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Order conditions for the semi-Lagrangian exponential integrators

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1 Introduction

Semi-Lagragian methods have been shown [1, 4, 2] to play an important role in the computation of flows of vector fields in exponential integrators designed for convection dominated problems of the convection-diffusion type. In this paper we examine some of the issues regarding the order conditions for the semi-Lagrangian exponential integrators, starting with a preliminary work by the authors in [2].

Suppose from the semi-discretization of a convection-diffusion model one obtains an ordinary differential equation (with initial data y_0) of the form

$$y_t = C(y)y + Ay, \quad y(0) = y_0, \tag{1.1}$$

with $y = y(t) \in \mathbb{R}^N$ for $t \in [0, T]$. The $N \times N$ matrices $C(y)$and A represents the discrete convection and linear diffusion operators respectively.

The methods then take the following general format

$$\begin{aligned}
&\text{for } i = 1 : s \text{ do}\\
&\quad Y_i = \varphi_i y_n + h \sum_j a_{i,j} \varphi_{i,j} A Y_j,\\
&\quad \varphi_i = \exp(h \sum_k \alpha_{i,J}^k C(Y_k)) \ldots \exp(h \sum_k \alpha_{i,1}^k C(Y_k)),\\
&\quad \varphi_{i,j} = \varphi_i \varphi_j^{-1}\\
&\text{end}\\
&y_{n+1} = \varphi_{n+1} y_n + h \sum_i b_i \varphi_{n+1,i} A Y_i,\\
&\varphi_{n+1} = \exp(h \sum_k \beta_J^k C(Y_k)) \ldots \exp(h \sum_k \beta_1^k C(Y_k)),\\
&\varphi_{n+1,i} = \varphi_{n+1} \varphi_i^{-1},
\end{aligned}$$

where $\{a_{i,j}, b_i\}$ are coefficients of a $s-$stage Runge-Kutta (RK) method and $\alpha_{i,l}^j$ and β_l^j are coefficients of a commuatator-free (CF) Lie group method (studied in [3, 6]) defined on a RK method with coefficients $\{\hat{a}_{i,j}, \hat{b}_i\}$ such that

$$\hat{a}_{i,j} = \sum_{l=1}^{J} \alpha_{i,l}^j, \quad \hat{b}_i = \sum_{l=1}^{J} \beta_l^j. \tag{1.2}$$

Thus given a partition RK method with Butcher tableaus

$$\begin{array}{c|c} \mathbf{c} & \mathcal{A} \\ \hline & \mathbf{b} \end{array}, \qquad \begin{array}{c|c} \hat{\mathbf{c}} & \hat{\mathcal{A}} \\ \hline & \hat{\mathbf{b}} \end{array}, \tag{1.3}$$

we treat the diffusion with the $s-$stage RK method $\{\mathcal{A}, \mathbf{b}, \mathbf{c}\}$ (preferably implicit) and the convection with a CF method based on the RK $\{\hat{\mathcal{A}}, \hat{\mathbf{b}}, \hat{\mathbf{c}}\}$.

Note: Here and in the rest of the literature, we shall write $\sum_j$ (without explicit limits of summation) to actually mean $\sum_{j=1}^{s}$. All tables have been put in the appendix.

In the study of the under conditions we treat (for the sake of convenience) the numerical solution y_{n+1} as an extra state value

$$Y_{s+1} = \varphi_{s+1} y_n + h \sum_j a_j \varphi_{s+1,j} A Y_j, \quad a_{s+1,j} = b_j,$$

with

$$\varphi_{s+1} = \exp(h \sum_k \alpha_{s+1,J}^k C(Y_k)) \dots \exp(h \sum_k \alpha_{s+1,1}^k C(Y_k)), \quad \alpha_{s+1,l}^k = \beta_l^k$$

and $\varphi_{s+1,j} = \varphi_{s+1} \varphi_j^{-1}$.

2 Deriving the order conditions

Taking the q^{th} derivatives with respect to h of the exact solution to (1.1) and of the stage values of the numerical solution we obtain the recursive formulas

$$y^{(q)} = \sum_{k=0}^{q-1} \binom{q-1}{k} \frac{d^{q-1-k}}{dh^{q-1-k}} \left(C(y) + A\right) y^{(k)}, \tag{2.1}$$

$$Y_i^{(q)} = \varphi_i^{(q)} y_0 + q \sum_j a_{i,j} \sum_{k=0}^{q-1} \binom{q-1}{k} \varphi_{i,j}^{(q-1-k)} A Y_j^{(k)}. \tag{2.2}$$

Order conditions for order $p = 1, 2, 3, \dots$ are recursively from the equations

$$Y_{s+1}^{(q)}|_{h=0} = y^{(q)}|_{h=0}, \quad q = 0, 1, \dots, p. \tag{2.3}$$

We often will simplify higher order conditions using conditions of lower order whenever neccessary. The computation of the derivatives of Y_i requires the use of φ_i and $\varphi_{i,j}$ and their derivatives.

Now let us consider the matrix-valued functions,

$$C_{i,J-l} := h \sum_k \alpha_{i,J-l}^k C(Y_k), \quad l = 0, 1, \dots, J-1,$$

and

$$\tilde{C}_{i,J-l} := -h \sum_k \alpha_{i,l+1}^k C(Y_k), \quad l = 0, 1, \dots, J-1$$

We donote by $B_{i,J-l}$ either of $C_{i,J-l}$ or $\tilde{C}_{i,J-l}$, for $l = 0, 1, \dots, J-1$, and consider

$$\psi_i(h) := \exp(B_{i,J}) \cdot \exp(B_{i,J-1}) \cdot \dots \cdot \exp(B_{i,1}).$$

Depending on the choice of $B_{i,J-l} = C_{i,J-l}$ or $\tilde{C}_{i,J-l}$, we have $\psi_i = \varphi_i$ or φ_i^{-1}, respectively. We will also make use of

$$\varphi_i^l(h) := \exp(B_{i,J}) \cdot \exp(B_{i,J-1}) \cdot \ldots \cdot \exp(B_{i,J-l}).$$

