme [1] to the singular perturbed system

$$\begin{aligned} \dot{y}_l &= w_l(x_l, x_a) \\ \varepsilon \dot{x}_l &= y_l - g_l(x_l) \end{aligned}$$

and setting $\varepsilon = 0$ leads to a scheme for the underlying DAE (7) (for simplicity we set the same stage number s for the latent and active part):

$$\begin{pmatrix} y_{l,1} \\ x_{l,1} \end{pmatrix} = \begin{pmatrix} y_{l,0} \\ x_{l,0} \end{pmatrix} + \sum_{i=1}^s b_i^L \begin{pmatrix} l_i^L \\ k_i^L \end{pmatrix} \quad (8a)$$

with weights $b^L := (b_1^L, \dots, b_s^L)^t$ and increments $k^L := (k_1^L, \dots, k_s^L)^t, l^L := (l_1^L, \dots, l_s^L)^t$ defined by

$$\begin{pmatrix} I_s & -\gamma^L h_l \frac{\partial w_l}{\partial x_l} \\ -\gamma^L I_s & \gamma^L \frac{\partial g_l}{\partial x_l} \end{pmatrix} \cdot \begin{pmatrix} l_i^L \\ k_i^L \end{pmatrix} = \begin{pmatrix} h_l \cdot w_l(x_{l,0} + \sum_{j=1}^{i-1} \alpha_{ij}^L k_j^L, x_{a,0} + \frac{h_l}{h_{a,1}} \sum_{j=1}^{i-1} \delta_{ij}^L k_j^A) + h_l \cdot \frac{\partial w_l}{\partial x_l} \sum_{j=1}^{i-1} \gamma_{ij}^L k_j^L \\ y_{l,0} - g_l(x_{l,0} + \sum_{j=1}^{i-1} \alpha_{ij}^L k_j^L) + \sum_{j=1}^{i-1} \beta_{ij}^L l_j^L - \frac{\partial g_l}{\partial x_l} \sum_{j=1}^{i-1} \gamma_{ij}^L k_j^L \end{pmatrix}, \quad (8b)$$

where the partial differentials are taken at the starting points $(x_l(t_0), x_a(t_0))$ and $x_l(t_0)$, and the method coefficients are characterized by

$$\begin{aligned} \mathcal{A}^L &= (\alpha_{ij}^L)_{i,j=1}^s, \alpha_{ij}^L = 0 \text{ for } i \geq j, \\ \mathcal{D}^L &= (\delta_{ij}^L)_{i,j=1}^s, \delta_{ij}^L = 0 \text{ for } i \geq j, \\ \mathcal{G}^L &= (\gamma_{ij}^L)_{i,j=1}^s, \gamma_{ij}^L = 0 \text{ for } i > j, \gamma_{ii}^L = \gamma^L \neq 0, \\ \mathcal{B}^L &= (\beta_{ij}^L)_{i,j=1}^s, \beta_{ij}^L = \alpha_{ij}^L + \gamma_{ij}^L. \end{aligned}$$

Due to the regularity of $\partial g_l / \partial x_l$ at $x_{l,0}$, l_i^L and k_i^L are uniquely determined for sufficiently small stepsizes h_l .

The second argument in the evaluation of w_l describes the coupling of the active part into the latent one according to the idea of *generalised multirate* by re-weighting the (already known) active increments k_1^A, \dots, k_{i-1}^A : the term $h_l/h_{a,1}$ projects the smaller interval $[t_0, t_0 + h_{a,1}]$ onto $[t_0, t_0 + h_l]$.

Now we make use of the linear structure (with respect to y_l) of the algebraic constraint of the reduced coupled Hessenberg system (7) and transform the multirate scheme (8a,b) by Block-Gaussian elimination into a scheme where the constraint on y_l is automatically fulfilled and which computes $x_{l,1}$ as a sum over weighted increments $\kappa^L := \mathcal{G}^L \cdot k^L$:

$$\begin{aligned} x_{l,1} &= x_{l,0} + \sum_{i=1}^s d_i^L \cdot \kappa_i^L, \\ y_{l,1} &= g_l(x_{l,1}), \end{aligned} \tag{9a}$$

with weights $d^L := (\mathcal{G}^L)^{-t} \cdot b^L$ and increments defined by

$$\begin{aligned} \left(\frac{\partial g_l}{\partial x_l} - h_l \gamma^L \frac{\partial w_l}{\partial x_l} \right) \kappa_i^L = \\ y_{l,0} - g_l(\tilde{a}_{L,i}) + h_l \sum_{j=1}^i \beta_{ij}^L w_l(\tilde{a}_{L,j}, \tilde{d}_{L,j}) + h_l \sum_{j=1}^{i-1} \beta_{ij}^L \frac{\partial w_l}{\partial x_l} \kappa_j^L \end{aligned} \tag{9b}$$

where

$$\begin{aligned} \tilde{a}_{L,i} &= x_{l,0} + \sum_{j=1}^{i-1} \sigma_{ij}^L \kappa_j^L & \mathcal{S}^L &= (\sigma_{ij}^L)_{i,j=1}^s = \mathcal{A}^L \cdot (\mathcal{G}^L)^{-1} \\ \tilde{d}_{L,i} &= x_{a,0} + \frac{h_l}{h_{a,1}} \sum_{j=1}^{i-1} \rho_{ij}^L \kappa_j^A & \mathcal{R}^L &= (\rho_{ij}^L)_{i,j=1}^s = \mathcal{D}^L \cdot (\mathcal{G}^A)^{-1} \end{aligned}$$

In order to get a multirate scheme for the coupled network equation (2) the linear transformations which led to the coupled Hessenberg system (6) have to be reversed. As we are interested solely in the node potentials x_l, x_a , the ‘‘charges’’ z_l, z_a are omitted. The full compound step is given in Fig. 2.

3.2 Later micro steps

The aim of the later micro steps is to integrate the active part of the coupled network equations (2) on the interval $[t_0 + h_{a,1}, t_0 + h_l]$. If exact values for $x_l(t)$ were available for this time span the problem would be reduced to a ‘‘simple’’ DAE

$$\begin{aligned} A_a \cdot \dot{z}_a &= f_a(x_l(t), x_a) \\ 0 &= z_a - q_a(x_a) \\ x_{a,1} &= x_a(t_0 + h_{a,1}) \end{aligned}$$

$$\begin{aligned}
x_{l,1} &= x_{l,0} + \sum_{i=1}^s d_i^L \cdot \kappa_i^L \\
x_{a,1} &= x_{a,0} + \sum_{i=1}^s d_i^A \cdot \kappa_i^A
\end{aligned} \tag{9c}$$

with:

$$\begin{aligned}
(A_l \frac{\partial q_l}{\partial x_l} - h_l \gamma^L \frac{\partial f_l}{\partial x_l}) \kappa_i^L &= A_l (q_l(x_{l,0}) - q_l(\tilde{a}_{L,i})) \\
&\quad + h_l \sum_{j=1}^i \beta_{ij}^L f_l(\tilde{a}_{L,j}, \tilde{d}_{L,j}) + h_l \sum_{j=1}^{i-1} \beta_{ij}^L \frac{\partial f_l}{\partial x_l} \kappa_j^L \\
(A_a \frac{\partial q_a}{\partial x_a} - h_a \gamma^A \frac{\partial f_a}{\partial x_a}) \kappa_i^A &= A_a (q_a(x_{a,0}) - q_a(\tilde{a}_{A,i})) \\
&\quad + h_a \sum_{j=1}^i \beta_{ij}^A f_l(\tilde{d}_{A,j}, \tilde{a}_{A,j}) + h_{a,1} \sum_{j=1}^{i-1} \beta_{ij}^A \frac{\partial f_a}{\partial x_a} \kappa_j^A \\
\tilde{a}_{L,i} &= x_{l,0} + \sum_{j=1}^{i-1} \sigma_{ij}^L \kappa_j^L \quad \left| \quad \tilde{d}_{L,i} = x_{a,0} + m \cdot \sum_{j=1}^{i-1} \varrho_{ij}^L \kappa_j^A \right. \\
\tilde{a}_{A,i} &= x_{a,0} + \sum_{j=1}^{i-1} \sigma_{ij}^A \kappa_j^A \quad \left| \quad \tilde{d}_{A,i} = x_{l,0} + m^{-1} \sum_{j=1}^{i-1} \varrho_{ij}^A \kappa_j^L \right. \\
&\quad m = h_l / h_{a,1}
\end{aligned}$$

Fig. 2. Compound step for coupled network equation (2)

which could be solved numerically with any index-1 integration scheme, e.g. CHORAL [3] developed for charge-oriented network equations, with stepsizes $h_{a,2}, \dots, h_{a,r}$, stage number s_C , increments κ^C , weights d^C and coefficients $\mathcal{B}^C, \mathcal{S}^C$. As we do not know the exact solution $x_l(t)$ but only one value $x_{l,1} \approx x_l(t_0 + h_l)$ and the increments κ^L that led to this approximation, we can employ dense output [5] to get x_l on the finer grid [1]:

$$\begin{aligned}
x_l^{\text{ds}}(\mu, \nu) &= x_{l,0} + \sum_{i=1}^s d_i^L(\theta_{\mu, \nu}) \cdot \kappa_i^L \quad (\approx x_l(t_0 + \theta_{\mu, \nu} h_l)) \\
\theta_{\mu, \nu} &= \frac{1}{h_l} (h_{a,1} + \dots + h_{a, \mu-1}) + \sigma_\nu^C \frac{h_{a, \mu}}{h_l}
\end{aligned} \tag{9d}$$

The weights $d_1^L(\cdot), \dots, d_s^L(\cdot)$ are polynomials in $\theta_{\mu, \nu} \in (0, 1]$ with $d_i^L(1) = d_i^L$ for all $i \in \{1, \dots, s\}$.

The method for the later microsteps can now be defined as a combination of CHORAL [3] and dense output (9d), see Fig. 3:

4 Order conditions

In simulating electrical networks numerically only the node potentials x_l, x_a are of interest. Thus consistency of the method is defined using these variables:

Definition 2 *A mixed multirate-type method is said to be consistent of order*

$$x_{a,\mu} = x_{a,\mu-1} + \sum_{i=1}^{s_C} d_i^C \cdot \kappa_i^C \quad (\mu = 2, \dots, r) \quad (9e)$$

with

$$\begin{aligned} (A_a \frac{\partial q_a}{\partial x_a} - h_{a,\mu} \gamma^C \frac{\partial f_a}{\partial x_a}) \kappa_i^C &= A_a (q_a(x_{a,\mu-1}) - q_a(\tilde{a}_{C,i})) \\ &+ h_{a,\mu} \sum_{j=1}^i \beta_{ij}^C f_a(x_l^{\text{ds}}(\mu, j), \tilde{a}_{C,j}) + h_{a,\mu} \sum_{j=1}^{i-1} \beta_{ij}^C \frac{\partial f_a}{\partial x_a} \kappa_j^C \end{aligned}$$

$$\tilde{a}_{C,i} = x_{a,\mu-1} + \sum_{j=1}^{i-1} \sigma_{ij}^C \kappa_j^C$$

$$x_l^{\text{ds}}(\mu, \nu) \text{ defined as in (9d)}$$

the partial derivatives are taken at the points $x_{a,\mu-1}$ and $(x_l^{\text{ds}}(\mu, 1), x_{a,\mu-1})$

Fig. 3. later micro steps for the coupled network equation (2)

p iff the following is fulfilled:

(1) compound step

$$\begin{aligned} \|x_i(t_0 + h_l) - x_{l,1}\| &= \mathcal{O}(h_l^{p+1}), \\ \|x_a(t_0 + h_{a,1}) - x_{a,1}\| &= \mathcal{O}(h_{a,1}^{p+1}) \end{aligned}$$

(2) later micro steps ($\mu = 2, \dots, r$)

$$\|x_a((t_0 + h_{a,1} + \dots + h_{a,\mu-1}) + h_{a,\mu}) - x_{a,\mu}\| = \mathcal{O}(h_{a,\max}^{p+1})$$

with $h_{a,\max} := \max_{\mu=1,\dots,r-1} h_{a,\mu}$.

Remark 3 It is easy to verify by standard arguments that consistency of order p implies global convergence of order p .

4.1 Order conditions for the compound step

The diagram (Fig. 4) shows how the compound step (9c) associated with the coupled network equations (2) has been developed.

Since ROW methods are invariant under linear transformations this diagram commutes, i. e. instead of investigating the consistency of the compound step (9c) concerning the coupled network equations (2) we can regard the method (8a,b) working with increments k^Λ, l^Λ ($\Lambda \in \{A, L\}$) and the reduced coupled Hessenberg system (7).

For further examination we assume that w_l, w_a, g_l and g_a are sufficiently often differentiable along the exact solution. We then expand both the analytical

solution $x_l(t), x_a(t)$ and the numerical approximation $x_{l,1}, x_{a,1}$ in Taylor series. To achieve consistency order p these series have to be equal up to order p , i. e. derivatives of the exact solution x_l, x_a and the increments k^L, k^A and l^L, l^A are needed. We introduce MDAT-trees which are related to B-trees and DAT-trees [4,5]. These allow to get a graphical representation of the process of differentiation and propose the definition of MDA-series to get the required derivatives.

Definition 4 (*Multirate differential algebraic trees*)

Let $\text{MDAT} = \text{MDAT}_{y_l} \cup \text{MDAT}_{x_l} \cup \text{MDAT}_{y_a} \cup \text{MDAT}_{x_a}$ be the set of all multirate differential algebraic trees. Each element of MDAT has exactly one root of the type $\bullet, \circ, \blacksquare$ or \square according to the indices y_l, x_l, y_a, x_a . Let $[\dots]_{y_l}$ describe the connection of all trees mentioned between “[” and “]” to one new root of the form “full circle” and in the same way for the other indices. Furthermore let $t^L \in \text{MDAT}_{y_l}, t^A \in \text{MDAT}_{y_a}, u^L \in \text{MDAT}_{x_l}, u^A \in \text{MDAT}_{x_a}$.

