Termination criteria for inexact fixed point schemes

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Abstract

We analyze inexact fixed point iterations where the generating function contains an inexact solve of an equation system to answer the question of how tolerances for the inner solves influence the iteration error of the outer fixed point iteration. Important applications are the Picard iteration and partitioned fluid structure interaction. We prove that the iteration converges irrespective of how accurate the inner systems are solved, provided that a specific relative termination criterion is employed, whereas standard relative and absolute criteria do not have this property. For the analysis, the iteration is modelled as a perturbed fixed point iteration and existing analysis is extended to the nested case $\mathbf{x} = \mathbf{F}(\mathbf{S}(\mathbf{x}))$.

Keywords: Fixed point iteration, Picard iteration, Transmission Problem, Dirichlet-Neumann iteration, Termination criteria

1 Introduction

The general problem that this article is about is the following: Consider a nonlinear equation system and an outer iteration method to solve it that consists of solving a subproblem at each step using a second, inner iteration method. Now we want to answer the following question: How can we efficiently control the iteration error of the outer iteration method? Or otherwise put: How accurate do we need to solve the inner systems to obtain a certain iteration error for the outer nonlinear equation?

For the case of the outer iteration being Newton's method, this problem has been successfully solved. The inner problem is a linear system and the concept of an inexact Newton's method was introduced in [3]. There, at each Newton step the inner iteration is terminated when a relative tolerance criterion in the linear residual is satisfied. Based on this, it is possible to give conditions on the sequence of relative tolerances to obtain linear, superlinear or quadratic convergence of the inexact Newton's method. Essentially, the sequence of tolerances has to converge to zero fast enough as the Newton scheme progresses and then quadratic convergence is obtained. Following up, a strategy that has this property and leads to a very efficient scheme was suggested in [4]. There, the point is that the initial systems are solved quite coarsely and these schemes are part of widely used software packages, for example of SUNDIALS [7].

Note that with this knowledge, the choice of iterative solver for the inner iteration obtains a better basis: If most of the systems are solved very coarsely and thus very few iterations are needed, it is more important that the method is cheap per iteration than how fast we can reach machine accuracy. In this setting, when looking at unsymmetric linear systems and Krylov subspace methods, GMRES [11] beats BiCGSTAB [13], since it needs only one matrix vector product per iteration instead of two.

Now when looking at fixed point iterations, an iteration typically consists of evaluating a function and not of solving a system. However, two prominent and important examples where this happens are the Picard iteration and fluid-structure interaction and thus we call these inexact fixed point schemes. Surprisingly, the problem framed in the first paragraph has not been analyzed for these.

For the Picard iteration, which is a common tool in the context of the incompressible Navier-Stokes equations, the evaluation of the right hand side corresponds to solving a linear system. Strategies for choosing a termination criterion for the inner iteration are empirically discussed for example in [5, 12].

In Fluid-Structure interaction, a standard approach are partitioned coupling schemes, where existing solvers for the subproblems are reused [6]. Commonly in the form of a Dirichlet-Neumann iteration, this consists of subsequently solving the fluid and the structure problem with appropriate boundary conditions and reasonable tolerances. It is common to formulate the coupling condition at the interface in the form of a fixed point equation. Recently, it was suggested to use a time adaptive implicit time integration scheme for fluid structure interaction [2], where the time step is chosen based on an error tolerance. As is common in this setting, the tolerances for the solvers for the appearing nonlinear equation systems are chosen such that the iteration error does not interfere with the error from the time integration scheme [1], but nevertheless as large as possible to avoid unnecessary computations. Thus, it is imperative to be able to control the iteration error.

To solve our problem, we proceed in the following way. First, we will review well known results on perturbations of fixed point schemes [9]. The general idea is then to quantify the iteration errors based on the termination criterion of the inner iteration such that the existing perturbation results can be applied. For the Dirichlet-Neumann iteration, we first have to extend the perturbation results to the case of a nested fixed point equation of the form $\mathbf{x} = \mathbf{F}(\mathbf{S}(\mathbf{x}))$.

As it turns out, the type of termination criterion chosen in the inner solver is crucial for the answer to our problem in that when using a non-standard relative criterion, we obtain convergence of the fixed point iteration to the exact solution independently of how accurate we solve the inner systems, leading to an efficient way of controlling the outer iteration error.

On the other hand, no general statement can be made on a standard relative or absolute termination criterion, but the analysis suggests that these do not have favorable properties. All of this is confirmed by numerical results, which show that the latter criteria cause convergence to a solution that is farther away from the exact one the less accurate we solve the linear systems or otherwise put, the less error we want in the fixed point equation, the more accurate we have to solve the linear systems.

2 Inexact Fixed Point Methods

2.1 Direct perturbation

Consider the fixed point equation

$$\mathbf{x} = \mathbf{f}(\mathbf{x}) \tag{1}$$

with $\mathbf{x} \in \Omega \subset \mathbb{R}^n$, Ω closed and where we assume that $\mathbf{f} : \Omega \to \Omega$ is Lipschitz continuous with Lipschitz constant $L < 1$. This implies by the Banach fixed point theorem that (1) has a unique solution $\mathbf{x}^*$.

