A Class of Multi-Derivative Spectral Deferred Correction Schemes

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Abstract

In this work, we present a class of multi-derivative spectral deferred correction schemes incorporating up to three derivatives. The new general class that utilizes higher-derivatives of the differential equations generalizes both the existing preconditioned one-derivative spectral deferred correction methods and the two-derivative Hermite–Birkhoff predictor–corrector methods. We show that an LU-based preconditioning strategy analogous to [M. Weiser, BIT Numerical Mathematics 55 (2015) 1219–1241] and [G. Čaklović et al., SIAM Journal on Scientific Computing 47 (2025) A430–A453] exhibits accelerated convergence and is verified on stiff differential equations. The order of convergence is illustrated numerically, and the numerical results for partial differential equations also support the convergence acceleration of the presented schemes.

Keywords: Multi-derivative, Spectral deferred corrections, Ordinary differential equations, Partial differential equations
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1. Introduction

Implicit schemes are essential in solving initial value problems, especially when it comes to stiff equations. The flexibility, stability, and higher order accuracy make *collocation schemes* appealing to solve stiff initial value problems. However, the dense Butcher tableaux corresponding to collocation schemes make them unfit for solving systems of large ordinary differential equations (ODEs) stemming from discretizing partial differential equations (PDEs). Hence, to reduce the complexity, an iterative solving strategy is used rather than solving the whole system of the collocation scheme. This iterative strategy can be developed and implemented using various approaches, most of which fall under the category of deferred correction (DC) schemes. These are higher-order numerical time-integration methods built from lower-order schemes. The iterative scheme is expected to converge to the underlying collocation solution as more correction steps are performed.

In the review paper [1], the authors classify the DC methods mainly into four classes based on the associated error equation formulations used. The classical deferred correction scheme (CDC) [2] and the method of Dutt, Greengard, and Rokhlin (DGR) [3] use error function initial value problems (IVP). In contrast, the spectral deferred correction methods (SDC) [4] and Integral Deferred Correction schemes (IDC) [5, 6] use the integral form of the error function. In each correction step, the error functions are solved and added to the previous corrected solution, and hence the accuracy is improved. The correction procedure repeats until it achieves its maximum consistency order. As the DC schemes have the potential to be parallelized, there are parallel DC schemes [7, 8, 9, 4, 10] in literature that use the idea of pipeline

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parallelism. Refer to articles [11, 12, 13, 14, 15, 16, 17] and the references therein for more insights on deferred correction schemes.

Introducing higher derivatives of the ODE's right-hand side into Runge-Kutta schemes can enhance the accuracy order without requiring additional stages. These schemes are termed multi-derivative Runge-Kutta schemes. Refer to [18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28] and the references therein for a non-exhaustive list of multi-derivative Runge-Kutta schemes. Based on two-derivative collocation schemes, two-derivative DC schemes were developed in [29], termed Hermite-Birkhoff Predictor-Corrector (HBPC) schemes. The schemes were improved in [30] to have $A(\alpha)$ stability with α close to 90^0, and parallelized in [28, 31]. Recently, a multi-step two-derivative DC scheme was also presented in [32].

In [14, 17], the authors have shown that the inclusion of free parameters does not affect the overall order of accuracy for one-derivative SDC schemes. The aforementioned free parameters were utilized to optimize the scheme in terms of stability [17, 30, 32] and to control the error constant growth [32]. When more derivatives are incorporated into the scheme, space for more free parameters will be created. Hence the available free parameters can be employed to design an optimized scheme without compromising on other essential properties. Taking into account the promising convergence and stability properties of the one-derivative SDC schemes [3, 4, 17] and the two-derivative HBPC schemes [29, 30], it is vital to study the broader category of SDC schemes involving higher order derivatives. In this work, we put the HBPC schemes into the framework of multiderivative SDC schemes and generalize them through the use of non-diagonal preconditioning [15, 4, 10].

Therefore, this paper investigates a class of multi-derivative SDC schemes. Specifically, we analyze the convergence properties of multi-derivative SDC schemes under various preconditioning strategies. The paper is structured as follows: The multi-derivative SDC schemes are introduced in Sec. 2, followed by the study of accelerated convergence in Sec. 3. In Sec. 3.1, the preconditioning strategies are studied on stiff differential equations for varying stiffness parameters. The convergence results for schemes up to three derivatives and order six are shown in Sec. 4.2. The schemes are applied to partial differential equations in Sec. 4.3, and the conclusion and outlook are provided in Sec. 5.

2. The multi-derivative SDC scheme

Consider the following initial value problem of form

$$y'(t) = f(y), \quad y(0) = y_0. \tag{1}$$

Let $\mathbf{Y} := \left(\mathbf{y}^{n,1}, \mathbf{y}^{n,2}, \cdots, \mathbf{y}^{n,s}\right)^T$ be the vector of approximate solutions at collocation points $(\tau_1, \tau_2, \ldots, \tau_s)$ and $f(\mathbf{Y})$ be the vector of function evaluations $\left(f\left(\mathbf{y}^{n,1}\right), f\left(\mathbf{y}^{n,2}\right), \cdots, f\left(\mathbf{y}^{n,s}\right)\right)^T$. Then, for the quadrature rule $\mathbf{Q} \in \mathbb{R}^{s\times s}$ corresponding to the given points $(\tau_1, \tau_2, \ldots, \tau_s)$, the collocation scheme [33, Sec. VII.4] is given by

$$\mathbf{Y} = \mathbf{y}^n \mathbb{1} + \Delta t \mathbf{Q} f(\mathbf{Y}), \tag{2}$$

$$\mathbf{y}^{n+1} = \mathbf{y}^n + \Delta t \mathbf{b}^T f(\mathbf{Y}), \tag{3}$$

where $\mathbf{b} \in \mathbb{R}^{s\times 1}$ are the quadrature weights. For a strategically chosen $\mathbf{Q}_\Delta \in \mathbb{R}^{s\times s}$ [4, 10], the preconditioned SDC corresponding to the above collocation scheme is given by

$$\mathbf{Y}^{k+1} - \Delta t \mathbf{Q}_\Delta f(\mathbf{Y}^{k+1}) = \mathbf{y}^n \mathbb{1} + \Delta t(\mathbf{Q} - \mathbf{Q}_\Delta) f(\mathbf{Y}^k), \quad k \geq 0, \tag{4}$$

where $\mathbf{Y}^k$ represents the vector of the corrected solution in each step k. The iterative scheme (4) starts with a predicted solution $\mathbf{Y}^0$. In our case, we use implicit Euler,

$$\mathbf{Y}^0 = \mathbf{y}^n \mathbb{1} + \Delta t\, \mathrm{Diag}\left(\tau_1, \tau_2, \ldots, \tau_s\right) f(\mathbf{Y}^0). \tag{5}$$

Then, for a given maximum correction step $k_{\max}$, the update is given by

$$\mathbf{y}^{n+1} := \mathbf{y}^n + \Delta t \mathbf{Q}_\Delta(s,:) \left(f(\mathbf{Y}^{k_{\max}}) - f(\mathbf{Y}^{k_{\max}-1}) \right) + \Delta t \mathbf{b}^T f(\mathbf{Y}^{k_{\max}-1}), \tag{6}$$

where $\mathbf{Q}_\Delta(s,:) \in \mathbb{R}^{1\times s}$ is the last row of the matrix $\mathbf{Q}_\Delta$.