We obtain[1]

$$\dot{\psi}_i = \sum_{l=0}^{J-1} \mathrm{Ad}_{\psi_i^l} \left(\mathrm{dexp}_{B_{i,J-l}}(\dot{B}_{i,J-l}) \right) \cdot \psi_i.$$

So we can write

$$\dot{\psi}_i = S_i(h)\psi_i \text{ with } S_i(h) := \sum_{l=0}^{J-1} \mathrm{Ad}_{\psi_i^l} \left(\mathrm{dexp}_{B_{i,J-l}}(\dot{B}_{i,J-l}) \right),$$

and as a direct consequence we have

$$\psi_i^{(r)} = \sum_{k=0}^{r-1} \binom{r-1}{k} \left(\frac{d^{r-1-k}}{dh^{r-1-k}} S_i(h) \right) \psi_i^{(k)}. \tag{2.4}$$

Now we have the following proposition for finding the derivatives of $S_i(h)$:

Proposition 2.1. *Given that $Z^0 = Z^0(h)$ and $W = W(h)$ are two matrix-valued differentiable functions then*

$$\frac{d^r}{dh^r} Ad_W Z^0 = Ad_W Z^r, \tag{2.5}$$

with

$$Z^r = [W^{-1}\dot{W}, Z^{r-1}] + \dot{Z}^{r-1}. \tag{2.6}$$

The proof is by induction.

By differentiating from (2.6) we obtain

$$\dot{Z}^r = [\dot{W}^{-1}\dot{W} + W^{-1}\ddot{W}, Z^{r-1}] + [W^{-1}\dot{W}, \dot{Z}^{r-1}] + \ddot{Z}^{r-1}, \tag{2.7}$$

and using (2.6) and (2.7), assuming $W(0) = I$, we obtain

$$\begin{cases} \frac{d}{dh}\mathrm{Ad}_W Z^0|_{h=0} &= Z^1(0) &= [\dot{W}(0), Z^0(0)] + \dot{Z}^0(0) \\ & \dot{Z}^1(0) &= [-\dot{W}(0)^2 + \ddot{W}(0), Z^0(0)] + [\dot{W}(0), \dot{Z}^0(0)] + \ddot{Z}^0(0) \\ \frac{d^2}{dh^2}\mathrm{Ad}_W Z^0|_{h=0} &= Z^2(0) &= [\dot{W}(0), Z^1(0)] + \dot{Z}^1(0) \\ & \dot{Z}^2(0) &= [-\dot{W}(0)^2 + \ddot{W}(0), Z^1(0)] + [\dot{W}(0), \dot{Z}^1(0)] + \ddot{Z}^1(0) \\ \frac{d^3}{dh^3}\mathrm{Ad}_W Z^0|_{h=0} &= Z^3(0) &= [\dot{W}(0), Z^2(0)] + \dot{Z}^2(0) \\ \vdots \end{cases} \tag{2.8}$$

[1]We recall that $\mathrm{dexp}_w(u) := \frac{e^z - 1}{z}\Big|_{z=\mathrm{ad}_w} (u) = u + 1/2![w,u] + 1/3![w,[w,u]] + \ldots,\ \mathrm{ad}_w(u) := [w,u]$ (matrix commutator of w and u) and $\mathrm{Ad}_\psi(u) := \psi u \psi^{-1}$.

Further assuming that $Z^0 = \mathrm{dexp}_{-B}(\dot{B})$ for some matrix-valued function $B = B(h)$, expanding the right-hand side and diffferentiating we obtain

$$\begin{cases} Z^0(0) = \dot{B}(0) \\ \dot{Z}^0(0) = \ddot{B}(0) \\ \ddot{Z}^0(0) = \dddot{B}(0) - \frac{1}{2}[\dot{B}(0), [\dot{B}(0), \ddot{B}(0)]] \\ \dddot{Z}^0(0) = B^{iv}(0) - [\dot{B}(0), \dddot{B}(0)] + \frac{1}{2}[\dot{B}(0), \ddot{B}(0)] \\ \vdots \end{cases} \tag{2.9}$$

We can now obtain derivatives of S_i and ψ_i. By setting $W = \psi_i^l$ and $B = B_i^{J-l}$ we can calculate the derivatives of S_i using the steps in (2.5)-(2.9). We obtain

$$\begin{cases} S_i(0) = \sum_{l=0}^{J-1} \dot{B}_i^{J-l}(0), \\ \left.\frac{dS_i}{dh}\right|_{h=0} = \sum_{l=0}^{J-1}\sum_{r=0}^{J-l-1} ([\dot{B}_i^{J-r}(0), \dot{B}_i^{J-l}(0)] + \ddot{B}_i^{J-l}(0)), \\ \left.\frac{d^2S_i}{dh^2}\right|_{h=0} = 2\sum_{l=0}^{J-1}\sum_{r=0}^{J-l-1} [\dot{B}_i^{J-r}(0), \ddot{B}_i^{J-l}(0)] + \sum_{l=0}^{J-1}\sum_{r=0}^{J-l-1} [\ddot{B}_i^{J-r}(0), \dot{B}_i^{J-l}(0)] + \\ \quad + \sum_{l=0}^{J-1} (\dddot{B}_i^{J-r}(0) - \frac{1}{2}[\dot{B}_i^{J-l}(0), \ddot{B}_i^{J-l}(0)]), \\ \vdots \end{cases} \tag{2.10}$$

Analogously the derivatives of $S_i^l := \sum_{r=0}^{J-l-1} \mathrm{Ad}_{\psi_i^r}\left(\mathrm{dexp}_{B_{i,J-r}}(\dot{B}_{i,J-r})\right)$ are obtained as in the forgoing formulae but substituting $J-1$ as upper index in the external summation with $J-l-1$. In table 1 we report the values of the derivatives of φ_i and φ_j^{-1} at $h=0$, which are obtained from (2.4) and (2.10) by recursion, starting with $\psi_i(0) = I$. In table 2 we report the values of the derivatives of $\varphi_{i,j}$ at $h=0$, which are obtained using table 1 and the formula

$$\varphi_{i,j}^{(m)} = \sum_{r=0}^{m} \binom{m}{r} \varphi_i^{(m-r)} (\varphi_j^{-1})^{(r)}. \tag{2.11}$$

The derivatives of Y_i, reported in table 3, are obtained using the results in tables 1 and 2, and the recursion formula (2.2), starting with $Y_i(0) = y_0$.