Furthermore, we consider the perturbed fixed point iteration

$$\mathbf{x}^{k+1} = \mathbf{f}(\mathbf{x}^k) + \epsilon, \tag{2}$$

where ϵ is a perturbation that could originate from an iterative solver and for simplicities sake we denote the norm of ϵ by ϵ as well. We furthermore assume for simplicities sake that $\mathbf{f} + \epsilon$ is also a self-map on Ω. Thus this iteration obtains a solution $\mathbf{x}_\epsilon$ of the perturbed fixed point equation

$$\mathbf{x} = \mathbf{f}(\mathbf{x}) + \epsilon. \tag{3}$$

The question is now: How far is the solution $\mathbf{x}_\epsilon$ of that equation away from $\mathbf{x}^*$? The answer is giving by the following theorem, see for example [9].

Theorem 1 *For the solutions* $\mathbf{x}_\epsilon$ *and* $\mathbf{x}^*$ *of problems* (3) *and* (1) *we have:*

$$\|\mathbf{x}_\epsilon - \mathbf{x}^*\| \leq \epsilon \frac{1}{1-L}. \tag{4}$$

This means that the error is of the order ϵ as is to be expected, but interestingly, it becomes larger, the closer the Lipschitz constant of $\mathbf{f}$ is to one or otherwise put, the less contractive the function is. This implies that in these cases, the error will be much larger than ϵ and thus a much smaller tolerance would have to be supplied to acchieve the desired error. Note that in practice, we typically do not know the Lipschitz constant and that in the nonlinear case, it depends on the definition of the domain Ω. Thus the important Lipschitz constant is the local one in the solution.

If we instead consider a sequence of perturbations ϵ_k, respectively a nonconstant perturbation, and thus the iteration

$$\mathbf{x}^{k+1} = \mathbf{f}(\mathbf{x}^k) + \epsilon_k, \tag{5}$$

the first question is when this sequence converges to $\mathbf{x}^*$. The answer is given by the next theorem, also from [9]:

Theorem 2 *The iteration* (5) *converges to the solution of the unperturbed problem* (1) *if and only if* $\lim_{k\to\infty} \epsilon_k = 0$.

A specific case is

$$\epsilon_k = cL^k \tag{6}$$

with $c > 0$, which we call the adaptive strategy.

2.2 Application: Picard iteration

As an application of the above theorems, we now analyze the convergence of the Picard iteration. This is often employed in the context of the incompressible Navier-Stokes equation and corresponds to a fixed point iteration for the equation

$$\mathbf{x} = \mathbf{A}^{-1}(\mathbf{x})\mathbf{b},$$

where $\mathbf{A}(\mathbf{x}) \in \mathbb{R}^{n\times n}$ is an approximation of a Jacobian in $\mathbf{x}$ [5]. Thus, the fixed point iteration

$$\mathbf{x}^{k+1} = \mathbf{A}^{-1}(\mathbf{x}^k)\mathbf{b} \tag{7}$$

is implemented by solving

$$\mathbf{A}(\mathbf{x}^k)\mathbf{x}^{k+1} = \mathbf{b} \tag{8}$$

for $\mathbf{x}^{k+1}$ up to a certain tolerance using an iterative scheme. The scheme (7) can be analyzed either as a fixed point scheme, which results in linear convergence provided that the Lipschitz constant L of $\mathbf{A}^{-1}(\mathbf{x})\mathbf{b}$ can be bounded from above away from one or as a method of Newton type where $\mathbf{A}(\mathbf{x})$ is an approximation of the exact Jacobian and we have linear convergence as long as this approximation is good enough.

When solving (8), either the relative termination criterion

$$\|\mathbf{A}(\mathbf{x}^k)\mathbf{x}^{k+1} - \mathbf{b}\| \leq \tau_r \|\mathbf{A}(\mathbf{x}^k)\mathbf{x}^k - \mathbf{b}\|, \tag{9}$$

the relative termination criterion

$$\|\mathbf{A}(\mathbf{x}^k)\mathbf{x}^{k+1} - \mathbf{b}\| \leq \tau_r \|\mathbf{b}\| \tag{10}$$

or the absolute criterion

$$\|\mathbf{A}(\mathbf{x}^k)\mathbf{x}^{k+1} - \mathbf{b}\| \leq \tau_a \tag{11}$$

are used, where τ_r and τ_a are relative and adaptive tolerances.