Remark 1. *If the collocation scheme is globally stiffly accurate (GSA), then it holds that*

$$\mathbf{b} = \mathbf{Q}(s,:).$$

Subsequently, the update step (6) *simplifies to* $\mathbf{y}^{n+1} := \mathbf{Y}^{k_{\max}}(s)$.

Consult articles [4, 10] and the references therein for more insights on preconditioning and efficiency of one-derivative SDC schemes. In the above case, the only way to increase the order of the scheme is to increase the number of collocation points. Instead, here we use multiple derivatives of the equations, which leads to m-Derivative SDC schemes (mD-SDC).

To extend the idea of SDC to mD-SDC schemes, we start with an m-derivative collocation scheme, given by

$$\mathbf{Y} = \mathbf{y}^n \mathbb{1} + \sum_{r=1}^{m} \Delta t^r \mathbf{Q}^{(r)} f^{(r)}(\mathbf{Y}), \tag{7}$$

$$\mathbf{y}^{n+1} = \mathbf{y}^n + \sum_{r=1}^{m} \Delta t^r {\mathbf{b}^{(r)}}^T f^{(r)}(\mathbf{Y}), \tag{8}$$

where $\mathbf{Q}^{(r)} \in \mathbb{R}^{s\times s}$ is the Butcher tableau for the rth derivative in the quadrature rule, $\mathbf{b}^{(r)} \in \mathbb{R}^{s\times 1}$ is the quadrature weight, and $f^{(r)}(\mathbf{Y})$ be the vector of function evaluations

$$\left(f^{(r)}(\mathbf{y}^{n,1}), f^{(r)}(\mathbf{y}^{n,2}), \cdots, f^{(r)}(\mathbf{y}^{n,s}) \right)^T,$$

corresponding to each derivative r. The derivatives $f^{(r)}$ are recursively defined as

$$f^{(r)}(y) := \left(\frac{d}{dy} f^{(r-1)}(y) \right) f(y), \; r \geq 2, \quad \text{and} \quad f^{(1)}(y) = f(y).$$

Definition 1. *For ease of representation in the upcoming sections, the exact stage solutions* $\left(\mathbf{y}^{n,1}, \mathbf{y}^{n,2}, \ldots, \mathbf{y}^{n,s}\right)^T$ *to the collocation problem* (7) *are denoted by* $\mathbf{Y}_{coll}$*, i.e.,*

$$\mathbf{Y}_{coll} = \mathbf{y}^n \mathbb{1} + \sum_{r=1}^{m} \Delta t^r \mathbf{Q}^{(r)} f^{(r)}(\mathbf{Y}_{coll}).$$

Then, the update (8) *is denoted as* y_{coll}.

Then, the algorithm for the preconditioned m-derivative SDC scheme is given as follows:

Algorithm 1. *The scheme starts with a predicted solution evaluated using an m-derivative Taylor method:*

1. ***Predict.*** *Solve the following expression for* $\mathbf{Y}^0$*:*

$$\mathbf{Y}^0 = \mathbf{y}^n \mathbb{1} + \sum_{r=1}^{m} (-1)^{r+1} \frac{\Delta t^r \operatorname{Diag}\left(\tau_1^r, \tau_2^r, \ldots, \tau_s^r\right)}{r!} f^{(r)}(\mathbf{Y}^0). \tag{9}$$

2. ***Correct.*** *Solve the following for* $\mathbf{Y}^{k+1}$*, for each* $0 \le k < k_{\max}$*:*

$$\mathbf{Y}^{k+1} - \sum_{r=1}^{m} \Delta t^r \mathbf{Q}_{\Delta}^{(r)} f^{(r)}(\mathbf{Y}^{k+1}) = \mathbf{y}^n \mathbb{1} + \sum_{r=1}^{m} \Delta t^r (\mathbf{Q}^{(r)} - \mathbf{Q}_{\Delta}^{(r)}) f^{(r)}(\mathbf{Y}^k). \tag{10}$$

3. ***Update.***

$$\mathbf{y}^{n+1} := \mathbf{y}^n + \sum_{r=1}^{m} \Delta t^r \mathbf{Q}_{\Delta}^{(r)}(s,:) \left(f^{(r)}(\mathbf{Y}^{k_{\max}}) - f^{(r)}(\mathbf{Y}^{k_{\max}-1}) \right) + \sum_{r=1}^{m} \Delta t^r {\mathbf{b}^{(r)}}^T f^{(r)}(\mathbf{Y}^{k_{\max}-1}), \tag{11}$$

where $\mathbf{Q}_{\Delta}^{(r)}(s,:) \in \mathbb{R}^{1\times s}$ *is the last row of the matrix* $\mathbf{Q}_{\Delta}^{(r)}$ *corresponding to each derivative* r*. If the collocation scheme is globally stiffly accurate (GSA), then the update step simplifies to* $\mathbf{y}^{n+1} := \mathbf{Y}^{k_{\max}}(s)$*.*

For the mD-SDC scheme outlined in Algorithm 1, the order of the scheme increases by one in each correction step, and at a correction step $k \le k_{\max}$, the order of accuracy is given by $\min(k+m, p)$, where p is the order of the underlying quadrature rule.

Remark 2. *In [29, 28], the authors have implemented a multi-derivative SDC type scheme that uses equally spaced collocation points in* $[t^n, t^{n+1}]$ *including the point* t^n *and use a specific* $\mathbf{Q}_{\Delta}^{(r)}$ *matrix of the following form*

$$\mathbf{Q}_{\Delta}^{(r)} = (-1)^{r+1} \frac{1}{r!} \operatorname{Diag}(0, 1, 1, \cdots, 1). \tag{12}$$

For the two-derivative case, these schemes were optimized to achieve $A(\alpha)$ *stability with* α *close to* 90^0 *in [30] using*

$$\mathbf{Q}_{\Delta}^{(r)} = (-1)^{r+1} \frac{1}{r!} \operatorname{Diag}(0, \theta_r, \theta_r, \cdots, \theta_r), \quad r = 1, 2. \tag{13}$$

