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CONVERGENCE OF MULTILEVEL SPECTRAL DEFERRED CORRECTIONS

GITTE KREMLING AND ROBERT SPECK

The spectral deferred correction (SDC) method is a class of iterative solvers for ordinary differential equations (ODEs). It can be interpreted as a preconditioned Picard iteration for the collocation problem. The convergence of this method is well known, for suitable problems it gains one order per iteration up to the order of the quadrature method of the collocation problem provided. This appealing feature enables an easy creation of flexible, high-order accurate methods for ODEs. A variation of SDC are multilevel spectral deferred corrections (MLSDC). Here, iterations are performed on a hierarchy of levels and an FAS correction term, as in nonlinear multigrid methods, couples solutions on different levels. While there are several numerical examples which show its capabilities and efficiency, a theoretical convergence proof is still missing. We address this issue. A proof of the convergence of MLSDC, including the determination of the convergence rate in the time-step size, will be given and the results of the theoretical analysis will be numerically demonstrated. It turns out that there are restrictions for the advantages of this method over SDC regarding the convergence rate.

1. Introduction

The original spectral deferred correction (SDC) method for solving ordinary differential equations (ODEs), a variant of the defect and deferred correction methods developed in the 1960s [3; 11; 27; 31], was introduced in [12] and subsequently improved, e.g., in [19; 21; 25; 26]. It relies on a discretization of the initial value problem in terms of a collocation problem which is then iteratively solved using a preconditioned fixed-point iteration. The iterative structure of SDC has been proven to provide many opportunities for algorithmic and mathematical improvements. These include the option of using Newton–Krylov schemes such as the Newton-GMRES method to solve the resulting preconditioned nonlinear systems, leading to the so-called Krylov deferred correction methods [21; 22]. Various semi-implicit and multi-implicit formulations have been explored [6; 15; 24; 25; 26]. In the last decade, SDC has been applied, e.g., to gas dynamics and incompressible or

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reactive flows [7; 26] as well as to fast-wave slow-wave problems [28] or particle dynamics [34]. The generalized integral deferred correction framework includes further variations of SDC, where the used discretization approach is not limited to collocation methods [9; 10]. Moreover, the SDC approach was used to derive efficient parallel-in-time solvers addressing the needs of modern high-performance computing architectures [13; 29]. Here, we will focus on the multilevel extension of SDC, namely multilevel spectral deferred corrections (MLSDC), which was introduced in [4]. It uses a multigrid-like approach to solve the collocation problem with SDC iterations (now called "sweeps" in this context) being performed on the individual levels. The solutions on the different levels are then coupled using the full approximation scheme (FAS) coming from nonlinear multigrid methods. This variation was designed to improve the efficiency of the method by shifting some of the work to coarser, less expensive levels. While there are several numerical examples which show the correctness and efficiency of MLSDC [14; 18; 30], a theoretical proof of its convergence is still missing. The convergence of SDC, however, was already extensively examined [8; 15; 19; 21; 32; 35]. It could be shown that, under certain conditions, the method gains one order per iteration up to the accuracy of the solution of the collocation problem. The aim of this work now is to prove statements on the convergence behavior of MLSDC using similar concepts and ideas as they were used in the convergence proof of SDC, in particular the one presented in [32].

For that, we first review SDC along with one of its existing convergence proofs, forming the basis for the following convergence analysis of MLSDC. Then, MLSDC is described and a first convergence theorem is provided. The theorem specifically states that MLSDC behaves at least as well as SDC does. Since this result contradicts our intuitive expectations in that we would assume the multilevel extension to be more efficient than the original one, we will again examine the convergence proof in greater detail, now for a specific choice of transfer operators between the different levels. As a result, a second theorem on the convergence of MLSDC will be derived, describing an improved behavior of the method if particular conditions are fulfilled. More specifically, we will provide theoretical guidelines for parameter choices in practical applications of MLSDC in order to achieve this improved efficiency. Finally, the theoretical results will be verified by numerical examples.

2. Spectral deferred corrections

In the following, SDC is presented as preconditioned Picard iterations for the collocation problem. The used approach and notations are substantially based on [4; 5]. First, the collocation problem for a generic initial value problem is explained. Then, SDC is described as a solver for this problem and compact notations are introduced. Finally, an existing theorem on the convergence of SDC, including its proof, is presented.

2A. *SDC and the collocation problem.* Consider the autonomous initial value problem (IVP)

$$u'(t) = f(u(t)), \quad t \in [t_0, t_1],$$

 $u(t_0) = u_0,$
(1)

with u(t), $u_0 \in \mathbb{C}^N$ and $f : \mathbb{C}^N \to \mathbb{C}^N$, $N \in \mathbb{N}$. To guarantee the existence and uniqueness of the solution, f is required to be Lipschitz continuous. Since a high-order method shall be used, f is additionally assumed to be sufficiently smooth.

The IVP can be written as

$$u(t) = u_0 + \int_{t_0}^t f(u(s)) ds, \quad t \in [t_0, t_1],$$

and choosing M quadrature nodes τ_1, \ldots, τ_M within the time interval such that $t_0 \le \tau_1 < \tau_2 < \cdots < \tau_M = t_1$, the integral is now approximated using a spectral quadrature rule like Gauss–Radau. This approach results in the discretized system of equations

$$u_m = u_0 + \Delta t \sum_{j=1}^{M} q_{m,j} f(u_j), \quad m = 1, \dots, M,$$
 (2)

where $u_m \approx u(\tau_m)$, $\Delta t = t_1 - t_0$ denotes the time step size and $q_{m,j}$ represent the quadrature weights for the unit interval with

$$q_{m,j} = \frac{1}{\Delta t} \int_{t_0}^{\tau_m} l_j(s) \, ds.$$

Here, l_j represents the j-th Lagrange polynomial corresponding to the set of nodes $(\tau_m)_{1 \le m \le M}$. We can combine these M equations into the following system of linear or nonlinear equations, defining the collocation problem:

$$C(U) := (I_{MN} - \Delta t(Q \otimes I_N)F)(U) = U_0, \tag{3}$$

where $U := (u_1, u_2, \dots, u_M)^T \in \mathbb{C}^{MN}$, $U_0 := (u_0, u_0, \dots, u_0)^T \in \mathbb{C}^{MN}$, $Q := (q_{m,j})_{1 \le m,j \le M}$ is the matrix gathering the quadrature weights, the vector function F is given by $F(U) := (f(u_1), f(u_2), \dots, f(u_M))^T$ and I_{MN} , I_N are the identity matrices of dimensions MN and N.

As described above, the solution U of the collocation problem approximates the solution of the initial value problem (1). With this in mind, the following theorem, referring to [16, Theorem 7.10], provides a statement on its order of accuracy.

Theorem 2.1. The solution $U = (u_1, u_2, ..., u_M)^T \in \mathbb{C}^{MN}$ of the collocation problem defined by (3) approximates the solution u of the IVP (1) at the collocation

nodes. In particular, for $\overline{U} := (u(\tau_1), \dots, u(\tau_M))^T$ the following error estimation applies:

$$\|\overline{U} - U\|_{\infty} \le C_1 \Delta t^{M+1} \|u\|_{M+1},$$

where C_1 is independent of Δt , M denotes the number of nodes and $||u||_{M+1}$ represents the maximum norm of $u^{(M+1)}$, the (M+1)-th derivative of u.

Interpreting the collocation problem as a discretization method with discretization parameter $n := \Delta t^{-1}$, the theorem shows that the discrete approximation U defined by the collocation problem converges with order M+1 to the solution \overline{U} of the corresponding IVP.

Since the system of equations (3) defining the collocation problem has an unfavorable structure with Q gathering the quadrature weights being fully populated, a direct solution is not advisable, in particular if the right-hand side of the ODE is nonlinear. An iterative method to solve the problem is SDC.

The standard Picard iteration for the collocation problem (3) is given by

$$U^{(k+1)} = U^{(k)} + (U_0 - C(U^{(k)}))$$

= $U_0 + \Delta t(Q \otimes I_N) F(U^{(k)}).$ (4)

As this method only converges for very small step sizes Δt , using a preconditioner to increase range and speed of convergence is reasonable. The SDC-type preconditioners are defined by

$$P(U) = (I_{MN} - \Delta t (Q_{\Delta} \otimes I_N) F)(U),$$

where the matrix $Q_{\Delta} = (q_{\Delta_{m,j}})_{1 \leq m,j \leq M} \approx Q$ is formed by the use of a simpler quadrature rule. In particular, Q_{Δ} is typically a lower triangular matrix, such that solving the system can be easily done by forward substitution.

Common choices for Q_{Δ} include the matrix

$$Q_{\Delta} = \frac{1}{\Delta t} \begin{pmatrix} \Delta \tau_1 & & \\ \Delta \tau_1 & \Delta \tau_2 & & \\ \vdots & \vdots & \ddots & \\ \Delta \tau_1 & \Delta \tau_2 & \dots & \Delta \tau_M \end{pmatrix}$$

with $\Delta \tau_m = \tau_m - \tau_{m-1}$ for m = 2, ..., M and $\Delta \tau_1 = \tau_1 - t_0$ representing the right-sided rectangle rule. Similarly, the left-sided rectangle rule [28] or a part of the LU decomposition of the matrix Q [33] are chosen. The theoretical considerations in the next chapters do not rely on a specific matrix Q_{Δ} . However, in the numerical examples the right-sided rectangle rule as given above is used.

By the use of such an operator to precondition the Picard iteration (4), the following iterative method for solving the collocation problem, which constitutes

the SDC iteration [12; 21], is obtained:

$$(I_{MN} - \Delta t(Q_{\Delta} \otimes I_N)F)(U^{(k+1)}) = U_0 + \Delta t((Q - Q_{\Delta}) \otimes I_N)F(U^{(k)}).$$
 (5)

Written down line-by-line, this formulation recovers the original SDC notation given in [12]. A more implicit formulation is given by

$$U^{(k+1)} = U_0 + \Delta t(Q_{\Lambda} \otimes I_N) F(U^{(k+1)}) + \Delta t((Q - Q_{\Lambda}) \otimes I_N) F(U^{(k)})$$
 (6)

and this will be used for the following convergence considerations.

2B. Convergence of SDC. There already exist several approaches proving the convergence of SDC, particularly those presented in [8; 15; 19; 21; 32; 35]. Here, we will focus on the idea of the proof from [32] as it uses the previously introduced matrix formulation of SDC, needed for an appropriate adaptation for a convergence proof of MLSDC, and simultaneously, provides a general result for linear and nonlinear initial value problems. We will review the idea of this proof in some detail to introduce the notation and the key ideas. This is followed by a concise discussion on stability and convergence of SDC in the sense of one-step ODE solvers.

The approach in [32] relies on a split of the local truncation error (LTE). The key concept used in the proof is a property of the operators QF(U) and $Q_{\Delta}F(U)$, respectively, which can be interpreted as a kind of extended Lipschitz continuity. It is presented in the following lemma using the previously introduced notation. For reasons of readability, the sizes of the identity matrices are no longer denoted here.

Lemma 2.2. If $f: \mathbb{C}^N \to \mathbb{C}^N$ is Lipschitz continuous, the following estimates apply:

$$\|\Delta t(Q \otimes I)(F(U_1) - F(U_2))\|_{\infty} \le C_2 \Delta t \|U_1 - U_2\|_{\infty},$$

$$\|\Delta t(Q_{\Delta} \otimes I)(F(U_1) - F(U_2))\|_{\infty} \le C_3 \Delta t \|U_1 - U_2\|_{\infty},$$

where the constants C_2 and C_3 are dependent on the Lipschitz constant L, but independent of Δt and $U_1, U_2 \in \mathbb{C}^{NM}$.

Proof. This can be shown directly using the definition of the maximum norm, the Lipschitz continuity of f and the compatibility between maximum absolute row sum norm for matrices and maximum norm for vectors.