To analyze the consequences of choosing one of these using theorems 1 and 2, we need to quantify the perturbation in the form (2). Thus, we define $\mathbf{f}(\mathbf{x}^k) = \mathbf{A}^{-1}(\mathbf{x}^k)\mathbf{b}$ to obtain

$$\mathbf{x}^{k+1} = \mathbf{A}^{-1}(\mathbf{x}^k)\mathbf{b} + \epsilon_k$$

and we can write

$$\epsilon_k = \mathbf{A}^{-1}(\mathbf{x}^k)(\mathbf{A}(\mathbf{x}^k)\mathbf{x}^{k+1} - \mathbf{b}). \tag{12}$$

In the case of the relative termination criterion (9), we can estimate the norm of the right hand side in (12) by

$$\|\epsilon_k\| \leq \|\mathbf{A}^{-1}(\mathbf{x}^k)\| \tau_r \|(\mathbf{A}(\mathbf{x}^k)\mathbf{x}^k - \mathbf{b})\|.$$

We furthermore have

$$\mathbf{A}(\mathbf{x}^k)\mathbf{x}^k - \mathbf{b} = \mathbf{A}(\mathbf{x}^k)(\mathbf{x}^k - \mathbf{A}^{-1}(\mathbf{x}^k)\mathbf{b}) = \mathbf{A}(\mathbf{x}^k)(\mathbf{f}(\mathbf{x}^{k-1}) - \mathbf{f}(\mathbf{x}^k)).$$

Thus,

$$\|(\mathbf{A}(\mathbf{x}^k)\mathbf{x}^k - \mathbf{b})\| \leq \|(\mathbf{A}(\mathbf{x}^k)\| L \|\mathbf{x}^{k-1} - \mathbf{x}^k\| \leq \|(\mathbf{A}(\mathbf{x}^k)\| L^k \|\mathbf{x}^1 - \mathbf{x}^0\|.$$

All in all, we obtain with the condition number $\kappa(\mathbf{A})$

$$\|\epsilon_k\| \leq \tau_r \kappa(\mathbf{A}(\mathbf{x}^k)) L^k \|\mathbf{x}^1 - \mathbf{x}^0\|. \tag{13}$$

With the additional and reasonable assumption that $\kappa(\mathbf{A}(\mathbf{x}))$ is bounded, this is a perturbation of the form (6) and ϵ_k converges to zero independent of the choice of τ_r! Thus by theorem 2 this iteration converges to the exact solution independently of how accurate we solve the linear equation systems. We now formulate this as a theorem.

Theorem 3 *Let $\mathbf{b} \in \mathbb{R}^n$ and the function $\mathbf{A}(\mathbf{x})$ be given that maps the closed set $\Omega \subset \mathbb{R}^n$ onto quadratic regular matrices. Assume that the function $\mathbf{A}^{-1}(\mathbf{x})\mathbf{b} : \Omega \to \Omega$ is Lipschitz continuous with Lipschitz constant $L < 1$ and correspondingly has a unique fixpoint $\mathbf{x}^*$. Furthermore assume that $\kappa(\mathbf{A}(\mathbf{x}))$ is bounded on Ω and that the inexact fixedpoint iteration defined by* (9) *converges to a limit $\mathbf{x}_\epsilon$. Then $\mathbf{x}_\epsilon = \mathbf{x}^*$, independent of the choice of τ_r.*

In case of the relative criterion (10), the estimate

$$\|\epsilon_k\| \leq \|\mathbf{A}^{-1}(\mathbf{x}^k)\|\tau_r\|\mathbf{b}\|$$

for the norm of the left hand side in (12) holds which is bounded away from zero provided that $\mathbf{A}^{-1}(\mathbf{x})$ is. Thus, it is not clear if this iteration satisfies theorem 2, but in the general case, the iteration will not converge to $\mathbf{x}^*$. Similarly if we use the absolute termination criterion (11), we obtain

$$\|\epsilon_k\| \leq \|\mathbf{A}^{-1}(\mathbf{x}^k)\|\tau_a$$

which is also bounded away from zero if $\mathbf{A}^{-1}(\mathbf{x})$ is.

Numerical results that confirm theorem 3 and demonstrate that the other two iterations behave like being of the form (1) can be found in section 3.1.2. We would like to point out that the criterion (9) is sometimes suggested in the literature on the Picard iteration, e.g. [8, 5], but that an absolute termination criterion is suggested in [12]. There it is suggested to just “gain one digit”, meaning to use a tolerance of 0.1.

2.3 Perturbed nested fixed point iteration

Now consider two functions $\mathbf{F} : \Omega_1 \to \Omega_2$ and $\mathbf{S} : \Omega_2 \to \Omega_1$ with $\Omega_1, \Omega_2 \subset \mathbb{R}^n$ closed and the fixed point equation

$$\mathbf{x} = \mathbf{S}(\mathbf{F}(\mathbf{x})) \tag{14}$$

again with solution $\mathbf{x}^*$. We now consider an iteration where both the evaluation of $\mathbf{F}$ and of $\mathbf{S}$ are perturbed, namely $\mathbf{S}$ is perturbed by δ_k and $\mathbf{F}$ by ϵ_k:

$$\mathbf{x}^{k+1} = \mathbf{S}(\mathbf{F}(\mathbf{x}^k) + \epsilon_k) + \delta_k. \tag{15}$$

Again, assume that this iteration is well defined and that this sequence has the limit $\mathbf{x}_\epsilon$. Then, we obtain the following theorem.