Then all regular trees are given recursively by:

- a) “Starting trees” $\bullet = \tau_{y_l}, \circ = \tau_{x_l}, \blacksquare = \tau_{y_a}, \square = \tau_{x_a}$,
- b) $[u_1^\Lambda, \dots, u_m^\Lambda, u_1^{\bar{\Lambda}}, \dots, u_n^{\bar{\Lambda}}]_{y_\lambda}$ where $n, m \in \mathbb{N}_0, (m, n) \neq (0, 0)$,
- c) $[t_1^\Lambda]_{x_\lambda}$,
- d) $[u_1^\Lambda, \dots, u_n^\Lambda]_{x_\lambda}$ where $n \in \mathbb{N}, n > 1$,

where $(\lambda, \Lambda) \in \{(l, L), (a, A)\}$ and $\{\Lambda, \bar{\Lambda}\} = \{L, A\}$.

Additionally the “empty” trees $\emptyset_{y_l}, \emptyset_{x_l}, \emptyset_{y_a}, \emptyset_{x_a}$ are needed to define the MDA-series later on.

Definition 5 (*Order of a tree*)

The order of a tree $t \in \text{MDAT}$, denoted by $\varrho(t)$, is the number of its full vertices (\bullet, \blacksquare)

Hence the empty trees $\emptyset_{y_l}, \emptyset_{x_l}, \emptyset_{y_a}, \emptyset_{x_a}$ are the only trees of order 0 and the

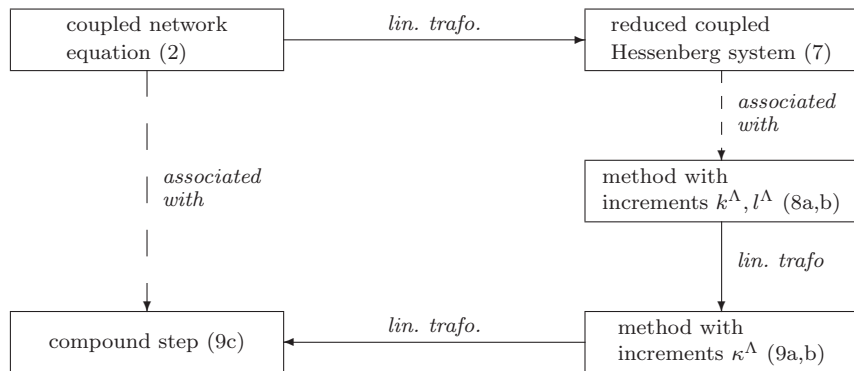


Fig. 4. schematical method construction

trees $\tau_{y_x}, \tau_{y_l}, \tau_{x_l}, \tau_{x_a}$ are the only ones of order 1.

Definition 6 (MDAT and elementary differentials)

The elementary differentials $F(\cdot)$ corresponding to regular trees in MDAT are defined as follows:

- a) $F(\emptyset_{y_\lambda}) = y_\lambda, \quad F(\emptyset_{x_\lambda}) = x_\lambda,$
- b) $F(\tau_{y_\lambda}) = w_\lambda, \quad F(\tau_{x_\lambda}) = \left(\frac{\partial g_\lambda}{\partial x_\lambda}\right)^{-1} w_\lambda,$
- c) $F([u_1^\Lambda, \dots, u_m^\Lambda, u_1^{\bar{\Lambda}}, \dots, u_n^{\bar{\Lambda}}]_{y_\lambda}) = \frac{\partial^{m+n} w_\lambda}{\partial x_\lambda^m \partial x_\lambda^n} \left(F(u_1^\Lambda), \dots, F(u_n^{\bar{\Lambda}})\right),$
- d) $F([t^\Lambda]_{x_\lambda}) = \left(\frac{\partial g_\lambda}{\partial x_\lambda}\right)^{-1} F(t^\Lambda),$
- e) $F([u_1^\Lambda, \dots, u_n^\Lambda]_{x_\lambda}) = -\left(\frac{\partial g_\lambda}{\partial x_\lambda}\right)^{-1} \frac{\partial^n g_\lambda}{\partial x_\lambda^n} \left(F(u_1^\Lambda), \dots, F(u_n^\Lambda)\right),$

where $(\lambda, \Lambda) \in \{(l, L), (a, A)\}, \{\Lambda, \bar{\Lambda}\} = \{L, A\}, \{\lambda, \bar{\lambda}\} = \{l, a\}$, functions and derivatives are evaluated at the starting point t_0 .

The elementary differentials are well defined due to the symmetry of the partial differentials, i. e. $F(\cdot)$ is not affected by permutations of the involved regular trees.

Example 7 (a tree of order $\rho = 3$)

$$F(\text{tree}) = F([\tau_{x_l}, \tau_{x_a}]_{y_l}) = \left(\frac{\partial g_l}{\partial x_l}\right)^{-1} \frac{\partial^2 w_l}{\partial x_l \partial x_a} \left(\left(\frac{\partial g_l}{\partial x_l}\right)^{-1} w_l, \left(\frac{\partial g_a}{\partial x_a}\right)^{-1} w_a\right)$$

Fig. 5 shows how all regular trees in MDAT can be obtained: if a regular tree is given then the application of each of the shown rules leads to another regular tree.

As each tree represents an elementary differential (Def. 6), these rules of attaching or splitting and attaching correspond to differentiation rules: (clockwise starting with the left upper rule in Fig. 5, $v_1, \dots \equiv \text{const}$)

- (1) derivation of $(\partial g_\lambda / \partial x_\lambda)^{-1} \cdot v_1$ with respect to x_λ and addition of the factor

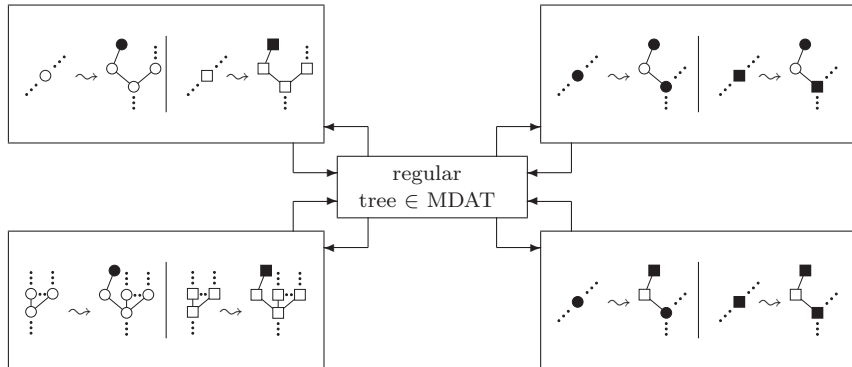


Fig. 5. from tree to tree: “graphical” differentiation

- $\dot{x}_\lambda = (\partial g_\lambda / \partial x_\lambda)^{-1} \cdot w_\lambda$
- (2) derivation of w_λ with respect to x_l and addition of the factor \dot{x}_l
 - (3) derivation of w_λ with respect to x_a and addition of the factor \dot{x}_a
 - (4) derivation of $\frac{\partial^n g_\lambda}{\partial x_\lambda^n}(v_1, \dots, v_n)$ with respect to x_λ and addition of the factor \dot{x}_λ . Note that $n \geq 2$.