Remark 2.3. For a system of ODEs stemming from a discretized PDE, the constants C_2 and C_3 may depend on the spatial resolution given by some grid spacing Δx , because the Lipschitz constant of f may depend on it. In this case we have $C_2 = C_2(\Delta x^{-d})$, $C_3 = C_3(\Delta x^{-d})$ for $d \in \mathbb{N}$. For example, using second-order finite differences in space for the heat equation results in the ODE system u' = Au with matrix $A \in \mathcal{O}(\Delta x^{-2})$, i.e., d = 2 in this case. This has to be kept in mind for most of the upcoming results and we will address this point separately in remarks

where appropriate. This will be particularly relevant for the convergence results in Section 3B, where the spatial discretization plays a key role. Note, however, that this is a rather pessimistic estimate. When focusing on spatial operators with more restrictive properties (e.g., linearity) or when using a specific matrix Q_{Δ} , the convergence results can be improved substantially, both in terms of constants and time-step size restrictions. For SDC, this has been already done; see, e.g., [33].

The following theorem provides a convergence statement for SDC using the presented lemma in the proof.

Theorem 2.4. Consider a generic initial value problem like (1) with a Lipschitz-continuous function f on the right-hand side.

If the step size Δt is sufficiently small, SDC converges linearly to the solution U of the collocation problem with a convergence rate in $\mathcal{O}(\Delta t)$, i.e., the following estimate for the error of the k-th iterate $U^{(k)}$ of SDC compared to the solution of the collocation problem is valid:

$$||U - U^{(k)}||_{\infty} \le C_4 \Delta t ||U - U^{(k-1)}||_{\infty},$$
 (7)

where the constant C_4 is independent of Δt .

If, additionally, the solution of the initial value problem u is (M+1)-times continuously differentiable, the LTE of SDC compared to the solution \overline{U} of the ODE can be bounded by

$$\|\overline{U} - U^{(k)}\|_{\infty} \le C_5 \Delta t^{k_0 + k} \|u\|_{k_0 + 1} + C_6 \Delta t^{M+1} \|u\|_{M+1}$$

$$= \mathcal{O}(\Delta t^{\min(k_0 + k, M + 1)}), \tag{8}$$

where the constants C_5 and C_6 are independent of Δt , k_0 denotes the approximation order of the initial guess $U^{(0)}$ and $\|u\|_p$ is defined by $\|u^{(p)}\|_{\infty}$.

Proof. We again closely follow [32] here. According to the definition of the collocation problem (3) and an SDC iteration (6),

$$\begin{split} \|U - U^{(k)}\|_{\infty} \\ &= \|\Delta t(Q \otimes I)(F(U) - F(U^{(k-1)})) + \Delta t(Q_{\Delta} \otimes I)(F(U^{(k-1)}) - F(U^{(k)}))\|_{\infty}. \end{split}$$

Combining this with the triangle inequality and Lemma 2.2, we obtain

$$||U - U^{(k)}||_{\infty} \le C_2 \Delta t ||U - U^{(k-1)}||_{\infty} + C_3 \Delta t ||U^{(k-1)} - U^{(k)}||_{\infty}.$$

Applying the triangle inequality again yields

$$||U - U^{(k)}||_{\infty} \le \widetilde{C}_1 \Delta t ||U - U^{(k-1)}||_{\infty} + C_3 \Delta t ||U - U^{(k)}||_{\infty},$$

where here and in the following, we use variables in the form of \widetilde{C}_i to denote

temporary arising constants. We continue by subtracting $C_3\Delta t \|U - U^{(k)}\|_{\infty}$ from both sides and dividing by $1 - C_3\Delta t$ which results in

$$\|U - U^{(k)}\|_{\infty} \le \frac{\widetilde{C}_1}{1 - C_3 \Delta t} \Delta t \|U - U^{(k-1)}\|_{\infty}.$$

If the step size is sufficiently small, in particular,

$$C_3 \Delta t < 1, \tag{9}$$

the estimate

$$\frac{\widetilde{C}_1}{1 - C_3 \Delta t} \le C_4 \tag{10}$$

is valid, which concludes the proof for (7).

Continuing with recursive insertion, we get

$$||U - U^{(k)}||_{\infty} \le \widetilde{C}_2 \Delta t^k ||U - U^{(0)}||_{\infty}.$$

Since $U^{(0)}$ is assumed to be an approximation of k_0 -th order, we further know that

$$\|\overline{U} - U^{(0)}\| \le \widetilde{C}_3 \Delta t^{k_0} \|u\|_{k_0+1}.$$

This estimation together with the triangle inequality and the error estimation for the solution of the collocation problem stated in Theorem 2.1 yields

$$||U - U^{(k)}||_{\infty} \le \widetilde{C}_2 \Delta t^k (||\overline{U} - U||_{\infty} + ||\overline{U} - U^{(0)}||_{\infty})$$

$$< \widetilde{C}_4 \Delta t^{M+k+1} ||u||_{M+1} + C_6 \Delta t^{k_0+k} ||u||_{k_0+1}. \tag{11}$$

Altogether,

$$\begin{split} \|\overline{U} - U^{(k)}\|_{\infty} &\leq \|\overline{U} - U\|_{\infty} + \|U - U^{(k)}\|_{\infty} \\ &\leq C_1 \Delta t^{M+1} \|u\|_{M+1} + \widetilde{C}_4 \Delta t^{M+k+1} \|u\|_{M+1} + C_6 \Delta t^{k_0+k} \|u\|_{k_0+1} \\ &= (C_1 + \widetilde{C}_4 \Delta t^k) \Delta t^{M+1} \|u\|_{M+1} + C_6 \Delta t^{k_0+k} \|u\|_{k_0+1}. \end{split}$$

Since the step size Δt is assumed to be sufficiently small, i.e., bounded above, the estimate

$$C_1 + \widetilde{C}_4 \Delta t^k \le C_5$$

is valid, which finally concludes the proof for (8).

Remark 2.5. Note that if the right-hand side of the ODE comes from a discretized PDE with a given spatial resolution, no additional restriction is posed. In this case, $C_3 = C_3(\Delta x^{-d}) = \widetilde{C}_5 \Delta x^{-d}$ for some constant \widetilde{C}_5 , so that the condition (9) becomes $\widetilde{C}_5 \Delta t < \Delta x^d$. Since we did not specify Q_Δ here, the SDC iterations can be explicit or implicit and it is natural to obtain such a restriction on the time-step size. Similar

restrictions can be found in other convergence results for SDC; see, e.g., [8; 15; 21]. Condition (10) then translates to

$$C_4 \ge \frac{\widetilde{C}_1}{1 - C_3 \Delta t} = \frac{\widetilde{C}_6 \Delta x^{-d}}{1 - \widetilde{C}_5 \Delta x^{-d} \Delta t} = \frac{\widetilde{C}_6}{\Delta x^d - \widetilde{C}_5 \Delta t}$$

for some constant \widetilde{C}_6 . Assuming a fixed distance between Δx^p and $\widetilde{C}_5\Delta t$ with $\Delta x^d - \widetilde{C}_5\Delta t = \delta$ we can write $C_4 = C_4(\delta^{-1})$ to indicate the dependence of C_4 on this distance and not Δx^p or Δt alone. Thus, C_4 does not pose an additional restriction to the convergence of SDC. Note that for C_5 we have $C_5 = C_5(\delta^{-(k+1)})$, so that the choice of δ can increase the constant in front of the Δt^{k_0+k} -term quite substantially, but it does not affect the Δt^{M+1} -term coming from the collocation problem itself.

Remark 2.6. More generally, the constant C_4 depends on the Lipschitz constant L of f with

$$C_4 = C_4(k) \approx \widetilde{C} \frac{L^k}{(1 - L\Delta t)^k} \in \mathcal{O}(L^k)$$

for iteration k and some constant \widetilde{C} , if $L\Delta t$ is small enough. Thus, for L>1 the "constant" $C_4=C_4(k)$ can grow significantly with k. When running numerical convergence studies for a fixed Δt , the gain in the error when going from one iterate $U^{(k)}$ to the next one $U^{(k+1)}$ may therefore be not as large as the asymptotic behavior in Δt suggests. This is true for all results found in this paper.

The theorem can be read as a convergence statement for SDC. In particular, the first estimation (7) shows that SDC, interpreted as an iterative method to solve the collocation problem, converges linearly to the solution of the collocation problem with a convergence rate of $\mathcal{O}(\Delta t)$ if $C_4\Delta t < 1$. The second part of the theorem, (8) shows that SDC, in the sense of a discretization method, converges with order $\min(k_0 + k, M + 1)$ to the solution of the initial value problem. In other words, the method gains one order per iteration, limited by the selected number of nodes used for discretization.

We can now immediately extend this result by looking at the right endpoint of the single time interval (which, in our case, is equal to the last collocation node). There, the convergence rate is limited not by the number of collocation nodes, but by the order of the quadrature.

Corollary 2.7. Consider a generic initial value problem like (1) with a Lipschitz-continuous function f on the right-hand side. Furthermore, let the solution of the initial value problem u be (2M)-times continuously differentiable.

Then, if the step size Δt is sufficiently small, the error of the k-th iteration of SDC, defined by (6), at the last collocation node $u_M^{(k)}$, compared to the exact value

at this point $u(\tau_M)$, can be bounded by

$$\|u(\tau_{m}) - u_{M}^{(k)}\|_{\infty}$$

$$\leq C_{7} \Delta t^{2M} \max(\|u\|_{2M}, \|u\|_{M+1}) + C_{8} \Delta t^{k_{0}+k} \max(\|u\|_{k_{0}+1}, \|u\|_{M+1})$$

$$= \mathcal{O}(\Delta t^{\min(k_{0}+k, 2M)}), \tag{12}$$

where the constants C_7 and C_8 are independent of Δt , k_0 denotes the approximation order of the initial guess $U^{(0)}$ and $\|u\|_p$ is defined by $\|u^{(p)}\|_{\infty}$.

Proof. The proof mainly relies on the interpretation of the solution of the collocation problem evaluated at the last node τ_M as the result of a Radau method with M stages. With this in mind, the well-known convergence, or in this case, consistency order of Radau methods yields the estimate [17]

$$\|u(\tau_M) - u_M\|_{\infty} \leq \widetilde{C}_1 \Delta t^{2M} \|u\|_{2M}$$

where \widetilde{C}_1 is independent of Δt . Here and in the following, temporary arising constants will again be denoted by symbols like \widetilde{C}_i . However, they are separately defined and thus, do not correspond to the ones used in previous proofs.

To use this estimation, we first have to apply the triangle inequality to the left-hand side of (12), in particular,

$$\|u(\tau_m) - u_M^{(k)}\|_{\infty} \le \|u(\tau_m) - u_M\|_{\infty} + \|u_M - u_M^{(k)}\|_{\infty}.$$
(13)

Then, with the definition of the vector $R := (0, ..., 0, 1) \in \mathbb{R}^{1 \times M}$ which, multiplied with another vector, only captures its last value, the second term on the right-hand side of the above equation can be transferred to

$$\begin{aligned} \|u_M - u_M^{(k)}\|_{\infty} &= \|RU - RU^{(k)}\|_{\infty} \le \|R\|_{\infty} \|U - U^{(k)}\|_{\infty} = \|U - U^{(k)}\|_{\infty} \\ &\le \widetilde{C}_2 \Delta t^{M+k+1} \|u\|_{M+1} + C_6 \Delta t^{k_0+k} \|u\|_{k_0+1}, \end{aligned}$$

where the last estimate comes from (11) in the proof of Theorem 2.4. Finally, by inserting all these results in (13), we obtain

$$\begin{split} \|u(\tau_m) - u_M^{(k)}\|_{\infty} &\leq \|u(\tau_m) - u_M\|_{\infty} + \|U - U^{(k)}\|_{\infty} \\ &\leq \widetilde{C}_1 \Delta t^{2M} \|u\|_{2M} + \widetilde{C}_2 \Delta t^{M+k+1} \|u\|_{M+1} + C_5 \Delta t^{k_0+k} \|u\|_{k_0+1}. \end{split}$$

Note that the leading order of this term is essentially independent of the summand corresponding to Δt^{M+k+1} . For Δt small enough, this result can be seen by a case analysis for k. For $k+1 \geq M$, the considered summand is dominated by $\Delta t^{2M} \geq \Delta t^{M+k+1}$ and thus can be disregarded in terms of leading order analysis. In the other case, i.e., for k+1 < M, the considered summand will, however, be greater than the one of order 2M. So, we will instead compare it to Δt^{k_0+k} in this case. Since the number of collocation nodes M is usually chosen to be greater than the

approximation order k_0 of the initial guess, the relation $\Delta t^{k_0+k} \ge \Delta t^{M+k+1}$ applies and hence, k_0+k will be the leading order for k < M. Thus, the considered summand Δt^{M+k+1} is again dominated by another term and can be disregarded concerning the overall asymptotic behavior. These considerations lead to the estimation

$$\|u(\tau_m) - u_M^{(k)}\|_{\infty} \le \widetilde{C}_3 \Delta t^{2M} \max(\|u\|_{2M}, \|u\|_{M+1}) + C_5 \Delta t^{k_0+k} \|u\|_{k_0+1}$$

for $k \ge M$ and

$$\|u(\tau_m) - u_M^{(k)}\|_{\infty} \le \widetilde{C}_1 \Delta t^{2M} \|u\|_{2M} + \widetilde{C}_4 \Delta t^{k_0 + k} \max(\|u\|_{k_0 + 1}, \|u\|_{M + 1})$$

for k < M, which can be combined to

$$||u(\tau_m) - u_M^{(k)}||_{\infty} \\ \leq C_7 \Delta t^{2M} \max(||u||_{2M}, ||u||_{M+1}) + C_8 \Delta t^{k_0+k} \max(||u||_{k_0+1}, ||u||_{M+1}),$$

concluding the proof.

