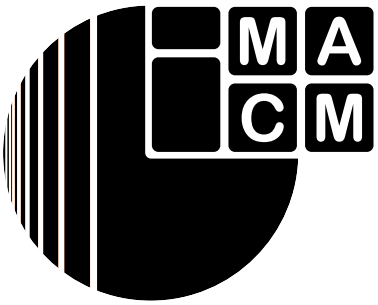

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Abstract

Multiphysical simulation tasks are often numerically solved by so-called dynamic iteration schemes. Usually, this demands the efficient and stable coupling of existing simulation software for the contributing physical subdomains or subsystem. Since the coupling is weakened by such a simulation strategy, iteration is needed to enhance the quality of the numerical approximation. By the means of error recursions, one obtains estimates for the approximation order and the reduction of error per iteration (convergence rate). It is know that the first iterations can be coarsely sampled (in time), but the last iterations need to be refined (h-refinement) to obtain the accuracy gain of latter iterations ('sweeps').
In this work we discuss an optimal choice of the approximation order p used in the time integration with respect to the iteration 'sweep' count. It is deduced from the analytical error recursion and yields a p-refinement strategy. Numerical experiments show that our estimates are sharp and give a precise prediction of the correct convergence.

1 Introduction

Today, the need for multiphysical simulations becomes more and more important in many engineering applications, e.g., in electromagnetic field/circuit coupling, [10]. For transient problems, e.g., after semi-discretization in space, one needs to solve a coupled system of differential algebraic equations (DAEs). Often separate software tools are available for each domain, but a framework to simulate the overall problem in an monolithic way (strong coupling) is missing. Thus simulation engineers want to couple those tools in an efficient and stable way, where subdomains are solved separately (weak coupling). This introduces a splitting error, which is mitigated by an iteration procedure (dynamic iteration). It has been shown that subdividing the time interval of interest into smaller time windows on which the iteration is carried out typically increases the efficiency [6, 11].

Dynamic iteration schemes for ordinary differential equations (ODEs) are globally convergent, but there are severe stability constraints for DAEs, which cannot be cured by a decrease of the window size. A fixed-point analysis reveals that a problem dependent contraction factor, [7], which measures the strength of the coupling of the

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algebraic variables, must be small to guarantee convergence, e.g. [1]. Then the error in a time window is reduced (super-)linearly within each iteration ('sweep'). Proceeding after a finite number of iterations to the next window, a splitting error remains and is transported, for details see e.g. [1, 2].

In practical applications each subproblem is solved by numerical integration and an discretization error is introduced, [4,5]. Often analytical investigations disregard it with respect to the splitting error. However, in practice computational cost increases with the demand of accuracy. Consequently, several authors have studied the usage of coarse or 'inexact' time discretization grids in early iterations that are refined in subsequent steps to increase the efficiency of the iterative method, e.g. [8, 9]. This can be interpreted as an h-refinement strategy where h is the micro time step size of the time integrator (in a subsystem). Thus it is also related to geometric multigrid approaches in classical domain decomposition.

In this paper we discuss a p-refinement strategy; given a fixed number of iterations we look for the minimal order p_k of the time integrators for each subproblem such that the overall convergence of the dynamic iteration scheme is optimal. The paper is organized as follows: in Section 2 we set up the basic formulations for a dynamic iteration of DAE systems; then we deduce the relation of splitting and time integration error (Section 3). In Section 4 we use an example with analytic dynamic iteration to verify that our estimates on the convergence rate are sharp (optimal).

2 Coupled DAE Systems and Dynamic Iteration Schemes

Following [2] we discuss in this paper the coupling of initial value problems (IVPs). We assume that all r subsystems can be rewritten in a semi-explicit form: $(i = 1, \dots, r)$

$$\dot{\mathbf{y}}_i = \mathbf{f}_i(\mathbf{y}, \mathbf{z}), \qquad \mathbf{y} := (\mathbf{y}_1, \dots, \mathbf{y}_r)^\top, \qquad \mathbf{y}(0) = \mathbf{y}_0 \in \mathbb{R}^{n_y}, \quad \text{(1a)}$$

$$0 = \mathbf{g}_i(\mathbf{y}, \mathbf{z}), \qquad \mathbf{z} := (\mathbf{z}_1, \dots, \mathbf{z}_r)^\top, \qquad \mathbf{z}(0) = \mathbf{z}_0 \in \mathbb{R}^{n_z}. \quad \text{(1b)}$$

