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DEFECT CORRECTION FOR GEOMETRIC INTEGRATORS

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Abstract. This paper deals with the defect correction principle used to estimate the error and to improve the accuracy of the numerical solution of ordinary differential equations. If the basic numerical method is designed for a special type of equation only, as is the case for many geometric integrators, a splitting approach enables the application of the defect correction principle in this case as well. We show experimental order results and fixed point properties of iterated defect correction when applied to various geometric integration methods in this setting.

1 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 [2]. Many of these methods are applicable to particular types of differential equations only.

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. The idea can also be used to successively improve the accuracy of the numerical solution ([1] 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. In this paper, we present *splitting methods* [2] to avoid such difficulties.

2 Splitting Defect Correction

First, we describe the classical version of *iterated defect correction* [1]. Consider an initial value problem

$$\dot{z} = f(t, z), \quad z(t_0) = z_0, \tag{1}$$

to be solved on the interval $[t_0, t_{\text{end}}]$. The approximate solution $z^{[0]} := (z_0, \ldots, z_N)$ is obtained by some discretization method Φ on a grid $(t_0, \ldots, t_N)$. Denote by $p^{[0]}(t)$ the polynomial of

degree N interpolating the values of $z^{[0]}$. Using this interpolating function, we construct a neighboring problem associated with (1) whose exact solution is $p^{[0]}(t)$:

$$\dot{z}(t) = f(t, z(t)) + d^{[0]}(t), \tag{2}$$

where $d^{[0]}(t) := \dot{p}^{[0]}(t) - f(t, p^{[0]}(t))$. We now solve (2) using the same numerical method Φ and obtain an approximate solution $\hat{p}^{[0]}$ for $p^{[0]}(t)$. This means that for the solution of the neighboring problem (2) we know the global error which is a good estimate for the unknown error of the original problem (1). This estimate can be used to improve the first solution,

$$z^{[1]} := z^{[0]} + \left(p^{[0]} - \hat{p}^{[0]}\right).$$

Now, these values are used to define a new interpolating polynomial $p^{[1]}(t)$ by requiring $p^{[1]}(t_j) = z_j^{[1]}$. Again, $p^{[1]}(t)$ defines a neighboring problem in the same manner as in (2), where again the exact solution is known, and the numerical solution of this neighboring problem serves to obtain the second improved solution $z^{[2]} := z^{[0]} + \left(p^{[1]} - \hat{p}^{[1]}\right)$. 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, piecewise functions composed of polynomials of (moderate) degree m are defined to specify 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.

If the basic method Φ is a geometric integrator, the neighboring problem (2) has a form to which the integrator cannot be applied straightforwardly. For example, if the Störmer-Verlet method is applied to a Hamiltonian system (see Section 3), (2) is no longer an autonomous, separated system. Another example is the exponential midpoint rule designed for linear homogeneous systems.

In order to be able to use iterated defect correction even in these cases, we employ splitting methods, cf. [2]. To apply *Strang splitting* to (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 Φ applied to (1) can be written as $\eta_{i+1} = \Phi_{t,h}(\eta_i)$. The numerical flow $\Delta_{t,h}$ of the other component $d^{[0]}(t)$ is defined by the quadrature rule

$$\Delta_{t,h}(y) = y + \int_t^{t+h} D^{[0]}(\tau) d\tau, \tag{3}$$

where $D^{[0]}(t)$ is a piecewise polynomial interpolant of degree $\leq m-1$ of $d^{[0]}(t)$. For the purpose of this paper, we use interpolation at Gaussian points in certain subintervals of length $H = mh$. The details of the procedure are given in [3]. Using $\Phi_{t,h}$ and $\Delta_{t,h}$, the numerical solution of (2) is computed using the numerical flow

$$\Psi_{t,h} = \Delta_{t+h/2,h/2} \circ \Phi_{t,h} \circ \Delta_{t,h/2}, \tag{4}$$

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)*.

3 The Störmer-Verlet Method

The Störmer-Verlet method is a geometric integration scheme of order two which is particularly suited for the solution of *Hamiltonian systems* of ODEs like Kepler's equations of planet motion (9), or more generally, *separated* ODEs. The method retains important conserved quantities of the exact flow like the angular momentum, see below.