3. Optimization of the coefficients

Here, we utilize an approach for an mD-SDC scheme similar to the one the authors employed in [10, Sec. 2.2] for one-derivative SDC schemes. Consider the Dahlquist test equation

$$y' = \lambda y, \quad \lambda \in \mathbb{C}.$$

Applying the above to Eq. (10) gives

$$\left(\mathbf{I} - \sum_{r=1}^{m} z^r \mathbf{Q}_{\Delta}^{(r)} \right) \mathbf{Y}^{k+1} = \mathbf{y}^n \mathbb{1} + \left(\sum_{r=1}^{m} z^r (\mathbf{Q}^{(r)} - \mathbf{Q}_{\Delta}^{(r)}) \right) \mathbf{Y}^k, \tag{14}$$

where $z := \lambda \Delta t$. Consider the exact solution $\mathbf{Y}_{coll}$ of the collocation problem (8) for the Dahlquist equation, given by

$$\mathbf{Y}_{coll} = \mathbf{y}^n \mathbb{1} + \left(\sum_{r=1}^{m} z^r \mathbf{Q}^{(r)} \right) \mathbf{Y}_{coll}. \tag{15}$$

Then, define the error to $\mathbf{Y}_{coll}$ as

$$\mathbf{E}^k := \mathbf{Y}^k - \mathbf{Y}_{coll}. \tag{16}$$

Subtract Eq. (15) from Eq. (14), and rearrange the terms as follows

$$\left(\mathbf{I} - \sum_{r=1}^{m} z^r \mathbf{Q}_{\Delta}^{(r)} \right) \mathbf{Y}^{k+1} - \mathbf{Y}_{coll} = \left(\sum_{r=1}^{m} z^r (\mathbf{Q}^{(r)} - \mathbf{Q}_{\Delta}^{(r)}) \right) \mathbf{Y}^k - \left(\sum_{r=1}^{m} z^r \mathbf{Q}^{(r)} \right) \mathbf{Y}_{coll},$$

$$\left(\mathbf{I} - \sum_{r=1}^{m} z^r \mathbf{Q}_{\Delta}^{(r)} \right) \mathbf{E}^{k+1} = \left(\sum_{r=1}^{m} z^r (\mathbf{Q}^{(r)} - \mathbf{Q}_{\Delta}^{(r)}) \right) \mathbf{E}^k.$$

Under the assumption that the matrix $\left(\mathbf{I} - \sum_{r=1}^{m} z^r \mathbf{Q}_\Delta^{(r)}\right)$ is invertible, we get

$$\mathbf{E}^{k+1} = \left(\mathbf{I} - \sum_{r=1}^{m} z^r \mathbf{Q}_\Delta^{(r)}\right)^{-1} \left(\sum_{r=1}^{m} z^r (\mathbf{Q}^{(r)} - \mathbf{Q}_\Delta^{(r)})\right) \mathbf{E}^k =: \mathbf{K}(z)\mathbf{E}^k,$$

where $\mathbf{K}(z)$ is the iteration matrix. The stiff limit of the iteration matrix function is defined by

$$\mathbf{K}_S := \lim_{|z|\to\infty} \mathbf{K}(z). \tag{17}$$

Upon realizing that for $z \neq 0$

$$\mathbf{K}(z) = \left(\frac{1}{z^m}\mathbf{I} - \sum_{r=1}^{m} \frac{z^r}{z^m} \mathbf{Q}_\Delta^{(r)}\right)^{-1} \left(\sum_{r=1}^{m} \frac{z^r}{z^m} (\mathbf{Q}^{(r)} - \mathbf{Q}_\Delta^{(r)})\right),$$

we can conclude that for an m-derivative SDC, the stiff limit is given by

$$\mathbf{K}_S = \mathbf{I} - \mathbf{Q}_\Delta^{(m)^{-1}} \mathbf{Q}^{(m)}, \tag{18}$$

if the matrix $\mathbf{Q}_\Delta^{(m)}$ is invertible.

In the stiff limit, if the matrix $\mathbf{K}_S$ is a nilpotent matrix, the error $\mathbf{E}^k$ will go to zero in a finite number of steps. Then, the matrix $\mathbf{Q}_\Delta^{(m)}$ has to be chosen wisely in Eq. (18) to generate a nilpotent matrix $\mathbf{K}_S$. We use the method of LU decomposition as done in [15] to choose such a matrix $\mathbf{Q}_\Delta^{(m)}$. Assume that an LU decomposition exists for $\mathbf{Q}^{(m)^T}$, where all diagonal entries of the lower-triangular matrix L are equal to one. Therefore,

$$\mathbf{Q}^{(m)^T} = \mathbf{L}^{(m)}\mathbf{U}^{(m)}. \tag{19}$$

Now, define the matrix $\mathbf{Q}_\Delta^{(m)}$ through

$$\mathbf{Q}_\Delta^{(m)} := \mathbf{U}^{(m)^T}. \tag{20}$$

Substituting the Eqs. (19) and (20) for $\mathbf{Q}^{(m)}$ and $\mathbf{Q}_\Delta^{(m)}$ in Eq. (18) gives

$$\mathbf{K}_S = \mathbf{I} - \mathbf{Q}_\Delta^{(m)^{-1}} \mathbf{Q}^{(m)} = \mathbf{I} - \left(\mathbf{U}^{(m)^T}\right)^{-1} \left(\mathbf{U}^{(m)^T} \mathbf{L}^{(m)^T}\right) = \mathbf{I} - \mathbf{L}^{(m)^T}, \tag{21}$$

which is an upper triangular with all the diagonal entries equal to zero, resulting into a nilpotent matrix. Therefore, in the stiff limit, the mD-SDC scheme with $\mathbf{Q}_\Delta^{(m)} = \mathbf{U}^{(m)^T}$ gives a faster convergence towards the collocation solution for the above mentioned test problem.

3.1. Preconditioning of the mD-SDC scheme

Using the stiff limit condition (18), for mD-SDC scheme, $\mathbf{Q}_\Delta^{(m)}$ should be assigned with $\mathbf{U}^{(m)^T}$. However a strategy has to be obtained for choosing the matrices $\mathbf{Q}_\Delta^{(r)}$ for $r < m$. Some of the possible preconditioning options are mentioned below.

- **Precond-1 :** Choose $\mathbf{Q}_\Delta^{(m)} = \mathbf{U}^{(m)^T}$, and for $r < m$, choose $\mathbf{Q}_\Delta^{(r)}$ as the lower triangular matrix with all entries equal to $(-1)^{r+1}\frac{1}{r!}$, see Rem. 2.
- **Precond-2 :** Choose $\mathbf{Q}_\Delta^{(r)} = \mathbf{U}^{(m)^T}$ for each $r \leq m$.
- **Precond-3 :** Choose $\mathbf{Q}_\Delta^{(r)} = \mathbf{U}^{(r)^T}$ for each $r \leq m$.

- **w/o Precond :** Choose $\mathbf{Q}_\Delta^{(r)}$ for all $1 \leq r \leq m$ as the lower triangular matrix with all entries equal to $(-1)^{r+1}\frac{1}{r!}$, see Rem. 2.

