

# Superconvergent Defect Correction Algorithms

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*Abstract:* In this paper we discuss several variants of the acceleration technique known as Iterated Defect Correction (IDeC) for the numerical solution of initial value problems for ODEs. A first approximation, computed by a low order basic method, is iteratively improved to obtain higher order solutions. We propose new versions of the IDeC algorithm with maximal achievable (super-)convergence order twice as high as in the classical setting. Moreover, if the basic numerical method is designed for a special type of ODE only, as it is the case for many geometric integrators, the idea of classical IDeC is not applicable in a straightforward way. Our approach enables the application of the defect correction principle in such cases as well.

*Key-Words:* Iterated defect correction, splitting methods, geometric integration, superconvergent collocation.

## 1 Introduction

We consider initial value problems

$$z'(t) = f(t, z(t)), \quad z(t_0) = z_0, \quad (1)$$

to be solved on the interval  $[t_0, t_{\text{end}}]$ . Let  $y(t)$  denote the exact solution to (1). We assume that a first approximate solution  $z_{\Gamma}^{[0]} = (z_0, \dots, z_N)$  is obtained by some discretization method on a grid  $\Gamma := (t_0, \dots, t_N)$ . For the time being, we consider the backward Euler scheme (BEUL), where  $z_{\Gamma}^{[0]}$  is computed from

$$\frac{z_k - z_{k-1}}{t_k - t_{k-1}} = f(t_k, z_k), \quad k = 1, \dots, N. \quad (2)$$

The technique of defect correction described here was first proposed by Zadunaisky in [8] in the context of Runge-Kutta schemes, see also Stetter [7] for a general formalism. We first give the basic ideas behind this approach. A more detailed specification of algorithmic components is given in Section 2.

Zadunaisky's original intention was to design an efficient and reliable global error estimate. To this end, a given numerical approximation  $z_{\Gamma}^{[0]}$  is interpolated by a polynomial function  $p^{[0]}(t)$ . This enables us to compute the defect, i.e. the residual of  $p^{[0]}(t)$  w.r.t. the given ODE, and to define a so-called neighboring problem to (1). Here the defect is added as an inhomogeneity such that the exact solution is simply  $p^{[0]}$ .

This provides an estimate for the global<sup>1</sup> error of  $z_{\Gamma}^{[0]}$  by means of applying the given scheme to the neighboring problem. Soon it became clear that the procedure can be iterated by considering the new approximation resulting from the computed error estimate and applying the same device again. The resulting method is called Iterated Defect Correction (IDeC), and it has been successfully applied to various classes of differential equations.

The purpose of the present paper is to demonstrate that, while the strategy *per se* is evident and plausible, the particular choice of the involved algorithmic components may be quite subtle. In particular, the way of evaluating the defect within an IDeC iteration is often crucial for success or failure of the method and for its convergence behavior. As will be demonstrated below, IDeC should in fact be considered as a rich *family* of iterative methods, each with its particular advantages. These include variable stepsizes, superconvergence effects, and suitability for geometric integration.

## 2 Classical IDeC

Let us now describe the technical details of the classical IDeC procedure. Using the polynomial  $p^{[0]}(t)$  of degree  $\leq N$  which interpolates the values of  $z_{\Gamma}^{[0]}$  we define the auxiliary neighboring problem

$$z'(t) = f(t, z(t)) + d^{[0]}(t), \quad z(t_0) = z_0, \quad (3)$$

<sup>1</sup>This approach enables also the estimation of local errors.