Obviously it is a split structure for the DAE system

$$\begin{array}{rll} \dot{\mathbf{y}} &= \mathbf{f}(\mathbf{y}, \mathbf{z}) & \text{with} \quad \mathbf{f} = (\mathbf{f}_1, \dots, \mathbf{f}_r)^\top \\ 0 &= \mathbf{g}(\mathbf{y}, \mathbf{z}) & \text{with} \quad \mathbf{g} = (\mathbf{g}_1, \dots, \mathbf{g}_r)^\top. \end{array} \tag{2}$$

Furthermore, let the overall problem (2) and each subsystem (1) be index-1 DAEs. Thus there is a unique solution

$$\mathbf{x} = (\mathbf{y}, \mathbf{z})^\top \in C^1([0,\, t_e], \mathbb{R}^{n_y}) \times C([0,\, t_e], \mathbb{R}^{n_z}) \quad \text{with} \quad \begin{array}{l} \mathbf{y} : [0, t_e] \to \mathbb{R}^{n_y}, \\ \mathbf{z} : [0, t_e] \to \mathbb{R}^{n_z}. \end{array}$$

System (1) may include also ODE subsystems with the trivial constraint $\mathbf{g}_i \equiv 0$ and no local algebraic variables (i.e., $\mathbf{z}_i(t) \in \mathbb{R}^{n_{z_i}}$ with $n_{z_i} = 0$). By the classical windowing technique, e.g. [6], the time interval of interest $[0, t_e]$ is subdivided into smaller (time-)windows $[t_n, t_{n+1}]$ with $0 = t_0 < t_1 < t_2 < \ldots < t_N = t_e$ and window sizes $H_n := t_{n+1} - t_n < 1$. We aim at computing a *sufficiently accurate* approximation $\tilde{\mathbf{x}} := (\tilde{\mathbf{y}}, \tilde{\mathbf{z}})^\top : [0, t_e] \to \mathbb{R}^{n_y} \times \mathbb{R}^{n_z}$ to the exact unique solution $\mathbf{x}$ of (1) that consists of waveforms on these windows

$$\tilde{\mathbf{x}}|_{(t_n, t_{n+1}]} \in C_n^{1,0} \quad \text{with} \quad C_n^{1,0} := C^1((t_n, t_{n+1}], \mathbb{R}^{n_y}) \times C((t_n, t_{n+1}], \mathbb{R}^{n_z}).$$

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In this paper we define *sufficiently accurate* as an p-th order approximation on each time window

$$\left\|\tilde{\mathbf{x}}|_{(t_n,t_{n+1}]} - \mathbf{x}|_{(t_n,t_{n+1}]}\right\| = \mathcal{O}(H_n^p),$$

with maximum-norm $\|\mathbf{u}|_{(t_n,t_{n+1}]}\| := \max_{t\in(t_n,t_{n+1}]} |\mathbf{u}(t)|$ for $\mathbf{u} \in C_n^{1,0}$ and any vector norm $|\cdot|$.

Now, given an approximation $\tilde{\mathbf{x}}$ on $[0, t_n]$, a dynamic iteration defines the approximations on the next window via an extrapolation map $\Phi_n : C_{n-1}^{1,0} \to C_n^{1,0}$ and a number of iterations using a solution operator $\Psi_n : C_n^{1,0} \to C_n^{1,0}$:

$$\Phi_n : \begin{pmatrix}\tilde{\mathbf{y}}|_{[t_{n-1},t_n]}\\ \tilde{\mathbf{z}}|_{[t_{n-1},t_n]}\end{pmatrix} \mapsto \begin{pmatrix}\tilde{\mathbf{y}}_n^{(0)}\\ \tilde{\mathbf{z}}_n^{(0)}\end{pmatrix} \qquad \Psi_n : \begin{pmatrix}\tilde{\mathbf{y}}_n^{(k-1)}\\ \tilde{\mathbf{z}}_n^{(k-1)}\end{pmatrix} \mapsto \begin{pmatrix}\tilde{\mathbf{y}}_n^{(k)}\\ \tilde{\mathbf{z}}_n^{(k)}\end{pmatrix} := \Psi_n \begin{pmatrix}\tilde{\mathbf{y}}_n^{(k-1)}\\ \tilde{\mathbf{z}}_n^{(k-1)}\end{pmatrix}.$$