Remark 3. *When the LU decomposition preconditioning is used, the matrices are generated only once for a particular scheme. The required matrices are saved and used in the time-stepping procedure as needed.*

Definition 2. *The mD-HBRK-p-ls method refers to an m-derivative collocation scheme of order p with l collocation points*

$$\mathbf{C} = (\tau_1, \tau_2, \ldots, \tau_{l-1}, 1), \qquad \tau_i \neq \tau_j \neq 1, \quad \forall i \neq j,$$

and quadrature matrices $\mathbf{Q}^{(r)}$ corresponding to each derivative $1 \leq r \leq m$. The construction of this scheme ensures at least an order of

$$p = ml$$

for any chosen nodes $0 \leq \tau_j < 1$ for $j < l$.

Remark 4. *Let us make the following comments on the choice of the collocation points:*

- *Since the right-most collocation point τ_l always equals one, the generated schemes are GSA. This is not a necessity for the schemes to work, but makes the update step considerably simpler.*
- *For the schemes presented in this paper, the initial node τ_1 is taken to be non-zero; otherwise, the LU preconditioning strategy cannot be applied to the generated quadrature matrices $\mathbf{Q}$ due to their zero first rows. The quadrature matrices and collocation nodes for the scheme used in this paper are given in Appendix A.*

Using specific collocation nodes, such as the Gauss-Radau nodes, leads to one-derivative collocation methods with improved order of accuracy [33]. Similarly, for odd values of m it is possible to identify collocation nodes that exhibit super-convergence. These schemes can achieve an accuracy order of $p > ml$.

4. Numerical results

4.1. Fixing the preconditioning strategy

We use the multi-derivative SDC schemes based on the collocation schemes 2D-HBRK-4-2s and 3D-HBRK-6-2s to compare the efficiencies of the above-mentioned preconditioning strategies. The schemes 2D-HBRK-4-2s and 3D-HBRK-6-2s correspond to the fourth-order two-derivative two-stage collocation scheme and the sixth-order three-derivative two-stage collocation scheme, respectively. The Butcher tableaux of these schemes are given in Appendix A. To analyze the behavior of mD-SDC schemes on various stiff conditions, we consider Van-der-Pol's problem. It is given by

$$y_1'(t) = y_2, \quad y_2'(t) = \frac{(1 - y_1^2)y_2 - y_1}{\varepsilon}, \quad y_0 = \left(2, -\frac{2}{3} + \frac{10}{81}\varepsilon\right), \tag{22}$$

where $\varepsilon > 0$ is the stiffness parameter.

In order to analyze the effect of different preconditioning strategies described in subsection 3.1, we have shown the plots of the 2D-SDC and 3D-SDC schemes in two different ways. We employ a damped Newton method to solve the nonlinear equations and utilize the standard backslash operator in Matlab to solve the associated linear system of equations. The Newton tolerance is set at a fine tolerance of 10^{-14}, with a maximum of 1000 allowable iterations.

The convergence of the mD-SDC schemes towards the collocation solution for increasing correction steps ($k_{\max}$) has been shown in Figs. 1 and 2 for three different fixed timesteps sizes (Δt). The error $\|y_{coll} - y_h\|_2$ is calculated at $T_{end} = 0.5$, where y_h is the mD-SDC solution and y_{coll} is the solution to the underlying collocation scheme. Each plot in Figs. 1 and 2 is given for different stiffness parameters and preconditioning strategies. It is evident from Figs. 1 and 2 that the schemes 2D-SDC and 3D-SDC with preconditioning strategy Precond-3 are more efficient than Precond-1 and Precond-2 in terms of its faster

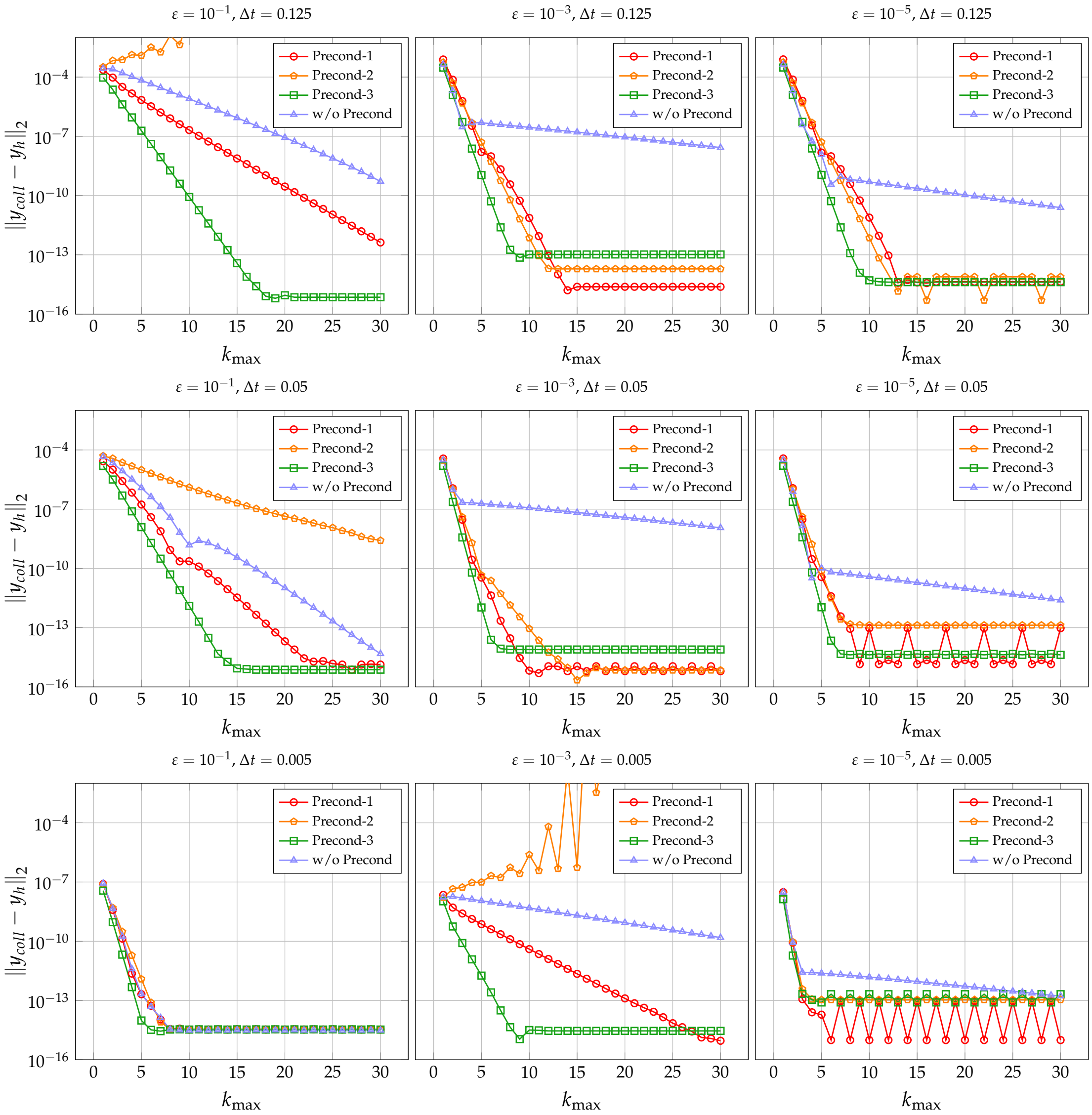

Figure 1: The error of the 2D-SDC scheme (based on 2D-HBRK-4-2s) for different preconditioning strategies in comparison to the exact solution of the corresponding collocation scheme. The error $\|y_{coll} - y_h\|_2$ is plotted against different $k_{\max}$ in each plots above. The errors are given for the Van-der-Pol equation, calculated at $T_{end} = 0.5$. Each column corresponds to a fixed stiffness parameter ε, and each row corresponds to a fixed timestep Δt.