Theorem 4 *Let $\mathbf{F}$ and $\mathbf{S}$ be Lipschitz continuous with Lipschitz constants L_F and L_S, respectively. Assume that $L_F L_S < 1$. Then we have, if $\epsilon_k = \delta_k = \epsilon$ for all k, that*

$$\|\mathbf{x}_\epsilon - \mathbf{x}^*\| \leq \epsilon \frac{1 + L_S}{1 - L_S L_F}. \tag{16}$$

In the case $\epsilon_k = \epsilon$ and $\delta_k = \delta$, we obtain

$$\|\mathbf{x}_\epsilon - \mathbf{x}^*\| \leq \frac{\epsilon L_S + \delta}{1 - L_S L_F}. \tag{17}$$

Finally, $\mathbf{x}_\epsilon = \mathbf{x}^*$ if and only if both δ_k and ϵ_k converge to zero.

Proof: The proof is technically identical to the one of theorem 1. We have due to the Lipschitz continuity

$$\begin{aligned}\|\mathbf{x}^{k+1} - \mathbf{x}^*\| = \|\mathbf{S}(\mathbf{F}(\mathbf{x}^k) + \epsilon_k) + \delta_k - \mathbf{x}^*\| &= \|\mathbf{S}(\mathbf{F}(\mathbf{x}^k) + \epsilon_k) + \delta_k - \mathbf{S}(\mathbf{F}(\mathbf{x}^*))\| \\ \leq L_S\|\mathbf{F}(\mathbf{x}^k) - \mathbf{F}(\mathbf{x}^*) + \epsilon_k\| + \delta_k &\leq L_S L_F\|\mathbf{x}^k - \mathbf{x}^*\| + L_S\epsilon_k + \delta_k \\ &\leq (L_S L_F)^2\|\mathbf{x}^{k-1} - \mathbf{x}^*\| + L_S^2 L_F \epsilon_{k-1} + L_S L_F \delta_{k-1} + L_S\epsilon_k + \delta_k \\ &\leq (L_S L_F)^{k+1}\|\mathbf{x}^0 - \mathbf{x}^*\| + \left(\sum_{j=0}^{k} L_S^{j+1} L_F^j \epsilon_{k-j}\right) + \left(\sum_{j=0}^{k} L_S^j L_F^j \delta_{k-j}\right)\end{aligned}$$

and thus in the limit $\mathbf{x}^{k+1} \to \mathbf{x}^*$,

$$\|\mathbf{x}_\epsilon - \mathbf{x}^*\| \leq L_S \lim_{k\to\infty} \sum_{j=0}^{k} (L_S L_F)^j \epsilon_{k-j} + \lim_{k\to\infty} \sum_{j=0}^{k} (L_S L_F)^j \delta_{k-j} \tag{18}$$

For a constant perturbation overall, e.g. $\epsilon_k = \delta_k = \epsilon$ for all k, we obtain in the limit

$$\|\mathbf{x}_\epsilon - \mathbf{x}^*\| \leq \epsilon(1 + L_S) \lim_{k\to\infty} \sum_{j=0}^{k} (L_S L_F)^j = \epsilon \frac{1 + L_S}{1 - L_S L_F},$$

which proves the inequality (16). If we have constant but separate perturbations ϵ and δ of $\mathbf{S}$ and $\mathbf{F}$, we obtain (17) from

$$\|\mathbf{x}_\epsilon - \mathbf{x}^*\| \leq \epsilon L_S \lim_{k\to\infty} \sum_{j=0}^{k} (L_S L_F)^j + \delta \lim_{k\to\infty} \sum_{j=0}^{k} (L_S L_F)^j = \frac{\epsilon L_S + \delta}{1 - L_S L_F}.$$

In the general case, due to positivity, the right hand side of (18) is zero if and only if both ϵ_k and δ_k are such that for $\phi_k = \epsilon_k$ or $\phi_k = \delta_k$,

$$\lim_{k\to\infty} \sum_{j=0}^{k} (L_S L_F)^j \phi_{k-j} = 0.$$

By an identical proof to theorem 2, this is the case if and only if both ϵ_k and δ_k converge to zero.

Note that this implies that the sequence ϵ_k perturbing the inner function $\mathbf{F}$ is less important by a factor of the Lipschitz constant L_S of the outer function. Thus, a possible strategy is to define

$$\epsilon_k = \delta_k / L_S, \tag{19}$$

meaning that we solve the fluid part less accurate by a factor of L_S. Unfortunately, L_S has to be known for this.

2.4 Application: Dirichlet-Neumann coupling for Transmission problem

As an application of the theory from section 2.3, we consider a problem that is a basic building block in fluid structure interaction, namely the transmission problem, where the Laplace equation with right hand side $f(x,y)$ on a domain Ω is cut into two domains $\Omega = \Omega_1 \cup \Omega_2$ using transmission conditions at the interface $\Gamma = \Omega_1 \cap \Omega_2$:

$$\begin{aligned}
\Delta u_i(x,y) &= f(x,y),\ (x,y) \in \Omega_i \subset \mathbb{R}^2,\ i = 1,2 \\
u_i(x,y) &= 0,\ (x,y) \in \partial\Omega_i\ \partial\Omega_1 \cap \Omega_2 \\
u_1(x,y) &= u_2(x,y),\ (x,y) \in \Gamma \\
\partial u_1(x,y) \cdot \mathbf{n} &= \partial u_2(x,y) \cdot \mathbf{n},\ (x,y) \in \Gamma
\end{aligned} \tag{20}$$