Subscript n denotes the n-th time window and superscript $k = 1, \ldots, k_n$ denotes the iteration count with (finite) integer k_n. To solve the split DAE (1) for $\tilde{\mathbf{y}}_n = (\tilde{\mathbf{y}}_{1,n}, \ldots, \tilde{\mathbf{y}}_{r,n})^\top$, $\tilde{\mathbf{z}}_n = (\tilde{\mathbf{z}}_{1,n}, \ldots, \tilde{\mathbf{z}}_{r,n})^\top$, operator Ψ_n maps given approximations with index $(k-1)$ to new ones $\tilde{\mathbf{y}}^{(k)}, \tilde{\mathbf{z}}^{(k)}$ of the decoupled initial-values problems. The operator encapsulates the (numerical) solution procedure for subproblems of the form (1). In particular, for a Gauss-Seidel-type scheme on the n-th time window and in the k-th iteration of the i-th subproblem, we need to solve:

$$\dot{\tilde{\mathbf{y}}}_i^{(k)} = \mathbf{f}_i(\mathbf{y}, \mathbf{z}), \quad \mathbf{y} := (\tilde{\mathbf{y}}_1^{(k)}, \ldots, \tilde{\mathbf{y}}_{i-1}^{(k)}, \bar{\mathbf{y}}_i^{(k)}, \tilde{\mathbf{y}}_{i+1}^{(k-1)} \ldots, \tilde{\mathbf{y}}_r^{(k-1)})^\top, \quad \bar{\mathbf{y}}_i(t_n) = \tilde{\mathbf{y}}_n, \tag{3a}$$

$$0 = \mathbf{g}_i(\mathbf{y}, \mathbf{z}), \quad \mathbf{z} := (\tilde{\mathbf{z}}_1^{(k)}, \ldots, \tilde{\mathbf{z}}_{i-1}^{(k)}, \bar{\mathbf{z}}_i^{(k)}, \tilde{\mathbf{z}}_{i+1}^{(k-1)} \ldots, \tilde{\mathbf{z}}_r^{(k-1)})^\top, \quad \bar{\mathbf{z}}_i(t_n) = \tilde{\mathbf{z}}_n, \tag{3b}$$

with respect to $\bar{\mathbf{x}}_i^{(k)}(t)$ on $(t_n, t_{n+1}]$. In practice one will not be able to obtain it exactly but a numerical approximation $\tilde{\mathbf{x}}_i^{(k)}$ by a time integration scheme. The scheme will further subdivide the time windows by a finite number $m_i^{(k)}$ of micro time steps to obtain the solution. Let us assume that the scheme has a variable order p_k and for simplicity that each time step is of constant size $h_{n,i}^{(k)} := H_n/m_i^{(k)}$ where H_n is the n-th time window size (or macro step size) as defined above. Thus, due to the *time integration error*, we obtain a solution of accuracy

$$\left\|\bar{\mathbf{x}}_i^{(k)}|_{(t_n,t_{n+1}]} - \tilde{\mathbf{x}}_i^{(k)}|_{(t_n,t_{n+1}]}\right\| = \mathcal{O}(h_{n,i}^{p_k}) = \mathcal{O}(H_n^{p_k}).$$

3 Relation of Splitting and Time Integration Errors

The sum of splitting error and time integration error on the n-the window after k iterations is defined as

$$\delta_{\mathbf{x},n}^{(k)} =: \max_{t\in(t_n,t_{n+1}]} \Delta_{\mathbf{x},n}^{(k)}(t) \quad \text{with} \quad \Delta_{\mathbf{x},n}^{(k)}(t) := \|\tilde{\mathbf{x}}^{(k)}(t) - \mathbf{x}(t)\| \text{ and } t \in (t_n, t_{n+1}].$$

The error in the differential variable $\delta_{\mathbf{y},n}^{(k)}$ and algebraic variable $\delta_{\mathbf{z},n}^{(k)}$ are defined analogously. Let a sufficiently accurate waveform $\tilde{\mathbf{x}}_n^{(k-1)}$ from a previous iteration be given, i.e.,

$$\Delta_{\mathbf{x},n}^{(k-1)}(t) = \mathcal{O}(H_n^{p_f\cdot[k-1]}) \quad \text{and} \quad \delta_{\mathbf{x},n}^{(k-1)} = \mathcal{O}(H_n^{p_f\cdot[k-1]}),$$