convergence towards the corresponding collocation solution y_{coll}. In particular, Precond-1 and Precond-3 demonstrate robustness across a range of stiffness parameters and timestep sizes, whereas Precond-2 does not. Similar results have been observed for the Pareschi-Russo problem with the abovementioned preconditioning strategies (results not shown here).

Therefore, Precond-3 can be considered a default preconditioning strategy for mD-SDC schemes if an LU-decomposition exists for each quadrature matrix $\mathbf{Q}^{(r)}$ associated with its underlying collocation scheme.

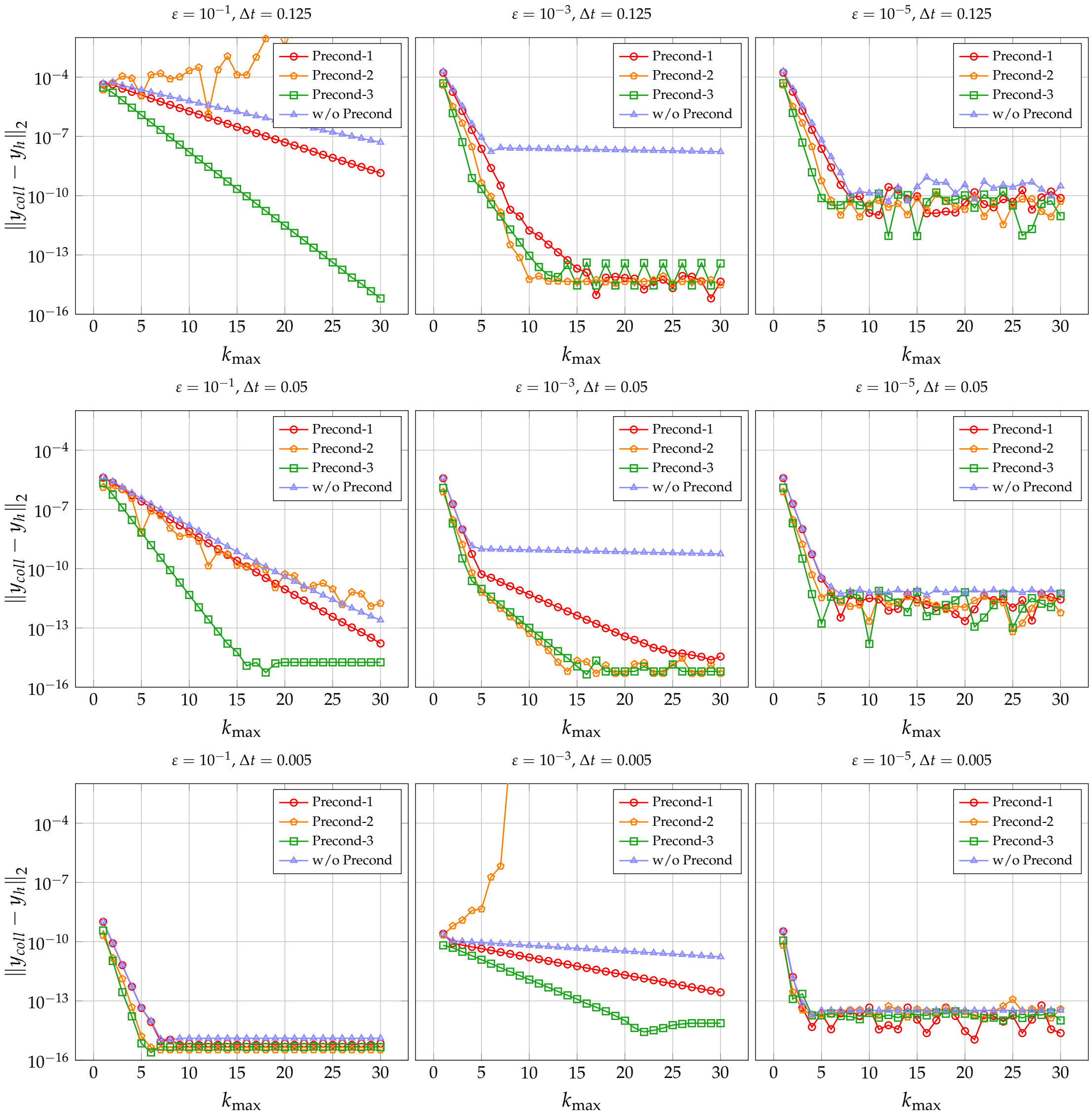

Figure 2: The error of the 3D-SDC scheme (based on 3D-HBRK-6-2s) for different preconditioning strategies in comparison to the exact solution of the corresponding collocation scheme. The error $\|y_{coll} - y_h\|_2$ is plotted against different $k_{\max}$ in each plots above. The errors are given for the Van-der-Pol equation, calculated at $T_{end} = 0.5$. Each column corresponds to a fixed stiffness parameter ε, and each row corresponds to a fixed timestep Δt.

4.2. Convergence testing of the MD-SDC schemes

We use the ordinary differential equation given by

$$u'(t) = -u^{-\frac{5}{2}}, \quad u_0 = 1, \tag{23}$$

to validate the convergence order of the introduced methods (with precond-3) numerically.

In Fig. 3, convergence plots of mD-SDC schemes based on the quadrature rules 2D-HBRK-4-2s, 3D-HBRK-6-2s and 3D-HBRK-7-2s are shown. The Newton tolerance is set at a fine tolerance of 10^{-14}, with a maximum of 1000 allowable iterations. The predictor step ($k_{\max} = 0$) exhibits second- and third-order convergence for the 2D-SDC and 3D-SDC schemes, respectively. The convergence order increases with the number of correction steps for all the schemes presented, reaching the maximum achievable value. Hence, for an mD-SDC scheme based on the mD-HBRK-p-ls quadrature rule, the convergence order at a correction step k is given by $\min(k+m, p)$.

