# Convergence Proof for Iterated Splitting Defect Correction

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# Introduction

In recent years, the importance of using special numerical integration schemes that reflect certain geometric properties or retain important conserved quantities of the flow of a differential equation has been widely recognized [13], [14]. Many of these methods are applicable to particular types of differential equations only. Examples of these are the Störmer/Verlet method and the exponential midpoint rule, but also higher order composition methods that we focus on in this report.

A cheap and efficient way to estimate the global error of a numerical method used to solve an ordinary differential equation (ODE) is the defect correction principle [22], [24]. The idea can also be used to successively improve the accuracy of the numerical solution ([3], [7], [8], [9], [10], [12], [20], and the references therein). In this acceleration technique, a number of *neighboring problems* have to be solved, which are not necessarily of the same type as the original problem. Therefore it may happen that the neighboring problems cannot be solved by the same geometric integrator as the original problem. Thus, in [17] and [18] we proposed the method of *splitting defect correction* to overcome this disadvantage, see also [4]. Here, we give a proof of the convergence of the iteration defined by this new approach to realize defect correction, which we denote by *iterated splitting defect correction (ISDeC)*. We estimate the error of each respective ISDeC iterate as compared with the fixed point of the iteration in terms of the previous solution approximation, and show that the global error of the numerical approximations decreases rapidly.

# Chapter 1

# Iterated Splitting Defect Correction

First, we describe the classical version of *iterated defect correction (IDeC)* [7], [8], [20]. Consider an initial value problem in $n$ dimensions

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0, \tag{1.1}$$

to be solved on the interval $[t_0, t_{\mathrm{end}}]$. Subsequently, we assume that a sufficiently smooth solution $y$ of the analytical problem exists on the whole interval. Moreover, we will require the existence of bounded Fréchet derivatives of $f$ at various points throughout the proofs given in Chapter 3. The approximate solution $\eta^{[0]} := (\eta_0, \ldots, \eta_N)$ is obtained by some discretization method $\Phi$ on a uniform grid[1] $\Gamma = (t_0, \ldots, t_N)$, where $t_{i+1} - t_i = h,\ i = 0, \ldots, N-1$. Denote by $p^{[0]}(t)$ the polynomial of degree $N$ interpolating the values of $\eta^{[0]}$. Using this interpolating function, called the *Zadunaisky polynomial*, we construct a neighboring problem associated with (1.1) whose exact solution is $p^{[0]}(t)$:

$$y'(t) = f(t, y(t)) + d^{[0]}(t), \quad y(t_0) = y_0, \tag{1.2}$$

where $d^{[0]}(t) := p^{[0]\prime}(t) - f(t, p^{[0]}(t))$. We now solve (1.2) using the same numerical method $\Phi$ and obtain an approximate solution $\pi^{[0]}$ for $p^{[0]}(t)$. This means that for the solution of the neighboring problem (1.2) we know the global error which is a good estimate for the unknown error of the original problem (1.1). This estimate can be used to improve the first solution,

$$\eta^{[1]} := \eta^{[0]} + \left(p^{[0]} - \pi^{[0]}\right). \tag{1.3}$$

Now, these values are used to define a new interpolating polynomial $p^{[1]}(t)$ by requiring $p^{[1]}(t_j) = \eta_j^{[1]}$. Again, $p^{[1]}(t)$ defines a neighboring problem in the same manner as in (1.2), where again the exact solution is known, and the numerical solution $\pi^{[1]}$ of this neighboring problem serves to obtain the second improved solution

$$\eta^{[2]} := \eta^{[0]} + \left(p^{[1]} - \pi^{[1]}\right).$$

[1] For the classical version of IDeC, piecewise equidistant grids are required for the classical order sequences to be observed, see for example [5], [6]. This restriction is not critical in our case, since many geometric integration methods rely on the assumption of equidistant grids to retain their advantageous properties [13]. We will indicate how our arguments formulated for equidistant grids can be extended to piecewise equidistant grids where appropriate.

This process can be continued iteratively. For obvious reasons one does not use one interpolating polynomial for the whole interval $[t_0, t_{\text{end}}]$ in practice. Instead, globally continuous piecewise functions composed of polynomials of (moderate) degree $m$ are defined as the Zadunaisky polynomials for the specification of the neighboring problems.

In many situations, the defect correction principle yields an asymptotically correct error estimate and a successive improvement in the convergence orders of the respective iterates, up to a certain limit determined by the smoothness of the problem data and the value of $m$, see for example [3], [7], [8], [9], [10], [12], [20].

If for the scheme described above the basic numerical solution method $\Phi$ is a geometric integrator, the neighboring problem (1.2) may have a form to which the integrator cannot be applied straightforwardly. For example, if the Störmer/Verlet method is applied to a Hamiltonian system, (1.2) is no longer an autonomous, separated system. Another example is the exponential midpoint rule designed for linear homogeneous systems, cf. [17].

In order to be able to use iterated defect correction even in these cases, we employ splitting methods, cf. [13]. To apply *Strang splitting* to (1.2), we split the time-dependent vector field into its components $f(t, y)$ and $d^{[0]}(t)$. We denote the numerical flow of $f(t, y)$ by $\Phi_{t,h}$, such that one step $(t, \eta_i) \mapsto (t + h, \eta_{i+1})$ with step size $h$ of the basic scheme $\Phi$ applied to (1.1) can be written as $\eta_{i+1} = \Phi_{t,h}(\eta_i)$. Note that for autonomous problems (1.1), we can write the flow independently of $t$, $\eta_{i+1} = \Phi_h(\eta_i)$. The numerical flow $\Delta_{t,h}$ of the other component $d^{[0]}(t)$ is defined by the quadrature rule

$$\Delta_{t,h}(y) = y + \int_t^{t+h} D^{[0]}(\tau) d\tau, \tag{1.4}$$

where $D^{[0]}(t)$ is a piecewise polynomial interpolant of degree $\leq m - 1$ of $d^{[0]}(t)$.

To explain this more precisely, we require some additional notation. Choose the grid $\Gamma = (t_0, \ldots, t_N)$ such that $N = mN_1$ for some integer $N_1$, and denote $t_{i,j} := t_{im+j}$, $j = 0, \ldots, m$, $\tau_i := t_{im}$, $i = 0, \ldots N_1 - 1$, $\tau_{N_1} := t_N$. We split the integration interval into subintervals $J_i := [\tau_i, \tau_{i+1}]$ of length $H$. On the interval $J_i$, we define interpolation nodes

$$\sigma_{i,j} := \tau_i + H\rho_j, \ j = 1, \ldots, m, \quad \text{where } 0 \leq \rho_1 < \rho_2 < \cdots < \rho_m \leq 1. \tag{1.5}$$

The highest attainable convergence orders for the ISDeC iterates result if we use interpolation at Gaussian points [2] in order to define $D^{[0]}(t)$. Thus the maximal convergence order of IDeC iterates is $O(H^{2m})$, see [17] and Chapter 3.

Using $\Phi_{t,h}$ and $\Delta_{t,h}$ from above, the numerical solution of (1.2) is computed using the numerical flow

$$\Psi_{t,h} = \Delta_{t+h/2,h/2} \circ \Phi_{t,h} \circ \Delta_{t,h/2}, \tag{1.6}$$

where $\circ$ denotes the *composition* of the numerical methods (which means that the result computed by one method is the starting value for the next method). We call the method where the solution of the neighboring problems is computed in this way *iterated splitting defect correction (ISDeC)*.

# Chapter 2

# High Order Geometric Integration Schemes

In the sequel, we introduce high order composition methods. When these are based on low order schemes with favorable geometric properties, as for example the Störmer/Verlet method for Hamiltonian systems, these properties are often inherited by the higher order scheme [13]. Let the basis for ISDeC be a composition method

$$\Phi = \Phi^{[s]} \circ \cdots \circ \Phi^{[2]} \circ \Phi^{[1]}. \tag{2.1}$$

Then, the numerical method $\Psi$ for the solution of the neighboring problem (1.2) can be defined by

$$\Psi_{t,h} = \Delta_{t+\hat{\delta}_{s+1}h,\delta_{s+1}h} \circ \Phi^{[s]} \circ \Delta_{t+\hat{\delta}_s h,\delta_s h} \circ \cdots \circ \Delta_{t+\hat{\delta}_2 h,\delta_2 h} \circ \Phi^{[1]} \circ \Delta_{t+\hat{\delta}_1 h,\delta_1 h}, \tag{2.2}$$

where $\delta_1, \ldots, \delta_{s+1}$ are given real numbers which satisfy

$$\delta_1 + \cdots + \delta_{s+1} = 1, \quad \hat{\delta}_j := \sum_{i=1}^{j-1} \delta_i,$$

and $\Delta_{t,h}$ is given by (1.4).

Subsequently we give some examples of composition methods we considered [17], [18]. First, we describe symmetric composition of symmetric methods [13, Sec. V.3]:

$$\Phi^{[j]} = \phi_{t+\hat{\gamma}_j h,\gamma_j h}, \quad j = 1, \ldots, s, \tag{2.3}$$

where $\phi$ is a symmetric second order method, the coefficients $\gamma_s = \gamma_1, \gamma_{s-1} = \gamma_2, \ldots$ are symmetric, and $\hat{\gamma}_j := \sum_{i=1}^{j-1} \gamma_j$. Examples of possible choices for $\phi$ are the Störmer/Verlet scheme, the implicit midpoint rule, the implicit trapezoidal rule, or the exponential midpoint rule [17]. The coefficients $\gamma_j$ may be chosen for example such as to yield Yoshida's method,

$$s = 3, \quad \gamma_1 = \gamma_3 = 1/(2 - 2^{1/3}), \quad \gamma_2 = -2^{1/3}/(2 - 2^{1/3}), \tag{2.4}$$

or Suzuki's method,

$$s = 5, \quad \gamma_1 = \gamma_2 = \gamma_4 = \gamma_5 = 1/(4 - 4^{1/3}), \quad \gamma_3 = -4^{1/3}/(4 - 4^{1/3}). \tag{2.5}$$

Both of these choices (in conjunction with a symmetric second-order basic scheme) yield methods of order 4, cf. [13, Sec. II.4]. A natural choice for the coefficients $\delta_j$ in the splitting (2.2) is

$$\delta_1 = \gamma_1/2, \qquad \delta_j = (\gamma_{j-1} + \gamma_j)/2, \quad j = 2, \ldots, s, \qquad \delta_{s+1} = \gamma_s/2, \tag{2.6}$$

since then $\Psi$ can be written as

$$\Psi = \Psi^{[s]} \circ \cdots \circ \Psi^{[1]}, \tag{2.7}$$

where

$$\Psi^{[j]} = \Delta_{t+\hat{\gamma}_j h+\gamma_j h/2, \gamma_j h/2} \circ \phi_{t+\hat{\gamma}_j h, \gamma_j h} \circ \Delta_{t+\hat{\gamma}_j h, \gamma_j h/2}. \tag{2.8}$$

Consequently, $\Psi^{[j]}$ is a symmetric second-order method and $\Psi$ has the same order as $\Phi$, see [13, Sec. II.4].

Alternatively, we also consider symmetric composition of first order methods. For $s$ even we choose

$$\Phi^{[2j-1]} = \phi_{t+\hat{\gamma}_{2j-1}h, \gamma_{2j-1}h}, \quad \Phi^{[2j]} = \phi^*_{t+\hat{\gamma}_{2j}h, \gamma_{2j}h}, \quad j = 1, \ldots, s/2, \tag{2.9}$$

where $\phi$ is an arbitrary first order method, $\phi^*$ the adjoint method of $\phi$, and the coefficients $\gamma_j$ satisfy

$$\gamma_s = \gamma_1, \gamma_{s-1} = \gamma_2, \ldots, \quad \hat{\gamma}_j := \sum_{i=1}^{j-1} \gamma_j.$$

A possible choice for the coefficients $\gamma_j$ is McLachlan's method (which yields a fourth-order method for suitable $\phi$),

$$\begin{aligned} s = 10, \quad & \gamma_1 = \gamma_{10} = (14 - \sqrt{19})/108, && \gamma_2 = \gamma_9 = (146 + 5\sqrt{19})/540, \\ & \gamma_3 = \gamma_8 = (-23 - 20\sqrt{19})/270, && \gamma_4 = \gamma_7 = (-2 + 10\sqrt{19})/135, \\ & \gamma_5 = \gamma_6 = 1/5, \end{aligned} \tag{2.10}$$

cf. [13, Sec. V.3.1]. Again, the choice of the coefficients $\delta_j$ in (2.2) according to (2.6) ensures that $\Psi$ has the same order as $\Phi$. As basic methods, we considered the explicit and the implicit Euler method, and the symplectic Euler method in conjunction with its adjoint method [17].