With this corollary, it can be concluded that SDC, in the sense of a single-step method to solve ODEs, is consistent of order $\min(k_0 + k - 1, 2M - 1)$. To extend this result towards a statement on the convergence order of the method an additional proof of its stability is needed. The following theorem provides an appropriate result for SDC.

Theorem 2.8. Consider a generic initial value problem like (1) with a Lipschitz-continuous function f on the right-hand side. If the step size Δt is sufficiently small and an appropriate initial guess is used, the SDC method, defined by (5), is stable.

Proof. As usual for single-step methods, we will prove the Lipschitz continuity of the increment function of SDC in order to prove the stability of the method.

A general single-step method is defined by the formula

$$u_{n+1} = u_n + \Delta t \phi(u_n),$$

where u_n denotes the approximation at the time step t_n and $\phi(u_n)$ is the increment function. Our aim now is to identify the specific increment function ϕ corresponding to SDC and to, subsequently, show its Lipschitz continuity, i.e., prove the validity of $|\phi(u_n) - \phi(v_n)| \le L_{\phi}|u_n - v_n|$.

First, note that the *k*-th iteration of SDC $u_m^{(k)}$ at an arbitrary collocation node τ_m $(1 \le m \le M)$ can be written as

$$u_m^{(k)} = u_n + r_m^{(k)}$$
 with
$$r_m^{(k)} := \Delta t (Q_\Delta F(U_n + r^{(k)}))_m + \Delta t ((Q - Q_\Delta) F(U_n + r^{(k-1)}))_m,$$

$$r^{(k)} := (r_1^{(k)}, \dots, r_M^{(k)})^T \quad \text{and} \quad U_n = (u_n, \dots, u_n)^T$$

for $k \ge 1$ according to a line-wise consideration of (5), where the subscript m denotes

the *m*-th line of the vectors. Consequently, the corresponding approximation at the time step $t_{n+1} = \tau_M$ can be written as

$$u_{n+1} = u_M^{(k)} = u_n + r_M^{(k)} =: u_n + \Delta t \phi^{(k)}(u_n) \quad \text{with } \phi^{(k)}(u_n) = \frac{1}{\Delta t} r_M^{(k)}.$$

Hence, we have found an appropriate, albeit implicit definition for the increment function $\phi^{(k)}$ of SDC.

As a second step, there follows an investigation on the Lipschitz continuity of this function. For that, we start by noting that

$$|\phi^{(k)}(u_n) - \phi^{(k)}(v_n)| = \frac{1}{\Delta t} |r_M^{(k)} - s_M^{(k)}| \le \frac{1}{\Delta t} ||r^{(k)} - s^{(k)}||_{\infty}, \tag{14}$$

where the r-terms belong to u_n and the s-terms to v_n . Now, we will further analyze the term $||r^{(k)} - s^{(k)}||$. With the insertion of the corresponding definitions and an application of the triangle inequality,

$$||r^{(k)} - s^{(k)}|| \le ||\Delta t Q_{\Delta}(F(U_n + r^{(k)}) - F(V_n + s^{(k)}))|| + ||\Delta t (Q - Q_{\Delta})(F(U_n + r^{(k-1)}) - F(V_n + s^{(k-1)}))||.$$

The use of Lemma 2.2 and a reapplication of the triangle inequality further yield

$$||r^{(k)} - s^{(k)}|| \le \widetilde{C}_1 \Delta t (|u_n - v_n| + ||r^{(k)} - s^{(k)}|| + ||r^{(k-1)} - s^{(k-1)}||).$$

Continuing with the same trick as in the proof of Theorem 2.4, namely a subtraction of $\widetilde{C}_1 \Delta t \| r^{(k)} - s^{(k)} \|$ and a subsequent division by $1 - \widetilde{C}_1 \Delta t$, we get

$$||r^{(k)} - s^{(k)}|| \le \frac{\widetilde{C}_1}{1 - \widetilde{C}_1 \Delta t} \Delta t (|u_n - v_n| + ||r^{(k-1)} - s^{(k-1)}||).$$

If the step size Δt is sufficiently small, the estimation

$$\frac{\widetilde{C}_1}{1 - \widetilde{C}_1 \Delta t} \le \widetilde{C}_2$$

applies and a subsequent iterative insertion further yields

$$||r^{(k)} - s^{(k)}|| \le \widetilde{C}_3 \sum_{l=1}^k \Delta t^l |u_n - v_n| + \widetilde{C}_4 \Delta t^k ||r^{(0)} - s^{(0)}||.$$

With the insertion of this result in (14), finally, we have

$$|\phi^{(k)}(u_n) - \phi^{(k)}(v_n)| \le C \sum_{l=0}^{k-1} \Delta t^l |u_n - v_n| + C \Delta t^{k-1} ||r^{(0)} - s^{(0)}||.$$

The value of $||r^{(0)} - s^{(0)}||$ depends on the initial guess for the SDC iterations. If, for example, the value at the last time step is used as the initial guess for all collocation

nodes, i.e., $U^{(0)} = U_n$ and $V^{(0)} = V_n$, we get $||r^{(0)} - s^{(0)}|| = 0 - 0 = 0$. If, by contrast, the initial guess is chosen to be zero, $||r^{(0)} - s^{(0)}|| = |u_n - v_n|$. Both variants, however, guarantee that $|\phi^k(u_n) - \phi^k(v_n)| \le C|u_n - v_n|$ which was to be shown.

Remark 2.9. Note that the assumed upper bound for the step size Δt in the previous theorem is the same as the one in Corollary 2.7, describing the consistency of SDC. Hence, there is no additional restriction for the convergence of the method.

Combined with Theorem 2.8, Corollary 2.7 can be extended towards a convergence theorem for SDC regarded in the context of single-step methods to solve ODEs. Specifically, the proven stability of the method allows a direct transfer of the order of consistency to the order of convergence. Consequently, it follows that SDC, in the sense of a single-step method, converges with order $\min(k_0 + k - 1, 2M - 1)$.

In the next section, MLSDC, a multilevel extension of SDC, is described. It is motivated by the assumption that additional iterations on a coarser level may increase the order of accuracy while keeping the costs rather low. In Section 5, we will investigate whether this assumption holds true, i.e., if the convergence order is indeed increased by the additional execution of relatively low-cost iterations on the coarse level.

3. Multilevel spectral deferred corrections

Multilevel SDC (MLSDC) is a method that uses a multigrid-like approach to solve the collocation problem (3). It is an extension of SDC in which the iterations, now called "sweeps" in this context, are computed on a hierarchy of levels and the individual solutions are coupled in the same manner as used in the full approximation scheme (FAS) for nonlinear multigrid methods.

The different levels are typically created by using discretizations of various resolutions. In this paper, only the two-level algorithm is considered. For this purpose, let Ω_h denote the fine level and Ω_H the coarse one. Then, U_h denotes the discretized vector on Ω_h . Furthermore, C_h , F_h and Q_h are the discretizations of the operators and the quadrature matrix. Likewise, U_H , C_H , F_H and Q_H represent the corresponding values for the discretization parameter H.

Here, we will consider two coarsening strategies. The first one is a rediscretization in time at the collocation problem, i.e., a reduction of collocation nodes. The second possibility, only applicable if a partial differential equation has to be solved, is a rediscretization in space, i.e., the use of fewer variables for the conversion into an ODE.

Since it is necessary to perform computations on different levels, a method to transfer vectors between the individual levels is needed. For this purpose, let I_H^h denote the operator that transfers a vector from the coarse level Ω_H to the fine

level Ω_h . This operator is called the interpolation operator. I_h^H , on the other hand, shall represent the operator for the reverse direction. It is called the restriction operator. Both operators together are called transfer operators.

In detail, the MLSDC two-level algorithm consists of these four steps. Note that for better readability, the enlargements of the matrices Q and Q_{Δ} by applying the Kronecker product with the identity matrix are no longer indicated.

(1) Compute the τ -correction as the difference between coarse and fine level:

$$\tau = C_H(I_h^H U_h^{(k)}) - I_h^H C_h(U_h^{(k)})$$

$$= I_h^H (\Delta t Q_h F_h(U_h^{(k)})) - \Delta t Q_H F_H(I_h^H U_h^{(k)}). \tag{15}$$

(2) Perform an SDC sweep to approximate the solution of the modified collocation problem on the coarse level

$$C_H(U_H) = U_{0,H} + \tau$$
 (16)

on Ω_H , beginning with $I_h^H U_h^{(k)}$:

$$U_H^{(k+1/2)} = U_{0,H} + \tau + \Delta t Q_{\Delta,H} F_H(U_H^{(k+1/2)}) + \Delta t (Q_H - Q_{\Delta,H}) F_H(I_h^H U_h^{(k)}). \tag{17}$$

(3) Compute the coarse level correction:

$$U_h^{(k+1/2)} = U_h^{(k)} + I_H^h(U_H^{(k+1/2)} - I_h^H U_h^{(k)}).$$
(18)

(4) Perform an SDC sweep to approximate the solution of the original collocation problem

$$C(U_h) = U_{0,h}$$

on Ω_h , beginning with $U_h^{(k+1/2)}$:

$$U_h^{(k+1)} = U_{0,h} + \Delta t Q_{\Delta,h} F_h(U_h^{(k+1)}) + \Delta t (Q_h - Q_{\Delta,h}) F_h(U_h^{(k+1/2)}).$$
 (19)

3A. A first convergence proof. Here, we will extend the existing convergence proof for SDC, as presented in Theorem 2.4, to prove the convergence of its multilevel extension MLSDC. The following theorem provides an appropriate convergence statement. In the proof, we use very similar ideas to those in the proof for the convergence of SDC.

Theorem 3.1. Consider a generic initial value problem like (1) with a Lipschitz-continuous function f on the right-hand side.

If the step size Δt is sufficiently small, MLSDC converges linearly to the solution of the collocation problem with a convergence rate in $\mathcal{O}(\Delta t)$, i.e., the following estimate for the error of the k-th iterate $U_h^{(k)}$ of MLSDC compared to the solution of

the collocation problem U_h is valid:

$$||U_h - U_h^{(k)}||_{\infty} \le C_9 \Delta t ||U_h - U_h^{(k-1)}||_{\infty}, \tag{20}$$

where the constant C_9 is independent of Δt .

If, additionally, the solution of the initial value problem u is (M+1)-times continuously differentiable, the LTE of MLSDC compared to the solution of the ODE can be bounded by

$$\|\overline{U} - U_h^{(k)}\|_{\infty} \le C_{10} \Delta t^{k_0 + k} \|u\|_{k_0 + 1} + C_{11} \Delta t^{M + 1} \|u\|_{M + 1}$$
(21)

$$= \mathcal{O}(\Delta t^{\min(k_0 + k, M + 1)}),\tag{22}$$

where the constants C_{10} and C_{11} are independent of Δt , k_0 denotes the approximation order of the initial guess $U^{(0)}$ and $\|u\|_p$ is defined by $\|u^{(p)}\|_{\infty}$.