We now employ a standard Dirichlet-Neumann iteration to solve it. Using any linear discretization, this corresponds to alternately solving the problems

$$\mathbf{A}\mathbf{u}_1^{k+1} = \mathbf{b}_1(\mathbf{u}_2^k) \tag{21}$$

and

$$\mathbf{B}\mathbf{u}_2^{k+1} = \mathbf{b}_2(\mathbf{u}_1^{k+1}) \tag{22}$$

were problem (21) corresponds to a discretization of the transmission problem (20) on Ω_1 only with Dirichlet data on Γ given by $\mathbf{u}_2^k$ on the coupling interface and problem (22) corresponds to a discretization of (20) on Ω_2 only with Neumann data on Γ given by the discrete normal derivative of $\mathbf{u}_1$ on Γ. It can be shown that convergence of the approximate solutions on the whole domain is equivalent to the convergence of the solution on the interface only [10].

By considering (21)-(22) as one iteration, we obtain a fixed point formulation

$$\mathbf{u}_\Gamma = \mathbf{S}(\mathbf{F}(\mathbf{u}_\Gamma))$$

where $\mathbf{u}_\Gamma$ is $\mathbf{u}_2$ on the interface, $\mathbf{F} = \mathbf{D}_{\mathbf{n}_\Gamma}\mathbf{A}^{-1}\mathbf{b}_1(\mathbf{u}_\Gamma)$ and $\mathbf{S} = \mathbf{P}_\Gamma\mathbf{B}^{-1}\mathbf{b}_2(\mathbf{u}_1)$. Hereby $\mathbf{D}_{\mathbf{n}_\Gamma}$ is the matrix that computes the discrete normal derivatives in Ω_1 on Γ and $\mathbf{P}_\Gamma$ is the discrete trace operator with respect to Γ. Otherwise put, $\mathbf{P}_\Gamma$ is the projection of the space that $\mathbf{u}_2$ is in onto the space of discrete unknowns on Γ.

In practice, the linear equation systems are solved iteratively, typically using the conjugate gradient method (CG) up to a relative tolerance of τ. Thus, we obtain a perturbed nested fixed point iteration of the form (15) and the question is now again if we can quantify this perturbation. We have

$$\mathbf{u}_{1_\epsilon}^{k+1} = \mathbf{A}^{-1}\mathbf{b}_1(\mathbf{u}_\Gamma^k) + \epsilon_k \tag{23}$$

and

$$\mathbf{u}_{2_\epsilon}^{k+1} = \mathbf{B}^{-1}\mathbf{b}_2(\mathbf{u}_{1_\epsilon}^{k+1}) + \delta_k. \tag{24}$$

For the iteration (23) we obtain

$$\|\epsilon_k\| = \|\mathbf{u}_{1_\epsilon}^{k+1} - \mathbf{A}^{-1}\mathbf{b}_1(\mathbf{u}_\Gamma^k)\| \leq \|\mathbf{A}^{-1}\|\|\mathbf{A}\mathbf{u}_{1_\epsilon}^{k+1} - \mathbf{b}_1(\mathbf{u}_\Gamma^k)\|.$$

Again, the second factor is what is tested in the termination criterion of CG. In the case of the relative criterion (9), here stated as

$$\|\mathbf{A}\mathbf{u}_{1_\epsilon}^{k+1} - \mathbf{b}_1(\mathbf{u}_\Gamma^k)\| \leq \tau_r\|\mathbf{A}\mathbf{u}_1^k - \mathbf{b}_1(\mathbf{u}_\Gamma^k)\|,$$

we obtain

$$\|\epsilon_k\| \leq \|\mathbf{A}^{-1}\|\tau_r\|\mathbf{A}\mathbf{u}_{1_\epsilon}^k - \mathbf{b}_1(\mathbf{u}_\Gamma^k)\| \leq \kappa(\mathbf{A})\tau_r\|\mathbf{u}_1^k - \mathbf{A}^{-1}\mathbf{b}_1(\mathbf{u}_\Gamma^k)\|$$

$$= \kappa(\mathbf{A})\tau_r\|\mathbf{u}_1^k - \mathbf{u}_1^{k+1}\|.$$

Now the point is that since the whole iteration is linear, we can write down a linear mapping that maps $\mathbf{u}_1^k$ onto $\mathbf{u}_1^{k+1}$ for arbitrary k. Let this have Lipschitz constant L_1, then we have

$$\|\epsilon_k\| \leq \tau_r\kappa(\mathbf{A})L_1^k\|\mathbf{u}_1^0 - \mathbf{u}_1^1\|.$$

Thus the perturbation has limit zero if $L_1 < 1$. This is the case if and only if the sequence $(\mathbf{u}_1^k)_k$ is convergent, which is in fact the case provided that $f(x, y)$ is sufficiently harmless, as can be seen from the literature on domain decomposition methods, e.g. [10, ch. 4].

Analagously to the Picard iteration, if we choose the absolute termination criterion (11) or the relative one based on the right hand side (10), we obtain a bound of the form

$$\|\epsilon_k\| \leq \|\mathbf{A}^{-1}\|\tau_r\|\mathbf{b}(\mathbf{u}_\Gamma^k)\|,$$

respectively

$$\|\epsilon_k\| \leq \|\mathbf{A}^{-1}\|\tau_a.$$

Again, we cannot make a statement on the limit of ϵ_k.