# Chapter 3

# Fixed Point Convergence

Without restriction of generality, we confine our analysis to autonomous problems

$$y'(t) = f(y(t)), \quad y(t_0) = y_0. \tag{3.1}$$

The neighboring problems

$$y'(t) = f(y(t)) + d(t), \quad y(t_0) = y_0 \tag{3.2}$$

are nonetheless nonautonomous. We use the standard procedure to rewrite this system as an autonomous differential equation by adding the trivial equation $s'(t) = 1$ with exact solution $s(t) = t$,

$$\tilde{y}'(t) = \tilde{f}(\tilde{y}(t)) + \tilde{d}(\tilde{y}(t)), \quad \tilde{y}(t_0) = \tilde{y}_0, \tag{3.3}$$

where

$$\tilde{y} = \begin{pmatrix} y \\ s \end{pmatrix}, \quad \tilde{f}(\tilde{y}) := \begin{pmatrix} f(y) \\ 0 \end{pmatrix}, \quad \tilde{d}(\tilde{y}) := \begin{pmatrix} d(s) \\ 1 \end{pmatrix}, \quad \tilde{y}_0 := \begin{pmatrix} y_0 \\ t_0 \end{pmatrix}. \tag{3.4}$$

Note that the right-hand side of the auxiliary equation $s'(t) = 1$ is appended to $d(s)$ and not to $f(y)$.

To achieve formal correspondence between the original equation and the augmented neighboring problem, we also add the trivial equation to (3.1) to obtain

$$\tilde{y}'(t) = \hat{f}(\tilde{y}(t)), \quad \tilde{y}(t_0) = \tilde{y}_0, \tag{3.5}$$

where

$$\hat{f}(\tilde{y}) := \begin{pmatrix} f(y) \\ 1 \end{pmatrix}.$$

To analyze the convergence of ISDeC introduced in Chapter 1, we consider one step of the iteration, starting from a grid vector $\eta = \eta_{i,j},\ j = 0,\dots,m,\ i = 0,\dots,N_1 - 1$, and estimate the *iteration error* of the new approximation in terms of the iteration error of $\eta_{i,j}$. $\eta_{i,j}$ is either the solution of (3.1) by the basic scheme $\Phi$, or an improved solution approximation computed in the course of the ISDeC iteration. For this type of analysis we use the fact that iterated defect correction converges to a fixed point $p^* = (p_0^*, p_1^*, \dots, p_{N_1-1}^*)$ under fairly general assumptions [6], [7], [11]. This fixed point is easily identified as the continuous collocating function consisting of polynomials of degree $\leq m$ which satisfies (1.1) at the points $\sigma_{i,j},\ i = 0,\dots,N_1-1, j = 1,\dots,m$, cf. (1.5). The *iteration error* $\eta - p^*$ is the error of the respective grid vector as compared with the fixed point, see also [21]. The results we obtain for the iteration error directly translate into order results for the global error of the numerical solution as compared with the exact solution $\tilde{y}$ of (3.1). Note that in our estimates, we usually neglect the last, trivial component of (3.3).

Denote by $p = (p_0, p_1, \dots, p_{N_1-1})$ the piecewise polynomial function of maximal degree $m$ interpolating $\eta_{i,j}$ at $t_{i,j},\ j = 0,\dots,m,\ i = 0,\dots,N_1-1$. One step of the ISDeC procedure yields a new grid function $\eta_{i,j}^{\text{new}}$ and a new Zadunaisky polynomial $p^{\text{new}} = (p_0^{\text{new}}, p_1^{\text{new}}, \dots, p_{N_1-1}^{\text{new}})$. Subsequently, we derive estimates of the current iteration error $e^{\text{new}} := p^{\text{new}} - p^*$ in terms of estimates for $e := p - p^*$.

$p_i(t),\ t \in J_i,\ i = 0,\dots,N_1-1$, is the exact solution of

$$y'(t) = f(y(t)) + d_i(t), \quad y(\tau_i) = p_i(\tau_i), \tag{3.6}$$

where the defect $d_i(t)$ is defined by

$$d_i(t) := p_i'(t) - f(p_i(t)). \tag{3.7}$$

Analogously as in (3.3), $\tilde{p}_i(t)$ is the exact solution of the augmented equations

$$\tilde{y}'(t) = \tilde{f}(\tilde{y}(t)) + \tilde{d}_i(\tilde{y}(t)), \quad \tilde{y}(\tau_i) = \tilde{\mathbf{p}}_i, \tag{3.8}$$

where $\tilde{\mathbf{p}}_i := \tilde{p}_i(\tau_i)$.

We now express all the quantities associated with one step of ISDeC using the calculus of Lie derivatives, cf. [13]. We start by rewriting the Zadunaisky polynomial $p$ and the fixed point $p^*$ in (3.9) and (3.16), and derive analogous expressions for the quantities computed numerically, the basic solution $\eta^{[0]}$ of (3.1) and the computational solution of the neighboring problem (3.2), see (3.28) and (3.29). Note that actually we use the flows for the autonomous formulations augmented by the trivial equations as in (3.5) or (3.3).

$\tilde{p}_i(t)$ can thus be written as

$$\tilde{p}_i(\tau_i + t) = \exp(t(\mathcal{F} + \mathcal{D}_i))\mathrm{Id}(\tilde{y})\Big|_{\tilde{y} = \tilde{\mathbf{p}}_i}, \tag{3.9}$$

where $\mathcal{F}$ and $\mathcal{D}_i$ are the differential operators (*Lie derivatives*)

$$\mathcal{F} = \sum_{j=1}^{n+1} \tilde{f}_j(\tilde{y}) \frac{\partial}{\partial \tilde{y}_j} = \sum_{j=1}^{n} f_j(y) \frac{\partial}{\partial y_j} \tag{3.10}$$

and

$$\mathcal{D}_i = \sum_{j=1}^{n+1} \tilde{d}_{i,j}(\tilde{y}) \frac{\partial}{\partial \tilde{y}_j} = \sum_{j=1}^{n} d_{i,j}(s) \frac{\partial}{\partial y_j} + \frac{\partial}{\partial s}, \tag{3.11}$$

see [13, Sec. III.5.1]. Here, $f_j$ and $d_{i,j}$ denote the $j$-th component of $f$ and $d_i$, respectively. With these definitions the exact flow $\tilde{\varphi}_t(\tilde{y})$ of the vector field $\tilde{f}(\tilde{y})$ is given by

$$\tilde{\varphi}_t(\tilde{y}) = \exp(t\mathcal{F})\mathrm{Id}(\tilde{y}), \tag{3.12}$$

and the exact flow

$$\tilde{\delta}_{i,t}(\tilde{y}) = \begin{pmatrix} y + \int_s^{s+t} d_i(\tau)d\tau \\ s+t \end{pmatrix} \tag{3.13}$$

of the vector field $\tilde{d}_i(\tilde{y})$ is given by

$$\tilde{\delta}_{i,t}(\tilde{y}) = \exp(t\mathcal{D}_i)\mathrm{Id}(\tilde{y}). \tag{3.14}$$

Now we derive a representation analogous to (3.9) for the fixed point $p^* = (p_0^*, p_1^*, \ldots, p_{N_1-1}^*)$. With $\tilde{p}^*$, $d^*$, and $\tilde{d}^*$ defined analogously as before, $\tilde{p}_i^*(t),\ t \in J_i$, is the exact solution of

$$\tilde{y}'(t) = \tilde{f}(\tilde{y}(t)) + \tilde{d}_i^*(\tilde{y}(t)), \quad \tilde{y}(\tau_i) = \tilde{\mathbf{p}}_i^*, \tag{3.15}$$

where $\tilde{\mathbf{p}}_i^* := \tilde{p}_i^*(\tau_i)$. Hence,

$$\tilde{p}_i^*(\tau_i + t) = \exp(t(\mathcal{F} + \mathcal{D}_i^*))\mathrm{Id}(\tilde{y})\Big|_{\tilde{y} = \tilde{\mathbf{p}}_i^*} \tag{3.16}$$

with

$$\mathcal{D}_i^* = \sum_{j=1}^{n+1} \tilde{d}_{i,j}^*(\tilde{y})\frac{\partial}{\partial \tilde{y}_j} = \sum_{j=1}^{n} d_{i,j}^*(s)\frac{\partial}{\partial y_j} + \frac{\partial}{\partial s}. \tag{3.17}$$

Choose as the basic method $\Phi$ for ISDeC a composition method according to Chapter 2. $\Phi$ is composed of substeps using the method $\phi$ and, if $\phi$ is a first order method, the adjoint method $\phi^*$. For all the methods we consider, the numerical flow defined by $\phi$ satisfies a *modified differential equation*

$$y' = f(y) + hF_1(y) + h^2F_2(y) + \ldots, \tag{3.18}$$

cf. [13, Chapt. IX]. Thus, the numerical flow of $\phi$ and $\phi^*$, respectively, can be written as

$$\phi_h(y) = \exp(h(\mathcal{F} + h\mathcal{F}_1 + h^2\mathcal{F}_2 + \ldots))\mathrm{Id}(y), \tag{3.19}$$

and

$$\phi_h^*(y) = \exp(h(\mathcal{F} - h\mathcal{F}_1 + h^2\mathcal{F}_2 - \ldots))\mathrm{Id}(y), \tag{3.20}$$

with the Lie derivatives

$$\mathcal{F}_\ell = \sum_{j=1}^{n} F_{\ell,j}(y)\frac{\partial}{\partial y_j}, \quad \ell = 1, 2, \ldots. \tag{3.21}$$

If we assume that $\Phi$ is a method of order $q$, then its numerical flow when applied to (3.1) can be written as

$$\Phi_h(y) = \exp(h(\mathcal{F} + h^q \mathcal{G}_q^* + h^{q+1}\mathcal{G}_{q+1}^* + \dots))\mathrm{Id}(y), \tag{3.22}$$

where the differential operators $\mathcal{G}_\ell^*$ are certain well defined elements of the free Lie algebra generated by $\{\mathcal{F}, \mathcal{F}_1, \mathcal{F}_2, \dots\}$, i. e., they are certain linear combinations of iterated commutators of elements of $\{\mathcal{F}, \mathcal{F}_1, \mathcal{F}_2, \dots\}$, see [13].

The corresponding numerical flow for the augmented equation (3.5) is given accordingly by

$$\tilde{\Phi}_h(\tilde{y}) = \exp(h(\mathcal{F} + \hat{\mathcal{D}}^* + h^q \mathcal{G}_q^* + h^{q+1}\mathcal{G}_{q+1}^* + \dots))\mathrm{Id}(\tilde{y}), \tag{3.23}$$

where

$$\hat{\mathcal{D}}^* := \frac{\partial}{\partial s} \tag{3.24}$$

only acts on the last component of $\tilde{y}$. The corresponding component of $\tilde{\Phi}_h(\tilde{y})$ is equal to $s + h$, whereas all other components are not affected by $\hat{\mathcal{D}}^*$.

The numerical flow $\tilde{\Delta}_{i,h}(\tilde{y})$ of the vector field $\tilde{d}_i(\tilde{y})$ of (3.8) is given by

$$\tilde{\Delta}_{i,h}(\tilde{y}) = \begin{pmatrix} y + \displaystyle\int_s^{s+h} D_i(\tau)d\tau \\ s+h \end{pmatrix} = \exp(h\hat{\mathcal{D}}_i)\mathrm{Id}(\tilde{y}), \tag{3.25}$$

where $D_i(t)$ is the polynomial of degree $\le m-1$ interpolating $d_i(t)$ at the collocation points $\sigma_{i,1}, \dots, \sigma_{i,m}$, cf. (1.4), (1.5). $\hat{\mathcal{D}}_i$ is defined similarly as in (3.11),

$$\hat{\mathcal{D}}_i = \sum_{j=1}^{n} D_{i,j}(s)\frac{\partial}{\partial y_j} + \frac{\partial}{\partial s}. \tag{3.26}$$

Note that $\tilde{\Delta}_{i,h}(\tilde{y})$ is the exact flow of the vector field $\tilde{D}_i(\tilde{y})$, which is defined as $D_i(s)$ augmented by the last component equal to 1.