We observe that the application of each of the rules to a tree of order q generates a regular tree of order $q + 1$. Hence all trees of the subset MDAT_{x_l} with order 2, i. e. all trees with root “o” and exactly two filled vertices are obtained by applying each of the rules (as far as possible) to the starting tree $\tau_{x_l}: \{\text{tree 1}, \text{tree 2}, \text{tree 3}\}$, all trees in MDAT_{x_l} of order 3 are obtained by applying each of the rules to these trees and so on. The set $\{u^L \in \text{MDAT}_{x_l} | \varrho(u^L) = 3\}$ has 13 different elements where some are generated two or three times. If we introduce a monotonic labelling of the trees, i. e. we enumerate the full vertices in the order of their generation corresponding to [4,5], there are 20 “empty circle”-rooted trees of order 3.

Reflecting the rules shown in Fig. 5 and the involved rules of differentiation we can easily conclude:

Theorem 8 (*Derivatives of the exact solution*)

For the exact solution $x_\lambda(t)$ $((\lambda, \Lambda) \in \{(l, L), (a, A)\})$ of (7) we have:

$$x_\lambda^{(q)}(t_0) = \sum_{\substack{u^\Lambda \in \text{LMDAT}_{x_\lambda} \\ \varrho(u^\Lambda) = q}} F(u^\Lambda) = \sum_{\substack{u^\Lambda \in \text{MDAT}_{x_\lambda} \\ \varrho(u^\Lambda) = q}} \alpha(u^\Lambda) \cdot F(u^\Lambda)$$

Here LMDAT is the set of trees in MDAT provided with all possible monotonic labellings as mentioned above and $\alpha(u^\Lambda)$ is the number of possible monotonic labellings of the tree u^Λ . Order ϱ and appropriate elementary differential F for trees in LMDAT are defined in the same way as for the elements of MDAT .

To get a similar theorem for the derivatives of k^L, \dots we introduce MDA-series.

Definition 9 (*MDA-series*)

Let $\mathbf{c}_{x_l}, \mathbf{c}_{x_a}, \mathbf{c}_{y_l}, \mathbf{c}_{y_a}$ be mappings from $\text{LMDAT}_{x_l}, \dots$ onto \mathbb{R} , i. e. a real number is assigned to every labelled tree of the corresponding subset. Then we call the following series – according to the index x_l, x_a, y_l, y_a – MDA_{x_l}, \dots -series:

$$\text{MDA}_\Psi(\mathbf{c}_\Psi) = \sum_{b \in \text{LMDAT}_\Psi} \mathbf{c}_\Psi \cdot F(b) \cdot \frac{h_l^{\varrho(b)}}{\varrho(b)!} \quad ((\Psi, b) \in \{(x_l, u^L), (y_l, t^L)\})$$

$$\text{MDA}_\Psi(\mathbf{c}_\Psi) = \sum_{b \in \text{LMDAT}_\Psi} \mathbf{c}_\Psi \cdot F(b) \cdot \frac{h_{a,1}^{\varrho(b)}}{\varrho(b)!} \quad ((\Psi, b) \in \{(x_a, u^A), (y_a, t^A)\})$$

For further investigation of the properties we set the stepsize relation $m =$

$h_l/h_{a,1}$. For a better understanding we denote in the following two lemmas trees with a “full” root with the letter t and those with an “empty” root as u . If they are additionally labelled with an L or A also the form (“circle” or “square”) is fixed, in the other cases it becomes clear from the context (all trees must be regular!).

Lemma 10

Let $a_l = \text{MDA}_{x_l}(\mathbf{a}_l), a_a = \text{MDA}_{x_a}(\mathbf{a}_a)$ such that $\mathbf{a}_l(\emptyset_{x_l}) = \mathbf{a}_a(\emptyset_{x_a}) = 1$. Then

$$\begin{aligned} h_l \cdot w_l(a_l, a_a) &= \text{MDA}_{y_l}(\mathbf{c}_l) \\ h_{a,1} \cdot w_a(a_l, a_a) &= \text{MDA}_{y_a}(\mathbf{c}_a) \end{aligned}$$

with $\mathbf{c}_l(\emptyset_{y_l}) = \mathbf{c}_a(\emptyset_{y_a}) = 0, \quad \mathbf{c}_l(\tau_{y_l}) = \mathbf{c}_a(\tau_{y_a}) = 1$

$$\mathbf{c}_\lambda(t) = \varrho(t) \cdot \mathbf{a}_l(u_1^L) \cdot \dots \cdot \mathbf{a}_l(u_l^L) \cdot \mathbf{a}_a(u_1^A) \cdot \dots \cdot \mathbf{a}_a(u_n^A) \cdot$$

$$\begin{cases} m^{-(\varrho(u_1^A) + \dots + \varrho(u_n^A))} & \text{if } \lambda = l \text{ \& } t = [u_1^L, \dots, u_l^L, u_1^A, \dots, u_n^A]_{y_l} \\ m^{(\varrho(u_1^L) + \dots + \varrho(u_l^L))} & \text{if } \lambda = a \text{ \& } t = [u_1^L, \dots, u_l^L, u_1^A, \dots, u_n^A]_{y_a} \end{cases}$$

and

$$\begin{aligned} h_l \cdot \frac{\partial w_l}{\partial x_l} \cdot a_l &= \text{MDA}_{y_l}(\mathbf{d}_l) \\ h_{a,1} \cdot \frac{\partial w_a}{\partial x_a} \cdot a_a &= \text{MDA}_{y_a}(\mathbf{d}_a) \end{aligned}$$

with $\mathbf{d}_\lambda(t) = \begin{cases} \varrho(t^\Lambda) \cdot \mathbf{a}_\lambda(u^\Lambda) & \text{if } t^\Lambda = [u^\Lambda]_{y_\lambda} \\ 0 & \text{otherwise} \end{cases} \quad (\lambda, \Lambda) \in \{(l, L), (a, A)\}$