3 Order conditions for orders $1-3$

We now present a detailed analysis for deriving the third order conditions.

From (2.4) we obtain that

$$\dot{\varphi}_i(0) = \sum_{l=0}^{J-1} \dot{B}_{i,J-l}(0) = \sum_{l=0}^{J-1} \dot{C}_{i,J-l}(0) \sum_{l=0}^{J-1}\sum_{k} \alpha_{i,J-l}^k C = (\sum_k \hat{a}_{i,k})C. \tag{3.1}$$

Analogously one computes $\dot{\varphi}_j^{-1}(0)$. These expressions are reported in table 1 and can be used to obtain

Table 1: Derivatives of φ_i and its inverse at $h=0$.

q	$\varphi_i^{(q)}(0)$
0	I
1	$C\hat{c}_i$
2	$2\sum_k \hat{a}_{i,k}C'(\hat{c}_k C y_0 + c_k A y_0) + \hat{c}_i^2 C^2$
3	$4\sum_{l=0}^{J-1}\sum_{r=0}^{J-1-l}\sum_k \alpha_{i,J-r}^k \sum_m \alpha_{i,J-l}^m [C, C'(\hat{c}_m C + c_m A)]+$ $2\sum_{l=0}^{J-1}\sum_{r=0}^{J-1-l}\sum_k \alpha_{i,J-r}^k \sum_m \alpha_{i,J-l}^m [C'(\hat{c}_k C + c_k A), C]+$ $-\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \sum_m \alpha_{i,J-l}^m [C, C'(\hat{c}_m C + c_m A)]+$ $3\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k C''(\hat{c}_k C + c_k A, \hat{c}_k C + c_k A)+$ $6\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \sum_j \hat{a}_{k,j} C'(C'(\hat{c}_j C + c_j A))+$ $3\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \hat{c}_k^2 C'(C"2)+$ $6\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k (\hat{c}_k c_k - \sum_j a_{k,j}\hat{c}_j) C'(CA)+$ $6\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \sum_j a_{k,j} C'(A(\hat{c}_j C + c_j A))+$ $4\hat{c}_i \sum_k a_{i,k}(C'(\hat{c}_k C + c_k A))C + 2\hat{c}_i \sum_k a_{i,k} C(C'(\hat{c}_k C + c_k A)) + \hat{c}_i^3 C^3$
q	$(\varphi_j^{-1})^{(q)}(0)$
0	I
1	$-C\hat{c}_j$
2	$-2\sum_k \hat{a}_{j,k}C'(\hat{c}_k C y_0 + c_k A y_0) + \hat{c}_j^2 C^2$
3	$4\sum_{l=0}^{J-1}\sum_{r=0}^{J-l-1}\sum_k \alpha_{j,r+1}^k \sum_m \alpha_{i,r+1}^m [C, C'(\hat{c}_m C + c_m A)]+$ $2\sum_{l=0}^{J-1}\sum_{r=0}^{J-l-1}\sum_k \alpha_{j,r+1}^k \sum_m \alpha_{i,r+1}^m [C'(\hat{c}_k C + c_k A), C]+$ $-\sum_{l=0}^{J-1}\sum_k \alpha_{j,l+1}^k \sum_r \alpha_{j,l+1}^r [C, C'(\hat{c}_r C + c_r A)]+$ $-3\sum_{l=0}^{J-1}\sum_k \alpha_{j,l+1}^k C''(\hat{c}_k C + c_k A, \hat{c}_k C + c_k A)+$ $-6\sum_{l=0}^{J-1}\sum_k \alpha_{j,l+1}^k \sum_j \hat{a}_{k,j} C'(C'(\hat{c}_j C + c_j A))+$ $-3\sum_{l=0}^{J-1}\sum_k \alpha_{j,l+1}^k \hat{c}_k^2 C'(C"2)+$ $-6\sum_{l=0}^{J-1}\sum_k \alpha_{j,l+1}^k (\hat{c}_k c_k - \sum_j a_{k,j}\hat{c}_j) C'(CA)+$ $-6\sum_{l=0}^{J-1}\sum_k \alpha_{i,l+1}^k \sum_r a_{k,r} C'(A(\hat{c}_r C + c_r A))+$ $4\hat{c}_j \sum_k a_{i,k}(C'(\hat{c}_k C + c_k A))C + 2\hat{c}_j \sum_k a_{j,k} C(C'(\hat{c}_k C + c_k A)) + \hat{c}_j^3 C^3$

$$\dot{Y}_i|_{h=0} = (\sum_k \hat{a}_{i,k})Cy_0 + (\sum_k a_{i,k})Ay_0 = \hat{c}_i C y_0 + c_i A y_0, \tag{3.2}$$

see table 3. Also from (2.1) we obtain

$$\dot{y}(0) = Cy_0 + Ay_0. \tag{3.3}$$

Imposing $\dot{Y}_{s+1}|_{h=0} = \dot{y}(0)$ we obtain the following order conditions for order 1,

$$\sum_k \hat{a}_{s+1,k} = 1, \sum_k a_{s+1,k} = 1.$$

These correspond to requiring that the two RK methods (1.3) are consistent.