The numerical solution method for the neighboring problem, $\Psi$, is constructed in such a way that a method of order $q$ results and the composition of the submethods is parallel to the definition of $\Phi$, see Chapter 2. Thus, the numerical flow $\tilde{\Psi}_{i,h}(\tilde{y})$ for (3.8) is given by

$$\tilde{\Psi}_{i,h}(\tilde{y}) = \exp(h(\mathcal{F} + \hat{\mathcal{D}}_i + h^q \mathcal{G}_{i,q} + h^{q+1}\mathcal{G}_{i,q+1} + \dots))\mathrm{Id}(\tilde{y}), \tag{3.27}$$

where the differential operators $\mathcal{G}_{i,\ell}$ are well defined elements of the free Lie algebra generated by $\{\mathcal{F}, \hat{\mathcal{D}}_i, \mathcal{F}_1, \mathcal{F}_2, \dots\}$. Note that if each occurrence of $\hat{\mathcal{D}}_i$ in the definition of $\mathcal{G}_{i,\ell}$ is replaced by $\hat{\mathcal{D}}^*$, the resulting differential operator coincides with $\mathcal{G}_\ell^*$ from (3.23).

Now we are in a position to write the numerical solutions of the original and the neighboring problem in terms of Lie derivatives as in (3.9) and (3.16).

The basic numerical solution $\tilde{\eta}^{[0]}_{i,j}$ of (3.5) is given by $\tilde{\eta}^{[0]}_{i,j} := \tilde{\pi}^*_i(\tau_i + jh)$, where the functions $\tilde{\pi}^*_i(t),\ t \in J_i$, are recursively defined by

$$\begin{aligned} &\tilde{\boldsymbol{\pi}}^*_0 = \tilde{y}_0, \\ &\tilde{\pi}^*_i(\tau_i + t) = \exp(t(\mathcal{F} + \hat{\mathcal{D}}^* + h^q \mathcal{G}^*_q + h^{q+1}\mathcal{G}^*_{q+1} + \dots))\mathrm{Id}(\tilde{y})\Big|_{\tilde{y} = \tilde{\boldsymbol{\pi}}^*_i}, \\ &\tilde{\boldsymbol{\pi}}^*_{i+1} = \tilde{\pi}^*_i(\tau_i + H), \end{aligned} \tag{3.28}$$

cf. (3.23).

Similarly, the numerical solution $\tilde{\pi}_{i,j}$ of the neighboring problem (3.3) is given by $\tilde{\pi}_{i,j} := \tilde{\pi}_i(\tau_i + jh)$, where

$$\begin{aligned} &\tilde{\boldsymbol{\pi}}_0 = \tilde{y}_0, \\ &\tilde{\pi}_i(\tau_i + t) = \exp(t(\mathcal{F} + \hat{\mathcal{D}}_i + h^q \mathcal{G}_{i,q} + h^{q+1}\mathcal{G}_{i,q+1} + \dots))\mathrm{Id}(\tilde{y})\Big|_{\tilde{y} = \tilde{\boldsymbol{\pi}}_i}, \\ &\tilde{\boldsymbol{\pi}}_{i+1} = \tilde{\pi}_i(\tau_i + H), \end{aligned} \tag{3.29}$$

cf. (3.27).

Now, one iteration step of the ISDeC method on the subinterval $J_i$ can be written as

$$p^{\mathrm{new}}_i(t_{i,j}) = \tilde{\pi}^*_i(t_{i,j}) + (\tilde{p}_i(t_{i,j}) - \tilde{\pi}_i(t_{i,j}))\,, \tag{3.30}$$

see (1.3).

This yields a representation of the iteration error $e^{\mathrm{new}} = p^{\mathrm{new}} - p^*$, which is the piecewise interpolant of degree $\le m$ at $t_{i,j}$ of the first $n$ components[1] of $\tilde{\varepsilon} = (\tilde{\varepsilon}_0, \tilde{\varepsilon}_1, \dots, \tilde{\varepsilon}_{N_1-1})$, where

$$\tilde{\varepsilon}_i(\tau_i + t) := (\tilde{\pi}^*_i(\tau_i + t) - \tilde{\pi}_i(\tau_i + t)) - (\tilde{p}^*_i(\tau_i + t) - \tilde{p}_i(\tau_i + t)). \tag{3.31}$$

Recall that the function $\tilde{\varepsilon}(t)$ is defined in a piecewise manner on the subintervals $J_i,\ i = 0, \dots, N_1 - 1$, cf. (3.28) and (3.29). Subsequently, we will derive estimates for the relevant quantities on each interval $J_i$, and use the following lemma to obtain global estimates on $[t_0, t_{\mathrm{end}}]$. We formulate the result for uniform grids, the modifications necessary for variable step sizes are indicated in [15, Sec. II.3].

**Lemma 1 (Discrete Gronwall Lemma)** *Let the sequence of nonnegative numbers $\xi_i,\ i = 0, 1 \dots$ satisfy*

$$\xi_0 = \delta_0, \quad \xi_{i+1} \le (1 + \omega)\xi_i + \delta, \quad i = 0, 1, \dots \tag{3.32}$$

[1]Note that the $(n + 1)$-st component of $\tilde{\varepsilon}$ is zero.

*with* $\omega > 0$ *and* $\delta \geq 0$*. Then the estimate*

$$\xi_i \leq \frac{e^{i\omega} - 1}{\omega}\delta + e^{i\omega}\delta_0 \tag{3.33}$$

*holds for all* $i$*.*

*Proof.* See for example [19] or [23]. □

Next, we introduce Sobolev-like norms by means of which we will estimate grid vectors or functions $X_H$ occurring in the course of the ISDeC step $p \mapsto p^{\text{new}}$. The index $H$ emphasizes that $X_H$ depends on the underlying grid and thus on the step size $H$. Frequently, our estimates will be written as

$$X_H = O(H^\ell \|e\|_k), \tag{3.34}$$

where this short-hand notation implies that there are constants $H_0 > 0$ and $C$ independent of $H$ and $p$ such that

$$\|X_H\| \leq CH^\ell \sum_{\kappa=0}^{k} \max_{i=0,\ldots,N_1-1} \max_{t\in J_i} |e_i^{(\kappa)}(t)| \tag{3.35}$$

for all $0 < H \leq H_0$, where $e := p - p^*$ is the iteration error of $p$. The following relations will be used in many of our arguments given below in the course of the convergence proof for ISDeC.

**Lemma 2** *If* $X_H$ *satisfies* (3.34)*, then*

$$X_H = O(H^{\ell-\kappa}\|e\|_{k-\kappa}), \quad \kappa = 0, \ldots, k, \tag{3.36}$$

$$X_H = O(H^\ell \|e\|_m), \quad \text{if } k \geq m. \tag{3.37}$$

*Proof.* Since $e$ is a polynomial of degree $\leq m$, (3.37) is clear. (3.36) can easily be shown if a representation of $e$ in terms of Lagrange polynomials is used, cf. for example [20], [21]. □

**Lemma 3** *Let* $p_i$ *be a polynomial of degree* $\leq m$ *interpolating a sufficiently smooth function* $y \in C^{m+1}[t_0, t_{\text{end}}]$ *on the interval* $J_i$*. Then the estimates*

$$\max_{t\in J_i} |p_i^{(\kappa)}(t) - y^{(\kappa)}(t)| \leq \text{const.} H^{m+1-\kappa} \max_{t\in J_i} |y^{(m+1)}(t)|, \quad \kappa = 0, \ldots, m+1, \tag{3.38}$$

$$\max_{t\in J_i} |p_i^{(\kappa)}(t) - y^{(\kappa)}(t)| \leq \text{const.} \max_{t\in J_i} |y^{(\kappa)}(t)|, \quad \kappa = 0, \ldots, m+1 \tag{3.39}$$

*hold.*

*Proof.* The proof for (3.38) is given in [16, Sec. 5.1], (3.39) can be found in [1], see also [7]. □

In the sequel, we formulate a number of lemmas necessary to estimate $\tilde{\varepsilon}$.

**Lemma 4** *For the quantities defined in* (3.9)*,* (3.16)*,* (3.28) *and* (3.29)*,*

$$|\tilde{\boldsymbol{\pi}}_i - \tilde{\mathbf{p}}_i| = O(H^{\min(q,m)}) \tag{3.40}$$

*and*

$$|\tilde{\boldsymbol{\pi}}_i^* - \tilde{\mathbf{p}}_i^*| = O(H^{\min(q,m)}) \tag{3.41}$$

*holds for* $i = 0, \ldots, N_1$.

*Proof.* We only prove (3.40), the proof of (3.41) is analogous. Expansion of (3.9) and (3.29) up to terms of order $O(H^q)$ yields

$$\begin{aligned} \tilde{\boldsymbol{\pi}}_{i+1} - \tilde{\mathbf{p}}_{i+1} &= \tilde{\pi}_i(\tau_i + H) - \tilde{p}_i(\tau_i + H) \\ &= \tilde{\boldsymbol{\pi}}_i - \tilde{\mathbf{p}}_i + \sum_{k=1}^{q} \frac{H^k}{k!}\Big((\mathcal{F} + \hat{\mathcal{D}}_i)^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i) - (\mathcal{F} + \mathcal{D}_i)^k \mathrm{Id}(\tilde{\mathbf{p}}_i)\Big) + O(H^{q+1}). \end{aligned} \tag{3.42}$$

Here and in the sequel, $\mathrm{Id}(\tilde{\mathbf{p}})$ denotes $\mathrm{Id}(\tilde{y})|_{\tilde{y}=\tilde{\mathbf{p}}}$.

As a prerequisite for the subsequent analysis, we describe the general form of terms occurring in the expansion of $\frac{H^k}{k!}(\mathcal{F} + \mathcal{D}_i)^k \mathrm{Id}(\tilde{\mathbf{p}}_i)$. We denote the generic form of the components of these terms by

$$\frac{H^k}{k!}\mathbf{f}(\mathbf{p}_i)\mathbf{d}_i(\tau_i), \tag{3.43}$$

where $\mathbf{f}(y)$ is either the constant function $\mathbf{f}(y) \equiv 1$ or a product of component functions $f_j(y)$ of $f(y)$ or derivatives thereof, all evaluated at $y = \mathbf{p}_i$ (the first $n$ components of $\tilde{\mathbf{p}}_i$). $\mathbf{d}_i(\tau_i)$ denotes expressions of the form

$$\mathbf{d}_i(\tau_i) = d_{i,j_1}^{(\kappa_1)}(\tau_i) \cdots d_{i,j_r}^{(\kappa_r)}(\tau_i), \tag{3.44}$$

where the derivatives are of order $\le k-1$ and $d_{i,j}$ denotes one component of the defect $d_i$. As an illustration, consider the first component of $\frac{H^2}{2}(\mathcal{F} + \mathcal{D}_i)^2 \mathrm{Id}(\tilde{\mathbf{p}}_i)$,

$$\begin{aligned} &\frac{H^2}{2}\Big((\mathcal{F}^2 + \mathcal{F}\mathcal{D}_i + \mathcal{D}_i\mathcal{F} + \mathcal{D}^2)\mathrm{Id}(\tilde{\mathbf{p}}_i)\Big)_1 \\ &\quad = \frac{H^2}{2}\left(\sum_{j=1}^{n} f_j(\mathbf{p}_i)\frac{\partial f_1(\mathbf{p}_i)}{\partial y_j} + 0 + \sum_{j=1}^{n} d_{i,j}(\tau_i)\frac{\partial f_1(\mathbf{p}_i)}{\partial y_j} + d'_{i,1}(\tau_i)\right). \end{aligned} \tag{3.45}$$

Clearly, the components of $\frac{H^k}{k!}(\mathcal{F}+\mathcal{D}_i)^k \mathrm{Id}(\tilde{\mathbf{p}}_i)$ can be expanded in this way for all $k=1,\dots,q$.