where  $d^{[0]}(t)$  denotes the defect w.r.t. (1),

$$d^{[0]}(t) := \frac{d}{dt}p^{[0]}(t) - f(t, p^{[0]}(t)). \quad (4)$$

We now solve (3) using the same numerical method as before to obtain an approximation  $p_\Gamma^{[0]}$  for the exact solution  $p^{[0]}(t)$  of (3). Note that for (3) the global error  $p_\Gamma^{[0]} - R_\Gamma p^{[0]}$  is known.<sup>2</sup> We expect this error to be a good estimate for the unknown error  $z_\Gamma^{[0]} - R_\Gamma y$  for the original problem (1), such that

$$z_\Gamma^{[1]} := z_\Gamma^{[0]} - (p_\Gamma^{[0]} - R_\Gamma p^{[0]}) \quad (5)$$

yields an improved numerical solution of (1).<sup>3</sup> Now, these values are used to define a new interpolating polynomial  $p^{[1]}(t)$  by requiring  $p^{[1]}(t_k) = z_k^{[1]}$ . Again,  $p^{[1]}(t)$  defines a neighboring problem analogous to (3), and the numerical solution of this neighboring problem serves to obtain the second improved solution  $z_\Gamma^{[2]} := z_\Gamma^{[0]} - (p_\Gamma^{[1]} - R_\Gamma p^{[1]})$ . This procedure can be continued iteratively in an obvious manner, yielding a sequence  $z_\Gamma^{[0]}, z_\Gamma^{[1]}, z_\Gamma^{[2]}, \dots$  of approximations for  $R_\Gamma y$ , which are recursively computed from

$$z_\Gamma^{[\nu]} := z_\Gamma^{[0]} - (p_\Gamma^{[\nu-1]} - R_\Gamma p^{[\nu-1]}) \quad (6)$$

for  $\nu = 1, 2, \dots$ . Note that each  $z_\Gamma^{[\nu]}$  also provides an estimate for the error of  $z_\Gamma^{[\nu-1]}$  via  $z_\Gamma^{[\nu-1]} - z_\Gamma^{[\nu]} \approx z_\Gamma^{[\nu-1]} - R_\Gamma y$ .

In practice one does not use one interpolating polynomial for the whole interval  $[t_0, t_{\text{end}}]$ . Instead, piecewise functions composed of polynomials of (moderate) degree  $m$  are used to specify the neighboring problem. Thus we choose the grid  $\Gamma = (t_0, \dots, t_N)$  such that  $N = N_1 m$  for some integer  $N_1$ , and split the integration interval into subintervals  $J_i := [t_{im}, t_{(i+1)m}]$ . The interpolants  $p^{[\nu]}(t)$  are continuous piecewise polynomial functions,  $p^{[\nu]}(t) = p_i^{[\nu]}(t)$ ,  $t \in J_i$ , where  $p_i^{[\nu]}(t)$  are polynomials of degree  $\leq m$ . Now, for sufficiently smooth data functions  $f(t, z)$  it can be shown that the approximations  $z_\Gamma^{[\nu]}$  satisfy

$$z_k^{[\nu]} - y(t_k) = O(\mathbf{h}^{\nu+1}), \quad \nu = 0, \dots, m-1, \quad (7)$$

if the backward Euler scheme (2) is carried out on a *piecewise equidistant* grid  $\Gamma$ , where  $t_{i,j} - t_{i,j-1} = h_i := (t_{i,m} - t_{i,0})/m$  for  $i = 0, \dots, N_1 - 1$  and

$j = 1, \dots, m$ . For convenience, here and in the sequel we use double indexing  $t_{i,j} := t_{im+j}$  for grid points and similarly for grid functions  $\zeta_\Gamma = (\zeta_0, \dots, \zeta_N)$ .  $\mathbf{h}$  denotes the maximal stepsize of  $\Gamma$ ,

$$\mathbf{h} := \max_{k=1, \dots, N} (t_k - t_{k-1}). \quad (8)$$

Note that further iterations do not improve the convergence order: For  $\nu \geq m$  only  $z_k^{[\nu]} - y(t_k) = O(\mathbf{h}^m)$  holds in general. To discuss this convergence behavior we write the global error in the form