Consider a system of two separated autonomous ODEs

$$\dot{p} = f(p,q), \quad \dot{q} = g(p,q). \tag{5}$$

One step of the Störmer-Verlet method for (5) is defined by

$$q_{i+1/2} = q_i + \frac{h}{2} g(p_i, q_{i+1/2}) \tag{6}$$

$$p_{i+1} = p_i + \frac{h}{2}\left(f(p_i, q_{i+1/2}) + f(p_{i+1}, q_{i+1/2})\right) \tag{7}$$

$$q_{i+1} = q_{i+1/2} + \frac{h}{2} g(p_{i+1}, q_{i+1/2}). \tag{8}$$

As a numerical example for the application of this method to a Hamiltonian system of differential equations consider the Kepler problem, i. e.,

$$\dot{p} = -H_q(p,q), \qquad \dot{q} = H_p(p,q), \tag{9}$$

where

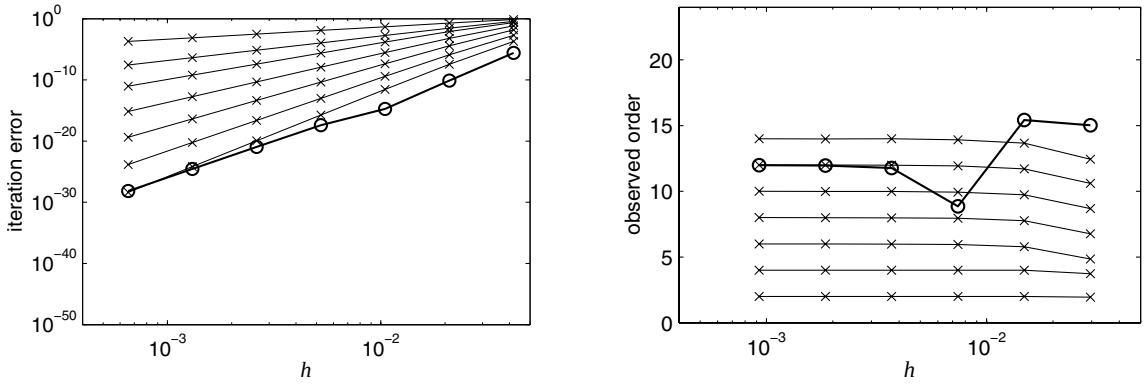
$$H(p_1,p_2,q_1,q_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}. \tag{10}$$

Note that the Hamiltonian H is constant along the exact flow of the problem. Moreover, the angular momentum $L(p_1,p_2,q_1,q_2) = q_1 p_2 - q_2 p_1$ is preserved.

Now, we discuss the asymptotic order of the iterates computed by ISDeC based on the Störmer-Verlet method. First, we remark that under certain circumstances, the ISDeC iteration converges to a fixed point p^*. This fixed point is a piecewise polynomial function, and from the definition of $\Delta_{t,h}$ it is clear that this fixed point is characterized by $\dot{p}^*(\tau_j) - f(\tau_j, p^*(\tau_j)) = 0$, where τ_j are the points where $D^{[0]}$ interpolates $d^{[0]}$ (in our case, Gaussian points). This means that in this situation the ISDeC iterates converge to a *collocation polynomial* [1].

Figure 1 gives the absolute errors of the respective ISDeC iterates with respect to the fixed point at $t_{\text{end}} = 2\pi$, using the particular initial values from [2] at $t = 0$ and polynomial degree $m = 6$. The left diagram shows these errors on a logarithmic scale plotted against the step size h, while the diagram on the right shows the empirical convergence orders of the iterates. The circles $\circ$ illustrate the error and the convergence order for the fixed point, i. e., a collocation solution of order 12. The convergence orders as compared to the fixed point are $O(h^2)$, $O(h^4)$, $O(h^6), \ldots$. This corresponds to classical theory which predicts the order to increase by two in every step if the data is sufficiently smooth [1]. From the triangle inequality it is clear that the global errors of the iterates as compared to the exact solution have orders $O(h^2)$, $O(h^4), \ldots,$ $O(h^{12})$, which does not increase further than the order of the fixed point.