Likewise, the components of $\frac{H^k}{k!}(\mathcal{F}+\hat{\mathcal{D}}_i)^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i)$ have expansions which contain terms

$$\frac{H^k}{k!}\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i), \tag{3.46}$$

where $\mathbf{f}(y)$ is evaluated at $y=\boldsymbol{\pi}_i$, and (3.44) is replaced by

$$\mathbf{D}_i(\tau_i) = D_{i,j_1}^{(\kappa_1)}(\tau_i)\cdots D_{i,j_r}^{(\kappa_r)}(\tau_i). \tag{3.47}$$

Combining corresponding terms in the expansions of $(\mathcal{F}+\mathcal{D}_i)^k \mathrm{Id}(\tilde{\mathbf{p}}_i)$ and $(\mathcal{F}+\hat{\mathcal{D}}_i)^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i)$ we obtain

$$\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i)-\mathbf{f}(\mathbf{p}_i)\mathbf{d}_i(\tau_i) = (\mathbf{f}(\boldsymbol{\pi}_i)-\mathbf{f}(\mathbf{p}_i))\mathbf{D}_i(\tau_i)+\mathbf{f}(\mathbf{p}_i)(\mathbf{D}_i(\tau_i)-\mathbf{d}_i(\tau_i)). \tag{3.48}$$

Using Lemma 3 applied to the interpolating polynomials $D_{i,j}(t)$ of $d_{i,j}(t)$ which have degree $\le m-1$, it is easy to show that

$$\mathbf{D}_i(\tau_i)-\mathbf{d}_i(\tau_i) = D_{i,j_1}^{(\kappa_1)}(\tau_i)\cdots D_{i,j_r}^{(\kappa_r)}(\tau_i)-d_{i,j_1}^{(\kappa_1)}(\tau_i)\cdots d_{i,j_r}^{(\kappa_r)}(\tau_i) = O(H^{m-k+1}), \tag{3.49}$$

if we recall that the highest derivatives occurring in this relation are of order $\le k-1$. Using a Lipschitz condition for $\mathbf{f}(y)$, (3.48) implies the estimate

$$\begin{aligned}\frac{H^k}{k!}\big|\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i)-\mathbf{f}(\mathbf{p}_i)\mathbf{d}_i(\tau_i)\big| &\le \text{const.}H^k|\tilde{\boldsymbol{\pi}}_i-\tilde{\mathbf{p}}_i|+O(H^{m+1})\\ &\le \text{const.}H|\tilde{\boldsymbol{\pi}}_i-\tilde{\mathbf{p}}_i|+O(H^{m+1}).\end{aligned} \tag{3.50}$$

Summation over all $k=1,\dots,q$ in (3.42) now yields

$$|\tilde{\boldsymbol{\pi}}_{i+1}-\tilde{\mathbf{p}}_{i+1}| \le (1+\text{const.}H)|\tilde{\boldsymbol{\pi}}_i-\tilde{\mathbf{p}}_i|+O(H^{\min(q,m)+1}). \tag{3.51}$$

The assertion of the lemma now follows from Lemma 1, on noting that $iH < N_1H = t_{\mathrm{end}}-t_0 = O(1)$. □

**Lemma 5** *The interpolant $D_{i,j}(t)$ of one component of the defect of $p$, $d_{i,j}(t) = p'_{i,j}(t)-f_j(p_i(t))$, satisfies*

$$D_{i,j}^{(k)}(\tau_i) = O(\|e\|_{k+1}), \quad k=0,\dots,m-1, \tag{3.52}$$

$$D_{i,j}^{(k)}(\tau_i) = 0, \quad k\ge m. \tag{3.53}$$

*Proof.* Let $F_{i,j}(t)$ and $F^*_{i,j}(t)$ be the polynomials of degree $\le m-1$ which interpolate the component functions $f_j(p_i(t))$ and $f_j(p^*_i(t))$, respectively, at the nodes

$\sigma_{i,1},\ldots,\sigma_{i,m}$. From the definition of $p^*(t)$ we conclude ${p^*}'_{i,j}(t) = F^*_{i,j}(t)$, and consequently

$$D^{(k)}_{i,j}(\tau_i) = (p^{(k+1)}_{i,j}(\tau_i) - p^{*(k+1)}_{i,j}(\tau_i)) - (F^{(k)}_{i,j}(\tau_i) - F^{*(k)}_{i,j}(\tau_i)). \tag{3.54}$$

Clearly,

$$p^{(k+1)}_{i,j}(\tau_i) - p^{*(k+1)}_{i,j}(\tau_i) = e^{(k+1)}_{i,j}(\tau_i) = O(\|e\|_{k+1}).$$

Using Lipschitz conditions for $f^{(\kappa)}_{i,j}(y)$, $\kappa = 0,\ldots,k$, and Lemma 3 for the interpolant $F_{i,j}(t) - F^*_{i,j}(t)$ of $f_j(p_i(t)) - f_j(p^*_i(t))$, it is straightforward to show that also

$$F^{(k)}_{i,j}(\tau_i) - F^{*(k)}_{i,j}(\tau_i) = O(\|e\|_k) = O(\|e\|_{k+1}).$$

□

**Lemma 6** *For each integer $u > 0$, the relation*

$$|\tilde{\boldsymbol{\pi}}^*_i - \tilde{\boldsymbol{\pi}}_i| = O(\|e\|_1) + O(H^u) \tag{3.55}$$

*holds.*

*Proof.* Expansion of (3.28) and (3.29) up to terms of order $O(H^u)$ and combination of like powers of $H$ yields

$$\begin{aligned} \tilde{\boldsymbol{\pi}}^*_{i+1} - \tilde{\boldsymbol{\pi}}_{i+1} &= \tilde{\pi}^*_i(\tau_i + H) - \tilde{\pi}_i(\tau_i + H) \\ &= \tilde{\boldsymbol{\pi}}^*_i - \tilde{\boldsymbol{\pi}}_i + \sum_{k=1}^{u} \frac{H^k}{k!}\Big(\mathcal{F}^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}^*_i) \;-\; (\mathcal{F} + \hat{\mathcal{D}}_i)^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i)\Big) \;+\; (0,\ldots,0,H)^T \\ &\quad + \big[\text{terms of order} \le u \text{ involving } \mathcal{G}^*_\ell \text{ or } \mathcal{G}_{i,\ell}\big] \;+\; O(H^{u+1}). \end{aligned} \tag{3.56}$$

Here we have used

$$\begin{aligned} &(\mathcal{F} + \hat{\mathcal{D}}^*)^k = \mathcal{F}^k + \hat{\mathcal{D}}^{*k}, \\ &\hat{\mathcal{D}}^* \mathrm{Id}(\tilde{y}) = (0,\ldots,0,1)^T \quad \text{and} \quad \hat{\mathcal{D}}^{*k} \mathrm{Id}(\tilde{y}) = 0,\ k \ge 2. \end{aligned}$$

The last component of the term $(0,\ldots,0,H)^T$ cancels with the corresponding term in the expansion of $(\mathcal{F} + \hat{\mathcal{D}}_i)^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i)$. Generally, the last component in (3.56) is zero and only the first $n$ components are subsequently considered. The terms involving $\mathcal{G}^*_\ell$ or $\mathcal{G}_{i,\ell}$ are treated below, see (3.60).

Similarly as in (3.46), the expansion of $\frac{H^k}{k!}(\mathcal{F}^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}^*_i) - (\mathcal{F} + \hat{\mathcal{D}}_i)^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i))$ consists of terms of the form

$$\frac{H^k}{k!}(\mathbf{f}(\boldsymbol{\pi}^*_i) - \mathbf{f}(\boldsymbol{\pi}_i)) \quad \text{or} \quad -\frac{H^k}{k!}\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i), \tag{3.57}$$

where the derivatives in $\mathbf{D}_i(\tau_i)$ are of order $\leq k-1$. Using a Lipschitz condition for $\mathbf{f}(y)$ we obtain

$$\frac{H^k}{k!}|\mathbf{f}(\boldsymbol{\pi}_i^*) - \mathbf{f}(\boldsymbol{\pi}_i)| \;\leq\; \text{const.}H^k|\tilde{\boldsymbol{\pi}}_i^* - \tilde{\boldsymbol{\pi}}_i| \;\leq\; \text{const.}H|\tilde{\boldsymbol{\pi}}_i^* - \tilde{\boldsymbol{\pi}}_i|, \tag{3.58}$$

and finally from Lemma 5 and Lemma 2 we conclude

$$\frac{H^k}{k!}\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i) \;=\; O(H^k\|e\|_k) \;=\; O(H\|e\|_1). \tag{3.59}$$

To estimate the terms in (3.56) not yet treated, we consider

$$\begin{aligned}&\Big(Hh^q\mathcal{G}_q^* + \frac{H^2h^q}{2}\big(\mathcal{F}\mathcal{G}_q^* + \mathcal{G}_q^*\mathcal{F}\big) + Hh^{q+1}\mathcal{G}_{q+1}^* + \dots\Big)\mathrm{Id}(\tilde{\boldsymbol{\pi}}_i^*) \\ &-\Big(Hh^q\mathcal{G}_{i,q} + \frac{H^2h^q}{2}\big((\mathcal{F}+\hat{\mathcal{D}}_i)\mathcal{G}_{i,q} + \mathcal{G}_{i,q}(\mathcal{F}+\hat{\mathcal{D}}_i)\big) + Hh^{q+1}\mathcal{G}_{i,q+1} + \dots\Big)\mathrm{Id}(\tilde{\boldsymbol{\pi}}_i),\end{aligned} \tag{3.60}$$

where we take into account that

$$\hat{\mathcal{D}}^*\mathcal{G}_\mu^* = \mathcal{G}_\mu^*\hat{\mathcal{D}}^* = 0, \quad \mu \geq q.$$

We now estimate terms of three different forms occurring in (3.60).

(i) $\mathcal{G}_\ell^*$ are elements of the free Lie algebra generated by $\{\mathcal{F}, \mathcal{F}_1, \mathcal{F}_2, \dots\}$. Thus for the corresponding terms appearing in (3.60) we introduce the notation

$$\frac{H^{k_1}h^{k_2}}{k_1!}\mathcal{A}_1^*\dots\mathcal{A}_r^*\mathrm{Id}(\tilde{\boldsymbol{\pi}}_i^*), \quad \text{where } \mathcal{A}_\ell^* \in \{\mathcal{F}, \mathcal{G}_q^*, \mathcal{G}_{q+1}^*, \dots\},\ \ell = 1,\dots,r. \tag{3.61}$$

The components of (3.61) are comprised of terms of the form

$$\frac{H^{k_1}h^{k_2}}{k_1!}\mathbf{f}(\boldsymbol{\pi}_i^*)\mathbf{f}_1(\boldsymbol{\pi}_i^*)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i^*), \tag{3.62}$$

where each $\mathbf{f}_\ell(\boldsymbol{\pi}_i^*)$ is either the constant function $\mathbf{f}_\ell(\boldsymbol{\pi}_i^*) \equiv 1$ or a product of component functions $F_{\ell,j}(y)$ of $F_\ell(y)$ (cf. (3.21) and (3.18)) or derivatives thereof, all evaluated at $y = \boldsymbol{\pi}_i^*$.

For each term (3.61) there is a corresponding term

$$-\frac{H^{k_1}h^{k_2}}{k_1!}\mathcal{A}_1\dots\mathcal{A}_r\mathrm{Id}(\tilde{\boldsymbol{\pi}}_i), \quad \text{where } \mathcal{A}_\ell \in \{\mathcal{F}, \mathcal{G}_{i,q}, \mathcal{G}_{i,q+1}, \dots\},\ \ell = 1,\dots,r \tag{3.63}$$

in (3.60), where every $\mathcal{G}_\ell^*$ has been replaced by $\mathcal{G}_{i,\ell}$.