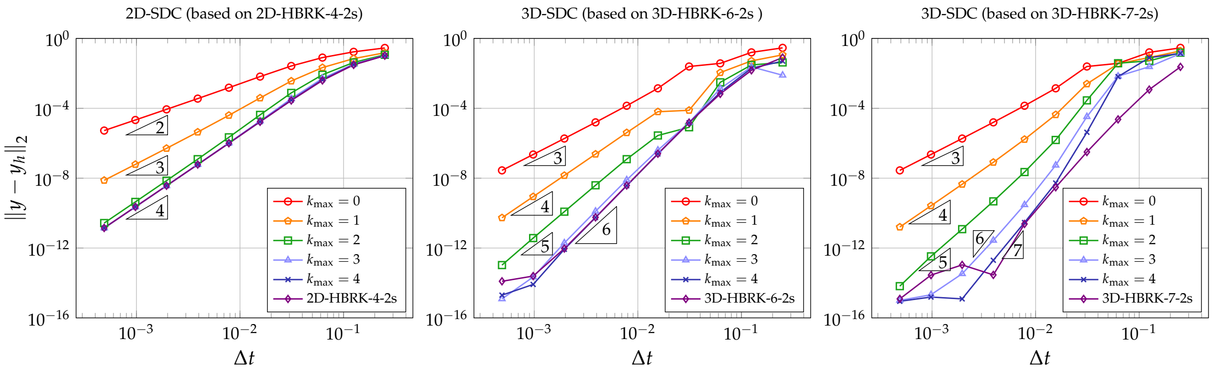

Figure 3: Convergence plot of the 2D-SDC (based on 2D-HBRK-4-2s) and 3D-SDC (based on 3D-HBRK-6-2s and 3D-HBRK-7-2s) schemes using the problem (23). The error $\|y - y_h\|_2$ is calculated at $T_{end} = 0.25$. The error is plotted against different Δt for correction steps $0 \le k_{\max} \le 4$ and the respective quadrature rule.

4.3. Benjamin–Bona–Mahony equation

In this section, we consider the Benjamin–Bona–Mahony (BBM) equation [34] to test the MD-SDC schemes on partial differential equations. It is given by

$$\partial_t u + \partial_x \left(\frac{u^2}{2} \right) - \partial^3_{txx} u = 0. \tag{24}$$

The initial conditions are derived from the solitary wave solution of Eq. (24) given by

$$u(x,t) = 1 + 3(c-1)\,\mathrm{sech}^2 \left(\frac{1}{2} \sqrt{\frac{c-1}{c}}\,(x - ct) \right), \tag{25}$$

where c is set to 1.2, see [35, Sec. 6.2]. The boundary conditions are periodic. We utilize summation-by-parts (SBP) operators [36] to derive the semi-discretization of Eq. (24). The semi-discretized equation can be formulated as

$$\partial_t u + D \left(\frac{u^2}{2} \right) - \partial_t D_+ D_- u = 0, \tag{26}$$

where $D_\pm$ are the high order periodic first-derivative upwind SBP operators [36] and

$$D := \frac{D_+ + D_-}{2}.$$

By rearranging the terms in Eq. (26), we obtain

$$\partial_t u = -\frac{1}{2} \left(I - D_+ D_- \right)^{-1} D u^2.$$

For more details on SBP operators and their applications, refer to [36, 37, 38, 35] and the references therein.

In Fig. 4, the convergence of $k_{\max}$ towards the collocation solution for the BBM equation is shown for the 1D-SDC scheme (based on 1D-HBRK-3-2s [4]), 2D-SDC scheme (based on 2D-HBRK-4-2s) and the 3D-SDC schemes (based on 3D-HBRK-6-2s and 3D-HBRK-7-2s). The Butcher tableaux of these schemes are given in Appendix A. The Newton tolerance is set at a fine tolerance of 10^{-10}, with a maximum of 20 allowable iterations. As observed for the one-derivative SDC (see the top-left plot in Fig. 4), the results clearly indicate that the preconditioned MD-SDC schemes (using precond-3) also converge more rapidly towards the underlying collocation solution than the schemes without preconditioning.

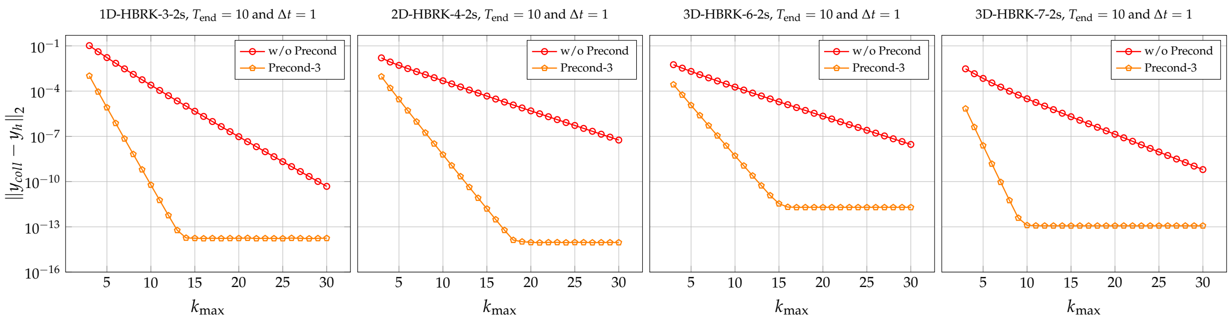

Figure 4: Plotted is the error of the 1D-SDC (based on 1D-HBRK-3-2s [4]), 2D-SDC (based on 2D-HBRK-4-2s) and 3D-SDC (based on 3D-HBRK-6-2s and 3D-HBRK-7-2s) schemes for different preconditioning strategies in comparison to the exact solution of the corresponding collocation scheme. The error $\|y_{coll} - y_h\|_2$ is plotted against different $k_{\max}$ in each plots above. The errors are given for the BBM equation (24), calculated at $T_{end} = 10$.

5. Conclusion and Outlook

In this paper, we have presented a class of multi-derivative spectral deferred correction schemes (MD-SDC). The new class of MD-SDC schemes utilizes higher derivatives of the differential equations to develop higher-order quadrature rules rather than increasing the number of stages. Hence, the existing preconditioned one-derivative spectral deferred correction methods [15, 4, 10], and the two-derivative Hermite–Birkhoff predictor–corrector methods [29, 28] are special cases of MD-SDC under different preconditioning strategies.

We have shown that an LU-based preconditioning strategy accelerates convergence towards the underlying collocation scheme. As multiple derivatives are used in the MD-SDC scheme, different preconditioning strategies have been analyzed on stiff ODEs and found that a preconditioning strategy using the LU decomposition for every derivative coefficient (precond-3, see Sec. 3.1) consistently shows faster convergence across various timesteps and stiffness values. The convergence of the presented fourth, sixth, and seventh-order schemes has been demonstrated numerically. The MD-SDC schemes were also applied to the Benjamin–Bona–Mahony equation discretized using summation-by-parts (SBP) operators. The findings validate that LU preconditioning also accelerates convergence in the context of partial differential equations.