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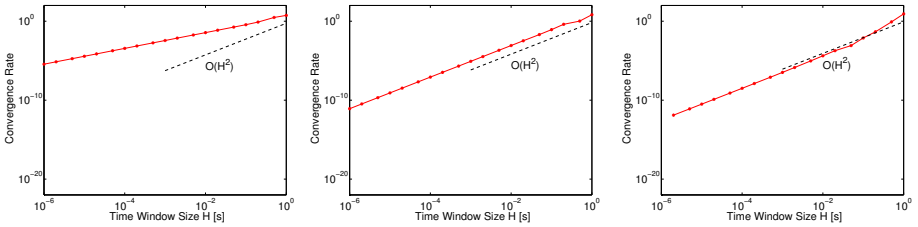

(a) Time integration error given by Taylor expansions of k-th order.

(b) Time integration error given by Taylor expansions of $(2 \cdot k)$-th order.

(c) Time integration error given by Taylor expansions of $(3 \cdot k)$-th order.

Figure 1: Convergence rate $\bar{\delta}$ per window size H_0, averaged over $k_0 = 5$ iterations. Experiments for the coupled Prothero-Robinson systems ($r = 2$) as given in Sec. 4. We depict the convergence rate versus window size H_0 computed according to our maximum-norm. Dashed lines show the expected 2nd-order convergence without time-integration error: from (a) to (c) the order of the time integration in the k-th iteration is increased from k to $3 \cdot k$.

where p_f is a problem dependent integer specified below. In [1,2] an error recursion has been deduced: for sufficiently small H, fixed k_n and sufficiently accurate waveforms $\tilde{\mathbf{y}}_n^{(k-1)}$ and $\tilde{\mathbf{z}}_n^{(k-1)}$, the iterates of the Gauss-Seidel-type scheme (1) fulfill the estimate:

$$\begin{pmatrix} \delta_{\mathbf{y}}^{(k)} \\ \delta_{\mathbf{z}}^{(k)} \end{pmatrix} \leq \mathbf{K} \begin{pmatrix} \delta_{\mathbf{y}}^{(k-1)} \\ \delta_{\mathbf{z}}^{(k-1)} \end{pmatrix} + \begin{pmatrix} 1 + CH_n \\ C \end{pmatrix} |\Delta_{\mathbf{y},n-1}^{(k-1)}(t_n)|, \tag{4}$$

where $C > 0$ is a problem dependent constant and $\mathbf{K}$ is an iteration matrix whose eigenvalues are $\lambda_K = \mathcal{O}(H_n^{p_f})$, i.e., p_f gives the convergence rate per iteration. Thus

$$\delta_{\mathbf{x},n}^{(k)} = \mathcal{O}(H_n^{p_f \cdot k}) \qquad \text{and} \qquad \Delta_{\mathbf{x},n}^{(k)}(t) = \mathcal{O}(H_n^{p_f \cdot k}).$$

The problem dependent parameter p_f is given by the type of coupling, see [3]: (a) for a coupled system of r DAEs with only differential coupling $p_f = r/(r-1)$, (b) for a DAE with no algebraic-to-algebraic coupling $p_f = 1$ and (c) for a general DAE $p_f = 0$. For eigenvalues $\lambda_K < 1$ the arguments in [1,2] guarantee convergence; While this is obvious in the first two cases (a) and (b) for small window size $H_n < 1$, the third case (c) exhibits an additional coupling constraint independent of H_n. This is well known, e.g., [7].

Finally, using the result above for the splitting error, we deduce that the *optimal order* for the numerical time integration reads:

$$p_k = p_f \cdot k.$$

Thus the time integration error is $\left\| \bar{\mathbf{x}}^{(k)}|_{(t_n,t_{n+1}]} - \tilde{\mathbf{x}}^{(k)}|_{(t_n,t_{n+1}]} \right\| = \mathcal{O}(H_n^{p_f \cdot k})$ and then we obtain as total approximation order

$$\left\| \tilde{\mathbf{x}}^{(k)}|_{(t_n,t_{n+1}]} - \mathbf{x}|_{(t_n,t_{n+1}]} \right\| = \mathcal{O}(H^{p_f \cdot k}) + \mathcal{O}(H^{p_f \cdot k}) = \mathcal{O}(H^{p_f \cdot k}).$$