$$z_k^{[\nu]} - y(t_k) = (z_k^{[\nu]} - z_k^*) + (z_k^* - y(t_k)), \quad (9)$$

where  $z_\Gamma^* = (z_0^*, \dots, z_N^*)$  denotes the fixed point of the iteration  $z_\Gamma^{[\nu]} \mapsto z_\Gamma^{[\nu+1]}$ , such that the global error is represented as the sum of the *iteration error*  $z_k^{[\nu]} - z_k^*$  and the global error  $z_k^* - y(t_k)$  of the fixed point. The fixed point  $z_\Gamma^*$  is easily characterized by the property that the defect vanishes at certain grid points, i.e., the fixed point is a certain collocation solution of (1). Indeed, let  $p^*(t)$  denote the continuous piecewise polynomial function defined by  $p^*(t_0) = p_0^*(t_0) = z_0$  and  $p^*(t) = p_i^*(t)$  for  $t \in J_i$ , where  $p_i^*(t)$  are polynomials of degree  $\leq m$  satisfying the collocation equations

$$\frac{d}{dt}p_i^*(t_{i,j}) = f(t_{i,j}, p_i^*(t_{i,j})), \quad j = 1, \dots, m. \quad (10)$$

The defect  $d^*(t) := \frac{d}{dt}p^*(t) - f(t, p^*(t))$  vanishes at all points  $t_{i,j}$  where the right-hand side of the according neighboring problem is evaluated in course of the backward Euler method. Thus, a defect correction step starting from  $z_\Gamma^* := R_\Gamma p^*$  maps  $z_\Gamma^*$  onto itself, and therefore  $z_\Gamma^*$  is indeed a fixed point of the defect correction iteration  $z_\Gamma^{[\nu]} \mapsto z_\Gamma^{[\nu+1]}$ .

From [3, Proposition 2] it follows that the sequence  $z_\Gamma^{[0]}, z_\Gamma^{[1]}, z_\Gamma^{[2]}, \dots$  actually converges to  $z_\Gamma^*$  with convergence rate  $O(\mathbf{h})$  such that (cf. (9))

$$z_k^{[\nu]} - y(t_k) = O(\mathbf{h}^{\nu+1}) + O(\mathbf{h}^p) = O(\mathbf{h}^{\min(\nu+1, p)}), \quad (11)$$

where  $p$  denotes the order of the fixed point. Note that the assumption of a piecewise equidistant grid  $\Gamma$  is essential in the proof of this proposition. For such a grid the order of the fixed point is  $p = m$  for all  $k$ .

On the other hand, for a grid

$$t_{i,j} = t_{i,0} + (t_{i,m} - t_{i,0})c_j, \quad j = 1, \dots, m \quad (12)$$

<sup>2</sup>Here,  $R_\Gamma$  denotes the restriction operator  $[t_0, t_{\text{end}}] \rightarrow \Gamma$ .

<sup>3</sup>For the construction of efficient error estimates for collocation schemes based on the idea of defect correction see [1].

$N_1$	BEUL	IDeC 1	IDeC 2	IDeC 3	IDeC 4	RadauIIa
2	$5.61 \cdot 10^{-2}$	$1.35 \cdot 10^{-2}$	$1.73 \cdot 10^{-2}$	$8.20 \cdot 10^{-5}$	$4.37 \cdot 10^{-3}$	$2.29 \cdot 10^{-6}$
4	$2.84 \cdot 10^{-2}$	$5.38 \cdot 10^{-3}$	$9.38 \cdot 10^{-3}$	$8.89 \cdot 10^{-4}$	$2.41 \cdot 10^{-3}$	$7.27 \cdot 10^{-8}$
8	$1.43 \cdot 10^{-2}$	$2.32 \cdot 10^{-3}$	$4.85 \cdot 10^{-3}$	$6.97 \cdot 10^{-4}$	$1.23 \cdot 10^{-3}$	$2.31 \cdot 10^{-9}$
16	$7.17 \cdot 10^{-3}$	$1.06 \cdot 10^{-3}$	$2.47 \cdot 10^{-3}$	$4.16 \cdot 10^{-4}$	$6.14 \cdot 10^{-4}$	$7.29 \cdot 10^{-10}$
2	0.98	1.33	0.88	-3.44	0.86	4.97
4	0.99	1.21	0.95	0.35	0.97	4.98
8	0.99	1.12	0.98	0.74	1.00	4.99
16						