In the second case, meaning the iteration with Neumann data (24), we obtain

$$\|\delta_k\| = \|\mathbf{u}_{2_\epsilon}^{k+1} - \mathbf{B}^{-1}\mathbf{b}_2(\mathbf{u}_{1_\epsilon}^{k+1})\| \leq \|\mathbf{B}^{-1}\| \|\mathbf{B}\mathbf{u}_{2_\epsilon}^{k+1} - \mathbf{b}_2(\mathbf{u}_{1_\epsilon}^{k+1})\|$$

and analogous arguments produce the same results for δ_k. Thus by theorem 4, we have that when using the relative criterion we obtain convergence to the exact solution for any τ_r.

2.5 A note on the termination criterion and convergence speed

It is important to note that under the assumptions, all sequences considered, wether perturbed or not, are convergent and therefore, the fixed point iteration will terminate when using the standard criterion

$$\|\mathbf{x}^{k+1} - \mathbf{x}^k\| \leq TOL. \tag{25}$$

However, as just shown, the perturbed iteration converges to an approximation of the unperturbed fixed point and thus, the algorithm can terminate when we are in fact not TOL-close to the solution.

A further difference between the different iterations that should be stressed is that the iterations perturbed by a constant are fixed point iterations, wheras the schemes with a variable perturbation are in fact, not. Thus, the convergence speed, which is otherwise linear with constant L, is not clear and numerical evidence suggests that it is in fact slower than for the other iteration.

Thus, we could argue to employ the schemes with constant perturbation, measure the Lipschitz constant numerically after a few iterations and then adjust the tolerance based on theorem 1 or 4. Unfortunately, it is not clear what the ϵ from these theorems is, respectively, it is based on quantities that are hard to measure like $\|\mathbf{A}^{-1}\|$. Thus, we cannot guarantee a certain iteration error in this way, to do this we must employ the nonstandard relative termination criterion.

Finally, it is important to note that this analysis is mostly relevant to the time independent case. Otherwise, when considering this inside an implicit time integration scheme, additional requirements on the solutions appear, namely that the solutions in the subdomains have a certain accuracy.

3 Numerical Results

For all numerical experiments, the fixed point iteration is terminated when the norm $\|\mathbf{x}^{k+1} - \mathbf{x}^k\|_2$ is smaller than 10^{-14}. Furthermore, with the exception of the results on the Picard iteration, all computations were performed

ϵ L	1e-1	1e-2	1e-3
0.009868	1.010e-1	1.010e-2	1.010e-3
0.101239	1.090e-1	1.089e-2	1.089e-3
0.899524	2.016e-1	1.827e-2	1.813e-3
0.996035	2.290e-1	1.981e-2	1.961e-3

Table 1: $|x_\epsilon - x^*|$ (left) and $\frac{\epsilon}{1-L}$ (right) for different values of ϵ and L for the solution of the scalar nonlinear equation (26)

in MATLAB, where MATLAB 2012a was used for all computations with the exception of the results in section 3.2.3, where MATLAB 2013a was employed.

3.1 Direct Perturbation

3.1.1 Testcase: Scalar nonlinear system

As a first example, we employ the nonlinear scalar equation

$$x = e^{\gamma x}/4 \tag{26}$$

with $x \in [0, 1]$ and $\gamma < 1$ given. Thus, the Lipschitz constant L on $[0, 1]$ is equal to $\gamma e^{\gamma}/4 < 1$. We solve this equation for $\gamma = 0.3, 1.145, 1.2$.

Employing the fixed point method with constant perturbation, we provide the values of $|x_\epsilon - x^*|$ in table 1. The difference in solutions is larger than one and proportional to ϵ, as suggested by theorem 1. However, the dependence on the Lipschitz constant is very weak and the error does not become worse when it approaches one. This is because the problem is nonlinear and thus, the Lipschitz constant is domain dependent. The local Lipschitz constant near the solution is actually well smaller than one, which reminds us that for nonlinear problems, the Lipschitz constant does not always describe a problem well.

Furthermore, we tested the adaptive strategy and there $|x_\epsilon - x^*|$ tends to machine accuracy, as predicted by the theory.

3.1.2 Testcase: Picard iteration

We now consider the Picard iteration (7). The equation system considered arises from the discretization of the incompressible Navier-Stokes equations on the unit square with homogeneous Dirichlet boundary conditions and a viscosity of $\nu = 1/1000$. The grid is cartesian with $128 \times 128 = 16384$ cells. For the computations, the code MooNMD by John et. al. [8] was used. The Finite Element discretization employs $Q_2 1/P_1$ elements, resulting in 181250

TOL	τ_r	Fixp. iter	GMRES it.	$\|res\|$
	1e-01	12	42	1.793e-15
	1e-02	9	48	8.559e-15
	1e-03	9	58	2.318e-15
1e-14	1e-04	8	57	2.121e-15
	1e-05	7	59	5.299e-15
	1e-06	7	64	5.266e-15
	1e-07	7	67	5.265e-15
1e-07	1e-01	4	11	5.66989e-08

Table 2: $\|res\|$, total number of GMRES iterations and fixpoint iterations for different values of τ_r when using termination criterion (9)

unknowns overall, thereof 66049 for each velocity component (including the Dirichlet nodes) and 49152 for the pressure.