Thus, for each term (3.62) there is also a term

$$-\frac{H^{k_1}h^{k_2}}{k_1!}\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{f}_1(\boldsymbol{\pi}_i)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i) \tag{3.64}$$

of the same structure. By using a Lipschitz condition for $\mathbf{f}(y)\mathbf{f}_1(y)\cdots\mathbf{f}_r(y)$ we obtain the estimate

$$\frac{H^{k_1}h^{k_2}}{k_1!}|\mathbf{f}(\boldsymbol{\pi}_i^*)\mathbf{f}_1(\boldsymbol{\pi}_i^*)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i^*) - \mathbf{f}(\boldsymbol{\pi}_i)\mathbf{f}_1(\boldsymbol{\pi}_i)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i)| \\ \leq \ \text{const.}H^{k_1+k_2}|\tilde{\boldsymbol{\pi}}_i^* - \tilde{\boldsymbol{\pi}}_i| \ \leq \ \text{const.}H|\tilde{\boldsymbol{\pi}}_i^* - \tilde{\boldsymbol{\pi}}_i|. \tag{3.65}$$

(ii) Additionally, (3.63) contains terms whose components take the form

$$-\frac{H^{k_1}h^{k_2}}{k_1!}\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{f}_1(\boldsymbol{\pi}_i)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i), \tag{3.66}$$

cf. (3.47). These originate from terms in the representation of $\mathcal{G}_{i,\ell}$ in the free Lie algebra generated by $\{\mathcal{F}, \hat{\mathcal{D}}_i, \mathcal{F}_1, \mathcal{F}_2, \dots\}$ in which the operator $\hat{\mathcal{D}}_i$ is involved. Note that the terms in (3.60) where $\hat{\mathcal{D}}_i$ appears explicitly are estimated later, here we only refer to occurences of $\hat{\mathcal{D}}_i$ in the definitions of $\mathcal{G}_{i,\ell}$. $\tilde{\Psi}_{i,h} = \exp(h(\mathcal{F} + \hat{\mathcal{D}}_i + h^q\mathcal{G}_{i,q} + h^{q+1}\mathcal{G}_{i,q+1} + \dots))$ is by construction a composition method for (3.8) of order $q$. According to the theory presented in [13], $\mathcal{G}_{i,\ell}$ are linear combinations of iterated commutators, denoted as *Lie brackets*, of maximal length $\ell + 1$ in which $\hat{\mathcal{D}}_i$ can occur at most $\ell$ times. It follows that the maximal number of factors $\hat{\mathcal{D}}_i$ in one term of (3.63) is

$$\sum_{j:\mathcal{A}_j=\mathcal{G}_{i,\ell}} \ell = k_2, \tag{3.67}$$

which implies that the derivatives in $\mathbf{D}_i(\tau_i)$ are of order $\leq k_2 - 1$. By Lemma 5 and Lemma 2, we obtain the estimate

$$\frac{H^{k_1}h^{k_2}}{k_1!}|\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{f}_1(\boldsymbol{\pi}_i)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i)| \\ = \ O(H^{k_1+k_2}\|e\|_{k_2}) \ = \ O(H^{q+1}\|e\|_q) \ = \ O(H\|e\|_1), \tag{3.68}$$

where we use $k_1 \geq 1$ and $k_2 \geq q$. Here and also in (3.69) below, the sharper bound $O(H^{q+1}\|e\|_q)$ is not needed at this point. However, this estimate is essential for the proof of Lemma 7 below.

(iii) Finally, there are terms in (3.60) involving $\hat{\mathcal{D}}_i$ explicitly, whose components again consist of terms of the form (3.66), where now the derivatives in $\mathbf{D}_i(\tau_i)$ are of order $\leq (k_1 - 1) + (k_2 - 1) = k_1 + k_2 - 2$. From Lemma 5 and Lemma 2 we conclude

$$\frac{H^{k_1}h^{k_2}}{k_1!}|\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{f}_1(\boldsymbol{\pi}_i)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i)| \\ = \ O(H^{k_1+k_2}\|e\|_{k_1+k_2-1}) \ = \ O(H^{q+1}\|e\|_q) \ = \ O(H\|e\|_1). \tag{3.69}$$

If we sum up all the estimates (3.58), (3.59), (3.65), (3.68), and (3.69) for terms in (3.56), we obtain

$$\|\tilde{\boldsymbol{\pi}}_{i+1} - \tilde{\boldsymbol{\pi}}_{i+1}^*\| \ \leq \ (1 + \text{const.}H)\|\tilde{\boldsymbol{\pi}}_i - \tilde{\boldsymbol{\pi}}_i^*\| + O(H\|e\|_1) + O(H^{u+1}). \tag{3.70}$$

Now, (3.55) follows by an application of Lemma 1. □

**Lemma 7** *Let*

$$\tilde{\boldsymbol{\varepsilon}}_i \ := \ \tilde{\varepsilon}_i(\tau_i) \ = \ (\tilde{\boldsymbol{\pi}}_i^* - \tilde{\boldsymbol{\pi}}_i) - (\tilde{\mathbf{p}}_i^* - \tilde{\mathbf{p}}_i). \tag{3.71}$$

*Then for each* $u \geq 0$ *the bound*

$$|\tilde{\boldsymbol{\varepsilon}}_i| \ = \ O(H^{\min(q,m)}\|e\|_{\min(q,m)}) + O(H^m\|e\|_m) + O(H^u) \tag{3.72}$$

*holds.*

*Proof.* Similarly as in the proof of Lemma 6 we obtain

$$\begin{aligned} \tilde{\boldsymbol{\varepsilon}}_{i+1} \ &= \ \tilde{\varepsilon}_i(\tau_i + H) \\ &= \ \tilde{\boldsymbol{\varepsilon}}_i + \sum_{k=1}^{u} \frac{H^k}{k!}\Big(\mathcal{F}^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i^*) \ - \ (\mathcal{F} + \hat{\mathcal{D}}_i)^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i) \ - \\ & \quad -(\mathcal{F} + \mathcal{D}_i^*)^k \mathrm{Id}(\tilde{\mathbf{p}}_i^*) \ + \ (\mathcal{F} + \mathcal{D}_i)^k \mathrm{Id}(\tilde{\mathbf{p}}_i)\Big) \ + \ (0, \ldots, 0, H)^T \\ & \quad +\big[\text{terms of order} \leq u \text{ involving } \mathcal{G}_\ell^* \text{ or } \mathcal{G}_{i,\ell}\big] \ + \ O(H^{u+1}), \end{aligned} \tag{3.73}$$

where the terms involving $\mathcal{G}_\ell^*$ or $\mathcal{G}_{i,\ell}$ are the same as in (3.56).
First, we treat the expansion of

$$\frac{H^k}{k!}(\mathcal{F}^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i^*) - (\mathcal{F} + \hat{\mathcal{D}}_i)^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i) - (\mathcal{F} + \mathcal{D}_i^*)^k \mathrm{Id}(\tilde{\mathbf{p}}_i^*) + (\mathcal{F} + \mathcal{D}_i)^k \mathrm{Id}(\tilde{\mathbf{p}}_i)),$$

which consists of terms of the form

$$\frac{H^k}{k!}\Big(\mathbf{f}(\boldsymbol{\pi}_i^*) - \mathbf{f}(\boldsymbol{\pi}_i) - \mathbf{f}(\mathbf{p}_i^*) + \mathbf{f}(\mathbf{p}_i)\Big) \tag{3.74}$$

or

$$\frac{H^k}{k!}\Big( - \mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i) - \mathbf{f}(\mathbf{p}_i^*)\mathbf{d}_i^*(\tau_i) + \mathbf{f}(\mathbf{p}_i)\mathbf{d}_i(\tau_i)\Big), \tag{3.75}$$

cf. (3.43), (3.46).
(i) Using the $(n \times 1)$-matrices

$$\hat{\mathbf{J}} := \int_0^1 \nabla\mathbf{f}(\boldsymbol{\pi}_i + \sigma(\boldsymbol{\pi}_i^* - \boldsymbol{\pi}_i))d\sigma, \quad \mathbf{J} := \int_0^1 \nabla\mathbf{f}(\mathbf{p}_i + \sigma(\mathbf{p}_i^* - \mathbf{p}_i))d\sigma, \tag{3.76}$$

where

$$\nabla\mathbf{f}(y) = (\frac{\partial}{\partial y_1}, \ldots, \frac{\partial}{\partial y_n})\mathbf{f}(y)$$

is the gradient of $\mathbf{f}(y)$, we can derive the bounds

$$\begin{aligned}\frac{H^k}{k!}|\mathbf{f}(\boldsymbol{\pi}_i^*) - \mathbf{f}(\boldsymbol{\pi}_i) - \mathbf{f}(\mathbf{p}_i^*) + \mathbf{f}(\mathbf{p}_i)| &= \frac{H^k}{k!}|\hat{\mathbf{J}} \cdot \boldsymbol{\varepsilon}_i + (\hat{\mathbf{J}} - \mathbf{J}) \cdot (\mathbf{p}_i^* - \mathbf{p}_i)| \\ &\le \text{const.} H^k |\tilde{\boldsymbol{\varepsilon}}_i| + O(H^{\min(q,m)+k} \|e\|_0) \\ &\le \text{const.} H |\tilde{\boldsymbol{\varepsilon}}_i| + O(H^{\min(q,m)+1} \|e\|_0). \qquad (3.77)\end{aligned}$$

For this estimate we have used $|\mathbf{p}_i^* - \mathbf{p}_i| \le \|e\|_0$ and

$$\|\hat{\mathbf{J}} - \mathbf{J}\| \;\le\; \text{const.}|\boldsymbol{\pi}_i - \mathbf{p}_i| + \text{const.}|\boldsymbol{\pi}_i^* - \mathbf{p}_i^*| \;=\; O(H^{\min(q,m)}), \qquad (3.78)$$

which follows from Lemma 4 using a Lipschitz condition for $\nabla \mathbf{f}(y)$.

(ii) Next, we derive an estimate for terms of the form (3.75). To this end we reformulate this expression as

$$\begin{aligned}&-\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i) - \mathbf{f}(\mathbf{p}_i^*)\mathbf{d}_i^*(\tau_i) + \mathbf{f}(\mathbf{p}_i)\mathbf{d}_i(\tau_i) \\ &\quad = \mathbf{f}(\boldsymbol{\pi}_i)(-\mathbf{D}_i(\tau_i) - \mathbf{d}_i^*(\tau_i) + \mathbf{d}_i(\tau_i)) \;+\; \mathbf{d}_i^*(\tau_i)(\mathbf{f}(\mathbf{p}_i) - \mathbf{f}(\mathbf{p}_i^*)) \;+ \\ &\quad\quad +(\mathbf{f}(\boldsymbol{\pi}_i) - \mathbf{f}(\mathbf{p}_i))(\mathbf{d}_i^*(\tau_i) - \mathbf{d}_i(\tau_i)). \qquad (3.79)\end{aligned}$$

In order to derive a bound for (3.79), we use the following estimates:

- Using a Lipschitz condition for $\mathbf{f}$ we obtain

$$\mathbf{f}(\mathbf{p}_i) - \mathbf{f}(\mathbf{p}_i^*) = O(\|e\|_0).$$

- Lemma 4 yields

$$\mathbf{f}(\boldsymbol{\pi}_i) - \mathbf{f}(\mathbf{p}_i) = O(H^{\min(q,m)}),$$

again using a Lipschitz condition for $\mathbf{f}$.

- 

$$\mathbf{d}_i^*(\tau_i) - \mathbf{d}_i(\tau_i) = O(\|e\|_k),$$

which follows easily using Lipschitz conditions for the derivatives of $f(y)$ on noting that the derivatives in

$$\mathbf{d}_i^*(\tau_i) - \mathbf{d}_i(\tau_i) \;=\; d_{i,j_1}^{*(\kappa_1)}(\tau_i) \cdots d_{i,j_r}^{*(\kappa_r)}(\tau_i) \;-\; d_{i,j_1}^{(\kappa_1)}(\tau_i) \cdots d_{i,j_r}^{(\kappa_r)}(\tau_i) \qquad (3.80)$$

are of order $\le k-1$. Here, $d_{i,j}^*(t) = p_{i,j}^{*'}(t) - f_j(p_i^*(t))$ and $d_{i,j}(t) = p_{i,j}'(t) - f_j(p_i(t))$ denote the components of the respective defect terms.

- 

$$\mathbf{d}_i^*(\tau_i) = O(H^{m-k+1})$$

follows from Lemma 3 similarly as in (3.49).

• Using induction over the number $r$ of factors in the products $\mathbf{D}_i(\tau_i)$, $\mathbf{d}_i^*(\tau_i)$ and $\mathbf{d}_i(\tau_i)$ we will subsequently prove that

$$-\mathbf{D}_i(\tau_i) - \mathbf{d}_i^*(\tau_i) + \mathbf{d}_i(\tau_i) = O(H^{m-k+1}\|e\|_m). \tag{3.81}$$

The first step of the induction for $r = 1$ is shown as follows: The polynomial $D_{i,j}(t)$ of degree $\le m-1$ interpolates $d_{i,j}(t) - d_{i,j}^*(t)$ at $\sigma_{i,1}, \ldots, \sigma_{i,m}$, since at these points $d_{i,j}^*$ vanishes. Thus, the derivatives of the interpolation error $D_{i,j}(t) - (d_{i,j}(t) - d_{i,j}^*(t))$ satisfy

$$\begin{aligned} \max_{t\in J_i}\left|D_{i,j}^{(\kappa)}(t) - (d_{i,j}^{(\kappa)}(t) - d_{i,j}^{*(\kappa)}(t))\right| &\le \text{const.} H^{m-\kappa} \max_{t\in J_i} |d_{i,j}^{(m)}(t) - d_{i,j}^{*(m)}(t)| \\ &= O(H^{m-\kappa}\|e\|_{m+1}) \\ &= O(H^{m-k+1}\|e\|_m), \end{aligned} \tag{3.82}$$

where Lemma 3 is used for $\kappa \le k-1$. This shows that (3.81) holds for $r = 1$.