For order 2 from (2.2) we have that

$$\ddot{Y}_i|_{h=0} = \varphi_i^{(2)}|_{h=0} y_0 + 2\sum_j a_{i,j}\left(\varphi_{i,j}^{(1)}(0) + \varphi_{i,j}(0)A\dot{Y}_j(0)\right)$$

Table 2: Derivatives of $\varphi_{i,j}$ at $h=0$.

q	$\varphi_{i,j}^{(q)}(0)$
0	I
1	$(\hat{c}_i - \hat{c}_j)C$
2	$2\sum_k(\hat{a}_{i,k} - \hat{a}_{j,k})C'(\hat{c}_k C + c_k A) + (\hat{c}_i - \hat{c}_j)^2 C^2$
3	$4\sum_{l=0}^{J-1}\sum_{r=0}^{J-l-1}(\sum_k \alpha_{i,J-r}^k \sum_m \alpha_{i,J-l}^m - \sum_k \alpha_{i,r+1}^k \sum_m \alpha_{i,l+1}^m)[C, C'(\hat{c}_m C + c_m A)]+$ $2\sum_{l=0}^{J-1}\sum_{r=0}^{J-l-1}(\sum_k \alpha_{i,J-r}^k \sum_m \alpha_{i,J-l}^m - \sum_k \alpha_{i,r+1}^k \sum_m \alpha_{i,l+1}^m)[C'(\hat{c}_k C + c_k A), C]+$ $-\sum_{l=0}^{J-1}(\sum_k \alpha_{i,J-l}^k \sum_m \alpha_{i,J-l}^m - \sum_k \alpha_{i,l+1}^k \sum_m \alpha_{i,l+1}^m)[C, C'(\hat{c}_m C + c_m A)]+$ $3\sum_k(\hat{a}_{i,k} - \hat{a}_{j,k})C''(\hat{c}_k C + c_k A, \hat{c}_k C + c_k A)+$ $6\sum_k(\hat{a}_{i,k}\sum_m \hat{a}_{k,m} - \hat{a}_{j,k}\sum_m \hat{a}_{k,m})C'(C'(\hat{c}_m C + c_m A))+$ $3\sum_k(\hat{a}_{i,k} - \hat{a}_{j,k})\hat{c}_k^2 C'(C^2)+$ $6\sum_k(\hat{a}_{i,k} - \hat{a}_{j,k})\sum_m a_{k,m}C'(A(\hat{c}_m C + c_m A))+$ $4\sum_k(\hat{c}_i\hat{a}_{i,k} + \hat{c}_j\hat{a}_{j,k})C'(\hat{c}_k C + c_k A)C + 2\sum_k(\hat{c}_i\hat{a}_{i,k} + \hat{c}_j\hat{a}_{j,k})CC'(\hat{c}_k C + c_k A)+$ $(\hat{c}_i^3 - \hat{c}_j^3)C^3 + 3(\hat{c}_i\hat{c}_j^2 - \hat{c}_j\hat{c}_i^2)C^3 - 6\hat{c}_j\sum_k \hat{a}_{i,k}C'(\hat{c}_k C + c_k A)C+$ $-6\hat{c}_i\sum_k \hat{a}_{j,k}CC'(\hat{c}_k C + c_k A)$

with $\varphi_{i,j}(0) = I$ and $\varphi_{i,j}^{(1)}(0) = \dot{\varphi}_i(0) - \dot{\varphi}_j(0) = (\hat{c}_i - \hat{c}_j)C$. Using $\dot{Y}_j(0)$ from table 3 we obtain

$$\ddot{Y}_i|_{h=0} = \varphi_i^{(2)}|_{h=0}y_0 + 2\sum_j a_{i,j}((\hat{c}_i - \hat{c}_j)CAy_0 + \hat{c}_j ACy_0 + c_j A^2 y_0). \tag{3.4}$$

From (2.4) and (2.10) we obtain

$$\begin{aligned}\varphi_i^{(2)}|_{h=0} &= \frac{dS_i(h)}{dh}\varphi_i(h)|_{h=0} + (S_i(h)^2\varphi_i(h))|_{h=0} \\ &= 2\sum_k \hat{a}_{i,k}\hat{c}_k C'(Cy_0) + 2\sum_k \hat{a}_{i,k}c_k C'(Ay_0) + (\sum_j \hat{a}_{i,j})^2 C^2,\end{aligned} \tag{3.5}$$

reported in table 1. Substituting the results in (3.4) we obtain

$$\begin{aligned}\ddot{Y}_i|_{h=0} &= (2\sum_k \hat{a}_{i,k}\hat{c}_k C'(Cy_0) + 2\sum_k \hat{a}_{i,k}c_k C'(Ay_0) + c_i^2 C^2)y_0 + \\ &\quad 2\sum_j a_{i,j}((\hat{c}_i - \hat{c}_j)CAy_0 + \hat{c}_j ACy_0 + c_j A^2 y_0,\end{aligned} \tag{3.6}$$

reported in table 3. Using (2.1) and substituting for $\dot{y}(0)$ from (3.3) we obtain

$$y^{(2)}|_{h=0} = C'(\dot{y}(0))y_0 + (C+A)^2 y_0 = C'((C+A)y_0)y_0 + (C+A)^2 y_0, \tag{3.7}$$

where $C'(y)(w)$ is obtained by differentiating $C(y)$ such that

$$(C'(y)(w))_{i,j} := \sum_{k=1}^N \frac{\partial c_{i,j}}{\partial y^k}(y)w_k, \quad c_{i,j} = (C(y))_{i,j}, \quad y = [y^1, \ldots, y^N]^T.$$

Taking $i = s+1$ and matching coefficients in $\ddot{Y}_i|_{h=0}$ and $y^{(2)}|_{h=0}$ we obtain the four order conditions for order 2,

$$\sum_j \hat{a}_{s+1,j}\hat{c}_j, \quad \sum_j a_{s+1,j}c_j,$$
$$\sum_j a_{s+1,j}\hat{c}_j, \quad \sum_j \hat{a}_{s+1,j}c_j.$$

Table 3: Derivatives of Y_i at $h = 0$.