The right hand side is chosen that the solution is given by $(u_1, u_2) = (d\psi/dy, -d\psi/dx)$ with $\psi = x^2(1-x)^2y^2(1-y)^2$, resulting in

$$u_1(x,y) = x^2(1-x)^2[2y(1-y)^2 - 2y^2(1-y)],$$
$$u_2(x,y) = [2x^2(1-x) - 2x(1-x)^2]y^2(1-y)^2,$$
$$p(x,y) = x^3 + y^3 - 1/2.$$

As initial guess for the Picard iteration, the zero vector is used. To solve the linear systems (8), GMRES is employed where the initial guess is the current Picard iterate. The Picard iteration is terminated either when the quantity

$$\|res\| = \|\mathbf{A}(\mathbf{u}^{n+1})\mathbf{u}^{n+1} - \mathbf{b}\|$$

is smaller than a tolerance TOL or when GMRES terminates immediately without performing an iteration, implying that $\mathbf{u}^{n+1} = \mathbf{u}^n$.

In the first block of table 2, $\|res\|$, as well as the total number of inner GMRES iterations and the number of Picard iterations needed to reach machine accuracy (TOL=10^{-14}) are shown for different values of the relative tolerance τ_r in GMRES, where the termination criterion (9) was used. As predicted by the theory, all schemes converge to the exact solution. Furthermore, it takes slightly more fixed point iterations to reach machine accuracy if the linear systems are solved very inaccurately. Nevertheless, the most efficient scheme is the one with $\tau_r = 1e-1$.

In table 3, we show the same quantities, but for the termination criterion (11). As can be seen, the Picard iteration does not converge to the exact solution, and how close we get is proportional to τ_a. This suggests that here,

TOL	τ_a	Fixp. iter	GMRES it.	$\|res\|$
1e-14	1e-01	1	0	8.212092e-03
	1e-02	1	0	8.212092e-03
	1e-03	1	4	6.356705e-04
	1e-04	1	6	2.131814e-05
	1e-05	1	7	4.018437e-06
	1e-06	2	11	3.016563e-07
	1e-07	2	14	6.249272e-08
	1e-14	7	70	5.916e-15

Table 3: $\|res\|$, total number of GMRES iterations and fixpoint iterations for different values of τ_a when using termination criterion (11)

the upper bound on the perturbation is accurate, thus having a situation as in theorem 1.

To illustrate the difference in efficiency, we can compare the last row of table 3 with the first row of table 2 which tells us that to reach machine accuracy, the method using the relative criterion is faster. A more realistic is obtained by choosing a less strict tolerance. Thus we performed a computation with $TOL = 10^{-7}$ and $\tau_r = 0.1$ for the first method, the result of which can be seen in the last line of table 2. To obtain the same accuracy with the second method, τ_a has to be chose as $1e - 0.7$. Again, the first method is slightly more accurate than the second.

3.2 Nested fixed point iteration

3.2.1 Testcase: Linear Equation System with Matrix Product

We now consider the linear problem

$$(\mathbf{I} - \mathbf{AB})\mathbf{x} = \mathbf{b} \Leftrightarrow \mathbf{x} = \mathbf{ABx} + \mathbf{b} \tag{27}$$

with

$$\mathbf{A} = \begin{pmatrix} \alpha & 0 \\ 0.001 & 0.001 \end{pmatrix}, \mathbf{B} = \begin{pmatrix} \beta & 0 \\ 0.001 & 0.001 \end{pmatrix}, \mathbf{b} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Thus, $\mathbf{S}(\mathbf{x}) = \mathbf{Ax} + \mathbf{b}$ with $L_S = \|\mathbf{A}\|_2 \approx \alpha$ and $\mathbf{F}(\mathbf{x}) = \mathbf{Bx}$ with $L_F = \|\mathbf{B}\|_2 \approx \beta$.

As a perturbation, we use a constant vector with eucledian norm $\epsilon = \delta$. The difference $\|\mathbf{x}_\epsilon - \mathbf{x}^*\|_2$ can be seen in table 4. As initial guess, the zero vector was used. The results demonstrate that (17) is a very good estimate of the true error and that the errors are perfectly proportional to ϵ. We furthermore tested the adaptive strategy and that iteration indeed converges to $\mathbf{x}^*$.