Lemma 11

Let $a_\lambda = \text{MDA}_{x_\lambda}(\mathbf{a}_\lambda), b_\lambda = \text{MDA}_{y_\lambda}(\mathbf{b}_\lambda)$ such that $\mathbf{a}_\lambda(\emptyset_{x_\lambda}) = \mathbf{b}_\lambda(\emptyset_{y_\lambda}) = 1$ and $\mathbf{a}_\lambda(\tau_{x_\lambda}) = \mathbf{b}_\lambda(\tau_{y_\lambda}) = 1$ for $(\lambda, \Lambda) \in \{(l, L), (a, A)\}$. Then

$$\begin{aligned} \left(\frac{\partial g_\lambda}{\partial x_\lambda}\right)^{-1} \cdot b_\lambda &= \text{MDA}_{x_\lambda}(\mathbf{c}_\lambda) \\ \left(\frac{\partial g_\lambda}{\partial x_\lambda}\right)^{-1} \cdot g_\lambda(a_\lambda) &= \text{MDA}_{x_\lambda}(\mathbf{d}_\lambda) \end{aligned}$$

with $\mathbf{c}_\lambda(u^\Lambda) = \begin{cases} \mathbf{b}_\lambda(t^\Lambda) & \text{if } u^\Lambda = [t^\Lambda]_{x_\lambda} \\ 0 & \text{otherwise} \end{cases}$

$$\mathbf{d}_\lambda(u^\Lambda) = \begin{cases} -\mathbf{a}_\lambda(u_1^\Lambda) \cdot \dots \cdot \mathbf{a}_\lambda(u_n^\Lambda) + \mathbf{a}_\lambda(u^\Lambda) & \text{if } u^\Lambda = [u_1^\Lambda, \dots, u_n^\Lambda]_{x_\lambda} \\ \mathbf{a}_\lambda(u) & \text{if } u^\Lambda = [t^\Lambda]_{x_\lambda} \\ 0 & \text{if } u^\Lambda = \emptyset_{x_\lambda} \end{cases}$$

Sketch of the proof for Lemmata 10 and 11

The MDA-series a_l, b_l, a_a, b_a can be understood as functions in the variables h_l and h_a : $a_l(h_l), b_l(h_l), a_a(h_{a,1}), b_a(h_{a,1})$. Then we expand the terms that are said to be MDA-series to Taylor series around zero, i. e. we need to compute derivatives with respect to h_l and $h_{a,1}$ respectively. In case of $h_l \cdot w_l(a_l, a_a)$ for example we have to look at $a_a(h_{a,1})$ as a function depending on h_l : $a_a(h_{a,1}) =$

$a_a(m^{-1} \cdot h_l)$. We then apply Leibniz' rule and the chain rule to get the differentials, take advantage of the linearity of the multilinear mappings, reflect in which way the involved trees and therefore the elementary differentials are constructed recursively and finally take into account, that $\varrho([u_1^\Lambda, \dots, u_n^\Lambda]_{x_\lambda}) = \varrho(u_1^\Lambda) + \dots + \varrho(u_n^\Lambda)$, $\varrho([t^\Lambda]_{x_\lambda}) = \varrho(t^\Lambda)$, $\varrho([u_1^\Lambda, \dots, u_n^\Lambda]_{y_\lambda}) = \varrho(u_1^\Lambda) + \dots + \varrho(u_n^\Lambda) + 1$.

□

Theorem 12 (*Derivatives of the compound step-increments*)

The increments k^L, k^A, l^L, l^A satisfy for $[(\lambda, \Lambda) \in \{(l, L), (a, A)\}, \{\Lambda, \bar{\Lambda}\} = \{L, A\}]$

$$\begin{aligned} (k_i^\Lambda)^{(q)}(0) &= \sum_{\substack{u^\Lambda \in \text{MDAT}_{x_\lambda} \\ \varrho(u^\Lambda) = q}} \alpha(u^\Lambda) \cdot \gamma(u^\Lambda) \cdot \Phi_i(u^\Lambda) \cdot F(u^\Lambda) \\ (l_i^\Lambda)^{(q)}(0) &= \sum_{\substack{t^\Lambda \in \text{MDAT}_{y_\lambda} \\ \varrho(t^\Lambda) = q}} \alpha(t^\Lambda) \cdot \gamma(t^\Lambda) \cdot \Phi_i(t^\Lambda) \cdot F(t^\Lambda) \end{aligned} \quad q \geq 1$$

with $\gamma(\cdot)$ defined as:

- $\gamma(\tau_{x_\lambda}) = \gamma(\tau_{y_\lambda}) = 1$
- $\gamma(u^\Lambda) = \begin{cases} \gamma(t^\Lambda) & \text{if } u = [t^\Lambda]_{x_\lambda} \\ \gamma(u_1^\Lambda) \cdot \dots \cdot \gamma(u_n^\Lambda) & \text{if } u^\Lambda = [u_1^\Lambda \dots, u_n^\Lambda]_{x_\lambda} \end{cases}$
- $\gamma(t^\Lambda) = \varrho(t^\Lambda) \cdot \gamma(u_1^L) \cdot \dots \cdot \gamma(u_n^A)$ if $t^\Lambda = [u_1^L, \dots, u_l^L, u_1^A, \dots, u_n^A]_{y_\lambda}$

and $\Phi_i(\cdot)$ defined as $[\Omega^\Lambda = (\omega_{ij}^\Lambda)_{i,j=1}^s = (\mathcal{B}^\Lambda)^{-1}, \chi(l) = 1, \chi(a) = -1]$:

- $\Phi_i(\tau_{x_\lambda}) = \Phi_i(\tau_{y_\lambda}) = 1$
- $\Phi_i(u^\Lambda) = \Phi_i(t^\Lambda)$ if $u^\Lambda = [t^\Lambda]_{x_\lambda}$
- $\Phi_i(u^\Lambda) = \sum_{j, \mu_1, \dots, \mu_n} \omega_{ij}^\Lambda \cdot \alpha_{j\mu_1}^\Lambda \cdot \dots \cdot \alpha_{j\mu_n}^\Lambda \cdot \Phi_{\mu_1}(u_1^\Lambda) \cdot \dots \cdot \Phi_{\mu_n}(u_n^\Lambda)$ if $u^\Lambda = [u_1^\Lambda \dots, u_n^\Lambda]_{x_\lambda}$
- $\Phi_i(t^\Lambda) = \sum_j \beta_{ij}^\Lambda \cdot \Phi_i(u_1^\Lambda)$ if $t^\Lambda = [u^\Lambda]_{y_\lambda}$
- $\Phi_i(t^\Lambda) = m^{\chi(\lambda) \cdot [n - (\varrho(u_1^\Lambda) + \dots + \varrho(u_n^\Lambda))]} \sum_{\mu_1, \dots, \mu_n} \alpha_{i\mu_1}^\Lambda \cdot \dots \cdot \alpha_{i\mu_l}^\Lambda \cdot \delta_{i\nu_1}^{\bar{\Lambda}} \cdot \dots \cdot \delta_{i\nu_n}^{\bar{\Lambda}} \cdot \Phi_{\mu_1}(u_1^\Lambda) \cdot \dots \cdot \Phi_{\nu_n}(u_n^\Lambda)$ if $t^\Lambda = [u_1^\Lambda, \dots, u_l^\Lambda, u_1^{\bar{\Lambda}}, \dots, u_n^{\bar{\Lambda}}]_{y_\lambda}$
($n + l > 1$) or ($l = 0$ and $n \geq 1$)
- $\Phi_i(u^\Lambda) = \sum_{j, \mu_1, \dots, \mu_n} \omega_{ij}^\Lambda \cdot \alpha_{j\mu_1}^\Lambda \cdot \dots \cdot \alpha_{j\mu_n}^\Lambda \cdot \Phi_{\mu_1}(u_1^\Lambda) \cdot \dots \cdot \Phi_{\mu_n}(u_n^\Lambda)$ if $u^\Lambda = [u_1^\Lambda, \dots, u_n^\Lambda]_{x_\lambda}$