q	$Y_i^{(q)}(0)$
0	y_0
1	$(\sum_j \hat{a}_{i,j})Cy_0 + (\sum_j a_{i,j})Ay_0$
2	$2\sum_j \hat{a}_{i,j}C'(\hat{c}_jC + c_jA)y_0 + \hat{c}_i^2C^2y_0 + 2\hat{c}_ic_iCAy_0 - 2(\sum_j a_{i,j}\hat{c}_j)CAy_0 + 2\sum_j a_{i,j}A(\hat{c}_jC + c_jA)y_0$
3	$4\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k \alpha_{i,J-r}^k \sum_m \alpha_{i,J-l}^m[C, C'(\hat{c}_mC + c_mA)]y_0+$ $2\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k \alpha_{i,J-r}^k \sum_m \alpha_{i,J-l}^m[C'(\hat{c}_kC + c_kA), C]y_0+$ $-\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \sum_r \alpha_{i,J-l}^r[C, C'(\hat{c}_rC + c_rA)]y_0+$ $3\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k C''(\hat{c}_kC + c_kA, \hat{c}_kC + c_kA)y_0+$ $6\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \sum_j \hat{a}_{k,j}C'(C'(\hat{c}_jC + c_jA))y_0+$ $3\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \hat{c}_k^2C'(C"2)y_0+$ $6\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k(\hat{c}_kc_k - \sum_j a_{k,j}\hat{c}_j)C'(CA)y_0+$ $6\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \sum_j a_{k,j}C'(A(\hat{c}_jC + c_jA))y_0+$ $4\hat{c}_i\sum_k a_{i,k}(C'(\hat{c}_kC + c_kA))Cy_0 + 2\hat{c}_i\sum_k a_{i,k}C(C'(\hat{c}_kC + c_kA))y_0 + \hat{c}_i^3C^3y_0$ $6\sum_k \hat{a}_{i,k}(\sum_j a_{i,j})C'(\hat{c}_kC + c_kA)Ay_0 + 3(\sum_k \hat{a}_{i,k})^2(\sum_j a_{i,j})C^2Ay_0+$ $6\sum_k \hat{a}_{i,k})(-\sum_j a_{i,j}\hat{c}_jC^2Ay_0 + \sum_j a_{i,j}CA(\hat{c}_jC + c_jA)y_0+$ $3\sum_j a_{i,j}\hat{c}_j^2C^2Ay_0 - 6\sum_j a_{i,j}\sum_k \hat{a}_{j,k}C'(\hat{c}_kC + c_kA)Ay_0 - 6\sum_j a_{i,j}\hat{c}_jCA(\hat{c}_jC + c_jA)y_0+$ $6\sum_j a_{i,j}\sum_m \hat{a}_{j,m}AC'(\hat{c}_mC + c_mA)y_0 + 3\sum_j a_{i,j}\hat{c}_j^2AC^2y_0+$ $6\sum_j a_{i,j}(\hat{c}_jc_j - \sum_m a_{j,m}\hat{c}_m)ACAy_0 + 6\sum_j a_{i,j}\sum_m a_{j,m}A^2(\hat{c}_mC + c_mA)y_0$

Note: The matrix-valued function $C = C(y)$ and it's derivatives are linear with respect to y.

For order 3 we proceed as follows:
First from (2.1) we have

$$\begin{aligned} y^{(3)}\|_{h=0} &= C''(y_0)(\dot{y}(0), \dot{y}(0))y_0+ \\ &\quad C'(y_0)(\ddot{y}(0))y_0 + 2C'(y_0)(\dot{y}(0))(C(y_0) + A)y_0+ \\ &\quad (C(y_0) + A)C'(y_0)(\dot{y}(0))y_0 + (C(y_0) + A)^3y_0, \end{aligned} \tag{3.8}$$

where we have used $C''(y)(w, z)$ obtained by differentiating $C(y)$ such that

$$(C''(y))(w, z))_{i,j} := \sum_{k=1}^{N}\sum_{m=1}^{N} \frac{\partial^2 c_{i,j}}{\partial y^k \partial y^m}(y)w_kz_m, \quad c_{i,j} = (C(y))_{i,j}.$$

In short we will write C, C', $C'', \dots$ for $C(y_0)$, $C'(y_0)$, $C''(y_0), \dots$ respectively. Substituting for $\dot{y}(0)$ and $\ddot{y}(0)$ from (3.3) and (3.7) respeclively, we obtain

$$\begin{aligned} y^{(3)}\|_{h=0} \quad = \quad & C''((C + A)y_0, (C + A)y_0)y_0 + C'(C'((C + A)y_0)y_0 + (C + A)^2y_0)y_0+ \\ & 2C'((C + A)y_0)(C + A)y_0 + (C + A)C'((C + A)y_0)y_0 + (C + A)^3y_0. \end{aligned} \tag{3.9}$$

We now consider the third derivative of the numerical solution. From (2.2) we obtain

$$\begin{aligned} Y_i^{(3)}\Big|_{h=0} &= \varphi_i^{(3)}\Big|_{h=0} y_0 + 3\sum_j a_{i,j}\, \varphi_i^{(2)}\Big|_{h=0} Ay_0+ \\ &\quad 6\sum_j a_{i,j}\, \varphi_i^{(1)}\Big|_{h=0} A\dot{Y}_j\|_{h=0} + 3\sum_j a_{i,j}A\, \ddot{Y}_j\Big|_{h=0}. \end{aligned} \tag{3.10}$$

We need to find $\varphi_i^{(3)}|_{h=0}$ via (2.4) using the expressions for $\varphi_i^{(2)}|_{h=0}$ and $\varphi_i^{(1)}|_{h=0}$ which have already been found and reported in table 1. Using earlier row entries of table 1 and (2.11) we also compute $\varphi_{i,j}^{(2)} = \varphi_i(0) + 2\ddot{\varphi}_i(0)\dot{\varphi}_j^{-1}(0) + \ddot{\varphi}_j^{-1}(0)$, reported in table 2.