Proof. For readability, the maximum norm $\|\cdot\|_{\infty}$ is denoted with the simple norm $\|\cdot\|$ within this proof. Besides, we consider $U_h^{(k+1)}$ instead of $U_h^{(k)}$ here, in order to enable consistent references to the definition of the MLSDC algorithm above.

As the last step of an MLSDC iteration, in particular (19), corresponds to an SDC iteration, we can use Theorem 2.4 to get an initial error estimation. Keeping in mind that the SDC iteration is based on $U_h^{(k+1/2)}$ as the initial guess here, the application of the mentioned theorem yields the estimation

$$||U_h - U_h^{(k+1)}|| \le C_4 \Delta t ||U_h - U_h^{(k+1/2)}||, \tag{23}$$

if the step size Δt is sufficiently small.

Now, the expression on the right-hand side of the above equation will be further examined. In this context, the definition of an MLSDC iteration, in particular (18), yields

$$||U_h - U_h^{(k+1/2)}|| = ||U_h - U_h^{(k)} - I_H^h (U_H^{(k+1/2)} - I_h^H U_h^{(k)})||$$

$$= ||U_h - U_h^{(k)} - I_H^h (U_H^{(k+1/2)} + U_H - U_H - I_h^H U_h^{(k)})||$$

$$= ||(I - I_H^h I_h^H) (U_h - U_h^{(k)}) + I_H^h (U_H - U_H^{(k+1/2)})||,$$

where in the last step we used the identity $U_H = I_h^H U_h$ which applies as a consequence of the τ -correction stemming from the usage of FAS. We get

$$||U_h - U_h^{(k+1/2)}|| \le ||(I - I_H^h I_h^H)(U_h - U_h^{(k)})|| + ||I_H^h (U_H - U_H^{(k+1/2)})||$$
 (24)

$$\leq \widetilde{C}_1 \|U_h - U_h^{(k)}\| + \widetilde{C}_2 \|U_H - U_H^{(k+1/2)}\|, \tag{25}$$

where here and in the following, temporary arising constants will again be denoted by symbols like \widetilde{C}_i .

Next, we have a further investigation of the newly emerged term, in particular the second summand of (25). An insertion of the corresponding definitions, namely

equations (3), (16) and (17), together with the application of the triangle inequality and Lemma 2.2 yields

$$||U_{H} - U_{H}^{(k+1/2)}||$$

$$= ||\Delta t Q_{H}(F_{H}(U_{H}) - F_{H}(I_{h}^{H}U_{h}^{(k)})) + \Delta t Q_{\Delta,H}(F_{H}(I_{h}^{H}U_{h}^{(k)}) - F_{H}(U_{H}^{(k+1/2)}))||$$

$$\leq C_{2,H} \Delta t ||U_{H} - I_{h}^{H}U_{h}^{(k)}|| + C_{3,H} \Delta t ||I_{h}^{H}U_{h}^{(k)} - U_{H}^{(k+1/2)}||$$

$$\leq \widetilde{C}_{3} \Delta t ||U_{H} - I_{h}^{H}U_{h}^{(k)}|| + C_{3,H} \Delta t ||U_{H} - U_{H}^{(k+1/2)}||.$$
(26)

Subtracting $C_{3,H}\Delta t \|U_H - U_H^{(k+1/2)}\|$ from both sides and dividing by $1 - C_{3,H}\Delta t$, results in

$$||U_H - U_H^{(k+1/2)}|| \le \frac{\widetilde{C}_3}{1 - C_{3H}\Delta t} \Delta t ||U_H - I_h^H U_h^{(k)}||.$$

With the same argumentation as above, given a sufficiently small step size,

$$||U_{H} - U_{H}^{(k+1/2)}|| \leq \widetilde{C}_{4} \Delta t ||U_{H} - I_{h}^{H} U_{h}^{(k)}||$$

$$< \widetilde{C}_{5} \Delta t ||U_{h} - U_{h}^{(k)}||, \tag{27}$$

where in the last step we used the identity $U_H = I_h^H U_h$.

By inserting (25) and this result subsequently into (23), we obtain

$$\begin{split} \|U_{h} - U_{h}^{(k+1)}\| &\leq C_{4} \Delta t \|U_{h} - U_{h}^{(k+1/2)}\| \\ &\leq C_{4} \Delta t (\widetilde{C}_{1} \|U_{h} - U_{h}^{(k)}\| + \widetilde{C}_{2} \|U_{H} - U_{H}^{(k+1/2)}\|) \\ &\leq \widetilde{C}_{6} \Delta t \|U_{h} - U_{h}^{(k)}\| + \widetilde{C}_{7} \Delta t (\widetilde{C}_{5} \Delta t \|U_{h} - U_{h}^{(k)}\|) \\ &= (\widetilde{C}_{6} + \widetilde{C}_{8} \Delta t) \Delta t \|U_{h} - U_{h}^{(k)}\|. \end{split}$$

Since the step size Δt is assumed to be sufficiently small, i.e., bounded above, the estimate

$$\widetilde{C}_6 + \widetilde{C}_8 \Delta t < C_9$$

is valid, which concludes the proof for (20).

The proof of (21) is similar to the one of (8) in Theorem 2.4, using the previous result. \Box

Remark 3.2. As before, if the Lipschitz constant of f depends on the spatial resolution, then constants \widetilde{C}_3 and $C_{3,H}$ do as well. In (27), the constant \widetilde{C}_5 then only depends on the original condition $1 - C_{3,H} < 1$, which is just the condition we know from SDC, but with a scaled constant if spatial coarsening is applied. As in Remark 2.5 we can write $\widetilde{C}_5 = \widetilde{C}_5(\delta^{-1})$. This only affects C_{10} in (21), where now $C_{10} = C_{10}(\delta^{-(k+1)})$.

Like Theorem 2.4, this theorem can also be read as a convergence statement. It shows that MLSDC, interpreted as an iterative method solving the collocation problem, converges linearly with a convergence rate in $\mathcal{O}(\Delta t)$ if $C_9\Delta t < 1$. Moreover, the second part of the theorem shows that MLSDC, in the sense of a discretization method for ODEs, converges with order $\min(k_0 + k, M + 1)$.

Remark 3.3. The results regarding consistency and stability of SDC, namely Corollary 2.7 and Theorem 2.8, can be easily adapted for MLSDC. Analogous to SDC, it can be proven that the error at the last collocation node can be bounded by $\mathcal{O}(\Delta t^{\min(k_0+k,2M)})$ and the increment function of MLSDC is Lipschitz continuous for Δt small enough.

Although Theorem 3.1 is the first general convergence theorem for MLSDC, its statement is rather disappointing: it merely establishes that MLSDC converges as least as fast as SDC, although more work is done per iteration.

A deeper look into the proof of the theorem gives an idea on the cause for the rather unexpected low convergence order. In particular, it is the estimate leading to (25) which is responsible for this issue. This equation implies that

$$||U_h - U_h^{(k+1/2)}|| \le C||U_h - U_h^{(k)}||,$$

which essentially means that the additional iteration on the coarse level does not gain any additional order in Δt compared to the previously computed solution $U_h^{(k)}$ on the fine level. More specifically, it is the estimation

$$||(I - I_H^h I_h^H)(U_h - U_h^{(k)})||_{\infty} \le C||U_h - U_h^{(k)}||_{\infty},$$

in (25) which leads to this result.

Thus, a possibly superior behavior of MLSDC seems to depend on the magnitude of $\|(I-I_H^hI_h^H)e_h\|_{\infty}$ with $e_h=U_h-U_h^{(k)}\in\mathbb{C}^{MN}$ which describes the difference between an original vector and the one which results from restricting and interpolating it. Consequently, the term can be interpreted as the quality of the approximation on the coarse level or the accuracy loss it causes, respectively. In the following, this term will be examined in detail, resulting in a new theorem for the convergence of MLSDC with a higher convergence order but additional assumptions which have to be met.

3B. An improved convergence result. For this purpose, we will mainly focus on a specific coarsening strategy here, in particular, coarsening in space. The differences occurring from coarsening in time will be discussed at the end of this section. Moreover, we will focus on particular methods used for the transfer operators. For I_H^h we consider a piecewise Lagrange interpolation of order p. This means that instead of using all N_H available values to approximate the value at a particular point $x_i \in \Omega_h$, only its p neighbors are taken into account for this purpose. Hence,

 I_H^h corresponds to the application of a p-th order Lagrange interpolation for each point. For the restriction operator I_h^H , on the other hand, we consider simple injection. Thereby, we can mainly focus on the interpolation order and disregard the restriction order.

The following lemma now provides an appropriate estimation for the considered term $\|(I-I_H^hI_h^H)e_h\|_{\infty}$.

Lemma 3.4. Let $E := (E_m)_{1 \le m \le M}$ denote the remainder of the truncated inverse discrete Fourier transformation of $U_h - U_h^{(k)}$, i.e.,

$$E_m := \sum_{\ell=N_0}^{N-1} |c_{m,\ell}|, \quad m = 1, \dots, M$$

for some cutoff index $N_0 \leq N$, with $c_{m,\ell} \in \mathbb{C}$ being the Fourier coefficients. Then, the estimate

$$\|(I - I_H^h I_h^H)(U_h - U_h^{(k)})\|_{\infty} \le (C_{11} \Delta x^p + C_{12}(E)) \|U_h - U_h^{(k)}\|_{\infty}$$

for this error is valid, where $I \equiv I_{MN}$ denotes the identity matrix of size MN, I_H^h is the piecewise spatial Lagrange interpolation of order p and I_h^H denotes the injection operator. Furthermore, $\Delta x \equiv \Delta x_H$ is defined as the resolution in space on the coarse level Ω_H of MLSDC.

Proof. First of all, we need to introduce some definitions. For ease of notation, the considered error vector $U_h - U_h^{(k)}$ will be denoted by e_h within the proof. In detail, the following definition is used:

$$e_{m,n} = e_{h,n}(\tau_m) = u_{h,n}(\tau_m) - u_{h,n}^{(k)}(\tau_m), \quad \text{for all } m = 1, \dots, M, \ n = 1, \dots, N,$$

where m denotes the temporal index identifying the particular collocation node τ_m and n represents the spatial index referring to some discretized points $(x_n)_{1 \le n \le N}$ within the considered interval in space [0, S]. Additionally, we assume the spatial steps to be equidistant here.

Another definition needed for the proof is $g_{m,p}(x)$. It denotes the Lagrangian interpolation polynomial of order p for the restricted vector $I_h^H e_h$ for each point in time τ_m , $m=1,\ldots,M$. As the two levels Ω_h and Ω_H differ in their spatial resolution, the transfer operators are applied at the spatial axis and thus can be considered separately for each component $e_h(\tau_m)$. More specifically, the restriction operator, corresponding to simple injection according to the assumptions, omits several values of $e_h(\tau_m) \in \mathbb{C}^N$ resulting in $(I_h^H e_h)(\tau_m) \in \mathbb{C}^{N_H}$, where N_H denotes the number of degrees of freedom at the coarse level. The subsequent application of the interpolation operator at this vector then leads to the M interpolating polynomials $(g_{m,p}(x))_{1 \leq m \leq M}$ with p referring to their order of accuracy.

Having introduced this notation, the considered term can be written as

$$(I - I_H^h I_h^H)(U_h - U_h^{(k)}) = (I - I_H^h I_h^H)e_h = (e_{m,n} - g_{m,p}(x_n))_{\substack{1 \le m \le M, \\ 1 \le n \le N}},$$

so that we can focus on $|e_{m,n} - g_{m,p}(x_n)|$.

Since $g_{m,p}(x)$ partially interpolates the points $(e_{m,n})_{1 \le n \le N}$, it seems very reasonable to use the general error estimation of Lagrangian interpolation to determine an estimate for the considered term. However, there is a crucial issue: the corresponding error bound, generally defined in [2; 20] by

$$\max_{x \in [a,b]} |f(x) - g_p(x)| \le \frac{\Delta x^p}{4p} |f^{(p)}(\xi)|, \quad \xi \in [a,b], \tag{28}$$

apparently depends on the function f from which the interpolation points are obtained. In our case, namely $|e_{m,n} - g_{m,p}(x_n)|$, we do not have a specific function directly available to which the error components $e_{m,n}$ correspond.