Proof Reformulating the compound step (8a,b) we get:

$$\begin{aligned} x_{l,1} &= x_{l,0} + \sum_{i=1}^s b_i^L k_i^L, \\ l_i^L &= h_l \cdot w_l(a_i^L, d_i^L) + h_l \frac{\partial w_l}{\partial x_l} \sum_{j=1}^i \gamma_{ij}^L k_j^L, \\ 0 &= g_l(x_{l,0}) - g_l(a_i^L) + \sum_{j=1}^i \beta_{ij}^L l_{ij}^L - \frac{\partial g_l}{\partial x_l} \sum_{j=1}^i \gamma_{ij}^L k_j^L, \\ a_i^L &= x_{l,0} + \sum_{j=1}^{i-1} \alpha_{ij}^L k_j^L, \\ d_i^L &= x_{a,0} + m \cdot \sum_{j=1}^{i-1} \delta_{ij}^L k_j^A. \end{aligned}$$

As a successive differentiation of (8a,b) shows, $x_{l,1}, k_i^L, l_i^L$ are MDA-series. We now assume $x_{l,1}, k_i^L, l_i^L, a_i^L, d_i^L$ to be MDA-series with coefficients $\mathbf{x}_{l,1}, \dots$

(and accordingly for the active part). Then the lemmas 10 and 11 and some algebraic calculus allow to transcribe k_i^L and l_i^L as we asserted. \square

Theorem 8 reveals that the exact solution x_λ is a MDA_{x_λ} -series with coefficients $\mathbf{x}_\lambda(u^\Lambda) = 1$ for all $u^\Lambda \in \text{MDAT}_{x_\lambda} [(\lambda, \Lambda) \in \{(l, L), (a, A)\}]$. As the derivatives of the exact solutions and the approximations have to be equal up to order p the order conditions are simply given by

Theorem 13 (*compound step order conditions*)

The compound step (8a,b) is consistent of order p iff

$$\begin{aligned} \sum_{i=1}^s b_i^L \cdot \Phi_i(u^L) &= \frac{1}{\gamma(u^L)} & \forall u^L \in \text{MDAT}_{x_l} & \text{ with } \varrho(u^L) \leq q, \\ \sum_{i=1}^s b_i^A \cdot \Phi_i(u^A) &= \frac{1}{\gamma(u^A)} & \forall u^A \in \text{MDAT}_{x_a} & \text{ with } \varrho(u^A) \leq q. \quad \square \end{aligned}$$

Remark 14 *The terms $\gamma(\cdot)$ and $\Phi_i(\cdot)$ are given recursively in Theorem 12. However, it is also possible to read off these values directly from the associated tree.*

Fig. 6 gives all elements of MDAT_{x_l} and MDAT_{x_a} up to order three and the corresponding order conditions.

4.2 Order conditions for the later micro steps

The later microsteps are integrated by combining a solver for single index-1 DAEs and a dense output scheme. The following lemma shows that the later micro steps are consistent of order p , if both the integration and dense output scheme are of order p .

Lemma 15 *The later micro steps (9e) are consistent of order p , i. e.*

$$\|x_a(t_\mu) - x_{a,\mu}\| \leq C \cdot h_{a,\max}^{p+1}$$

for $\mu = 2, \dots, r$, if an integration scheme of order p is used and a dense output scheme for x_l with error

$$\|x_l(t_0 + \theta h_l) - x_l^{\text{ds}}(\theta)\| \leq c_1 \cdot h_l^p \quad \forall \theta \in [0, 1]$$

of order p .



































	$\sum b_i^L = 1$		$\sum b_i^A = 1$
	$\sum b_i^L \omega_{ij}^L (\alpha_j^L)^2 = 1$		$\sum b_i^A \omega_{ij}^A (\alpha_j^A)^2 = 1$
	$\sum b_i^L \beta_i^L = \frac{1}{2}$		$\sum b_i^A \beta_i^A = \frac{1}{2}$
	$\sum b_i^L \delta_i^L = \frac{1}{2}$		$\sum b_i^A \delta_i^A = \frac{1}{2}$
	$\sum b_i^L (\alpha_i^L)^2 = \frac{1}{3}$		$\sum b_i^A (\alpha_i^A)^2 = \frac{1}{3}$
	$\sum b_i^L \alpha_i^L \delta_i^L = \frac{1}{3}$		$\sum b_i^A \alpha_i^A \delta_i^A = \frac{1}{3}$
	$\sum b_i^L (\delta_i^L)^2 = \frac{1}{3}$		$\sum b_i^A (\delta_i^A)^2 = \frac{1}{3}$
	$\sum b_i^L \beta_{ij}^L \beta_j^L = \frac{1}{6}$		$\sum b_i^A \beta_{ij}^A \beta_j^A = \frac{1}{6}$
	$\sum b_i^L \beta_{ij}^L \delta_j^L = \frac{1}{6}$		$\sum b_i^A \beta_{ij}^A \delta_j^A = \frac{1}{6}$
	$\sum b_i^L \cdot \frac{1}{m} \cdot \delta_{ij}^L \beta_j^A = \frac{1}{6}$		$\sum b_i^A \cdot m \cdot \delta_{ij}^A \beta_j^L = \frac{1}{6}$
	$\sum b_i^L \cdot \frac{1}{m} \cdot \delta_{ij}^L \delta_j^A = \frac{1}{6}$		$\sum b_i^A \cdot m \cdot \delta_{ij}^A \delta_j^L = \frac{1}{6}$
	$\sum b_i^L \omega_{ij}^L \alpha_j^L \alpha_{jk}^L \beta_k^L = \frac{1}{2}$		$\sum b_i^A \omega_{ij}^A \alpha_j^A \alpha_{jk}^A \beta_k^A = \frac{1}{2}$
	$\sum b_i^L \omega_{ij}^L \alpha_j^L \alpha_{jk}^L \delta_k^L = \frac{1}{2}$		$\sum b_i^A \omega_{ij}^A \alpha_j^A \alpha_{jk}^A \delta_k^A = \frac{1}{2}$
	$\sum b_i^L \omega_{ij}^L (\alpha_j^L)^3 = 1$		$\sum b_i^A \omega_{ij}^A (\alpha_j^A)^3 = 1$
	$\sum b_i^L \omega_{ij}^L \alpha_j^L \alpha_{jk}^L \omega_{kl}^L (\alpha_l^L)^2 = 1$		$\sum b_i^A \omega_{ij}^A \alpha_j^A \alpha_{jk}^A \omega_{kl}^A (\alpha_l^A)^2 = 1$
	$\sum b_i^L \beta_{ij}^L \omega_{jk}^L (\alpha_k^L)^2 = \frac{1}{3}$		$\sum b_i^A \beta_{ij}^A \omega_{jk}^A (\alpha_k^A)^2 = \frac{1}{3}$
	$\sum b_i^L \cdot \frac{1}{m} \cdot \delta_{ij}^L \omega_{jk}^A (\alpha_k^A)^2 = \frac{1}{3}$		$\sum b_i^A \cdot m \cdot \delta_{ij}^A \omega_{jk}^L (\alpha_k^L)^2 = \frac{1}{3}$