Table 1: Classical IDeC based on RadauIIa nodes (degree  $m = 3$ ) for the problem  $z'(t) = -(z(t) - \sin(t) - 2) + \cos(t)$ ,  $z(0) = 2$ , with exact solution  $z(t) = \sin(t) + 2$ . Global error and observed order are displayed at  $t_{\text{end}} = 3.0$ .  $N_1$  denotes the number of subintervals  $J_i \subset [0, t_{\text{end}}]$  each having the same length  $t_{\text{end}}/N_1$ .

based on RadauIIa nodes  $0 < c_1 < \dots < c_m = 1$ , superconvergence  $z_{i,m}^* - y(t_{i,m}) = O(\mathbf{h}^{2m-1})$  holds for the fixed point  $z_\Gamma^*$  at the endpoints  $t_{i,m}$  of the subintervals  $J_i$ . This means that in case of fixed point convergence with convergence rate  $O(\mathbf{h})$  we would have  $p = 2m - 1$  in (11) at these points. Unfortunately, we do not observe this convergence rate for such nonequidistant grids. Convergence, if present at all, occurs at a much slower rate, as demonstrated in Table 1.

### 3 Modified IDeC

In the following sections we consider certain modifications of the IDeC procedure, which eventually will enable rapid fixed point convergence to arbitrary (including superconvergent) collocation solutions. The common idea behind these modifications will be to use some kind of splitting for the numerical solution of the respective neighboring problems, which are all of the generic form

$$z'(t) = f(t, z(t)) + d(t), \quad z(t_0) = z_0. \quad (13)$$

Here, we split the time-dependent vector field into its components  $f(t, z)$  and  $d(t)$ . We denote the numerical flow of  $f(t, z)$  by  $\Phi_{t,h}$ , such that one step  $(t, z_k) \mapsto (t+h, z_{k+1})$  with step size  $h$  of the basic scheme applied to (1) can be written as  $z_{k+1} = \Phi_{t,h}(z_k)$ . The numerical flow  $\Delta_{t,h}$  of the other component  $d(t)$  is given by a suitable quadrature rule,

$$\Delta_{t,h}(z) \approx z + \int_t^{t+h} d(\tau) d\tau. \quad (14)$$

A method  $\Psi_{t,h}$  for the numerical solution of (13) is then given by a splitting scheme, i.e.,  $\Psi_{t,h}$  is a com-

position of the numerical flows  $\Phi_{t,h}$  and  $\Delta_{t,h}$ , cf. [4, Section II.5].

Note that also the classical version of IDeC described in Section 2 can be interpreted within this framework, namely if we use *Lie-Trotter splitting* [4],

$$\Psi_{t,h} = \Phi_{t,h} \circ \Delta_{t,h}, \quad (15)$$

where  $\Delta_{t,h}$  is defined by the simple quadrature rule

$$\Delta_{t,h}(z) = z + hd(t+h). \quad (16)$$

### 4 Defect Quadrature (IQDeC)

For our first modification of classical IDeC, we retain the splitting scheme (15) but replace the simple quadrature rule (16) by

$$\Delta_{t,h}(z) = z + \int_t^{t+h} D(\tau) d\tau, \quad (17)$$

where  $D(t) = D_i(t)$  for  $t \in J_i$  is the piecewise polynomial interpolant of degree  $\leq m - 1$  of  $d(t)$ , defined by  $D_i(t_{i,j}) = d(t_{i,j})$ ,  $j = 1, \dots, m$ . If the grid  $\Gamma$  is given by (12) with arbitrary nodes  $0 < c_1 < \dots < c_m = 1$ , then

$$\begin{aligned} \int_{t_{i,j-1}}^{t_{i,j}} D_i(\tau) d\tau &= h_{i,j} \sum_{\ell=1}^m \alpha_{j,\ell} d(t_{i,\ell}) \\ &= z_{i,j} - z_{i,j-1} - h_{i,j} \sum_{\ell=1}^m \alpha_{j,\ell} f(t_{i,\ell}, z_{i,\ell}) \end{aligned}$$

holds with  $h_{i,j} = t_{i,j} - t_{i,j-1}$  and well-defined coefficients  $\alpha_{j,\ell}$  independent of  $i$ . Here, the latter identity easily follows, if the function  $d(t)$  is given by