To fill this gap, we will now derive an appropriate function for this purpose, using a continuous extension of the inverse discrete Fourier transformation (iDFT). The iDFT at the spatial axes for the points $e_{m,n}$ is given by

$$e_{m,n} = \frac{1}{\sqrt{N}} \sum_{\ell=0}^{N-1} c_{m,\ell} \exp\left(i\frac{2\pi}{N}(n-1)\ell\right), \quad m = 1, \dots, M, \quad n = 1, \dots, N,$$

with $c_{m,\ell}$ as Fourier coefficients and i symbolizing the imaginary unit [23].

A continuous extension $\tilde{e}_m(x)$, $x \in [0, S]$, on the whole spatial interval can then be derived by enforcing $\tilde{e}_m(x_n) = e_{m,n}$ for all m and n. With the transformation $x_n = \frac{S}{N}(n-1)$, i.e., $n = \frac{N}{S}x_n + 1$, implied by an equidistant spatial discretization, we have

$$\tilde{e}_m(x_n) = \frac{1}{\sqrt{N}} \sum_{\ell=0}^{N-1} c_{m,\ell} \exp\left(i\frac{2\pi}{S}\ell x_n\right)$$

and hence

$$\tilde{e}_m(x) := \frac{1}{\sqrt{N}} \sum_{\ell=0}^{N-1} c_{m,\ell} \exp\left(i\frac{2\pi}{S}\ell x\right), \quad x \in [0, S], \quad m = 1, \dots, M.$$

Consequently, we have found a function describing the points $e_{m,n}$. Thus, an interpretation of $g_{m,p}(x)$ as the interpolation polynomial of p points stemming from $\tilde{e}_m(x)$ is possible and the error estimation for Lagrange interpolation, presented in (28), can now be applied. As a result, we get

$$|e_{m,n} - g_{m,p}(x_n)| = |\tilde{e}_m(x_n) - g_{m,p}(x_n)| \le \frac{\Delta x^p}{4p} |\tilde{e}_m^{(p)}(\xi)|$$
 (29)

with $\xi \in [0, S]$.

With the insertion of the definition of $\tilde{e}_m(x)$ and its p-th derivative, we have

$$|\tilde{e}_{m}(x_{n}) - g_{m,p}(x_{n})| \leq \frac{\Delta x^{p}}{4p} |*| \frac{1}{\sqrt{N}} \sum_{\ell=0}^{N-1} c_{m,\ell} \left(i \frac{2\pi}{S} \ell \right)^{p} \exp\left(i \frac{2\pi}{S} \ell \xi \right)$$

$$= \frac{1}{\sqrt{N}} \frac{\Delta x^{p}}{4p} \left(\frac{2\pi}{S} \right)^{p} |*| \sum_{\ell=0}^{N-1} c_{m,\ell} \ell^{p} \exp\left(i \frac{2\pi}{S} \ell \xi \right),$$

so that with $\widetilde{C}(p) := \frac{1}{4p} \left(\frac{2\pi}{S}\right)^p$, we have

$$|\tilde{e}_{m}(x_{n}) - g_{m,p}(x_{n})| \leq \frac{1}{\sqrt{N}} \widetilde{C}(p) \Delta x^{p} \sum_{\ell=0}^{N-1} |*|c_{m,\ell} \ell^{p} \exp\left(i\frac{2\pi}{S}\ell\xi\right)$$
$$\leq \frac{1}{\sqrt{N}} \widetilde{C}(p) \Delta x^{p} \sum_{\ell=0}^{N-1} |c_{m,\ell}| \ell^{p}.$$

We now choose $N_0 \le N$ such that

$$\sum_{\ell=0}^{N_0-1} |c_{m,\ell}| \ge \epsilon_m > 0 \quad \text{for all } m$$

for given ϵ_m . Note that this is not possible if there exists an m for which the coefficients $(c_{m,\ell})_{\ell=0,\dots,N-1}$ are all 0. This would imply that for this particular m the error $e_{m,n}$ equals 0 for all $n=1,\dots,N$. However, the respective error $e_h(\tau_m)$ would then be 0 and could just be disregarded in our particular context as it does not have an impact on the considered maximum norm. Therefore, the assumption does not lead to a loss of generality. Finally, we define the remainders of the sums as

$$E_m := \sum_{\ell=N_0}^{N-1} |c_{m,\ell}|, \quad m=1,\ldots,M.$$

Now, the sum in the previous estimation will be split at N_0 resulting in the estimate

$$|\tilde{e}_m(x_n) - g_{m,p}(x_n)| \le \frac{1}{\sqrt{N}} \widetilde{C}(p) \Delta x^p \left(\sum_{\ell=0}^{N_0-1} |c_{m,\ell}| \ell^p + \sum_{\ell=N_0}^{N-1} |c_{m,\ell}| \ell^p \right).$$

With the simple estimation $\ell \le N_0$ for the first sum and $\ell \le N$ for the second one, the following formulation using the definition of the remainder E_m is obtained:

$$|\tilde{e}_{m}(x_{n}) - g_{m,p}(x_{n})| \leq \frac{1}{\sqrt{N}} \widetilde{C}(p) \Delta x^{p} \left(N_{0}^{p} \sum_{\ell=0}^{N_{0}-1} |c_{m,\ell}| + N^{p} \sum_{\ell=N_{0}}^{N-1} |c_{m,\ell}| \right)$$

$$= \frac{1}{\sqrt{N}} \widetilde{C}(p) \Delta x^{p} \left(N_{0}^{p} \sum_{\ell=0}^{N_{0}-1} |c_{m,\ell}| + N^{p} E_{m} \right).$$

Now, we will have a look at the norm of the whole vector $(I - I_H^h I_h^H)e_h$, but instead of the maximum norm, we first consider the squared 2-norm given by

$$||(I - I_H^h I_h^H)e_h||_2^2 = \sum_{n=1}^N \sum_{m=1}^M |\tilde{e}_m(x_n) - g_{m,p}(x_n)|^2.$$

By the insertion of the previous estimation, it follows that

$$\|(I-I_H^hI_h^H)e_h\|_2^2 \leq \sum_{n=1}^N \sum_{m=1}^M \left[\frac{1}{\sqrt{N}} \widetilde{C}(p) \Delta x^p \left(N_0^p \sum_{\ell=0}^{N_0-1} |c_{m,\ell}| + N^p E_m \right) \right]^2.$$

Since the summands are independent of the running index n, the equation can be simplified to

$$\|(I - I_H^h I_h^H) e_h\|_2^2 \le \widetilde{C}(p)^2 \Delta x^{2p} \sum_{m=1}^M \left(N_0^p \sum_{\ell=0}^{N_0 - 1} |c_{m,\ell}| + N^p E_m \right)^2.$$
 (30)

Now, each inner summand can be written as

$$\left(N_0^p \sum_{\ell=0}^{N_0-1} |c_{m,\ell}| + N^p E_m\right)^2 = N_0^{2p} \left(\sum_{\ell=0}^{N_0-1} |c_{m,\ell}|\right)^2 + 2N_0^p N^p E_m \sum_{\ell=0}^{N_0-1} |c_{m,\ell}| + N^{2p} E_m^2 \\
=: S_1 + S_2 + S_3. \tag{31}$$

While S_1 is an intended component (it contains the squared sum of $c_{m,\ell}$ which we will need to get back to the norm of e_h), the other two summands S_2 and S_3 are inconvenient. Therefore, we will now eliminate them by searching a $T(E_m)$ such that

$$S_1 + S_2 + S_3 \le S_1 + T(E_m) \left(\sum_{\ell=0}^{N_0 - 1} |c_{m,\ell}| \right)^2 = (N_0^{2p} + T(E_m)) \left(\sum_{\ell=0}^{N_0 - 1} |c_{m,\ell}| \right)^2.$$
 (32)

This is true if

$$S_2 + S_3 - T(E_m) \left(\sum_{\ell=0}^{N_0-1} |c_{m,\ell}| \right)^2 \le 0,$$

which in turn leads to

$$T(E_m) \ge \frac{2N_0^p N^p}{\sum_{\ell=0}^{N_0-1} |c_{m,\ell}|} E_m + \frac{N^{2p}}{\left(\sum_{\ell=0}^{N_0-1} |c_{m,\ell}|\right)^2} E_m^2,$$

after using the definitions of S_2 and S_3 . Thus, for

$$T(E_m) := \frac{2N_0^p N^p}{\epsilon_m} E_m + \frac{N^{2p}}{\epsilon_m^2} E_m^2$$
 (33)

we can bound

$$S_1 + S_2 + S_3 \le (N_0^{2p} + T(E_m)) \left(\sum_{\ell=0}^{N_0 - 1} |c_{m,\ell}| \right)^2.$$

Using the Cauchy-Schwarz inequality we have

$$\left(\sum_{\ell=0}^{N_0-1} |c_{m,\ell}|\right)^2 = \left(\sum_{\ell=0}^{N_0-1} |c_{m,\ell}| \cdot 1\right)^2 \le \sum_{\ell=0}^{N_0-1} |c_{m,\ell}|^2 \cdot \sum_{\ell=0}^{N_0-1} 1^2 = N_0 \sum_{\ell=0}^{N_0-1} |c_{m,\ell}|^2,$$

so that with (30), (31) and (32) we get

$$\|(I - I_H^h I_h^H)e_h\|_2^2 \le \widetilde{C}(p)^2 \Delta x^{2p} N_0 \sum_{m=1}^M (N_0^{2p} + T(E_m)) \sum_{\ell=0}^{N_0 - 1} |c_{m,\ell}|^2.$$

Further, it follows from Parseval's theorem [23] that

$$\sum_{\ell=0}^{N_0-1} |c_{m,\ell}|^2 \le \sum_{\ell=0}^{N-1} |c_{m,\ell}|^2 = \sum_{n=1}^{N} |e_{m,n}|^2$$

and thus

$$\begin{aligned} \|(I - I_H^h I_h^H) e_h\|_2^2 &\leq \widetilde{C}(p)^2 \Delta x^{2p} N_0 \sum_{m=1}^M (N_0^{2p} + T(E_m)) \sum_{n=1}^N |e_{m,n}|^2 \\ &= \widetilde{C}(p)^2 \Delta x^{2p} N_0 (N_0^{2p} + \max_{m=1,\dots,M} T(E_m)) \|e_h\|_2^2. \end{aligned}$$

Since it is the maximum norm we are interested in and not the Euclidean one, an appropriate transformation is required, given by

$$||x||_{\infty} \le ||x||_2 \le \sqrt{n} ||x||_{\infty}$$
 for all $x \in \mathbb{C}^n$,

so that

$$\begin{split} \|(I - I_H^h I_h^H) e_h\|_{\infty} &\leq \|(I - I_H^h I_h^H) e_h\|_2 \\ &\leq \widetilde{C}(p) \Delta x^p \sqrt{N_0 (N_0^{2p} + \max_{m=1,...,M} T(E_m))} \|e_h\|_2 \\ &\leq \widetilde{C}(p) \Delta x^p \sqrt{N_0 M N} \sqrt{N_0^{2p} + \max_{m=1,...,M} T(E_m)} \|e_h\|_{\infty}. \end{split}$$

Using the triangle inequality for square roots, the sum can be split as

$$\|(I - I_H^h I_h^H)e_h\|_{\infty} \le \widetilde{C}(p)\Delta x^p \sqrt{N_0 M N} \Big(N_0^p + \sqrt{\max_{m=1,\dots,M} T(E_m)}\Big) \|e_h\|_{\infty}.$$

With the insertion of the definition of $T(E_m)$ presented in (33), we get

$$\|(I - I_{H}^{h} I_{h}^{H}) e_{h}\|_{\infty} \leq \widetilde{C}(p) \sqrt{N_{0} M N} N_{0}^{p} \Delta x^{p} \cdot \left(N_{0}^{p} + \sqrt{\max_{m=1,\dots,M} \frac{2N_{0}^{p} N^{p}}{\epsilon_{m}}} E_{m} + \frac{N^{2p}}{\epsilon_{m}^{2}} E_{m}^{2} \right) \|e_{h}\|_{\infty}.$$
(34)