Fig. 6. Order conditions for compound step up to order 3

Proof Let \tilde{x}_a be the exact solution of the perturbed problem

$$\begin{aligned} \dot{y}_a &= w_a(x_l^{\text{ds}}(t), x_a), & \tilde{x}_a(t_1) &= x_{a,1}, \\ 0 &= y_a - g_a(x_a) \end{aligned}$$

which is approximated numerically by $x_{a,2}, \dots, x_{a,r}$ at time points $t_2, \dots, t_r = t_0 + h_l$. The triangle inequality now yields

$$\|x_a(t_\mu) - x_{a,\mu}\| \leq \|x_a(t_\mu) - \tilde{x}_a(t_\mu)\| + \|\tilde{x}_a(t_\mu) - x_{a,\mu}\|.$$

Gronwall's Lemma then allows to estimate the first term and the second is just the error made, applying the solver to the perturbed problem above. Taking into account, that the stepsize relation $h_l/h_{a,\mu}$ should be reasonably bounded, i. e. the microstepsizes should not become too small in relation to the macro stepsize h_l , the proof is finished. \square

To get a mixed multirate-type method of consistency order p according to Def. 1, we have to adjust the dense-output scheme (9d) to get an error of magnitude $\mathcal{O}(h_l^p)$. We therefore use the transformed formulation with $b_i^L(\cdot)$ instead of $d_i^L(\cdot)$ and k_i^L instead of κ_i^L and follow the instructions of [5, II.6] where the values Φ_i and $\gamma^\Lambda(\cdot)$ ($\Lambda \in \{L, A\}$) are those we defined previously.

5 Implementation

For test purposes MDAE23, a stiffly accurate mixed multirate method of local (and therefore global) accuracy order 3 and stage number $s = 4$ with an embedded method of order 2 with stage number $\hat{s} = 3$, has been implemented in MATLAB. This scheme is suitable for nonautonomous coupled index-1 systems of the type

$$\begin{aligned} A_l \cdot \dot{z}_l &= f_l(x_l, x_a, t) & A_a \cdot \dot{z}_a &= f_a(x_l, x_a, t) \\ 0 &= z_l - q_l(x_l, t), & 0 &= z_a - q_a(x_a, t). \\ x_{l,0} &= x_l(t_0) & x_{a,0} &= x_a(t_0) \end{aligned}$$

Details of the implementation (including coefficient sets) can be found in the appendix. First promising numerical results for the generalised Prothero-Robinson-equation, introduced by A. Kværnø [6] can be found in [8].

6 Conclusion

To exploit the multirate potential in full chip design, multirate schemes have to be tailored to partitioned systems of differential-algebraic equations. In this paper we have described first steps towards this goal and shown the feasibility of the approach. Future work has to concentrate on more sophisticated DAE network systems and partitioning techniques. For the first aim, the MDA-series theory has to be generalised. The second goal may be achieved by using the mixed multirate-type scheme in a recursive manner based on a hierarchical description of the network.

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A MDAE23

A.1 Computation of the numerical approximation

- *compound step* $[(\lambda, \Lambda, \bar{\lambda}, \bar{\Lambda}) \in \{(l, L, a, A), (a, A, l, L)\}$ here $h_a = h_{a,1}$]

$$x_{\lambda,1} = x_{\lambda,0} + \sum_{i=1}^s d_i^\Lambda \cdot \kappa_i^\Lambda, \quad \hat{x}_{\lambda,1} = x_{\lambda,0} + \sum_{i=1}^{\hat{s}} \hat{d}_i^\Lambda \cdot \kappa_i^\Lambda,$$

with increments κ_i^Λ given by

$$\begin{aligned} (A_\lambda \frac{\partial q_\lambda}{\partial x_\lambda} - h_\lambda \gamma^\Lambda \frac{\partial f_i}{\partial x_i}) \kappa_i^\Lambda &= A_\lambda (q_\lambda(x_{\lambda,0}, t_0) - q_\lambda(\tilde{a}_{\Lambda,i}, t_0 + \alpha_i^\Lambda h_\lambda)) \\ &+ h_\lambda \sum_{j=1}^i \beta_{ij}^\Lambda f_\lambda(\tilde{a}_{\Lambda,j}, \tilde{d}_{\Lambda,j}, t_0 + \alpha_j^\Lambda h_\lambda) + h_\lambda \sum_{j=1}^{j-1} \frac{\partial f_i}{\partial x_i} \kappa_j^\Lambda \\ &+ h_\lambda^2 \tau_i^\Lambda \frac{\partial f_\lambda}{\partial t} - h_\lambda \gamma_i^\Lambda A_\lambda \frac{\partial q_\lambda}{\partial t} \quad \text{and} \end{aligned}$$

$$\begin{aligned}
\tilde{a}_{L,i} &= x_{l,0} + \sum_{j=1}^{i-1} \sigma_{ij}^L \kappa_j^L, & \tilde{d}_{L,i} &= x_{a,0} + m \cdot \sum_{j=1}^{i-1} \varrho_{ij}^L \kappa_j^A, \\
\tilde{a}_{A,i} &= x_{l,0} + m^{-1} \cdot \sum_{j=1}^{i-1} \varrho_{ij}^A \kappa_j^L, & \tilde{d}_{A,i} &= x_{a,0} + \sum_{j=1}^{i-1} \sigma_{ij}^A \kappa_j^A, \\
\alpha_i^\Lambda &= \sum_{j=1}^{i-1} \alpha_{ij}^\Lambda, & \gamma_i^\Lambda &= \sum_{j=1}^{i-1} \gamma_{ij}^\Lambda, & \tau_i^\Lambda &= \sum_{j=1}^{i-1} \beta_{ij}^\Lambda \gamma_{ij}^\Lambda, & m &= h_l/h_{a,1}.
\end{aligned}$$

• *later micro steps*

$$x_{a,\mu} = x_{a,\mu-1} + \sum_{i=1}^{s_C} d_i^C \cdot \kappa_i^C \quad (\mu = 2, \dots, r),$$

with increments κ_i^C given by

$$\begin{aligned}
(A_a \frac{\partial q_a}{\partial x_a} - h_{a,\mu} \gamma^C \frac{\partial f_a}{\partial x_a}) \kappa_i^C &= A_a (q_a(x_{a,\mu-1}, t_{0,\mu}) - q_a(\tilde{a}_{C,i}, t_{0,\mu} + \alpha_i^C \cdot h_{a,\mu})) \\
&+ h_{a,\mu} \sum_{j=1}^i \beta_{ij}^C f_a(x_l^{\text{ds}}(\mu, j), \tilde{a}_{C,j}, t_{0,\mu} + \alpha_i^C \cdot h_{a,\mu}) + h_{a,\mu} \sum_{j=1}^{i-1} \beta_{ij}^C \frac{\partial f_a}{\partial x_a} \kappa_j^C \\
&+ h_{a,\mu}^2 \tau_i^C \frac{\partial f_a}{\partial t} - h_{a,\mu} \gamma_i^C A_a \frac{\partial q_a}{\partial t} \quad \text{and} \\
\tilde{a}_{C,i} &= x_{a,\mu-1} + \sum_{j=1}^{i-1} \sigma_{ij}^C \kappa_j^C \quad \left| \quad x_l^{\text{ds}}(\mu, \nu) \text{ defined as in (9d)} \right. \\
t_{0,\mu} &= t_0 + \sum_{i=1}^{\mu-1} h_{a,\mu} \quad \left| \quad \text{with } d_i^L(\theta) = d_{i1}^L \theta^2 + d_{i2}^L \theta \right. \\
\alpha_i^C &= \sum_{j=1}^{i-1} \alpha_{ij}^C, \quad \gamma_i^C = \sum_{j=1}^{i-1} \gamma_{ij}^C, \quad \tau_i^C = \sum_{j=1}^{i-1} \beta_{ij}^C \gamma_{ij}^C
\end{aligned}$$