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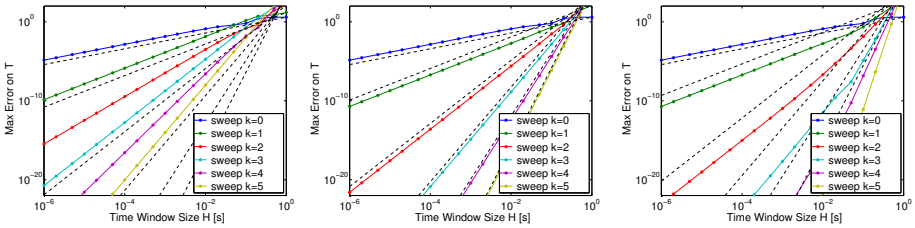

(a) Time integration error given by Taylor expansions of k-th order.

(b) Time integration error given by Taylor expansions of $(2 \cdot k)$-th order.

(c) Time integration error given by Taylor expansions of $(3 \cdot k)$-th order.

Figure 2: Convergence per window size H_0 for various $k = k_0$. Experiments for $r = 2$ coupled Prothero-Robinson systems. We depict the convergence rate versus window size H_0 computed according to our maximum-norm. Dashed lines show the expected 2nd-order convergence without time-integration error: from (a) to (c) the order of the time integration in the k-th iteration is increased from k to $3 \cdot k$.

4 Example

To analyze the dynamic iteration scheme, we study a linear DAE test case from [3], which is an extension of the classical Prothero-Robinson test equation:

$$\begin{pmatrix} \dot{\mathbf{y}} \\ 0 \end{pmatrix} = \begin{pmatrix} \mathbf{A} - \mathbf{BF} & \mathbf{B} \\ \mathbf{C} - \mathbf{DF} & \mathbf{D} \end{pmatrix} \begin{pmatrix} \mathbf{y} \\ \mathbf{z} \end{pmatrix} + \begin{pmatrix} -\mathbf{A}\eta(t) - \mathbf{B}\zeta(t) + \eta'(t) \\ -\mathbf{C}\eta(t) - \mathbf{D}\zeta(t) \end{pmatrix}$$
$$\text{with } \mathbf{A} = \begin{pmatrix} 4 & 3 \\ 2 & 5 \end{pmatrix},\ \mathbf{D} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \mathbf{B} = \mathbf{C} = \mathbf{F} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{5}$$

and $\eta(t) = (\sin(2\pi t),\ 2\cos(4\pi t) + 100)^\top, \zeta(t) = 0$. Thus our example problem is rather an ODE with solution $\mathbf{y}(t) = \eta(t)$ and the trivial algebraic component $\mathbf{z}(t) = 0$ but this example is particularly interesting because of a dynamic iteration convergence rate $p_f = 2$. Nonetheless, other DAEs will behave also as predicted above.

We solve the differential equations analytically using Mathematica and perform a dynamic iteration on the first time window $[0, H_0]$ for various window sizes H_0. The $r = 2$ scalar DAE subsystems are solved in the obvious sequence $(y_1, z_1)^\top \rightarrow (y_2, z_2)^\top$ using the Gauss-Seidel-type scheme (3) with $k_0 = 5$ iterations.

For the given example we estimate the error reduction per iteration by averaging the quotient of the errors after k iterations $\bar{\delta} := (\delta^k_{y,z}/\delta^0_{y,z})^{1/k}$. The dependency of the convergence rate on the window size H is depicted in Fig. 1, where the time integration error has been modeled by a Taylor expansion of varying order (k to $3 \cdot k$). Fig. 2 depicts the the same result but for each iteration k separately. Both figures show that an time integration order $\mathcal{O}(H^{2k})$ is optimal. Using less accuracy (a) reduces the overall convergence order of the dynamic iteration scheme (time integration errors dominate), while higher order time integration (c) does not improve the overall order (splitting errors dominate). Other version of our test case (5) with different coupling structure and convergence rate (see above) showed exactly the same optimality behavior.

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5 Conclusion

In this paper we have discussed an optimal p-refinement strategy for time-integration methods in dynamic iteration schemes of coupled DAEs. The optimal order of p is closely linked to a problem dependent convergence rate p_f, which is fixed by the problem specific coupling structure. Such a p-refinement strategy increases the effectivity of dynamic iteration schemes. Practical implementations of such a p-refinement strategy, which can be based on extrapolation strategies or deferred correction schemes, will be a topic of future work.

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