At the first sight, it looks like Δx^p is the dominating term in this equation. However, a closer look reveals that the root term is in $\mathcal{O}(N^p)$ which shifts the dominance of this summand towards the remainder E_m . To see this, we first transform the root term by extracting N^{2p} :

$$\sqrt{\max_{m=1,\dots,M} \frac{2N_0^p N^p}{\epsilon_m} E_m + \frac{N^{2p}}{\epsilon_m^2} E_m^2} \le \sqrt{\max_{m=1,\dots,M} N^{2p} \left(\frac{2N_0^p}{\epsilon_m} E_m + \frac{1}{\epsilon_m^2} E_m^2\right)} \\
= N^p \sqrt{\max_{m=1,\dots,M} \frac{2N_0^p}{\epsilon_m} E_m + \frac{1}{\epsilon_m^2} E_m^2}.$$

Then, we consider the definition of the step size on the fine level, namely $\Delta x_h = \frac{S}{N}$, which allows the representation of N^p as $\left(\frac{S}{\Delta x_h}\right)^p$. From this representation, we get

$$\Delta x^p \sqrt{\max_{m=1,\dots,M} \frac{2N_0^p N^p}{\epsilon_m} E_m + \frac{N^{2p}}{\epsilon_m^2} E_m^2} \leq S^p \left(\frac{\Delta x_H}{\Delta x_h}\right)^p \sqrt{\max_{m=1,\dots,M} \frac{2N_0^p}{\epsilon_m} E_m + \frac{1}{\epsilon_m^2} E_m^2}.$$

The insertion of this estimation into (34) finally leads to the overall result

$$\begin{split} \|(I - I_H^h I_h^H) e_h\|_{\infty} &\leq \widetilde{C}(p) \sqrt{N_0 M N} N_0^{2p} \Delta x^p \|e_h\|_{\infty} \\ &+ \frac{(2\pi)^p}{4p} \left(\frac{\Delta x_H}{\Delta x_h}\right)^p \left(\sqrt{\max_{m=1,...,M} \frac{2N_0^p}{\epsilon_m} E_m + \frac{1}{\epsilon_m^2} E_m^2}\right) \|e_h\|_{\infty}, \end{split}$$

where we used the definition of $\widetilde{C}(p)$ to eliminate S^p in the second summand.

In this estimation, we can finally see that Δx^p does not dominate the second summand anymore. It is replaced by the relation between the step size on the coarse and on the fine level which can be regarded as constant. As a result, the remainder E_m is now the dominating item in the term. Hence, a formulation like

$$||(I - I_H^h I_h^H)e_h||_{\infty} \le C_{11} \Delta x^p ||e_h||_{\infty} + C_{12}(E) ||e_h||_{\infty}$$

with $E := (E_m)_{1 \le m \le M}$ is reasonable and concludes the proof.

Remark 3.5. The splitting of the sum and the consideration of the vector of remainders E is needed since the constant C_{11} would otherwise depend on N^p . Considering the relation $\frac{N}{S} = \frac{1}{\Delta x}$, this would mean that the approximated boundary would not depend on Δx anymore. As a result, we would not obtain a better estimation than the simple one $\|(I - I_H^h I_h^H)(e_h)\|_{\infty} \le C \|e_h\|_{\infty}$, which was already used in the proof of Theorem 3.1. By the applied split of the series, the term N^p is replaced by N_0^p which yields a more meaningful estimation as it keeps the dependence on the term Δx^p while adding another on the smoothness of the error.

Remark 3.6. Note that ideally the error only has a few, low-frequency Fourier coefficients, i.e., $\tilde{e}_m(x)$ can be written as

$$\tilde{e}_m(x) := \frac{1}{\sqrt{N}} \sum_{\ell=0}^{N_0-1} c_{m,\ell} \exp\left(i\frac{2\pi}{S}\ell x\right), \quad x \in [0, S], \quad m = 1, \dots, M,$$

using N_0 summands only. Then, $E_m = 0$ and the estimate

$$||(I - I_H^h I_h^H)e_h||_{\infty} \le C_{11} \Delta x^p ||e_h||_{\infty} + C_{12}(E) ||e_h||_{\infty}$$

reduces to

$$||(I - I_H^h I_h^H)e_h||_{\infty} \le C_{11} \Delta x^p ||e_h||_{\infty}.$$

The following theorem uses Lemma 3.4 to extend Theorem 3.1. In particular, the provided estimation for $\|(I-I_H^hI_h^H)(U_h-U_h^{(k)})\|_{\infty}$ is used in the corresponding proof which results in a new convergence theorem for MLSDC.

Theorem 3.7. Consider a generic initial value problem like (1) with a Lipschitz-continuous function f on the right-hand side. Furthermore, let the conditions of Lemma 3.4 be met.

Then, if the step size Δt is sufficiently small, MLSDC converges linearly to the solution of the collocation problem with a convergence factor in

$$\mathcal{O}((\Delta x^p + C(E))\Delta t + \Delta t^2),$$

i.e., the estimate

$$||U_h - U_h^{(k)}||_{\infty} \le ((C_{13}\Delta x^p + C_{14}(E))\Delta t + C_{15}\Delta t^2)||U_h - U_h^{(k-1)}||_{\infty}$$
 (35)

for the error is valid, where $\Delta x \equiv \Delta x_H$ is defined as the resolution in space on the coarse level Ω_H of MLSDC and the constants C_{13} , $C_{14}(E)$ and C_{15} are independent of Δt .

If, additionally, the solution of the initial value problem u is (M+1)-times continuously differentiable, the LTE of MLSDC compared to the solution of the

ODE can be bounded by

$$\|\bar{U}_{h} - U_{h}^{(k)}\|_{\infty} \leq C_{17} \Delta t^{M+1} \|u\|_{M+1} + \sum_{l=0}^{k} C_{l+18} (\Delta x^{p} + C_{14}(E))^{k-l} \Delta t^{k_{0}+k+l} \|u\|_{k_{0}+1}$$
 (36)

where the constants C_{17}, \ldots, C_{k+18} are independent of Δt , k_0 denotes the approximation order of the initial guess $U_h^{(0)}$ and $\|u\|_p$ is defined by $\|u^{(p)}\|_{\infty}$.

Proof. The proof is similar to that of Theorem 3.1 but differs in the estimation used for $\|(I - I_H^h I_h^H)(U_h - U_h^{(k)})\|_{\infty}$. Here, Lemma 3.4 instead of the simple norm compatibility inequality is used for this purpose. Based on the estimations (23), (24) and (27) arising in the proof of the mentioned theorem,

$$||U_h - U_h^{(k+1)}||_{\infty} \le \widetilde{C}_1 \Delta t ||(I - I_H^h I_h^H)(U_h - U_h^{(k)})||_{\infty} + C_{15} \Delta t^2 ||U_h - U_h^{(k)}||_{\infty}.$$

As already mentioned, we will now apply Lemma 3.4, namely,

$$\|(I - I_H^h I_h^H)(U_h - U_h^{(k)})\|_{\infty} \le (C_{11} \Delta x^p + C_{12}(E)) \|U_h - U_h^{(k)}\|_{\infty},$$

which yields

$$\begin{split} \|U_h - U_h^{(k+1)}\|_{\infty} &\leq (C_{13} \Delta x^p + C_{14}(E)) \Delta t \|U_h - U_h^{(k)}\|_{\infty} \\ &\quad + C_{15} \Delta t^2 \|U_h - U_h^{(k)}\|_{\infty} \\ &\quad = ((C_{13} \Delta x^p + C_{14}(E)) \Delta t + C_{15} \Delta t^2) \|U_h - U_h^k\|_{\infty}. \end{split}$$

This concludes the proof of (35).

The proof of (36) is again similar to that of the second equation in Theorem 2.4, using the previous result. Additionally, the binomial theorem is applied to simplify the arising term $((C_{13}\Delta x^p + C_{14}(E))\Delta t + C_{15}\Delta t^2)^k$.

Remark 3.8. It is here that a possible dependency of f's Lipschitz constant on Δx plays a key role. Similar to the observations before, we find that in this case (35) needs to be replaced with

$$||U_h - U_h^{(k)}||_{\infty} \le ((C_{13} \Delta x^p + C_{14}(E))C(\delta^{-1})\Delta t + C_{15}(\delta^{-2})\Delta t^2)||U_h - U_h^{(k-1)}||_{\infty},$$

where δ denotes the difference between spatial and temporal resolution (up to constants) and comes from the initial step size restriction of SDC. The term $C_{13}\Delta x^p + C_{14}(E)$ itself does not depend on δ , since it comes from the remainder of the interpolation estimate in Lemma 3.4, where f and therefore its Lipschitz constant as well as the step size does not play a role. As before, (36) has to be modified, now including the term $\delta^{-(k-l+1)}$ in the sum. The constant C_{17} is still independent of δ .

Remark 3.9. Similar to Corollary 2.7, it can be proven that the order limit M + 1 in Theorem 3.7 can be replaced by 2M if only the error at the last collocation node is considered.

The theorem states that, under the named conditions, MLSDC converges linearly with a convergence rate of $\mathcal{O}((\Delta x^p + C(E))\Delta t + \Delta t^2)$ to the collocation solution if $(C_{13}\Delta x^p + C_{14}(E))\Delta t + C_{15}\Delta t^2 < 1$. This means that if Δx^p and the vector of remainders E are sufficiently small, the error of MLSDC decreases by two orders of Δt with each iteration, which indeed represents an improved convergence behavior compared to the one described in Theorem 3.1. Otherwise, i.e., if Δx^p and E are not that small, it only decreases by one order in Δt which is equivalent to the result of the previous theorem.

In the second equation of the theorem, it can be seen that again, Δx^p and E are the crucial factors here. If they are small enough such that Δt^{k_0+2k} is the leading order, MLSDC converges with order $\min(k_0+2k-1,2M-1)$ and thus gains two orders per iteration. Otherwise, the convergence order is only $\min(k_0+k-1,2M-1)$, i.e., the error decreases by one order in Δt in each iteration.

Note that, as a result, it is advisable to use a high interpolation order p and a small spatial step size Δx on the coarse level in practical applications of MLSDC. This theoretical result matches the numerical observations described in [30]. In Section 2.2.5 of that paper, it is mentioned that the convergence properties of MLSDC seem to be highly dependent on the used interpolation order and resolution in space. Moreover, it was said that in the considered numerical examples a high resolution in space, i.e., a small Δx , led to a lower sensitivity on the interpolation order p. Our theoretical investigation provides an explanation for this behavior.

It seems reasonable to use a similar approach to determine the conditions for a higher convergence order of MLSDC if coarsening in time instead of space is used. Analogous to (28) in the proof of Lemma 3.4, the Lagrangian error estimation could be used for this purpose, resulting in the estimation

$$\|(I - I_H^h I_h^H)(U_h - U_H^{(k)})\|_{\infty} \le \frac{\Delta \tau^p}{4p} \|e^{(p)}(t)\|_{\infty},\tag{37}$$

where I_H^h and I_h^H denote temporal transfer operators now and e(t) is defined as the continuous error of MLSDC compared to the collocation solution. In this case, however, the function e(t) is implicitly known and thus does not have to be approximated by an iDFT. In particular, it is a polynomial of degree $M \equiv M_h$ as both the collocation solution U and each iterate $U_h^{(k)}$ of MLSDC are polynomials of that degree, respectively. This can be seen by considering that $\Delta t \, Q \, F(U)$ as well as $\Delta t \, Q_\Delta F(U)$ essentially represent a sum of integrals of Lagrange polynomials which apparently results in a polynomial. Consequently, the p-th derivative of e(t) is a polynomial of degree $M_h - p$. The maximal interpolation order p is the number

of collocation nodes M_H on the coarse level. Here, we will assume that $p = M_H$, i.e., the maximal interpolation order is used. Note that $e^{(p)}(t) = 0$ for $p > M_h$ and hence $\|(I - I_H^h I_h^H)(U_h - U_H^{(k)})\|_{\infty} = 0$ for $M_H = M_h$ which is consistent with the expected behavior as it means that no coarsening is used at all. As a conclusion, it can be said that, according to (37) the improved convergence behavior of MLSDC using coarsening in time is dependent on the used time step size $\Delta \tau = C \Delta t$ and the number of collocation nodes on the coarse level M_H . Note that it is also dependent on the specific coefficients of $e^{(p)}(t)$. However, these are highly dependent on the right-hand side f of the IVP and thus cannot be controlled by any method parameters.