Finally, we discuss the conservation of the angular momentum L. It is well known that both the Störmer-Verlet method and the fixed point of ISDeC, defined by collocation at Gaussian



Obr. 1: ISDeC based on Störmer-Verlet, $m = 6$.

h	Störmer	ISDeC 1	ISDeC 2	ISDeC 3	ISDeC 4	ISDeC 5	ISDeC 6
$\pi/600$	0.00	$8.90{\cdot}10^{-5}$	$7.39{\cdot}10^{-7}$	$6.00{\cdot}10^{-9}$	$1.59{\cdot}10^{-11}$	$4.03{\cdot}10^{-14}$	$6.48{\cdot}10^{-17}$
$\pi/1200$	0.00	$5.55{\cdot}10^{-6}$	$1.17{\cdot}10^{-8}$	$2.37{\cdot}10^{-11}$	$1.58{\cdot}10^{-14}$	$9.99{\cdot}10^{-18}$	$4.02{\cdot}10^{-21}$
$\pi/2400$	0.00	$3.47{\cdot}10^{-7}$	$1.83{\cdot}10^{-10}$	$9.27{\cdot}10^{-14}$	$1.55{\cdot}10^{-17}$	$2.45{\cdot}10^{-21}$	$2.46{\cdot}10^{-25}$
$\pi/4800$	0.00	$2.17{\cdot}10^{-8}$	$2.86{\cdot}10^{-12}$	$3.62{\cdot}10^{-16}$	$1.51{\cdot}10^{-20}$	$5.98{\cdot}10^{-25}$	$1.51{\cdot}10^{-29}$
$\pi/600$							
$\pi/1200$		4.00	5.98	7.98	9.97	11.98	13.98
$\pi/2400$		4.00	6.00	8.00	9.99	11.99	14.00
$\pi/4800$		4.00	6.00	8.00	10.00	12.00	13.99

Tabuľka 1: Error in the angular momentum for ISDeC based on Störmer-Verlet.

points, preserve this quantity exactly [2]. This is not precisely the case for the ISDeC iterates, however. Table 1 shows that the angular momentum is preserved up to terms of the order of the iteration error (as compared with the fixed point p^*).

3.1 Composition Methods

The results for the Störmer-Verlet method in Section 3 are encouraging, but we would also like to be able to use higher order schemes as basic methods for ISDeC to increase the gain in every step of the iteration. This is possible to some extent.

The *Suzuki method* uses the composition of five steps of the Störmer-Verlet method to define a method of order 4 which has similarly favorable geometric properties as the original method, see [2]. If we use the resulting integrator $\Phi_{t,h}$ as in (4), the observed order sequence is $O(h^4)$, $O(h^6)$, $O(h^8), \ldots, O(h^{2m})$. We can modify our approach in order to obtain $O(h^4)$, $O(h^8)$, $O(h^{10}), \ldots$, however.

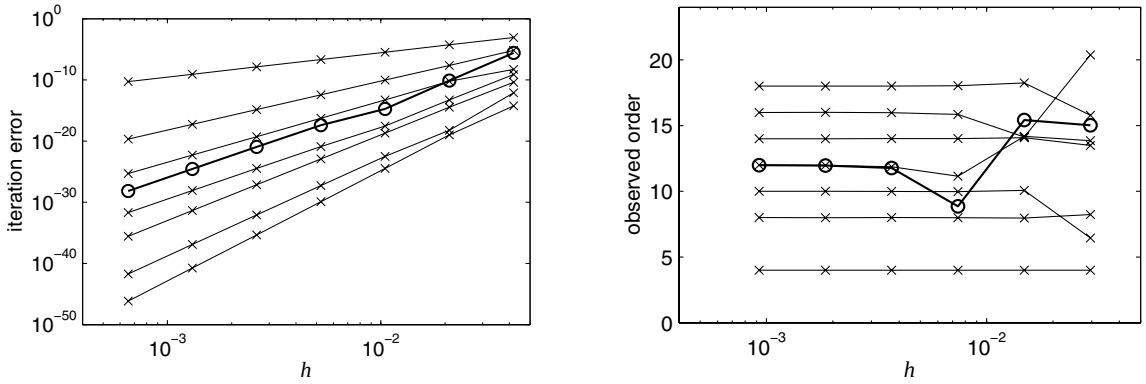
If the composition method is

$$\Phi = \Phi^{[1]} \circ \cdots \circ \Phi^{[k]}, \tag{11}$$

the ISDeC solution method for the neighboring problem (2) can be chosen as

$$\Psi = \Psi^{[1]} \circ \cdots \circ \Psi^{[k]}, \tag{12}$$

where $\Psi^{[j]}$ is a splitting method analogous to (4), see [3]. This new approach yields favorable results, see Figure 2. Using $m = 6$, the order sequence of the iteration error to the fixed point



Obr. 2: ISDeC based on Suzuki, $m = 6$.

is $O(h^4)$, $O(h^8)$, $O(h^{10}), \ldots$. Up to the order of the fixed point, which is again a collocation solution of order 12, this is equal to the order of the global error.