From (2.4) it follows that

$$\left.\varphi_i^{(3)}\right|_{h=0} = \left.\frac{d^2 S_i}{dh^2}\right|_{h=0} + 2\left.\frac{dS_i}{dh}\right|_{h=0}\left.\varphi_i^{(1)}\right|_{h=0} + S_i|_{h=0}\left.\varphi_i^{(2)}\right|_{h=0}. \tag{3.11}$$

We obtain

$$\begin{aligned}\left.\varphi_i^{(3)}\right|_{h=0} &= \left.\frac{d^2 S_i}{dh^2}\right|_{h=0} + \\ &2(2\sum_k \hat{a}_{i,k}\hat{c}_k C'(Cy_0) + 2\sum_k \hat{a}_{i,k}c_k C'(Ay_0))\sum_k \hat{a}_{i,k}C \quad + \\ &2\sum_k \hat{a}_{i,k}C(\sum_k \hat{a}_{i,k}\hat{c}_k C'(Cy_0) + \sum_k \hat{a}_{i,k}c_k C'(Ay_0)) + \sum_k \hat{a}_{i,k}C(\sum_j \hat{a}_{i,j})^2 C^2.\end{aligned} \tag{3.12}$$

We have

$$\begin{aligned}\dot{C}_{i,J-l}(0) &= \sum_k \alpha_{i,J-l}^k C, \\ \ddot{C}_{i,J-l}(0) &= 2\sum_k \alpha_{i,J-l}^k C'(\hat{c}_k C + c_k A), \\ \dddot{C}_{i,J-l}(0) &= 3\sum_k \alpha_{i,J-l}^k C''(\hat{c}_k C + c_k, \hat{c}_k C + c_k) + C'(\ddot{Y}_k(0)).\end{aligned} \tag{3.13}$$

We use (2.10) to find $\frac{d^2 S_i}{dh^2}|_{h=0}$, setting $B_{i,J-l} = C_{i,J-l}$, and using the derivatives computed in (3.13) with $\ddot{Y}_k(0)$ from table 3.

Finally we get

$$\begin{aligned}\frac{d^2 S_i}{dh^2}|_{h=0} &= 4\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k \alpha_{i,J-r}^k \sum_m \alpha_{i,J-l}^m [C, C'(\hat{c}_m C + c_m A)] \quad + \\ &2\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k \alpha_{i,J-r}^k \sum_m \alpha_{i,J-l}^m [C'(\hat{c}_k C + c_k A), C] \quad + \\ &3\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k C''(\hat{c}_k C + c_k A, \hat{c}_k C + c_k A) \quad + \\ &6\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \sum_j \hat{a}_{k,j} C'(C'(\hat{c}_j C + c_j A)) \quad + \\ &3\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \hat{c}_k^2 C'(C^2) \quad + \\ &6\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k (\hat{c}_k c_k - \sum_j a_{k,j}\hat{c}_j) C'(CA) \quad + \\ &6\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \sum_j a_{k,j} C'(A(\hat{c}_j C + c_j A)) \quad + \\ &-\sum_{l=0}^{J-1}\sum_k \alpha_{i,J-l}^k \sum_r \alpha_{i,J-l}^r [C, C'(\hat{c}_r C + c_r A)].\end{aligned} \tag{3.14}$$

Using (3.11) we obtain $\varphi_i^{(3)}(0)$ as reported in table 1 and from (3.10) we obtain $Y_i^{(3)}(0)$ reported in table 3.

By imposing $Y_{s+1}^{(3)}|_{h=0} = y^{(3)}|_{h=0}$ we obtain the conditions for order 3 (recalling that $\alpha_{s+1,J-l}^k = \beta^k$ and $\sum_{l=0}^{J-1} \beta_{J-l}^k = \hat{b}_k$) reported in table 4.

Table 4: Conditions of order 3

condition	elementary differential
commutators	
$4\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k \beta_{J-r}^k \sum_m \beta_{J-l}^m \hat{c}_m +$ $-2\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k \beta_{J-r}^k \sum_m \beta_{J-l}^m \hat{c}_k +$ $-\sum_{l=0}^{J-1}\sum_k \beta_{J-l}^k \sum_r \beta_{J-l}^r \hat{c}_r = 0$	$[C'(C), C]$
$4\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k \beta_{J-r}^k \sum_m \beta_{J-l}^m c_m +$ $-2\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k \beta_{J-r}^k \sum_m \beta_{J-l}^m c_k +$ $-\sum_{l=0}^{J-1}\sum_k \beta_{J-l}^k \sum_r \beta_{J-l}^r c_r = 0$	$[C'(A), C]$
higher order differentials	
$3\sum_k \hat{b}_k \hat{c}_k^2 = 1$	$C''(C,C)$
$3\sum_k \hat{b}_k \hat{c}_k c_k = 1$	$C''(C,A)$
$3\sum_k \hat{b}_k \hat{c}_k c_k^2 = 1$	$C''(A,A)$
$3\sum_k \hat{b}_k c_k \hat{c}_k = 1$	$C''(A,C)$
$6\sum_k \hat{b}_k \sum_j \hat{a}_{k,j}\hat{c}_j = 1$	$C'(C'(C))$
$6\sum_k \hat{b}_k \sum_j \hat{a}_{k,j} c_j = 1$	$C'(C'(A))$
$3\sum_k \hat{b}_k \hat{c}_k^2 = 1$	$C'(C^2)$
$6\sum_k \hat{b}_k (\hat{c}_k c_k - \sum_j a_{k,j}\hat{c}_j) = 1$	$C'(CA)$
$6\sum_k \hat{b}_k \sum_j a_{k,j}\hat{c}_j = 1$	$C'(AC)$
$6\sum_k \hat{b}_k \sum_j a_{k,j} c_j = 1$	$C'(A^2)$
products of lower order differentials	
$6\sum_k \hat{b}_k (\sum_j b_j)\hat{c}_k - 6\sum_j b_j \sum_k \hat{a}_{j,k}\hat{c}_k = 2$	$C'(C)A$
$6\sum_k \hat{b}_k (\sum_j b_j) c_k - 6\sum_j b_j \sum_k \hat{a}_{j,k} c_k = 2$	$C'(A)A$
$3 - 6\sum_j b_j \hat{c}_j + 3\sum_j b_j \hat{c}_j^2 = 1$	$C^2 A$
$6\sum_j b_j \hat{c}_j - 6\sum_j b_j \hat{c}_j^2 = 1$	CAC
$6\sum_j b_j c_j - 6\sum_j b_j \hat{c}_j c_j = 1$	CA^2
$6\sum_j b_j \sum_m \hat{a}_{j,m}\hat{c}_m = 1$	$AC'(C)$
$6\sum_j b_j \sum_m \hat{a}_{j,m} c_m = 1$	$AC'(A)$
$3\sum_j b_j \hat{c}_j^2 = 1$	AC^2
$6\sum_j b_j (\hat{c}_j c_j \sum_m a_{j,m}\hat{c}_m) = 1$	ACA
$6\sum_j b_j \sum_m a_{j,m}\hat{c}_m = 1$	$A^2 C$
$6\sum_j b_j \sum_m a_{j,m} c_m = 1$	A^3