In summary, two convergence theorems for MLSDC were established in this section. While the first one, Theorem 3.1, represents a general statement on the convergence of the method, the second one, Theorem 3.7, provides theoretically established guidelines for the parameter choice in practical applications of MLSDC in order to achieve an improved convergence behavior of the method. In the next section, we will examine numerical examples of MLSDC to check if the resulting errors match those theoretical predictions.

4. Numerical results

In this section, the convergence behavior of MLSDC, theoretically analyzed in the previous section, is verified by numerical examples. The method is applied to three different initial value problems and the results are compared to those from classical, single-level SDC. The key question here is whether the conditions derived in the previous sections (smoothness, high spatial/temporal resolution and high interpolation order) are actually sharp, i.e., whether MLSDC does indeed show only low order convergence if any of these conditions are violated. The corresponding programs were written in Python using pySDC.¹

4A. *Heat equation.* The first numerical example is the one-dimensional heat equation defined by the following initial value problem:

$$\frac{\partial}{\partial t}u(x,t) = v\frac{\partial^2}{\partial x^2}u(x,t), \quad \text{for all } t \in [0, t_{\text{end}}], x \in [0, 1]$$

$$u(0,t) = 0, \quad u(1,t) = 0, \quad u(x,0) = u_0(x),$$
(38)

where u(x, t) represents the temperature at the location x and time t and v > 0 defines the thermal diffusivity of the medium. This partial differential equation is discretized in space using standard second-order finite differences with N degrees of freedom.

As the initial value, a sine wave with frequency κ is selected, i.e., $u_0(x) = \sin(\kappa \pi x)$. Under these conditions, the analytical solution of the spatially discretized initial

¹http://parallel-in-time.org/pySDC/

value problem is given by

$$\vec{u}(t) = \sin(\kappa \pi \vec{x})e^{-t\nu\rho}$$
 with $\rho = \frac{1}{\Delta x^2}(2 - 2\cos(\pi \nu \vec{x}))$

with $\vec{x} := (x_n)_{1 \le n \le N}$ and an elementwise application of the trigonometric functions. For the tests, we choose $\kappa = 4$, $\nu = 0.1$ and M = 5 Gauss–Radau collocation nodes.

Note that we are using this linear ODE for our tests even though the linearity of the right-hand side f is not a necessary condition in Theorems 2.4, 3.1 or 3.7. In fact, f is just assumed to be Lipschitz continuous. However, we will consider the heat equation here since it is well studied and has a convenient exact solution needed to compute the errors of SDC and MLSDC.

The following tests are structured in a particular way: In the first one, we will adjust the method parameters according to the results of Theorem 3.7 to observe an improved convergence of MLSDC over SDC. More specifically, we will use a small spatial step size Δx , a high interpolation order p and try to generate smooth errors using smooth initial guesses for the iteration. In a second step, we will subsequently change these parameters leading to a lower convergence order of MLSDC as described in Theorem 3.1. Thereby, we will reveal the dependence of MLSDC's convergence behavior on those parameters and simultaneously verify the general minimal achievable convergence order of the method. Altogether, this will confirm the theoretical results of the previous section.

For the first test, the number of degrees of freedom was set to $N_h = 255$ on the fine and $N_H = 127$ on the coarse level of MLSDC. This parameter particularly determines the spatial grid size $\Delta x = \frac{1}{N+1}$. As discussed before, we use injection as restriction and a piecewise p-th order Lagrange interpolation as interpolation, for now with p = 8. Moreover, the smooth initial value $u_0(x) = \sin(4\pi x)$ was spread across the different nodes τ_m to form the initial guess.

An illustration of the corresponding numerical results is shown in Figure 1(c), with the reference SDC result in Figure 1(a). MLSDC was applied with different step sizes Δt and numbers of iterations k to the considered problem and the resulting errors were plotted as points in the respective graphs. The drawn lines, on the other hand, represent the expected behavior, i.e., the predicted convergence orders of the method according to Theorem 3.7. In particular, we assume that the terms Δx^p and C(E) are sufficiently small such that Δt^{k_0+2k} is the leading order in the corresponding error estimation. As a result, MLSDC is expected to gain two orders per iteration. In the figure, it can be seen that nearly all of the computed points lie on the expected lines (except when the errors hit the precision limit at approximately 10^{-14}) which always start at the error resulting for the largest step size. Therefore, the numerical results match the theoretical predictions.

Note that the gain in accuracy when comparing two runs with k and k+1 for a fixed Δt is not as high as one might expect. As mentioned in Remark 2.6, this is

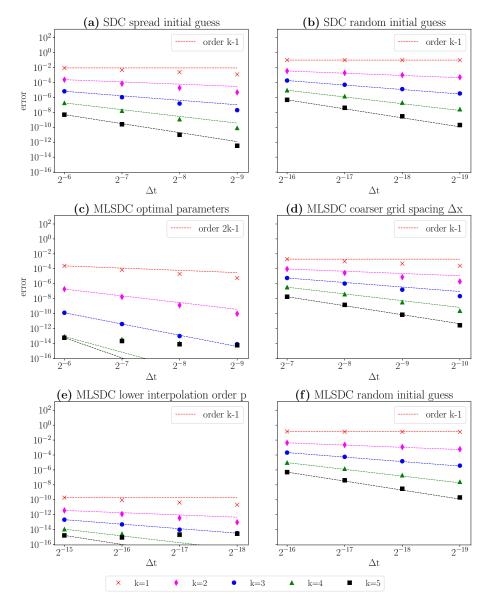


Figure 1. Convergence behavior of SDC and MLSDC applied to the discretized onedimensional heat equation with coarsening in space (for MLSDC) and different parameters.

due to the fact that the error is multiplied with L^k , where L > 1 is the Lipschitz constant of the discretized right-hand side of the ODE (38).

If, by contrast, the spatial grid size Δx is chosen to be significantly larger, in particular as large as $\frac{1}{16}$ on the fine and $\frac{1}{8}$ on the coarse level, the leading order in Theorem 3.7, presenting an error estimation for MLSDC, changes to Δt^{k_0+k} . Hence, in this example, we expect MLSDC to only gain one order in Δt with each

iteration, as SDC does and as it was described in the general convergence theorem (Theorem 3.1). The corresponding numerical results, presented in Figure 1(d), confirm this prediction. For both methods, the error decreases by one order in Δt with each iteration.

Another possible modification of the first example is a decrease of the interpolation order p. Figure 1(e) shows the numerical results if this parameter is changed to p=4. Apparently, this also leads to an order reduction of MLSDC compared to Figure 1(c). According to Theorem 3.7, this is a reasonable behavior. In particular, the leading order in the presented error estimation is again reduced to Δt^{k_0+k} due to the higher magnitude of Δx^p . Besides, it should be noted that the considered values of Δt are significantly smaller here. This is caused by the fact that MLSDC does not converge for greater values of this parameter, i.e., the upper bound for Δt , implicitly occurring in the assumptions of the respective theorem, seems to be lower here. The smaller step sizes Δt also entail overall smaller errors. As a result, the accuracy of the collocation solution is reached earlier which explains the outliers in the considered plots.

The third necessary condition for the improved convergence of MLSDC is the magnitude of the remainders E_m or, in other words, the smoothness of the error. In this context, we will now have a look at the changes which result from a higher oscillatory initial guess. In particular, we will assign random values to $U^{(0)}$. The corresponding errors are shown in Figure 1(b) for SDC and Figure 1(f) for MLSDC. It can be seen that this change results again in a lower convergence order of MLSDC, in particular it gains one order per iteration as SDC. Since this time, as the crucial term Δx^p is left unchanged, the result can only be assigned to a higher value of C(E) and thus to an insufficient smoothness of the error. This may lead to the assumption that for this problem type a smooth initial guess is a sufficient condition for the smoothness of the error and thus, a low value of C(E).

4B. *Allen–Cahn equation.* The second test case is the nonlinear, two-dimensional Allen–Cahn equation

$$u_t = \Delta u + \frac{1}{\epsilon^2} u(1 - u^2)$$
 on $[-0.5, 0.5]^2 \times [0, T], T > 0,$ (39)
 $u(x, 0) = u_0(x), x \in [-0.5, 0.5]^2,$

with periodic boundary conditions and scaling parameter $\epsilon > 0$. We use again second-order finite differences in space and choose a sine wave in 2D as the initial condition, i.e., $u_0(x) = \sin(\kappa \pi x) \sin(\kappa \pi y)$. There is no analytical solution, neither for the continuous nor for the spatially discretized equations. Therefore, reported errors are computed against a numerically computed high-order reference solution. For the tests, we choose $\kappa = 4$, $\epsilon = 0.2$ and M = 3 Gauss–Radau collocation nodes.

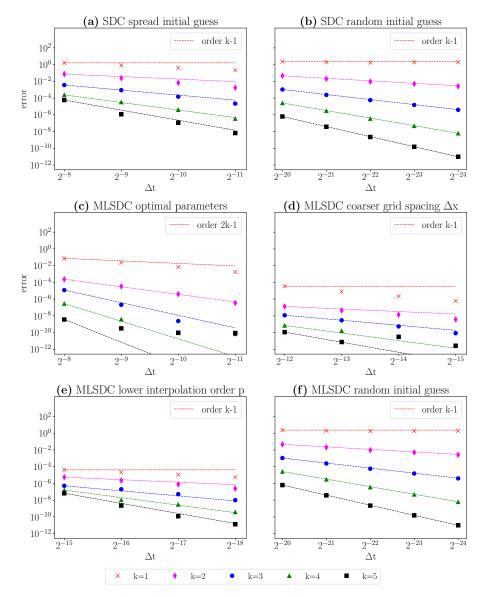


Figure 2. Convergence behavior of SDC and MLSDC applied to the discretized two-dimensional Allen–Cahn equation with coarsening in space (for MLSDC) and different parameters.

The tests are structured precisely as for the heat equation: we first show secondorder convergence factors using appropriate parameters and then test the sharpness of the conditions on smoothness, the resolution and the interpolation order. For the first test, the number of degrees of freedom per dimension was set to $N_h = 128$ on the fine and $N_H = 64$ on the coarse level of MLSDC. Transfer operators are the same as before. Figure 2 shows the results of our tests for the Allen–Cahn equation for both SDC and MLSDC. The main conclusion here is the same as before: using fewer degrees of freedom (here N=32 on the fine level instead of 128), a lower interpolation order (here p=2 instead of 8) or a nonsmooth (here random) initial guess leads to a degraded order of the convergence factor.

4C. *Auzinger's test case.* The third test case is the following two-dimensional ODE introduced in [1]:

$$\dot{u} = \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} -y - \lambda x (1 - x^2 - y^2) \\ x - \lambda \rho y (1 - x^2 - y^2) \end{pmatrix}, \text{ for all } t \in [0, t_{\text{end}}],$$

$$u(0) = u_0,$$
(40)

where $\lambda < 0$ determines the stiffness of the problem and $\rho > 0$ is a positive parameter. For the tests, we choose $\lambda = -0.75$, $\rho = 3$ and $u_0 = (1, 0)^T$. The analytical solution of this initial value problem is known. It is given by

$$u(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} \cos(t) \\ \sin(t) \end{pmatrix}, \quad t \in [0, t_{\text{end}}].$$

The corresponding tests are structured in a similar way as before but this time the ODE version of Theorem 3.7, given by (37), is considered. So, first appropriate parameters are used to reach second-order convergence of MLSDC, and then the sharpness of the implied conditions is tested. In particular, the improved convergence behavior of MLSDC is expected to depend on the time step size $\Delta \tau = C \Delta t$, the (now temporal) interpolation order p and the smoothness of the error in time. In our tests, we always used the maximal interpolation order $p = M_H$ corresponding to the number of collocation nodes on the coarse level, since otherwise it was not possible to get a second order convergence at all. The number of nodes on the fine grid was chosen to be $M_h = 8$.