$N_1$	BEUL	IQDeC 1	IQDeC 2	IQDeC 3	IQDeC 4	IQDeC 5	Gauss
2	$4.83 \cdot 10^{-2}$	$1.46 \cdot 10^{-5}$	$9.53 \cdot 10^{-5}$	$7.53 \cdot 10^{-6}$	$3.27 \cdot 10^{-7}$	$4.99 \cdot 10^{-8}$	$6.25 \cdot 10^{-8}$
4	$2.44 \cdot 10^{-2}$	$1.64 \cdot 10^{-6}$	$1.27 \cdot 10^{-5}$	$5.13 \cdot 10^{-7}$	$1.25 \cdot 10^{-8}$	$7.06 \cdot 10^{-10}$	$9.30 \cdot 10^{-10}$
8	$1.22 \cdot 10^{-2}$	$1.09 \cdot 10^{-6}$	$1.64 \cdot 10^{-6}$	$3.34 \cdot 10^{-8}$	$4.30 \cdot 10^{-10}$	$1.06 \cdot 10^{-11}$	$1.43 \cdot 10^{-11}$
16	$6.13 \cdot 10^{-3}$	$3.60 \cdot 10^{-7}$	$2.08 \cdot 10^{-7}$	$2.14 \cdot 10^{-9}$	$1.40 \cdot 10^{-11}$	$1.63 \cdot 10^{-13}$	$2.23 \cdot 10^{-13}$
2	0.99	3.15	2.91	3.88	4.71	6.14	6.07
4	0.99	0.59	2.95	3.94	4.87	6.06	6.02
8	1.00	1.60	2.98	3.97	4.94	6.02	6.00
16							

Table 2: Modified IQDeC based on Gauss nodes ( $m = 3$ ). Problem data as in Table 1.

$d(t) = p'(t) - f(t, p(t))$ , where  $p(t) = p_i(t)$  for  $t \in J_i$  is the piecewise interpolant of degree  $\leq m$  of some grid function  $z_\Gamma$ . The equations defining the numerical solution  $p_\Gamma$  of the neighboring problems (13) now read

$$\frac{p_{i,j} - p_{i,j-1}}{h_{i,j}} = f(t_{i,j}, p_{i,j}) + d_{i,j} \quad (18)$$

with

$$\begin{aligned} d_{i,j} &= \frac{1}{h_{i,j}} \int_{t_{i,j-1}}^{t_{i,j}} D_i(\tau) d\tau \\ &= \frac{z_{i,j} - z_{i,j-1}}{h_{i,j}} - \sum_{\ell=1}^m \alpha_{j,\ell} f(t_{i,\ell}, z_{i,\ell}), \end{aligned} \quad (19)$$

which explains the term ‘‘IDeC with defect quadrature’’ (IQDeC) for this variant of classical IDeC.<sup>4</sup>

For sufficiently smooth  $f(t, z)$ , convergence towards the fixed point  $z_\Gamma^*$  with convergence rate  $O(\mathbf{h})$  can be shown for the IQDeC-iterates  $z_\Gamma^{[\nu]}$ , which ensures the validity of (11) for this IDeC variant, cf. [3, Proposition 1]. Note that this result holds for *arbitrary nodes*  $0 < c_1 < \dots < c_m = 1$  in (12). In particular, for RadauIIa nodes  $c_j$  we now have

$$z_{i,m}^{[\nu]} - y(t_{i,m}) = O(\mathbf{h}^{\min(\nu+1, 2m-1)}), \quad (20)$$

i.e., superconvergence at the points  $t_{i,m}$ .

## 5 Modified IQDeC

Despite superconvergence, IQDeC is not completely satisfactory for the following reasons:

- (i) The nodes  $c_j$  are arbitrary with the restriction that  $c_m = 1$  must hold. This excludes the usage of e.g. Gauss nodes.