Related Work: In [4], an IDeC iteration was analyzed which can be reformulated such as to fit into the context of the above discussion. The basic method is

$$\Phi_{t,h} = \phi_{t+h/2,h/2} \circ \phi^*_{t,h/2},$$

where ϕ^* and ϕ are the explicit and the implicit Euler methods, respectively. Consequently, Φ is the implicit trapezoidal rule. ISDeC is realized as

$$\Psi_{t,h} = \phi_{t+h/2,h/2} \circ \Delta_{t,h} \circ \phi^*_{t,h/2}.$$

In [4] it has been demonstrated for linear problems that the usage of Gaussian points in the quadrature rule leads to an order sequence $O(h^2)$, $O(h^4), \ldots$ for the iteration error, which means that the order of the global error increases by two up to the convergence order of the fixed point, i. e. $O(h^{2m})$. This asymptotic behavior is the same as for the geometric integrators of this paper.

4 Exponential Integrators

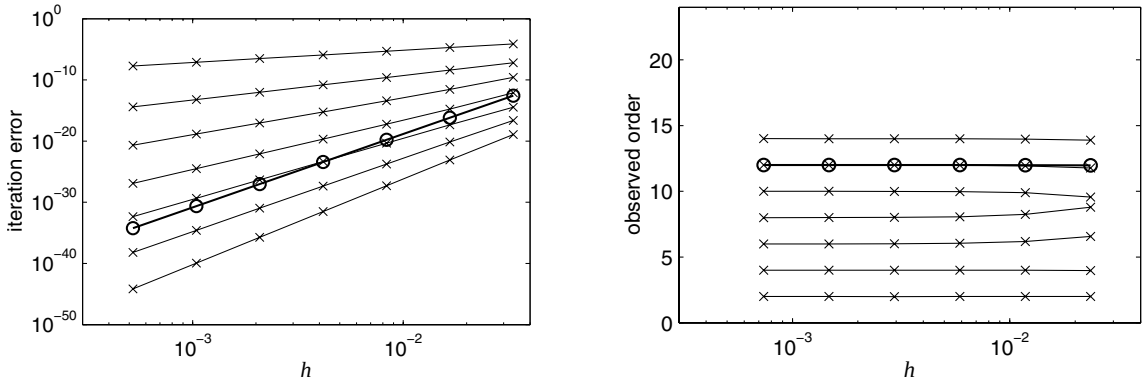
First, we consider the exponential midpoint rule, which is a second order method defined for linear homogeneous ODEs $\dot{y} = A(t)y$ by

$$\Phi_{t,h}(y) = \exp\left(hA(t + h/2)\right) y. \tag{13}$$

If ISDeC based on the exponential midpoint rule is applied to smooth problems, the same behavior as for the Störmer-Verlet method can be observed. Results for

$$A(t) = \begin{pmatrix} 0 & t & -0.4\cos(t) \\ -t & 0 & 0.1t \\ 0.4\cos(t) & -0.1t & 0 \end{pmatrix} \tag{14}$$

are given in Figure 3. In this case the exact flow of the differential equation preserves the norm of the solution. The solution by the exponential midpoint rule shares this property, while this



Obr. 3: ISDeC based on exponential midpoint rule, $m = 6$.

conservation law is violated for the ISDeC iterates, which preserve the norm up to terms of the order of the iteration error. Note that collocation at Gaussian points also preserves the norm for (14). Unfortunately, ISDeC in conjunction with the exponential midpoint rule can only be used successfully if smooth problems are to be solved. This can be demonstrated using the simple *test equation* $\dot{y} = \lambda y$. In this case the solution obtained by the exponential midpoint rule corresponds to the exact flow, $y(t+h) = \exp(\lambda h)y(t)$. Nonetheless we may formally apply ISDeC for this problem. It turns out that for moderate values of $\lambda \in \mathbb{C}$ the iteration error successively increases up to its theoretical maximum given by the fixed point [3]. If, however, the problem is non-smooth in the sense that the modulus of λ is large, ISDeC fails already for reasonable step sizes. Only if $|h\lambda| \ll 1$, the expected order sequences can be observed. In [3] we demonstrate that for $\lambda = 1000\mathrm{i}$, the error of the ISDeC iterates is unacceptably large for reasonable h. Consequently, ISDeC needs some modification to become useful for error estimation for the time-dependent Schrödinger equation after space (semi-)discretization. The favorable results presented in this paper are a starting point for finding a successful ISDeC version for this important class of problems.

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