As future work, we are interested in extending MD-SDC into various directions. As efficiency is a major concern in solving large systems such as the Navier-Stokes equations, exploring convergence-accelerated parallel MD-SDC is a promising future direction. One of the main advantages of MD-SDC schemes is their ease in deriving an IMEX version, which requires only an IMEX predictor. However, a detailed analysis of the IMEX MD-SDC schemes is necessary, particularly in their application to specific stiff problems, the splitting methods used, and their asymptotic preserving property.

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References

[1] B. W. Ong, R. J. Spiteri, Deferred correction methods for ordinary differential equations, Journal of Scientific Computing 83 (2020) Paper No. 60, 29.

[2] P. Zadunaisky, On the estimation of errors propagated in the numerical integration of ordinary differential equations., Numerische Mathematik 27 (1976/1977) 21–40. URL: http://eudml.org/doc/132429.
[3] A. Dutt, L. Greengard, V. Rokhlin, Spectral deferred correction methods for ordinary differential equations, BIT. Numerical Mathematics 40 (2000) 241–266.
[4] R. Speck, Parallelizing spectral deferred corrections across the method, Computing and Visualization in Science 19 (2018) 75–83. URL: https://doi.org/10.1007/s00791-018-0298-x. doi:10.1007/s00791-018-0298-x.
[5] A. Christlieb, B. Ong, J.-M. Qiu, Comments on high-order integrators embedded within integral deferred correction methods, Communications in Applied Mathematics and Computational Science 4 (2009) 27 – 56. URL: https://doi.org/10.2140/camcos.2009.4.27. doi:10.2140/camcos.2009.4.27.
[6] A. Christlieb, B. Ong, J.-M. Qiu, Integral deferred correction methods constructed with high order Runge-Kutta integrators, Mathematics of Computation 79 (2010) 761–783.
[7] A. J. Christlieb, C. B. Macdonald, B. W. Ong, Parallel high-order integrators, SIAM Journal on Scientific Computing 32 (2010) 818–835.
[8] A. Christlieb, B. Ong, Implicit parallel time integrators, Journal of Scientific Computing 49 (2011) 167–179.
[9] A. J. Christlieb, C. B. Macdonald, B. W. Ong, R. J. Spiteri, Revisionist integral deferred correction with adaptive step-size control, Communications in Applied Mathematics and Computational Science 10 (2015) 1–25.
[10] G. Čaklović, T. Lunet, S. Götschel, D. Ruprecht, Improving efficiency of parallel across the method spectral deferred corrections, SIAM Journal on Scientific Computing 47 (2025) A430–A453. URL: https://doi.org/10.1137/24M1649800. doi:10.1137/24M1649800. arXiv:https://doi.org/10.1137/24M1649800.
[11] K. Böhmer, P. W. Hemker, H. J. Stetter, The Defect Correction Approach, Springer Vienna, Vienna, 1984, pp. 1–32. URL: https://doi.org/10.1007/978-3-7091-7023-6_1. doi:10.1007/978-3-7091-7023-6_1.
[12] M. Minion, Semi-implicit spectral deferred correction methods for ordinary differential equations, Communications in Mathematical Sciences 1 (2003) 471–500.
[13] J. Huang, J. Jia, M. Minion, Accelerating the convergence of spectral deferred correction methods, Journal of Computational Physics 214 (2006) 633–656. URL: http://dx.doi.org/10.1016/j.jcp.2005.10.004. doi:10.1016/j.jcp.2005.10.004.
[14] Y. Xia, Y. Xu, C.-W. Shu, Efficient time discretization for local discontinuous galerkin methods, Discrete and Continuous Dynamical Systems - B 8 (2007) 677–693. URL: https://www.aimsciences.org/article/id/547a34a0-eba5-43df-9e6f-ca0378ffe601. doi:10.3934/dcdsb.2007.8.677.
[15] M. Weiser, Faster sdc convergence on non-equidistant grids by dirk sweeps, BIT Numerical Mathematics 55 (2015) 1219–1241. URL: https://doi.org/10.1007/s10543-014-0540-y. doi:10.1007/s10543-014-0540-y.
[16] R. Speck, D. Ruprecht, M. Emmett, M. Minion, M. Bolten, R. Krause, A multi-level spectral deferred correction method, BIT Numerical Mathematics 55 (2015) 843–867. URL: https://doi.org/10.1007/s10543-014-0517-x. doi:10.1007/s10543-014-0517-x.
[17] M. F. Causley, D. C. Seal, On the convergence of spectral deferred correction methods, Communications in Applied Mathematics and Computational Science 14 (2019) 33–64.
[18] R. Chan, A. Tsai, On explicit two-derivative Runge-Kutta methods, Numerical Algorithms 53 (2010) 171–194.
[19] R. L. Brown, Multi-derivative numerical methods for the solution of stiff ordinary differential equations, Technical Report UIUCDCS-R-74-672, Department of Computer Science, University of Illinois, 1974.
[20] D. Seal, Y. Güçlü, A. Christlieb, High-order multiderivative time integrators for hyperbolic conservation laws, Journal of Scientific Computing 60 (2014) 101–140.
[21] A. J. Christlieb, S. Gottlieb, Z. J. Grant, D. C. Seal, Explicit strong stability preserving multistage two-derivative time-stepping schemes, Journal of Scientific Computing 68 (2016) 914–942.
[22] D. Yakubu, A. Kwami, Implicit two-derivative runge–kutta collocation methods for systems of initial value problems, Journal of the Nigerian Mathematical Society 34 (2015) 128–142.
[23] A. Jaust, J. Schütz, D. C. Seal, Implicit multistage two-derivative discontinuous Galerkin schemes for viscous conservation laws, Journal of Scientific Computing 69 (2016) 866–891.
[24] Z. Grant, S. Gottlieb, D. C. Seal, A strong stability preserving analysis for explicit multistage two-derivative time-stepping schemes based on Taylor series conditions, Communications on Applied Mathematics and Computation 1 (2019) 21–59.
[25] I. B. Aiguobasimwin, R. I. Okuonghae, A class of two-derivative two-step Runge-Kutta methods for non-stiff ODEs, Journal of Applied Mathematics (2019) Art. ID 2459809, 9.
[26] S. Gottlieb, Z. J. Grant, J. Hu, R. Shu, High order strong stability preserving multiderivative implicit and IMEX Runge–Kutta methods with asymptotic preserving properties, SIAM Journal on Numerical Analysis 60 (2022) 423–449.
[27] J. Schütz, D. Seal, A. Jaust, Implicit multiderivative collocation solvers for linear partial differential equations with discontinuous Galerkin spatial discretizations, Journal of Scientific Computing 73 (2017) 1145–1163.
[28] J. Schütz, D. C. Seal, J. Zeifang, Parallel-in-time high-order multiderivative IMEX solvers, Journal of Scientific Computing 90 (2022) 1–33.
[29] J. Schütz, D. Seal, An asymptotic preserving semi-implicit multiderivative solver, Applied Numerical Mathematics 160 (2021) 84–101.
[30] J. Zeifang, J. Schütz, D. Seal, Stability of implicit multiderivative deferred correction methods, BIT Numerical Mathematics (2022).
[31] J. Zeifang, A. Thenery Manikantan, J. Schütz, Time parallelism and Newton-adaptivity of the two-derivative deferred correction discontinuous Galerkin method, Applied Mathematics and Computation 457 (2023) 128198.
[32] A. Thenery Manikantan, J. Schütz, Multi-step hermite-birkhoff predictor-corrector schemes, Applied Numerical Mathematics 205 (2024) 281–295. URL: https://www.sciencedirect.com/science/article/pii/S0168927424001910. doi:https://doi.org/10.1016/j.apnum.2024.07.011.