To prove the inductive step $r \to r+1$, we need to show that for $\kappa \le k-1$

$$-D_{i,j}^{(\kappa)}(\tau_i)\mathbf{D}_i(\tau_i) - d_{i,j}^{*(\kappa)}(\tau_i)\mathbf{d}_i^*(\tau_i) + d_{i,j}^{(\kappa)}(\tau_i)\mathbf{d}_i(\tau_i) = O(H^{m-k+1}\|e\|_m), \tag{3.83}$$

where $\mathbf{D}_i(\tau_i)$, $\mathbf{d}_i^*(\tau_i)$ and $\mathbf{d}_i(\tau_i)$, are products of $r$ factors respectively for which (3.81) holds by the induction hypothesis. Using an identity analogous to (3.79) and the estimates derived above, we obtain

$$\begin{aligned} &-D_{i,j}^{(\kappa)}(\tau_i)\mathbf{D}_i(\tau_i) - d_{i,j}^{*(\kappa)}(\tau_i)\mathbf{d}_i^*(\tau_i) + d_{i,j}^{(\kappa)}(\tau_i)\mathbf{d}_i(\tau_i) \\ &= D_{i,j}^{(\kappa)}(\tau_i)\Big(-\mathbf{D}_i(\tau_i) - \mathbf{d}_i^*(\tau_i) + \mathbf{d}_i(\tau_i)\Big) + \mathbf{d}_i^*(\tau_i)\Big(d_{i,j}^{(\kappa)}(\tau_i) - d_{i,j}^{*(\kappa)}(\tau_i)\Big) \\ &\quad + \Big(D_{i,j}^{(\kappa)}(\tau_i) - d_{i,j}^{(\kappa)}(\tau_i)\Big)\Big(\mathbf{d}_i^*(\tau_i) - \mathbf{d}_i(\tau_i)\Big) \\ &= O(H^{m-k+1}\|e\|_m) \;+\; O(H^{m-k+1}\|e\|_{\kappa+1}) \;+\; O(H^{m-k+1}\|e\|_k) \\ &= O(H^{m-k+1}\|e\|_m), \end{aligned} \tag{3.84}$$

which completes the proof of (3.81).

Applying the estimates from above, we obtain

$$\begin{aligned} &-\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i) - \mathbf{f}(\mathbf{p}_i^*)\mathbf{d}_i^*(\tau_i) + \mathbf{f}(\mathbf{p}_i)\mathbf{d}_i(\tau_i) \\ &\qquad = O(H^{m-k+1}\|e\|_m) + O(H^{\min(q,m)}\|e\|_k). \end{aligned} \tag{3.85}$$

Hence, terms of the form (3.75) can be estimated as

$$\begin{aligned} &\frac{H^k}{k!}\left|-\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i) - \mathbf{f}(\mathbf{p}_i^*)\mathbf{d}_i^*(\tau_i) + \mathbf{f}(\mathbf{p}_i)\mathbf{d}_i(\tau_i)\right| \\ &\qquad = O(H^{m+1}\|e\|_m) + O(H^{\min(q,m)+k}\|e\|_k) \\ &\qquad = O(H^{m+1}\|e\|_m) + O(H^{\min(q,m)+1}\|e\|_1), \end{aligned} \tag{3.86}$$

where in the last step Lemma 2 is used.

(iii) The terms (3.60) involving $\mathcal{G}_\ell^*$ or $\mathcal{G}_{i,\ell}$ in (3.73) are the same as in (3.56). Thus they can be estimated using (3.65), (3.68) and (3.69). We apply Lemma 6 to (3.65), which yields the estimate

$$\begin{aligned}
&\frac{H^{k_1}h^{k_2}}{k_1!}|\mathbf{f}(\boldsymbol{\pi}_i^*)\mathbf{f}_1(\boldsymbol{\pi}_i^*)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i^*)-\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{f}_1(\boldsymbol{\pi}_i)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i)| \\
&\qquad = O(H^{k_1+k_2}\|e\|_1)+O(H^{u+k_1+k_2}) = O(H^{q+1}\|e\|_1)+O(H^{u+1}), \qquad (3.87)
\end{aligned}$$

on noting that $k_1+k_2 \geq q+1 \geq 1$.

Collecting all the terms in (3.73) and using the bounds (3.68), (3.69), (3.77), (3.86) and (3.87), we finally obtain

$$\|\tilde{\boldsymbol{\varepsilon}}_{i+1}\| \leq (1+\text{const.}H)\|\tilde{\boldsymbol{\varepsilon}}_i\|+O(H^{\min(q,m)+1}\|e\|_q)+O(H^{m+1}\|e\|_m)+O(H^{u+1}). \qquad (3.88)$$

(3.72) now follows from Lemma 1. □

**Lemma 8** *Let $\tilde{\varepsilon}_{i;u}(\tau_i+t)$ for $0 \leq t \leq H$ denote the part of the expansion of $\tilde{\varepsilon}_i(\tau_i+t)$ consisting of the terms of order up to $O(H^u)$. For the derivatives*

$$\tilde{\varepsilon}_{i;u}^{(\kappa)}(\tau_i+t)=\frac{d^\kappa}{dt^\kappa}\tilde{\varepsilon}_{i;u}(\tau_i+t), \quad \kappa=0,\ldots,m, \quad 0\leq t\leq H,$$

*the estimates*

$$\begin{aligned}
&|\tilde{\varepsilon}_{i;u}^{(\kappa)}(\tau_i+t)| \\
&= \begin{cases} O(H^m\|e\|_m) + O(H^q\|e\|_q) + O(H^u), & \kappa=0, \\ O(H^{m+1-\kappa}\|e\|_m) + O(H^q\|e\|_{q-1+\kappa}) + O(H^u), & \kappa=1,\ldots,m-q, \\ O(H^{m+1-\kappa}\|e\|_m) + O(H^u), & \kappa=m-q+1,\ldots,m \end{cases} \qquad (3.89)
\end{aligned}$$

*hold in the case $q<m$. For $q\geq m$,*

$$|\varepsilon_{i;u}^{(\kappa)}(\tau_i+t)| = \begin{cases} O(H^m\|e\|_m) + O(H^u), & \kappa=0, \\ O(H^{m+1-\kappa}\|e\|_m) + O(H^u), & \kappa=1,\ldots,m. \end{cases} \qquad (3.90)$$

*Proof.* $\tilde{\varepsilon}_{i;u}(\tau_i+t)$ is given by

$$\begin{aligned}
\tilde{\varepsilon}_{i;u}(\tau_i+t) &= \tilde{\boldsymbol{\varepsilon}}_i+\sum_{k=1}^{u}\frac{t^k}{k!}\Big(\mathcal{F}^k\mathrm{Id}(\tilde{\boldsymbol{\pi}}_i^*) - (\mathcal{F}+\hat{\mathcal{D}}_i)^k\mathrm{Id}(\tilde{\boldsymbol{\pi}}_i) - \\
&\quad - (\mathcal{F}+\mathcal{D}_i^*)^k\mathrm{Id}(\tilde{\mathbf{p}}_i^*) + (\mathcal{F}+\mathcal{D}_i)^k\mathrm{Id}(\tilde{\mathbf{p}}_i)\Big) + (0,\ldots,0,t)^T \\
&\quad +\big[\text{terms of order} \leq u \text{ involving } \mathcal{G}_\ell^* \text{ or } \mathcal{G}_{i,\ell}\big]. \qquad (3.91)
\end{aligned}$$

Now, terms not involving $\mathcal{G}_\ell^*$ or $\mathcal{G}_{i,\ell}$ can be estimated using estimates analogous to (3.77) and (3.86). For the derivative of order $\kappa$, where $\kappa \le k$, terms $\frac{H^k}{k!}$ are replaced by $\frac{t^{k-\kappa}}{(k-\kappa)!}$, and consequently the order of the bounds in terms of $H$ is decreased in the same way.

(i) Thus, (3.77) is replaced by

$$\begin{aligned}\frac{t^{k-\kappa}}{(k-\kappa)!}&|\mathbf{f}(\boldsymbol{\pi}_i^*) - \mathbf{f}(\boldsymbol{\pi}_i) - \mathbf{f}(\mathbf{p}_i^*) + \mathbf{f}(\mathbf{p}_i)| \\ &= O(H^{m+k-\kappa}\|e\|_m) + O(H^{\min(q,m)+k-\kappa}\|e\|_q) + O(H^{u+k-\kappa}) \\ &= O(H^m\|e\|_m) + O(H^{\min(q,m)}\|e\|_q) + O(H^u), \end{aligned} \qquad (3.92)$$

where Lemma 7 is used.

(ii) Similarly, instead of (3.86)

$$\begin{aligned}\frac{t^{k-\kappa}}{(k-\kappa)!}&|-\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i) - \mathbf{f}(\mathbf{p}_i^*)\mathbf{d}_i^*(\tau_i) + \mathbf{f}(\mathbf{p}_i)\mathbf{d}_i(\tau_i)| \\ &= O(H^{m+1-\kappa}\|e\|_m) + O(H^{\min(q,m)+k-\kappa}\|e\|_k) \\ &= O(H^{m+1-\kappa}\|e\|_m) + O(H^{\min(q,m)}\|e\|_\kappa) \end{aligned} \qquad (3.93)$$

holds.

(iii) Likewise, terms involving $\mathcal{G}_\ell^*$ or $\mathcal{G}_{i,\ell}$ can be estimated using estimates corresponding to (3.68), (3.69) and (3.87), where $\frac{H^{k_1}}{k_1!}$ replaced by $\frac{t^{k_1-\kappa}}{(k_1-\kappa)!}$ for $k_1 \ge \kappa$, and the bounds are adjusted accordingly. In this way, using $k_1 \ge 1$ and $k_2 \ge q$, (3.68) and (3.69) are replaced by

$$\begin{aligned}\frac{t^{k_1-\kappa}h^{k_2}}{(k_1-\kappa)!}&|\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{f}_1(\boldsymbol{\pi}_i)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i)\mathbf{D}(\tau_i)| \\ &= O(H^{k_1+k_2-\kappa}\|e\|_{k_1+k_2-1}) = O(H^q\|e\|_{q-1+\kappa}), \end{aligned} \qquad (3.94)$$

and instead of (3.87)

$$\begin{aligned}\frac{t^{k_1-\kappa}h^{k_2}}{(k_1-\kappa)!}&|\mathbf{f}(\boldsymbol{\pi}_i^*)\mathbf{f}_1(\boldsymbol{\pi}_i^*)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i^*) - \mathbf{f}(\boldsymbol{\pi}_i)\mathbf{f}_1(\boldsymbol{\pi}_i)\cdots\mathbf{f}_r(\boldsymbol{\pi}_i)| \\ &= O(H^{k_1+k_2-\kappa}\|e\|_1) + O(H^{u+k_1+k_2-\kappa}) = O(H^q\|e\|_1) + O(H^{u+q}), \end{aligned} \qquad (3.95)$$

can be shown if we note that $k_2 \ge q$ and $k_1 \ge \kappa$.

Now we discuss the bounds derived above in the case where $q < m$. It is easy to verify that (3.92), (3.93), (3.94) and (3.95) can all be estimated according to (3.89) for $\kappa \le m-q$. For $\kappa \ge m-q+1$, we note that

$$k \ge \kappa \ge m-q+1 \implies q+k-\kappa \ge m+1-\kappa \qquad (3.96)$$

and

$$k_1 \geq \kappa \geq m - q + 1,\ k_2 \geq q \implies k_1 + k_2 - \kappa \geq m + 1 - \kappa. \tag{3.97}$$

Hence, the bound $O(H^{m+1-\kappa}) + O(H^{u-\kappa})$ holds in this case, and (3.89) is shown in the case $q < m$.

In the case $q \geq m$, (3.90) is obtained similarly, where Lemma 3 is used where appropriate. □

The next lemma is used to obtain sharper bounds than in Lemma 8 for special choices of the points $\sigma_{i,j}$ used for defect interpolation, see (1.4). The assumption of the lemma holds for instance if the points $\rho_j$ from (1.5) are symmetric in the interval $[0, 1]$.