4 Extra coupling conditions for order 4

We consider coefficients of elementary differentials preceeded by an A in both the expressions for the fourth derivatives ($q = 4$) of the exact and numerical solutions (2.1) and (2.2) respectively. That means matching the terms in $Ay^{(3)}\big|_{h=0}$ and $4\sum_j \sum_j a_{i,j}\varphi_{i,j}(0)AY_j^{(3)}(0)$, since $\varphi_{i,j}(0) = I$. We obtain

$$\begin{aligned} Ay^{(3)}\Big|_{h=0} &= A[C''(C,C) + C''(C,A) + C''(A,C) + C''(A,A) + C'(C'(C)) + C'(C'(A)) \\ &+ C'(C^2) + C'(CA) + C'(AC) + C'(A^2) + 2C'(C)C + 2C'(C)A + 2C'(A)C \\ &+ 2C'(A)A + CC'(C) + CC'(A) + AC'(C) + AC'(A) + (C+A)^3]y_0. \end{aligned} \tag{4.1}$$

We substitute for $\varphi_{i,j}(0)$ and $Y_j^{(3)}(0)$ in $4\sum_j \sum_j a_{i,j}\varphi_{i,j}^{(0)} AY_j^{(3)}(0)$, and select elementary diffentials whose coefficients contain the CF coefficients $\alpha_{s+1,J-l}^k := \beta_{J-l}^k$. These include $ACC'(C)y_0,\ ACC'(A)y_0,\ AC'(C)Cy_0,\ AC'(A)Cy_0$, arising from the terms

$$\begin{aligned} &16\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k \sum_m a_{i,j}\alpha_{j,J-r}^k \alpha_{j,J-l}^m A[C, C'(\hat{c}_m C + c_m A)]y_0 \quad + \\ &8\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k \sum_m a_{i,j}\alpha_{j,J-r}^k \alpha_{j,J-l}^m A[C, C'(\hat{c}_k C + c_k A)]y_0 \quad + \\ &-4\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k a_{i,j}\alpha_{j,J-l}^k \alpha_{j,J-l}^r A[C, C'(\hat{c}_r C + c_r A)]y_0 \quad + \\ &16\sum_j \sum_k a_{i,j}\hat{c}_j \hat{a}_{j,k} AC'(\hat{c}_k C + c_k A)Cy_0 + 8\sum_j \sum_k a_{i,j}\hat{c}_j \hat{a}_{j,k} ACC'(\hat{c}_k C + c_k A)y_0 \end{aligned} \tag{4.2}$$

Comparing coefficients of elementary differentials $ACC'(C)y_0,\ ACC'(A)y_0,\ AC'(C)Cy_0,\ AC'(A)Cy_0$ we obtain respectively the order conditions

$$\begin{aligned} &16\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k \sum_m a_{i,j}\alpha_{j,J-r}^k \alpha_{j,J-l}^m \hat{c}_m - 8\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k \sum_m a_{i,j}\alpha_{j,J-r}^k \alpha_{j,J-l}^m \hat{c}_k \\ &-4\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k a_{i,j}\alpha_{j,J-l}^k \alpha_{j,J-l}^r \hat{c}_r + 8\sum_j \sum_k a_{i,j}\hat{c}_j \hat{a}_{j,k}\hat{c}_k = 1, \end{aligned} \tag{4.3}$$

$$\begin{aligned} &16\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k \sum_m a_{i,j}\alpha_{j,J-r}^k \alpha_{j,J-l}^m c_m - 8\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k \sum_m a_{i,j}\alpha_{j,J-r}^k \alpha_{j,J-l}^m c_k \\ &-4\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k a_{i,j}\alpha_{j,J-l}^k \alpha_{j,J-l}^r c_r + 8\sum_j \sum_k a_{i,j}\hat{c}_j \hat{a}_{j,k} c_k = 1, \end{aligned} \tag{4.4}$$

$$\begin{aligned} &-16\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k \sum_m a_{i,j}\alpha_{j,J-r}^k \alpha_{j,J-l}^m \hat{c}_m + 8\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k \sum_m a_{i,j}\alpha_{j,J-r}^k \alpha_{j,J-l}^m \hat{c}_k \\ &+4\sum_j \sum_{l=0}^{J-1} \sum_{r=0}^{l} \sum_k a_{i,j}\alpha_{j,J-l}^k \alpha_{j,J-l}^r \hat{c}_r + 16\sum_j \sum_k a_{i,j}\hat{c}_j \hat{a}_{j,k}\hat{c}_k = 2, \end{aligned} \tag{4.5}$$

$$
-16\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k\sum_m a_{i,j}\alpha^k_{j,J-r}\alpha^m_{j,J-l}c_m + 8\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k\sum_m a_{i,j}\alpha^k_{j,J-r}\alpha^m_{j,J-l}c_k
+4\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k a_{i,j}\alpha^k_{j,J-l}\alpha^r_{j,J-l}c_r + 16\sum_j\sum_k a_{i,j}\hat{c}_j\hat{a}_{j,k}c_k = 1, \tag{4.6}
$$