The numerical results are shown in Figure 3. Again, they agree with our theoretical predictions: All of the three conditions implied by (37) need to be fulfilled to reach second-order convergence of MLSDC. A larger time step size (here, $\Delta t \in [2^{-1}, 2^{-4}]$ instead of $[2^{-3}, 2^{-6}]$), a lower interpolation order (here, $p = M_H = 2$ instead of 6) or a nonsmooth (here, random) initial guess immediately led to a decrease in the order.

However, there are a few oddities in the graphs that we would like to discuss here. First of all, the orders shown in Figure 3 (a), (c) and (d) are not 2k - 1 and k - 1 as we would expect, but rather 2k and k. This behavior is probably related to the k_0 -term in the estimates which stems from the initial guess of SDC and MLSDC. This explanation would also agree with the result that this additional order gets lost if a random initial guess is used (see Figure 3 (b), (f)). Aside from

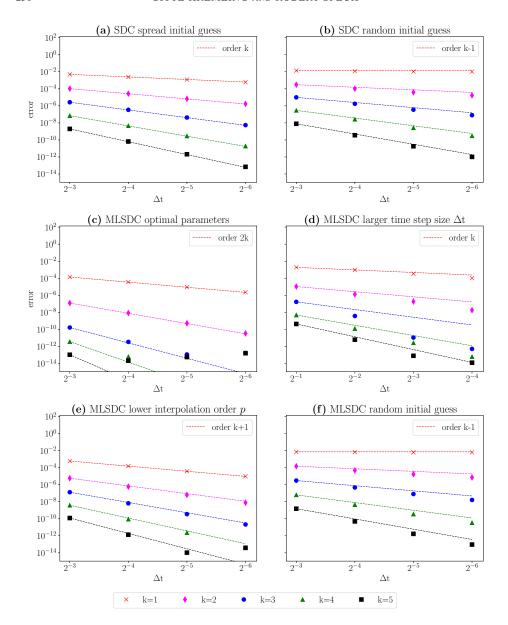


Figure 3. Convergence behavior of SDC and MLSDC applied to the Auzinger problem with coarsening in the collocation nodes (for MLSDC) and different parameters.

that, it should be noted that the use of a lower interpolation order (Figure 3(e)) led to a convergence order of k + 1 instead of k as we would have expected. The reason for this is not clear but could be related to (36) which implies that all orders between k and 2k can potentially be reached. In any case, the result shows that the second-order convergence is lost if the interpolation order is decreased. Finally,

example	method	order in Δt		
		$2^{-6} \rightarrow 2^{-7}$	$2^{-7} \rightarrow 2^{-8}$	$2^{-8} \rightarrow 2^{-9}$
Heat1D	SDC	0.844	0.928	0.969
	MLSDC	0.196	-0.442	-1.064
	MLSDC (k = 1, 2)	1.632	1.754	0.443
		$2^{-8} \rightarrow 2^{-9}$	$2^{-9} \rightarrow 2^{-10}$	$2^{-10} \rightarrow 2^{-11}$
Allen-Cahn	SDC	1.537	0.574	0.749
	MLSDC	-0.247	-3.341	-1.097
	MLSDC (k = 1, 2)	2.7652	2.719	1.629
		$2^{-3} \rightarrow 2^{-4}$	$2^{-4} \rightarrow 2^{-5}$	$2^{-5} \rightarrow 2^{-6}$
Auzinger	SDC	0.968	0.988	0.976
	MLSDC	-2.762	-2.062	-0.413
	MLSDC (k = 1, 2)	1.799	1.202	-4.125

Table 1. Order of convergence in Δt , computing the error at iteration k vs. the error at iteration k+1, taking the mean over these ratios for a fixed Δt and then computing the order of convergence when going from one Δt to a finer one $\Delta t/2$ (which is indicated by the " \rightarrow "). Ideally, SDC shows order 1, MLSDC order 2. The third row for each example only considers the first two iterations to avoid noise from stalling convergence.

we want to discuss the plot in Figure 3(d) resulting from the use of a larger time step size Δt . It can be seen that the data points do not perfectly agree with the predicted lines here. Apparently, the numerical results are often much better than expected. However, they do not reach order 2k and hence confirm our theory that the second-order convergence of MLSDC is also dependent on a small time step size. The deviations in the data are, in fact, not too surprising here, considering that the time step size is a very crucial parameter for the convergence of MLSDC in general. As described in Theorems 3.1 and 3.7, Δt has to be small enough in order for MLSDC to converge at all. For that reason, the possible testing scope for the time step size is rather small, making it difficult to find appropriate parameters where MLSDC converges exactly with order k.

4D. Further observations. The artifacts described above shed some light on the "robustness" of the results, a fact that we would like to share here: during the tests with all three examples, we saw that it is actually very hard to get these more or less consistent results. All model and method parameters had to be chosen carefully in order to support the theory derived above so clearly. In many cases the results were much more inconsistent, showing, e.g., convergence orders somewhere between k and 2k, changing convergence orders or stagnating results close to machine precision or discretization errors. None of the tests we did contradicted our theoretical results, but they revealed that the bounds we obtained are indeed rather pessimistic.

In Table 1 we show the order of convergence in Δt for the three test problems.

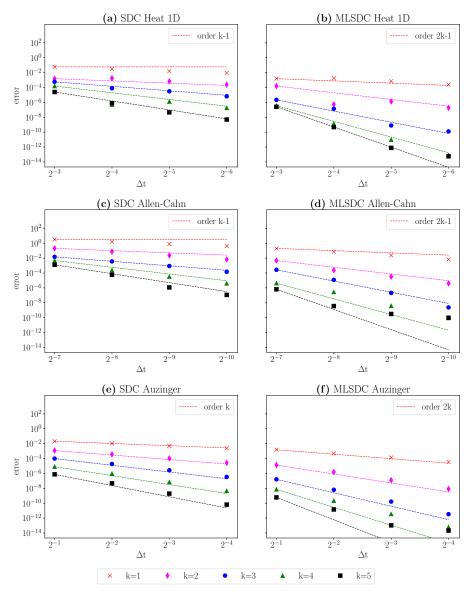


Figure 4. Convergence behavior of SDC and MLSDC for all three examples, now with larger Δt .

More precisely, we compute for a fixed Δt the ratio between the error at iteration k and the error at iteration k+1. This corresponds, in a sense, to the convergence order in k and in order to check whether this is indeed of order Δt for SDC (i.e., gaining one order of accuracy per iteration) and of order Δt^2 for MLSDC (i.e., gaining two orders of accuracy per iteration), we take the mean over the ratios for a fixed Δt and compute the order by comparing two different Δt . The results can be seen in Table 1 and they clearly indicate how noisy the convergence results are. While for

SDC we do indeed see orders around 1, the results for MLSDC are far from clear or consistent. This is due to stalling convergence and outliers, as we have already seen in the plots above. When considering only the first two iterations (the third row in each example), the results get closer to order 2. Again, this shows that obtaining consistent results is a rather delicate task.

In addition, one may wonder why the time step sizes are chosen so small in many of the tests above, especially since we deal with implicit time stepping schemes. In Figure 4 we show the results for the same three equations as before, but now with larger Δt . On the left, SDC is shown, while the right column shows MLSDC with otherwise ideal parameter choices. The measured errors still follow the lines indicating the expected orders, but the results are less consistent. We see, e.g., outliers in Figure 4 (a) and (b), early stagnation because of large Δt in (d) as well as a somewhat unclear order in (f). Still, even for these choices of Δt both SDC and MLSDC converge reasonably well and fast. However, this is beyond the range of the convergence proofs presented here, so that convergence, convergence bounds and orders of accuracy cannot be guaranteed. For applying the convergence theorems both of SDC and MLSDC, certain bounds on Δt must be taken into account, although actual results suggest that these bounds are much too restrictive. These bounds are present for most SDC convergence results (see, e.g., [15; 21; 8]), at least those relying on the matrix formulation we used as our starting point. Removing or at least relaxing these bounds in this approach is a promising further research direction for both SDC and MLSDC.

5. Conclusions and outlook

In this paper, we established two convergence theorems for multilevel spectral deferred correction (MLSDC) methods, using similar concepts and ideas as those presented in [32] for the proof of the convergence of SDC. In the first of these, namely Theorem 3.1, it was shown that with each iteration of MLSDC the error compared to the solution of the initial value problem decreases by at least one order of the chosen step size Δt , limited by the accuracy of the underlying collocation solution. The corresponding theorem only requires the operator on the right-hand side of the considered initial value problem to be Lipschitz-continuous, not necessarily linear, and the chosen time step size Δt to be sufficiently small. Consequently, we found a first theoretical convergence result for MLSDC proving that it converges as well as SDC does. However, we would expect, and numerical results have indicated, that the additional computations on the coarse level, more specifically the SDC iterations performed there, would lead to an improved convergence behavior of the method.

For that reason, we analyzed the errors in greater detail, leading to a second theorem on the convergence of MLSDC, namely Theorem 3.7. Here, we focused on a specific coarsening strategy and transfer operators. In particular, we considered

MLSDC using coarsening in space with Lagrangian interpolation. Given these assumptions, we could prove that, if particular conditions are met, the method can even gain two orders of Δt in each iteration until the accuracy of the collocation problem is reached. This consequently led us to theoretically established guidelines for the parameter choice in practical applications of MLSDC in order to achieve the described improved convergence behavior of the method. More specifically, the corresponding theorem says that for this purpose the spatial grid size on the coarse level has to be small, the interpolation order has to be high and the errors have to be smooth. We presented numerical examples which confirm these theoretical results. In particular, it could be observed that the change of one of those crucial parameters immediately led to a decrease in the order of accuracy. Essentially, it resulted in a convergence behavior as it was described in the first presented theorem.

Besides the research direction mentioned in Section 4D, there are several open questions related to the presented work which have not yet been investigated. Three of them are briefly discussed here.

More information, better results. The results presented here are quite generic. As a consequence, since we only assume Lipschitz continuity of the right-hand side of the ODE and do not pose conditions on the SDC preconditioner, both constants and step size restrictions are rather pessimistic. Using more knowledge of the right-hand side or the matrix Q_{Δ} will yield better results, as it already did for SDC. Since the goal of this paper is to establish a baseline for convergence of MLSDC, exploiting this direction, especially with respect to the treatment of convergence in the stiff limit as done in [33] for SDC, is left for future work.

Smoothness of the error. The second theorem, describing conditions for an improved convergence behavior of MLSDC, has a drawback regarding its practical significance. The way Theorem 3.7 is currently proven requires a smooth error after its periodic extension. This occurring condition of a smooth error does not always apply and is in particular not easy to control. Essentially, something like a smoothing property would be needed to ensure that the error always becomes smooth after enough iterations. Numerical results indicate that this property apparently does not hold for SDC, though [5]. In this context, however, it would be sufficient if we could at least control this condition, i.e., derive particular criteria for the parameters of the method ensuring the errors to be smooth. The numerical examples presented in Section 4 particularly lead to the assumption that the selection of a smooth initial guess $U^{(0)}$ would result in smooth errors for $U^{(k)}$, $k \ge 1$, at least for a particular set of problems.

Other extensions of SDC. Furthermore, one could try to adapt the presented convergence proofs of MLSDC to other extensions and variations of SDC, as for example the parallel-in-time method PFASST (parallel full approximation scheme

in space and time) [13] or general semi-implicit and multi-implicit formulations of SDC (SISDC/MISDC) [25; 26]. Whereas an adaptation to SISDC and MISDC methods seems to be rather straightforward [8], we found that the application of similar concepts and ideas to prove the convergence of PFASST may involve some difficulties. In particular, the coupling of the different time steps, i.e., the use of the approximation at the endpoint of the last subinterval for the start point of the next one, could cause a problem in this context since the corresponding operator is independent of Δt and would thus add a constant term to our estimations.

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GITTE KREMLING: g.kremling@fz-juelich.de

Juelich Supercomputing Centre, Forschungszentrum Juelich GmbH, Juelich, Germany

ROBERT SPECK: r.speck@fz-juelich.de

Juelich Supercomputing Centre, Forschungszentrum Juelich GmbH, Juelich, Germany