**Lemma 9** *Let $y(t)$ be an $(m+2)$ times continuously differentiable function on $[t_0, t_0+H]$. Let $p(t)$ be the interpolation polynomial of degree $\leq m$ which is defined by*

$$p(t_0 + jh) = y(t_0 + jh), \quad j = 0, \ldots, m, \tag{3.98}$$

*and let $q(t)$ be any polynomial of degree $\leq m$ which satisfies*

$$q'(t_0 + \rho_j H) = y'(t_0 + \rho_j H), \quad j = 1, \ldots, m. \tag{3.99}$$

*If $\rho_j$ satisfy*

$$\sum_{j=1}^{m} \rho_j = \frac{m}{2}, \tag{3.100}$$

*then for the $m$-th derivatives of $p(t) - q(t)$ we have*

$$p^{(m)}(t_0 + t) - q^{(m)}(t_0 + t) \ = \ O(H^2 \|y^{(m+2)}\|), \quad 0 \leq t \leq H, \tag{3.101}$$

*where $\|y^{(\kappa)}\| := \max_{t \in [t_0, t_0+H]} |y^{(\kappa)}(t)|$.*

*Proof.* Using the Lagrange interpolation formula with the Lagrange polynomials

$$L_j(\tau) = \prod_{\substack{i=0 \\ i \neq j}}^{m} \frac{\tau - i}{j - i} \tag{3.102}$$

and the Taylor expansion

$$y(t_0 + jh) = \sum_{k=0}^{m+1} \frac{h^k j^k y^{(k)}(t_0)}{k!} + O(H^{m+2} \|y^{(m+2)}\|), \tag{3.103}$$

we obtain

$$\begin{aligned} p(t_0+\tau h) &= \sum_{j=0}^{m} y(t_0+jh)L_j(\tau) \\ &= \sum_{j=0}^{m}\sum_{k=0}^{m} \frac{h^k j^k y^{(k)}(t_0)}{k!} L_j(\tau) + \sum_{j=0}^{m} \frac{h^{m+1} j^{m+1} y^{(m+1)}(t_0)}{(m+1)!} L_j(\tau) + O(H^{m+2}\|y^{(m+2)}\|) \\ &= \sum_{k=0}^{m} \frac{h^k \tau^k y^{(k)}(t_0)}{k!} + \frac{h^{m+1} y^{(m+1)}(t_0)}{(m+1)!}\Big(\tau^{m+1} - \prod_{j=0}^{m}(\tau - j)\Big) + O(H^{m+2}\|y^{(m+2)}\|). \end{aligned}$$

In the last step we have used $\sum_{j=0}^{m} j^k L_j(\tau) = \tau^k$ and the fact that the interpolation polynomial $\sum_{j=0}^{m} j^{m+1} L_j(\tau)$ of $\tau^{m+1}$ at the nodes $0,\dots,m$ is given by $\tau^{m+1} - \prod_{j=0}^{m}(\tau - j)$. Similarly, we obtain

$$\begin{aligned} q'(t_0+\tau h) &= \sum_{k=0}^{m-1} \frac{h^k \tau^k y^{(k+1)}(t_0)}{k!} + \frac{h^m y^{(m+1)}(t_0)}{m!}\Big(\tau^m - \prod_{j=1}^{m}(\tau - \rho_j m)\Big) \\ &\quad + O(H^{m+1}\|y^{(m+1)}\|) \end{aligned} \tag{3.104}$$

and

$$\begin{aligned} q(t_0+\tau h) &= q(t_0) + \sum_{k=1}^{m} \frac{h^k \tau^k y^{(k)}(t_0)}{k!} + \\ &+ \frac{h^{m+1} y^{(m+1)}(t_0)}{(m+1)!}\Big(\tau^{m+1} - (m+1)\int_0^\tau \prod_{j=1}^{m}(\sigma - \rho_j m)d\sigma\Big) + O(H^{m+2}\|y^{(m+1)}\|) \end{aligned}$$

by integration. Using

$$\frac{d^m}{d\tau^m}\prod_{j=0}^{m}(\tau - j) = (m+1)!\tau - m!\sum_{j=0}^{m} j = (m+1)!(\tau - \frac{m}{2}) \tag{3.105}$$

and

$$(m+1)\frac{d^{m-1}}{d\tau^{m-1}}\prod_{j=1}^{m}(\tau - \rho_j m) = (m+1)!\Big(\tau - \sum_{j=1}^{m}\rho_j\Big), \tag{3.106}$$

and noting that the $O(H^{m+2}\|y^{(\kappa)}\|)$ remainder terms from above are of the form $H^{m+2}R(\tau,H)$ with smooth functions $R(\tau,H)$ (which are actually polynomials in $\tau$ of degree $\le m$, with $\frac{\partial^k}{\partial\tau^k}R(\tau,H) = O(H^{-k}\|y^{(\kappa)}\|)$) we conclude

$$\begin{aligned} & p^{(m)}(t_0+\tau h) - q^{(m)}(t_0+\tau h) \\ &\quad = hy^{(m+1)}(t_0)\Big(\frac{m}{2} - \sum_{j=1}^{m}\rho_j\Big) + O(H^2\|y^{(m+1)}\|) + O(H^2\|y^{(m+2)}\|). \end{aligned} \tag{3.107}$$

Using

$$|y^{(m+1)}(t_0+t)| = \left| \int_{t_0}^{t_0+t} y^{(m+2)}(\sigma) d\sigma \right| \le H \|y^{(m+2)}\|,$$

the statement of the lemma follows. □

Now, we are in a position to prove the central convergence result for the iteration error of ISDeC.

**Theorem 1** *In the case where $q < m$, the iteration error $e^{\text{new}} = p^{\text{new}} - p^*$ satisfies estimates*

$$\left| \frac{d^\kappa}{dt^\kappa} e^{\text{new}}(\tau_i + t) \right|$$
$$= \begin{cases} O(H^m \|e\|_m) & +O(H^q \|e\|_q) & +O(H^u), & \kappa = 0, \\ O(H^{m+1-\kappa} \|e\|_m) & +O(H^q \|e\|_{q-1+\kappa}) & +O(H^{u+1-\kappa}), & \kappa = 1, \dots, m-q, \\ O(H^{m+1-\kappa} \|e\|_m) & & +O(H^{u+1-\kappa}), & \kappa = m-q+1, \dots, m \end{cases} \tag{3.108}$$

*for each $u \ge 0$. Conversely, for $q \ge m$*

$$\left| \frac{d^\kappa}{dt^\kappa} e^{\text{new}}(\tau_i + t) \right| = \begin{cases} O(H^m \|e\|_m) & +O(H^u), & \kappa = 0, \\ O(H^{m+1-\kappa} \|e\|_m) & +O(H^{u+1-\kappa}), & \kappa = 1, \dots, m \end{cases} \tag{3.109}$$

*holds. If the collocation abscissae $\rho_j$ from* (1.5) *satisfy the condition* (3.100)*, then the estimates* (3.108) *and* (3.109) *for $\kappa = m$ can be replaced by the sharper bounds*

$$\left| \frac{d^m}{dt^m} e^{\text{new}}(\tau_i + t) \right| = O(H^2 \|e\|_m) + O(H^{u+1-m}). \tag{3.110}$$

*Proof.* Let $e^{\text{new}} = (e_0^{\text{new}}, e_1^{\text{new}}, \dots, e_{N_1-1}^{\text{new}})$, where $e_i^{\text{new}}(t)$, $i = 1, \dots, N_1 - 1$, is the polynomial of degree $\le m$ which interpolates $\varepsilon_i(t)$ at $t_{i,0}, \dots, t_{i,m}$. Here $\varepsilon_i(t)$ denotes the first $n$ components of $\tilde{\varepsilon}_i(t)$, where the last, vanishing component is neglected. We rewrite $e_i^{\text{new}}(t)$ as

$$e_i^{\text{new}}(t) = e_{i;u}^{\text{new}}(t) + (e_i^{\text{new}}(t) - e_{i;u}^{\text{new}}(t)),$$

where $e_{i;u}^{\text{new}}(t)$ interpolates $\varepsilon_{i;u}(t)$, the first $n$ components of $\tilde{\varepsilon}_{i;u}(t)$, and $e_i^{\text{new}}(t) - e_{i;u}^{\text{new}}(t)$ interpolates the remainder term $\varepsilon_i(t) - \varepsilon_{i;u}(t) = O(H^{u+1})$, cf. Lemma 8. From Lemma 3 we conclude

$$|e_{i;u}^{\text{new}(\kappa)}(t) - \varepsilon_{i;u}^{(\kappa)}(t)| \le \text{const.} \max_{t \in J_i} |\varepsilon_{i;u}^{(\kappa)}(t)|, \quad t \in J_i,$$

whence

$$\frac{d^\kappa}{dt^\kappa} e_{i;u}^{\text{new}}(t) \le \text{const.} \max_{t \in J_i} \left| \varepsilon_{i;u}^{(\kappa)}(t) \right|, \quad t \in J_i, \; \kappa = 0, \dots, m, \tag{3.111}$$

follows by the triangle inequality.

For the interpolant of the remainder $\varepsilon_i(t) - \varepsilon_{i;u}(t) = O(H^{u+1})$ Lemma 3 implies

$$\frac{d^\kappa}{dt^\kappa}(e_i^{\text{new}}(t) - e_{i;u}^{\text{new}}(t)) = O(H^{u+1-\kappa}), \quad t \in J_i,\ \kappa = 0, \ldots, m. \tag{3.112}$$

From (3.111) and (3.112) together with Lemma 8, (3.108) and (3.109) now follow.

Finally, we prove (3.110). The bound $O(H\|e\|_m)$ in (3.108) and (3.109) for $\kappa = m$ is a consequence of (3.81), (3.86) and (3.93). Note that (3.79) reduces to (3.81) when the lowest order estimate for (3.86) and (3.93) holds. All other contributions to (3.108) and (3.109) are actually $O(H^2\|e\|_m)$.

In (3.81) the lowest possible order $O(H^{m-k+1}\|e\|_m)$ occurs only in the case where derivatives of order $k-1$ occur in $\mathbf{D}_i(\tau_i)$, $\mathbf{d}_i^*(\tau_i)$ and $\mathbf{d}_i(\tau_i)$. This is only possible if

$$\mathbf{D}_i(\tau_i) = D_{i,j}^{(k-1)}(\tau_i),\ \mathbf{d}_i^*(\tau_i) = d_{i,j}^{*(k-1)}(\tau_i),\ \text{and } \mathbf{d}_i(\tau_i) = d_{i,j}^{(k-1)}(\tau_i). \tag{3.113}$$

In all other cases,

$$-\mathbf{D}_i(\tau_i) - \mathbf{d}_i^*(\tau_i) + \mathbf{d}_i(\tau_i) = O(H^{m-k+2}\|e\|_m) \tag{3.114}$$

follows by a simple modification of the arguments leading to (3.81). We may conclude that, except for the case characterized by (3.113),

$$\frac{t^{k-m}}{(k-m)!}\left|-\mathbf{f}(\boldsymbol{\pi}_i)\mathbf{D}_i(\tau_i) - \mathbf{f}(\mathbf{p}_i^*)\mathbf{d}_i^*(\tau_i) + \mathbf{f}(\mathbf{p}_i)\mathbf{d}_i(\tau_i)\right| \;=\; O(H^2\|e\|_m) \tag{3.115}$$

holds instead of the estimate given in (3.93).