[33] E. Hairer, G. Wanner, Solving ordinary differential equations II, Springer Series in Computational Mathematics, 1991.
[34] T. B. Benjamin, J. L. Bona, J. J. Mahony, Model equations for long waves in nonlinear dispersive systems, Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences 272 (1972) 47–78. URL: http://www.jstor.org/stable/74079.
[35] S. Bleecke, A. Biswas, D. I. Ketcheson, H. Ranocha, J. Schütz, Asymptotic-preserving and energy-conserving methods for a hyperbolic approximation of the bbm equation, 2025. URL: https://arxiv.org/abs/2511.10044. arXiv:2511.10044.
[36] K. Mattsson, Diagonal-norm upwind sbp operators, Journal of Computational Physics 335 (2017) 283–310. URL: https://www.sciencedirect.com/science/article/pii/S002199911730058X. doi:https://doi.org/10.1016/j.jcp.2017.01.042.
[37] H. Ranocha, A. R. Winters, M. Schlottke-Lakemper, P. Öffner, J. Glaubitz, G. J. Gassner, On the robustness of high-order upwind summation-by-parts methods for nonlinear conservation laws, Journal of Computational Physics 520 (2025) 113471. URL: https://www.sciencedirect.com/science/article/pii/S0021999124007198. doi:https://doi.org/10.1016/j.jcp.2024.113471.
[38] A. Biswas, D. I. Ketcheson, H. Ranocha, J. Schütz, Traveling-wave solutions and structure-preserving numerical methods for a hyperbolic approximation of the korteweg-de vries equation, Journal of Scientific Computing 103 (2025) 90. URL: https://doi.org/10.1007/s10915-025-02898-x. doi:10.1007/s10915-025-02898-x.

Appendix A. Butcher tableau and collocation points

The vector of collocation points and the quadrature matrices corresponding to an m-derivative collocation scheme are denoted as $\mathbf{C}$ and $\mathbf{Q}^{(r)}$ for each $r \leq m$, respectively, in the following subsections. The values are rounded to five decimal places. The collocation points and the quadrature matrices for the below mentioned schemes can also be found in the supplementary material.

Appendix A.1. Collocation scheme: 1D-HBRK-3-2s [4]

$$\mathbf{C} = \begin{pmatrix} \frac{1}{3} \\ 1 \end{pmatrix}, \quad \mathbf{Q}^{(1)} = \begin{pmatrix} \frac{5}{12} & -\frac{1}{12} \\ \frac{3}{4} & \frac{1}{4} \end{pmatrix}.$$

Appendix A.2. Collocation scheme: 2D-HBRK-4-2s

$$\mathbf{C} = \begin{pmatrix} \frac{1}{3} \\ 1 \end{pmatrix}, \quad \mathbf{Q}^{(1)} = \begin{pmatrix} \frac{11}{48} & \frac{5}{48} \\ \frac{9}{16} & \frac{7}{16} \end{pmatrix}, \quad \mathbf{Q}^{(2)} = \begin{pmatrix} -\frac{43}{432} & -\frac{11}{432} \\ -\frac{1}{16} & -\frac{1}{16} \end{pmatrix}.$$

Appendix A.3. Collocation scheme: 3D-HBRK-6-2s

$$\mathbf{C} = \begin{pmatrix} \frac{1}{3} \\ 1 \end{pmatrix}, \quad \mathbf{Q}^{(1)} = \begin{pmatrix} \frac{49}{96} & -\frac{17}{96} \\ \frac{27}{32} & \frac{5}{32} \end{pmatrix}, \quad \mathbf{Q}^{(2)} \begin{pmatrix} \frac{17}{1440} & \frac{73}{1440} \\ \frac{9}{160} & \frac{1}{160} \end{pmatrix}, \quad \mathbf{Q}^{(3)} = \begin{pmatrix} \frac{211}{12960} & -\frac{59}{12960} \\ \frac{3}{160} & -\frac{1}{480} \end{pmatrix}.$$

Appendix A.4. Collocation scheme: 3D-HBRK-7-2s

A general three derivative collocation scheme with collocation points $\tau \neq 1$ is given by

$$\mathbf{C} = \begin{pmatrix} \tau \\ 1 \end{pmatrix}, \quad \mathbf{Q}^{(1)} = \begin{pmatrix} \frac{\tau}{2} - \frac{5\tau^2 - 4\tau + 1}{2(\tau-1)^5} - \frac{1}{2} & \frac{\tau^4(\tau^2 - 4\tau + 5)}{2(\tau-1)^5} \\ -\frac{5\tau^2 - 4\tau + 1}{2(\tau-1)^5} & \frac{5\tau^2 - 4\tau + 1}{2(\tau-1)^5} + 1 \end{pmatrix},$$

$$\mathbf{Q}^{(2)} = \begin{pmatrix} -\frac{\tau^2(\tau^4 - 6\tau^3 + 15\tau^2 - 20\tau + 5)}{10(\tau-1)^4} & \frac{\tau^4(\tau^2 - 6\tau + 10)}{10(\tau-1)^4} \\ \frac{10\tau^2 - 6\tau + 1}{10(\tau-1)^4} & \frac{15\tau^2 - 14\tau + 4}{10(\tau-1)^4} - \frac{1}{2} \end{pmatrix},$$

$$\mathbf{Q}^{(3)} = \begin{pmatrix} \frac{\tau^3(\tau^3 - 6\tau^2 + 15\tau - 20)}{120(\tau-1)^3} & \frac{\tau^4(\tau^2 - 6\tau + 15)}{120(\tau-1)^3} \\ -\frac{15\tau^2 - 6\tau + 1}{120(\tau-1)^3} & \frac{45\tau^2 - 54\tau + 19}{120(\tau-1)^3} + \frac{1}{6} \end{pmatrix}.$$

This is a sixth-order scheme in general, and the scheme 3D-HBRK-6-2s from above is obtained for $\tau = \frac{1}{3}$. If we choose τ such that

$$-\frac{\tau^3}{2880} + \frac{\tau^2}{4800} - \frac{\tau}{14400} + \frac{1}{100800} = 0, \tag{A.1}$$

the scheme is of order seven, which defines the scheme 3D-HBRK-7-2s. For the numerical results, we used an approximation (error level: 10^{-16}) to τ from (A.1) given by $\tau = \frac{9333740}{36594761}$.