- (ii) For stiff problems the implicit equations (2) and (18) are usually solved by (some variant of) Newton’s method. To minimize the computational effort in the involved linear algebra, it is desirable to reuse the LU-decomposition of the respective Jacobians as far as possible. But this is only possible as long as the stepsize does not change.

To find a remedy for both drawbacks, we note that it is not necessary that the interpolation points for the definition of  $D(t)$  in (17) are identical to the points  $t_{i,j} \in \Gamma$ . Instead, we now introduce a second grid  $\tilde{\Gamma} = (\tilde{t}_{i,j})$  by

$$\tilde{t}_{i,j} = t_{i,0} + (t_{i,m} - t_{i,0})\tilde{c}_j, \quad j = 1, \dots, m \quad (21)$$

for arbitrary nodes  $0 < \tilde{c}_1 < \dots < \tilde{c}_m \leq 1$ , and let  $D_i(t)$  be defined by  $D_i(\tilde{t}_{i,j}) = d(\tilde{t}_{i,j})$ ,  $j = 1, \dots, m$ . The original grid  $\Gamma$ , on which the basic scheme operates, is assumed to be piecewise equidistant, exactly as in the case of the classical IDeC procedure.

For this new IDeC variant the fixed point  $z_\Gamma^*$  is given by  $R_\Gamma p^*$ , where now  $p^*(t)$  is the piecewise collocation polynomial corresponding to the collocation points  $\tilde{t}_{i,j} \in \tilde{\Gamma}$ . Again, convergence towards the fixed point  $z_\Gamma^*$  with convergence rate  $O(\mathbf{h})$  can be shown for the iterates  $z_\Gamma^{[\nu]}$  by a straightforward adaptation of the proof of [3, Proposition 1]. In particular, for Gauss nodes  $\tilde{c}_j$  in (21) we have

$$z_{i,m}^{[\nu]} - y(t_{i,m}) = O(\mathbf{h}^{\min(\nu+1, 2m)}), \quad (22)$$

i.e., superconvergence at the points  $t_{i,m}$ . This is illustrated by a numerical example in Table 2.

<sup>4</sup>For the idea to replace the pointwise evaluation of the defect by locally integrated values (19) see [2].

## 6 Defect Interpolation (IPDeC)

Let us consider a slight variant of the modified IQDeC procedure from Section 5. Namely, we do not integrate the interpolated defect  $D(t)$  exactly for the definition of  $\Delta_{t,h}$  as in (17), but apply the quadrature rule (16) to  $D(t)$ ,

$$\Delta_{t,h}(z) = z + hD(t+h). \quad (23)$$

This IDeC variant can be characterized by the fact that now the basic scheme is not applied to the neighboring problems (13) as is the case for classical IDeC, but to

$$z'(t) = f(t, z(t)) + D(t), \quad z(t_0) = z_0, \quad (24)$$

where the defect  $d(t)$  has been replaced by its interpolant  $D(t)$ . Hence, we call this IDeC variant ‘‘IDeC with defect interpolation’’ (IPDeC).

The convergence behavior of the IPDeC procedure is very similar to that of the modified IQDeC procedure, cf. [3, Proposition 2].

## 7 Splitting Defect Correction (ISDeC)

In this section we generalize the splitting approach from Section 3 in two respects:

- (i) We consider other basic methods  $\Phi_{t,h}$  instead of the backward Euler method, namely methods of higher order, and geometric integrators, which are suited for problems (1) with special structure.
- (ii) We replace Lie-Trotter splitting (15) for the numerical solution of the neighboring problems (13) by other schemes, e.g. by *Strang splitting*,

$$\Psi_{t,h} = \Delta_{t+\frac{h}{2}, \frac{h}{2}} \circ \Phi_{t,h} \circ \Delta_{t, \frac{h}{2}}. \quad (25)$$

Throughout this section, the numerical flow  $\Delta_{t,h}$  for the component  $d(t)$  of (13) is defined as in Section 5,

$$\Delta_{t,h}(z) = z + \int_t^{t+h} D(\tau) d\tau, \quad (26)$$

where  $D(t)$  is the piecewise polynomial of degree  $\leq m-1$  which interpolates  $d(t)$  at the points  $\tilde{t}_{i,j}$ , cf. (21). This choice of  $\Delta_{t,h}$  ensures that the fixed point  $z_\Gamma^*$  of the IDeC iteration is given by  $z_\Gamma^* = R_\Gamma p^*$ , where

<sup>5</sup>A Hamiltonian system  $p' = -H_q(p, q)$ ,  $q' = H_p(p, q)$  is of this special form if the Hamiltonian function  $H(p, q)$  can be written as  $H(p, q) = V(p) + U(q)$ .