The terms given by (3.113) constitute components of

$$\begin{aligned}
\tilde{\varepsilon}_{i;\mathcal{D}}(\tau_i + t) \;&:=\; \sum_{k=1}^{\infty} \frac{t^k}{k!}\Big( -\hat{\mathcal{D}}_i^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i) - \mathcal{D}_i^{*k}\mathrm{Id}(\tilde{\boldsymbol{\pi}}_i^*) + \mathcal{D}_i^k \mathrm{Id}(\tilde{\boldsymbol{\pi}}_i)\Big) \\
&=\; \sum_{k=1}^{\infty} \frac{t^k}{k!}\Big( -\tilde{D}_i^{(k-1)}(\tau_i) - \tilde{d}_i^{*(k-1)}(\tau_i) + \tilde{d}_i^{(k-1)}(\tau_i)\Big) \\
&=\; \int_{\tau_i}^{\tau_i+t} \Big( -\tilde{D}_i(\sigma) - \tilde{d}_i^*(\sigma) + \tilde{d}_i(\sigma)\Big) d\sigma
\end{aligned} \tag{3.116}$$

in (3.91). Now we rewrite the first $n$ components of $\tilde{\varepsilon}_i(\tau_i + t)$ as

$$\varepsilon_i(\tau_i + t) = \varepsilon_{i;\mathcal{D}}(\tau_i + t) + (\varepsilon_i(\tau_i + t) - \varepsilon_{i;\mathcal{D}}(\tau_i + t)),$$

and treat the two terms separately in the interpolation process outlined above. Thus, let $e_{i;\mathcal{D}}^{\text{new}}(t)$ be the polynomial of degree $\le m$ which interpolates $\varepsilon_{i;\mathcal{D}}(t)$ at $t_{i,0}, \ldots, t_{i,m}$. Clearly,

$$\frac{d^m}{dt^m}(e_i^{\text{new}}(\tau_i+t) - e_{i;\mathcal{D}}^{\text{new}}(\tau_i+t)) \;=\; O(H^2\|e\|_m) + O(H^{u+1-m}), \quad 0 \le t \le H. \tag{3.117}$$

Noting that $D_i(t)$ is the interpolation polynomial of $d_i(t) - d_i^*(t)$ at $\sigma_{i,1}, \ldots, \sigma_{i,m}$, we now apply Lemma 9 component-wise with

$$\begin{aligned}
t_0 &= \tau_i, \\
y(\tau_i + t) &= \int_{\tau_i}^{\tau_i+t} (d_{i,j}(\sigma) - d_{i,j}^*(\sigma))d\sigma, \\
q(\tau_i + t) &= \int_{\tau_i}^{\tau_i+t} D_{i,j}(\sigma)d\sigma, \\
p(\tau_i + t) - q(\tau_i + t) &= e_{i,j;\mathcal{D}}^{\text{new}}(t_i + t).
\end{aligned}$$

We conclude that

$$\frac{d^m}{dt^m} e_{i,j;\mathcal{D}}^{\text{new}}(\tau_i + t) \;=\; O(H^2\|e\|_m), \quad j = 1, \ldots, n, \quad 0 \le t \le H, \tag{3.118}$$

if condition (3.100) is satisfied, since

$$y^{(m+2)}(t) = \frac{d^{m+1}}{dt^{m+1}}(d_{i,j}(t) - d_{i,j}^*(t)) = \frac{d^{m+1}}{dt^{m+1}}(f_j(p_i(t)) - f_j(p_i^*(t))) = O(\|e\|_m) \tag{3.119}$$

for $t \in J_i$, using Lipschitz conditions for the derivatives of $f_j(y)$.

Together with (3.117) this completes the proof of (3.110). □

As a corollary to Theorem 1, we now derive the sequence of convergence orders of ISDeC iterates, where any of the fourth-order symmetric composition methods described in Chapter 2 serves as the basis for the iteration. First, we discuss the iteration error of the basic solution and its derivatives in the following lemma.

**Theorem 2** *The interpolant $e^{[0]}$ of the iteration error*

$$\varepsilon^{[0]} = \eta^{[0]} - p^*$$

*for the basic solution $\eta^{[0]}$ of* (3.1) *computed by a numerical method $\Phi$ of order $q$ satisfies*

$$\begin{aligned}
&\|e^{[0]}\|_k = O(H^q), \quad k = 0, \ldots, m - q + 1, \\
&\|e^{[0]}\|_k = O(H^{m+1-k}), \quad k = m - q + 2, \ldots, m - 1, \\
&\|e^{[0]}\|_m = \begin{cases} O(H^2) & \text{if } \rho_j \text{ satisfy (3.100)}, \\ O(H) & \text{otherwise}, \end{cases}
\end{aligned} \tag{3.120}$$

*if ISDeC is defined by polynomials of degree $m$.*

*Proof.* For reasons of simplicity we assume $m \ge q$, since this is the natural choice for ISDeC. The estimates above follow from

$$\|g\|_k = O(H^q), \quad k = 0, \ldots, m,$$

where $g$ is the piecewise polynomial interpolant of degree $\leq m$ of the global error $\eta^{[0]} - y$. This can be proven by means of an asymptotic expansion of the global error of $\Phi$: If a sufficiently long error expansion exists, then there is a smooth function $E(t, H)$ such that

$$\eta_{i,j}^{[0]} - y(t_{i,j}) = E(t_{i,j}, H)H^q,$$

with $\frac{\partial^k}{\partial t^k} E(t, H) = O(1),\ k = 0, \ldots, m$. Consequently, we conclude

$$\begin{aligned} \left|\frac{d^k}{dt^k} g_i(t)\right| &\leq \left|\frac{d^k}{dt^k} g_i(t) - \frac{\partial^k}{\partial t^k} E(t, H)H^q\right| + \left|\frac{\partial^k}{\partial t^k} E(t, H)H^q\right| \\ &\leq O(H^{m+q+1-k}) + O(H^q) = O(H^q), \quad k = 0, \ldots, m, \end{aligned}$$

which follows from Lemma 3. Moreover, we use the relations

$$\begin{aligned} \|Q\|_0 &= \begin{cases} O(H^{m+1}) & \text{if } \rho_j \text{ define a collocation scheme of order } \geq m+1, \\ O(H^m) & \text{otherwise,} \end{cases} \\ \|Q\|_k &= O(H^{m+1-k}), \quad k = 1, \ldots, m-1, \\ \|Q\|_m &= \begin{cases} O(H^2) & \text{if } \rho_j \text{ satisfy (3.100),} \\ O(H) & \text{otherwise} \end{cases} \end{aligned}$$

for the piecewise polynomial interpolant $Q$ of $p^* - y$ at $t_{i,j},\ j = 0, \ldots, m$. These are standard results for collocation methods [2], again taking into account Lemma 3. The improved estimate $\|Q\|_m = O(H^2)$ when (3.100) holds follows from

$$|Q^{(m)}(t)| = O(H^2), \quad \text{if } \rho_j \text{ satisfy (3.100),} \tag{3.121}$$

which is shown as follows: Let $z_i(t),\ t \in J_i$, denote the exact solution of

$$z_i'(t) = f(z_i(t)), \quad z_i(\tau_i) = \mathbf{p}_i^* = p_i^*(\tau_i).$$

Using the estimate $|\mathbf{p}_i^* - y(\tau_i)| = O(H^m)$ for the global error of the collocation solution it is easy to show that

$$\left|\frac{d^k}{dt^k}(z_i(t) - y(t))\right| = O(H^m), \quad t \in J_i, \quad k = 0, \ldots, m. \tag{3.122}$$

Let $q_i(t)$ be a polynomial of degree $\leq m$ which satisfies

$$q_i'(\sigma_{i,j}) = z_i'(\sigma_{i,j}) = f(z_i(\sigma_{i,j})), \quad j = 1, \ldots, m, \tag{3.123}$$

and let $P_i(t)$ denote the polynomial of degree $\leq m$ which interpolates $z_i(t)$ at $t_{i,j},\ j = 0, \ldots, m$. An application of Lemma 9 yields

$$|P_i^{(m)}(t) - q_i^{(m)}(t)| = O(H^2), \quad t \in J_i. \tag{3.124}$$

The polynomial $q_i'(t) - p_i^{*\prime}(t)$ of degree $\le m-1$ interpolates $f(z_i(t)) - f(p_i^*(t))$ at $\sigma_{i,j},\ j = 1, \dots, m$, where

$$|f(z_i(t)) - f(p_i^*(t))| \le \text{const.}|z_i(t) - p_i^*(t)| = O(H^{m+1}), \quad t \in J_i,$$

see [13, Lemma II.1.6]. From Lemma 3 we conclude

$$|q_i^{(m)}(t) - p_i^{*(m)}(t)| = O(H^2), \quad t \in J_i, \tag{3.125}$$

and, combining this estimate with (3.124),

$$|P_i^{(m)}(t) - p_i^{*(m)}(t)| = O(H^2), \quad t \in J_i. \tag{3.126}$$

Finally, let $u_i(t)$ denote the polynomial of degree $\le m$ interpolating $z_i(t) - y(t)$ at $t_{i,j},\ j = 0, \dots, m$. From (3.122) and Lemma 3 we conclude

$$|u_i^{(m)}(t)| = O(H^m), \quad t \in J_i,$$

and (3.121) follows by noting that

$$Q = (p_i^* - P_i) + u_i, \quad t \in J_i.$$

□

Using this result for the basic approximation and Theorem 1, we can easily conclude the sequence of iteration errors for the respective ISDeC iterates. To illustrate the procedure, we give the results for the case where $m = 6$, and $\Phi$ is any of the fourth order composition methods described in Chapter 2.

If the condition (3.100) is not satisfied, the iteration errors satisfy

| | $k=0$ | $k=1$ | $k=2$ | $k=3$ | $k=4$ | $k=5$ | $k=6$ |
|---|---|---|---|---|---|---|---|
| $\|e^{[0]}\|_k$ | $O(H^4)$ | $O(H^4)$ | $O(H^4)$ | $O(H^4)$ | $O(H^3)$ | $O(H^2)$ | $O(H^1)$ |
| $\|e^{[1]}\|_k$ | $O(H^7)$ | $O(H^7)$ | $O(H^6)$ | $O(H^5)$ | $O(H^4)$ | $O(H^3)$ | $O(H^2)$ |
| $\|e^{[2]}\|_k$ | $O(H^8)$ | $O(H^8)$ | $O(H^7)$ | $O(H^6)$ | $O(H^5)$ | $O(H^4)$ | $O(H^3)$ |

The resulting order sequences for $\|e^{[\nu]}\|_0$ are given below for the values of $m = 6, \dots, 9$:

$$\begin{aligned}
m = 6: &\quad O(H^4),\ O(H^7),\ O(H^8),\ O(H^9),\ O(H^{10}),\ O(H^{11}), \dots \\
m = 7: &\quad O(H^4),\ O(H^8),\ O(H^9),\ O(H^{10}),\ O(H^{11}),\ O(H^{12}), \dots \\
m = 8: &\quad O(H^4),\ O(H^8),\ O(H^{10}),\ O(H^{11}),\ O(H^{12}),\ O(H^{13}), \dots \\
m = 9: &\quad O(H^4),\ O(H^8),\ O(H^{11}),\ O(H^{12}),\ O(H^{13}),\ O(H^{14}), \dots
\end{aligned}$$

which are also observed in the numerical experiments reported in [17].

If conversely (3.100) is satisfied, the case $m = 6$ results in

| | $k=0$ | $k=1$ | $k=2$ | $k=3$ | $k=4$ | $k=5$ | $k=6$ |
|---|---|---|---|---|---|---|---|
| $\|e^{[0]}\|_k$ | $O(H^4)$ | $O(H^4)$ | $O(H^4)$ | $O(H^4)$ | $O(H^3)$ | $O(H^2)$ | $O(H^2)$ |
| $\|e^{[1]}\|_k$ | $O(H^7)$ | $O(H^7)$ | $O(H^6)$ | $O(H^6)$ | $O(H^5)$ | $O(H^4)$ | $O(H^4)$ |
| $\|e^{[2]}\|_k$ | $O(H^9)$ | $O(H^9)$ | $O(H^8)$ | $O(H^8)$ | $O(H^7)$ | $O(H^6)$ | $O(H^6)$ |

The resulting order sequences for $m = 6, \ldots, 9$ for $\|e^{[\nu]}\|_0$ are

$$\begin{aligned}
m = 6: &\quad O(H^4),\ O(H^7),\ O(H^9),\ O(H^{11}),\ O(H^{13}),\ O(H^{15}), \ldots \\
m = 7: &\quad O(H^4),\ O(H^8),\ O(H^{10}),\ O(H^{12}),\ O(H^{14}),\ O(H^{16}), \ldots \\
m = 8: &\quad O(H^4),\ O(H^8),\ O(H^{10}),\ O(H^{12}),\ O(H^{14}),\ O(H^{16}), \ldots \\
m = 9: &\quad O(H^4),\ O(H^8),\ O(H^{11}),\ O(H^{13}),\ O(H^{15}),\ O(H^{17}), \ldots \\
&\vdots
\end{aligned}$$

Note that the actually observed orders for $m = 6$ and $m = 9$ in the case where (3.100) holds were in fact higher in the numerical experiments reported in [17] than the orders concluded from the considerations reported above. We actually observed the following order sequences:

$$\begin{aligned}
m = 6: &\quad O(H^4),\ O(H^8),\ O(H^{10}),\ O(H^{12}),\ O(H^{14}),\ O(H^{16}), \ldots \\
m = 9: &\quad O(H^4),\ O(H^8),\ O(H^{12}),\ O(H^{14}),\ O(H^{16}),\ O(H^{18}), \ldots
\end{aligned}$$

These experimental results are no contradiction to the theory, however, since we only give sufficient conditions for our estimates to hold.

So far, we have considered the *iteration error* of ISDeC. The global error of the ISDeC iterates as compared with the exact solution of (3.1) is of course closely linked to this quantity. Namely, it follows from the triangle equality that the global error has the same order as the iteration error up to the order defined by the fixed point $p^*$. If we use Gaussian points $\sigma_{i,j}$ for the interpolation of the defect, see (1.4), (1.5), the maximally attainable order of the global error of ISDeC iterates is $2m$, cf. [17].

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