Simplifying (4.3)-(4.6) via the use of third order conditions we obtain the order conditions (4.7)-(4.10). Assuming that the RK tableaus (1.3) fulfill the order conditions for a classical partitioned RK method of order 4, and that the b's are different from the $\hat{b}$'s, i.e., $b_j \neq \hat{b}_j$ for some $j = 1, \dots, s$, then the order conditions in (4.7)-(4.10) will result in a new or extra set of coupling conditions (involving the α and β coefficients) for our method, which are not included in the set of order conditions for the classical partioned RK methods and CF methods. This is not the case for orders 1 through 3 where all our order conditions are only a subset of those for the partioned RK and CF methods.

$$
16\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k\sum_m a_{i,j}\alpha^k_{j,J-r}\alpha^m_{j,J-l}\hat{c}_m - 8\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k\sum_m a_{i,j}\alpha^k_{j,J-r}\alpha^m_{j,J-l}\hat{c}_k
-4\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k a_{i,j}\alpha^k_{j,J-l}\alpha^r_{j,J-l}\hat{c}_r = 0, \tag{4.7}
$$

$$
16\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k\sum_m a_{i,j}\alpha^k_{j,J-r}\alpha^m_{j,J-l}c_m - 8\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k\sum_m a_{i,j}\alpha^k_{j,J-r}\alpha^m_{j,J-l}c_k
-4\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k a_{i,j}\alpha^k_{j,J-l}\alpha^r_{j,J-l}c_r = 0, \tag{4.8}
$$

$$
-16\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k\sum_m a_{i,j}\alpha^k_{j,J-r}\alpha^m_{j,J-l}\hat{c}_m + 8\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k\sum_m a_{i,j}\alpha^k_{j,J-r}\alpha^m_{j,J-l}\hat{c}_k
+4\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k a_{i,j}\alpha^k_{j,J-l}\alpha^r_{j,J-l}\hat{c}_r = 0, \tag{4.9}
$$

$$
-16\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k\sum_m a_{i,j}\alpha^k_{j,J-r}\alpha^m_{j,J-l}c_m + 8\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k\sum_m a_{i,j}\alpha^k_{j,J-r}\alpha^m_{j,J-l}c_k
+4\sum_j\sum_{l=0}^{J-1}\sum_{r=0}^{l}\sum_k a_{i,j}\alpha^k_{j,J-l}\alpha^r_{j,J-l}c_r = 0, \tag{4.10}
$$

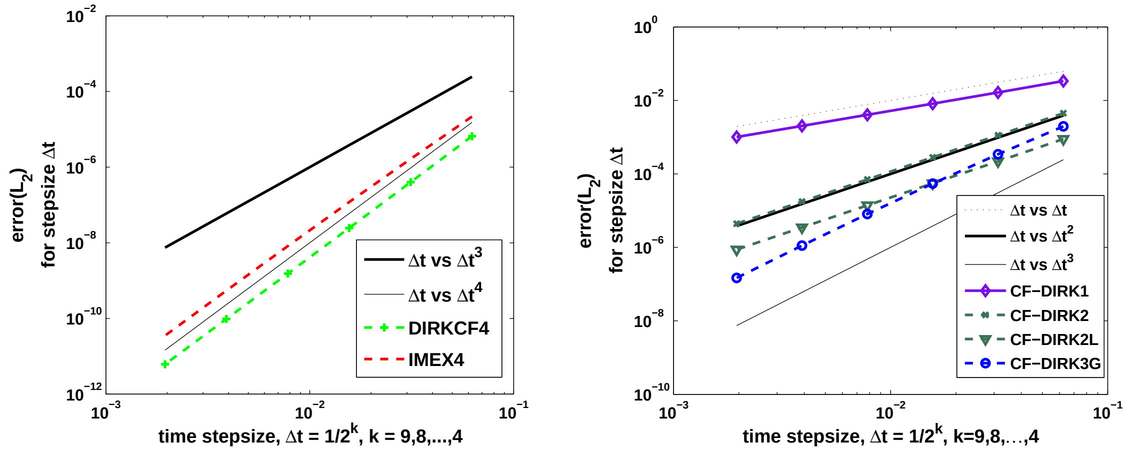
where $i = s+1$ so that $a_{i,j} = a_{s+1,j} = b_j,\ j = 1, \dots, s$.

In figure 1(a) we have a numerical test showing the order in time for a fourth order method (DIRK-CF4). This method is constructed using the additive partioned IMEX RK method of Kennedy and Carpenter [5] (here named as IMEX4) wherein we derive from the corresponding explicit tableau the commutator-free coefficients via (1.2) satifying the

CF order conditions as described by Owren [6]. It is mportant to note, however, that our new method DIRK-CF4 automatically satisfy the coupling conditions (4.7)-(4.10) as part of the partioned RK order conditions since in this choice of IMEX RK scheme the b's and $\hat{b}$'s are the same (see [5]). The figure also shows a comparison between the DIRK-CF4 and its counterpart IMEX4. The numerical experiment is performed on the viscous Burgers equation

$$u_t + uu_x = \nu u_{xx}$$

over a domain $[0, 1]$ with initial condition $u(x, 0) = u_0(x) = \sin(\pi x)$, and Dirichlet homogenoues boundary conditions. We integrate on the interval $[0, T]$ $(T = 1, \nu = 0.05$ in this case) with time steps in the range $\{\Delta t = 2^{-n} | n = 4, 5, \ldots, 9\}$. The spatial discretization is the standard centered differences on a uniform grid of mesh step $\Delta x = 1/32$. The error is measured as a grid-point error in the 2−norm, and the reference (exact) solution is computed as in [2]. Figure 1(b) shows the numerical order tests performed for some of the first to third order methods derived in [2].



(a) Order 4 (b) Orders $1, 2, 3$

Figure 1: Numerical order tests using Burgers equation, $u_t + uu_x = \nu u_{xx}$, on Dirichlet homogeneous BCs, $x \in [0, 1], \nu = 0.05, u_0 = sin\pi x, T = 1, \Delta x = 1/32$. Plot of the 2− norm error as a function of $\Delta t = 2^{-n}, n = 4, 5, \ldots, 9$. (a)Order test for the fourth order DIRK-CF4 and IMEX4 (b) Order test for first order DIRK-CF1, second order DIRK-CF2 and DIRK-CF2L, third order DIRK-CF3G.

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