$p^*(t)$  is the collocation solution corresponding to the grid (21).

### 7.1 Schild’s Method

In [6] an IDeC variant was analyzed which can be reformulated such as to fit into the context of the present discussion. The basic method  $\Phi_{t,h}$  is the implicit trapezoidal rule, which can be written as

$$\Phi_{t,h} = \phi_{t+\frac{h}{2}, \frac{h}{2}} \circ \phi_{t, \frac{h}{2}}^*, \quad (27)$$

where  $\phi^*$  and  $\phi$  are the forward and backward Euler methods, respectively. Splitting for the neighboring problems (13) is realized as

$$\Psi_{t,h} = \phi_{t+\frac{h}{2}, \frac{h}{2}} \circ \Delta_{t,h} \circ \phi_{t, \frac{h}{2}}^*. \quad (28)$$

In [6] it has been demonstrated that the usage of Gauss nodes  $\tilde{c}_j$  in (21) leads to a convergence rate  $O(\mathbf{h}^2)$  for this IDeC variant. Consequently,

$$z_{i,m}^{[\nu]} - y(t_{i,m}) = O(\mathbf{h}^{\min(2\nu+2, 2m)}) \quad (29)$$

holds for the global errors of the iterates  $z_\Gamma^{[\nu]}$  at the points  $t_{i,m}$ .

### 7.2 Geometric Integrators

In the context of geometric integration [4] it is common to study ODEs of special structure. For example, consider a system of two autonomous ODEs of the special form<sup>5</sup>

$$y' = f(z), \quad z' = g(y). \quad (30)$$

An explicit 2nd order method  $\Phi_{t,h}$  for (30) is given by the *Störmer-Verlet* scheme

$$\begin{aligned} z_{k+\frac{1}{2}} &= z_k + \frac{h}{2}g(y_k), \\ y_{k+1} &= y_k + hf(z_{k+\frac{1}{2}}), \\ z_{k+1} &= z_{k+\frac{1}{2}} + \frac{h}{2}g(y_{k+1}). \end{aligned} \quad (31)$$

Note that now the original IDeC idea cannot be applied in a straightforward way, because the nonautonomous neighboring problems (13) are not of the form (30). On the other hand, the splitting idea using Strang splitting (25) and  $\Delta_{t,h}$  given by (26) is evidently applicable. By means of numerical experiments, it is demonstrated in [5] that this IDeC variant

$N_1$	Störmer	ISDeC 1	ISDeC 2	ISDeC 3	ISDeC 4	ISDeC 5	Gauss
100	$4.97 \cdot 10^{-2}$	$1.80 \cdot 10^{-3}$	$1.49 \cdot 10^{-4}$	$2.93 \cdot 10^{-6}$	$4.38 \cdot 10^{-8}$	$3.84 \cdot 10^{-10}$	$1.82 \cdot 10^{-15}$
200	$1.24 \cdot 10^{-2}$	$1.12 \cdot 10^{-4}$	$2.40 \cdot 10^{-6}$	$1.18 \cdot 10^{-8}$	$4.46 \cdot 10^{-11}$	$9.84 \cdot 10^{-14}$	$3.93 \cdot 10^{-18}$
400	$3.10 \cdot 10^{-3}$	$7.03 \cdot 10^{-6}$	$3.78 \cdot 10^{-8}$	$4.66 \cdot 10^{-11}$	$4.40 \cdot 10^{-14}$	$2.43 \cdot 10^{-17}$	$1.12 \cdot 10^{-21}$
800	$7.76 \cdot 10^{-4}$	$4.39 \cdot 10^{-7}$	$5.91 \cdot 10^{-10}$	$1.83 \cdot 10^{-13}$	$4.31 \cdot 10^{-17}$	$5.96 \cdot 10^{-21}$	$2.84 \cdot 10^{-25}$
100	2.00	4.00	5.96	7.95	9.94	11.93	8.85
200	2.00	4.00	5.99	7.99	9.99	11.98	11.78
400	2.00	4.00	6.00	8.00	10.00	12.00	11.95
800							