A.2 Coefficients (zero, if not stated)

compound step

$$\begin{aligned}
\gamma^\Lambda &= \gamma_1^\Lambda = \gamma_2^\Lambda = 0.2928932188135 & \gamma_3^\Lambda &= 1.2692039481916 \\
d_1^\Lambda &= 3.1761423749154 & d_2^\Lambda &= 4.6765488185427 & d_3^\Lambda &= -1.0242640687119 & d_4^\Lambda &= 1 \\
\hat{d}_1^\Lambda &= 3.1761423749154 & \hat{d}_2^\Lambda &= 4.6765488185427 & \hat{d}_3^\Lambda &= -1.0242640687119 \\
\beta_{11}^\Lambda &= \beta_{22}^\Lambda = \beta_{33}^\Lambda = \beta_{44}^\Lambda = \gamma^\Lambda \\
\beta_{21}^\Lambda &= 0.5857864376269 \\
\beta_{31}^\Lambda &= 1.6271845489636 & \beta_{32}^\Lambda &= 0.3254369097927 \\
\beta_{41}^\Lambda &= 0.2121320343560 & \beta_{42}^\Lambda &= 0.7071067811866 & \beta_{43}^\Lambda &= -0.2121320343560 \\
\sigma_{21}^\Lambda &= 2.0 \\
\sigma_{31}^\Lambda &= 2.2761423749154 & \sigma_{32}^\Lambda &= 1.0571909584179 \\
\sigma_{41}^\Lambda &= 3.1761423749154 & \sigma_{42}^\Lambda &= 4.6765488185427 & \sigma_{43}^\Lambda &= -1.0242640687119 \\
\varrho_{21}^L &= 2.0 \\
\varrho_{31}^L &= 17.8858627082946 + 2.1011418665042 \cdot m & \varrho_{32}^L &= -14.5525293749612 - 2.1011418665042 \cdot m \\
\varrho_{41}^L &= 18.5225484931711 - 1.794800932260 \cdot m & \varrho_{42}^L &= -7.5313796686280 + 1.7948009322599 \cdot m \\
\varrho_{43}^L &= -1.7485281374239 \\
\varrho_{21}^A &= 2.0 \\
\varrho_{31}^A &= 17.8858627082946 + 2.1011418665042/m & \varrho_{32}^A &= -14.5525293749612 - 2.1011418665042/m \\
\varrho_{41}^A &= 18.5225484931711 - 1.794800932260/m & \varrho_{42}^A &= -7.5313796686280 + 1.7948009322599/m
\end{aligned}$$

$$\begin{aligned}
\varrho_{43}^A &= -1.7485281374239 \\
\alpha_2^A &= 0.5857864376269 & \alpha_3^A &= 0.9763107293782 & \alpha_4^A &= 1.0 \\
\tau_1^A &= 0.0857864376269 & \tau_2^A &= 0.2573593128807 & \tau_3^A &= 0.9436508138960
\end{aligned}$$

later micro steps (CHORAL)

$$\begin{aligned}
\gamma^C &= 0.5728160624821 & \beta_{21}^C &= -2.0302139317498 \\
d_1^C &= \hat{d}_1^C = \sigma_{21}^C = \sigma_{31}^C = \sigma_{41}^C = 1/\gamma^C & \beta_{31}^C &= 0.2707896390840 \\
d_2^C &= \hat{d}_2^C = \sigma_{32}^C = \sigma_{42}^C = 0.0 & \beta_{32}^C &= 0.1563942984339 \\
d_3^C &= \hat{d}_3^C = \sigma_{43}^C = 1.0 & \beta_{41}^C &= 2/3 \\
d_4^C &= 1.0 & \beta_{42}^C &= 0.08757666432972 \\
\alpha_2^C &= \alpha_3^C = \alpha_4^C = 1.0 & \beta_{43}^C &= -0.3270593934785 \\
\tau_1^C &= 0.3281182414375 & \gamma_1^C &= \gamma^C \\
\tau_2^C &= -2.5705761218072 & \gamma_2^C &= -2.457397870 \\
\tau_3^C &= -0.2292103609160 & \sigma_2^C &= \sigma_3^C = 1/\gamma^C \\
\tau_4^C &= 1/6 & \sigma_4^C &= 1 + 1/\gamma^C
\end{aligned}$$

dense output

$$\begin{aligned}
d_{11}^L &= -2.9142135623731 & d_{12}^L &= 6.090355937288 \\
d_{21}^L &= 2.914213562373 & d_{22}^L &= 1.7623352561696 \\
d_{32}^L &= -1.0242640687119
\end{aligned}$$

A.3 Error control and step size prediction

As proposed in [4] and applied in [3] we use the following error estimation $[(\lambda, \Lambda) \in \{(l, L), (a, A)\}]$:

$$\begin{aligned}
\text{err}_\Lambda &= (A_\lambda \frac{\partial q_\lambda}{\partial x_\lambda} - h_\lambda \gamma^\Lambda \frac{\partial f_\lambda}{\partial x_l})^{-1} (x_{\lambda,1} - \hat{x}_{\lambda,1}) \\
&\quad \text{with } \hat{x}_{\lambda,1} = x_{\lambda,0} + \sum_{i=1}^{\hat{s}} \hat{d}_i^\Lambda \kappa_i^\Lambda \quad \text{and } h_a = h_{a,1} \\
\text{err}_C &= (A_a \frac{\partial q_a}{\partial x_a} - h_{a,\mu} \gamma^\Lambda \frac{\partial f_a}{\partial x_a})^{-1} (x_{a,\mu} - \hat{x}_{a,\mu}) \\
&\quad \text{with } \hat{x}_{a,\mu} = x_{a,\mu-1} + \sum_{j=1}^{\hat{s}} \hat{d}_j^C \kappa_j^C \quad \text{and } \mu = 2, 3, \dots
\end{aligned}$$

Further on we apply the *standard step size prediction* ([4, IV.8]) with safety factors $\text{fac} = 0.8$, $\text{facmax} = 5$, $\text{facmin} = 0.2$ and the tolerances $\text{atol} = \text{rtol} = 10^{-4}$.

The most significant point is, that the error estimation and stepsize control is based directly on the relevant values, the node potentials x_l, x_a and not has to be derived from the charges z_l, z_a .