Table 3: ISDeC based on Störmer-Verlet (31), Strang splitting (25), and Gauss nodes ( $m = 6$ ) for the Kepler problem [4, Section I.2.2]. Global error and observed order are displayed at  $t_{\text{end}} = 2\pi$ .

again leads to a fixed point convergence rate  $O(\mathbf{h}^2)$ , if a Gauss grid  $\tilde{\Gamma}$  is used. Consequently, superconvergence as in (29) can be observed. This is illustrated by a numerical example in Table 3.

In the context of geometric integration it is often desirable that certain invariants of the original ODE are preserved by the numerical solution as well. For example, the Störmer-Verlet scheme (31) preserves quadratic invariants of the form  $Q(y, z) = y^T D z$  with some matrix  $D$ , cf. [4, Section IV.2.2]. Unfortunately, these invariants are not exactly preserved by the iterates  $z_{\Gamma}^{[\nu]}$  in general. But as they are preserved by the fixed point  $z_{\Gamma}^*$  corresponding to a Gauss collocation method, it makes sense to continue the IDeC iteration beyond  $\nu \geq m$ , because then these invariants are preserved by  $z_{\Gamma}^{[\nu]}$  up to terms of the order of the iteration error  $z_{\Gamma}^{[\nu]} - z_{\Gamma}^*$  which is  $O(\mathbf{h}^{2\nu+2})$ , in contrast to the global error which is only  $O(\mathbf{h}^{2m})$ .

## 8 Conclusion

Whereas the convergence order of the classical version of IDeC is restricted to  $O(\mathbf{h}^m)$ , we have demonstrated in this paper how to overcome this restriction. We have presented modifications of the algorithm for which superconvergence order up to  $O(\mathbf{h}^{2m})$  is obtained. All these modifications were based on the idea to solve the respective neighboring problems by a splitting scheme, which leads to alternative ways of evaluating the defect compared to classical IDeC. Defect quadrature and defect interpolation are techniques which can be effectively applied in this context.

The splitting approach can also be successfully adapted to even more general situations, cf. [5].

## References

- [1] W. Auzinger, O. Koch, and E. Weinmüller, Efficient Collocation Schemes for Singular Boundary Value Problems, *Numer. Algorithms* 31 (2002), pp. 5–25.
- [2] W. Auzinger, O. Koch, and E. Weinmüller, New Variants of Defect Correction for Boundary Value Problems in Ordinary Differential Equations, in *Current Trends in Scientific Computing*, Z. Chen, R. Glowinski, K. Li (eds), Publ. of AMS, *Cont. Math. Series*, 329 (2003), pp. 43–50.
- [3] W. Auzinger, H. Hofstätter, W. Kreuzer and E. Weinmüller, Modified Defect Correction Algorithms for ODEs. Part I: General Theory, submitted to *Numer. Algorithms*.
- [4] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration*, Springer-Verlag, Berlin-Heidelberg-New York, 2002.
- [5] H. Hofstätter and O. Koch, Defect Correction for Geometric Integrators, Proceedings of APLIMAT 2004, pp. 465–470.
- [6] K.H. Schild, Gaussian Collocation via Defect Correction, *Numer. Math.* 58 (1990), pp. 369–386.
- [7] H.J. Stetter, The Defect Correction Principle and Discretization Methods, *Numer. Math.* 29 (1978), pp. 425–443.
- [8] P.E. Zadunaisky, On the Estimation of Errors Propagated in the Numerical Integration of ODEs, *Numer. Math.* 27 (1976), pp. 21–39.