ϵ	α \ β	0.1	0.9	0.99
1e-1	0.1	1.111e-1	1.209e-1	1.221e-1
		1.058e-1	1.111e-1	1.117e-1
	0.9	2.087e-1	1.000e-0	1.743e-0
		1.638e-1	7.107e-1	1.235e-0
	0.99	2.209e-1	1.826e-1	1.000e+1
		1.715e-1	1.293e-1	7.071e-0
1e-2	0.1	1.111e-2	1.209e-2	1.221e-2
		1.058e-2	1.111e-2	1.117e-2
	0.9	2.088e-2	1.000e-1	1.743e-1
		1.638e-2	7.107e-2	1.235e-1
	0.99	2.209e-2	1.826e-1	1.000e-0
		1.715e-2	1.293e-1	7.071e-1
1e-3	0.1	1.111e-3	1.209e-3	1.221e-3
		1.058e-3	1.111e-3	1.117e-3
	0.9	2.088e-3	1.000e-2	1.743e-2
		1.638e-3	7.107e-3	1.235e-3
	0.99	2.209e-3	1.826e-2	1.000e-1
		1.715e-3	1.293e-3	7.071e-2

Table 4: Estimate (17) and $\|\mathbf{x}_\epsilon - \mathbf{x}^*\|_2$ for different values of ϵ, L_S and L_F for equation (27)

3.2.2 Testcase: Scalar nonlinear system

As a second example, we employ the nonlinear scalar problem

$$x = 0.25\gamma_1 e^{\gamma_2 x^2} \tag{28}$$

with $x \in [0,1]$, $S(x) = 0.25\gamma_1 e^x$ and $L_S = 0.25\gamma_1 e$ and $F(x) = \gamma_2 x^2$ and $L_F = 2\gamma_2$.

The initial guess in the following numerical experiments is $x^0 = 0.5$. In table 5, we show several quantities for different values of ϵ, L_S and L_F where a constant perturbation $\epsilon = \delta$ is employed. First, the estimate (16) using the Lipschitz constants on the interval [0,1], which is referred to as the global estimate. Then the local estimate, which is (16) using the derivatives in the solution, giving an estimate of a local Lipschitz constant. This is reasonable, since all functions are monotonic. Finally, the difference $|x_\epsilon - x^*|$ itself.

As can be seen, we again have the proportionality to ϵ. Furthermore, we see that only when both L_F and L_S are close to one, an influence on

ϵ	L_F L_S	0.01	0.1	0.9	0.99
1e-1	0.1	1.101e-1	1.111e-1	1.209e-1	1.221e-1
		1.038e-1	1.038e-1	1.039e-1	1.040e-1
		1.039e-1	1.039e-1	1.042e-1	1.042e-1
	0.9	1.917e-1	2.088e-1	1.000e-0	1.743e-0
		1.463e-1	1.485e-1	1.724e-1	1.760e-1
		1.350e-1	1.370e-1	1.618e-1	1.658e-1
	0.99	2.010e-1	2.209e-1	1.826e-0	1.000e+1
		1.527e-1	1.555e-1	1.896e-1	1.949e-1
		1.386e-1	1.411e-1	1.746e-1	1.806e-1
1e-2	0.1	1.101e-2	1.111e-2	1.209e-2	1.221e-2
		1.038e-2	1.038e-2	1.040e-2	1.040e-2
		1.037e-2	1.037e-2	1.038e-2	1.039e-2
	0.9	1.917e-2	2.088e-2	1.000e-1	1.743e-1
		1.463e-2	1.485e-2	1.725e-2	1.760e-2
		1.334e-2	1.350e-2	1.525e-2	1.551e-2
	0.99	2.010e-2	2.209e-2	1.826e-1	1.000e-0
		1.527e-2	1.556e-2	1.896e-2	1.949e-2
		1.368e-2	1.388e-2	1.621e-2	1.658e-2
1e-3	0.1	1.101e-3	1.111e-3	1.209e-3	1.221e-3
		1.038e-3	1.038e-3	1.039e-3	1.040e-3
		1.037e-3	1.037e-3	1.038e-3	1.038e-3
	0.9	1.917e-3	2.088e-3	1.000e-2	1.743e-2
		1.463e-3	1.485e-3	1.725e-3	1.760e-3
		1.333e-3	1.348e-3	1.518e-3	1.542e-3
	0.99	2.010e-3	2.209e-3	1.826e-2	1.000e-1
		1.527e-3	1.555e-3	1.896e-3	1.949e-3
		1.366e-3	1.386e-3	1.612e-3	1.646e-3

Table 5: Global estimate, local estimate and $|x_\epsilon - x^*|$ for different values of ϵ, L_S and L_F for equation (28)

the error can be observed, as suggested by theorem 4. Finally, we test the adaptive strategy as an example of perturbations converging to zero and again, we obtain convergence of the new sequence to x^*.

3.2.3 Testcase: Transmission Problem

We now consider the transmission problem (20). Specifically, we use $\Omega_1 = [0,1] \times [0,1]$, $\Omega_2 = [1,2] \times [0,1]$ and

$$\begin{aligned} f(x,y) = &\quad \sin \pi y^2 (\pi \cos \tfrac{\pi}{2} x^2 - \pi^2 x^2 \sin \tfrac{\pi}{2} x^2) \\ & + \sin \tfrac{\pi}{2} x^2 (2\pi \cos \pi y^2 - 4\pi^2 y^2 \sin \pi y^2). \end{aligned}$$

This was chosen such that the solution is

$$u(x,y) = \sin \pi y^2 \sin \frac{\pi}{2} x^2, \qquad (29)$$

which satisfies the boundary conditions.

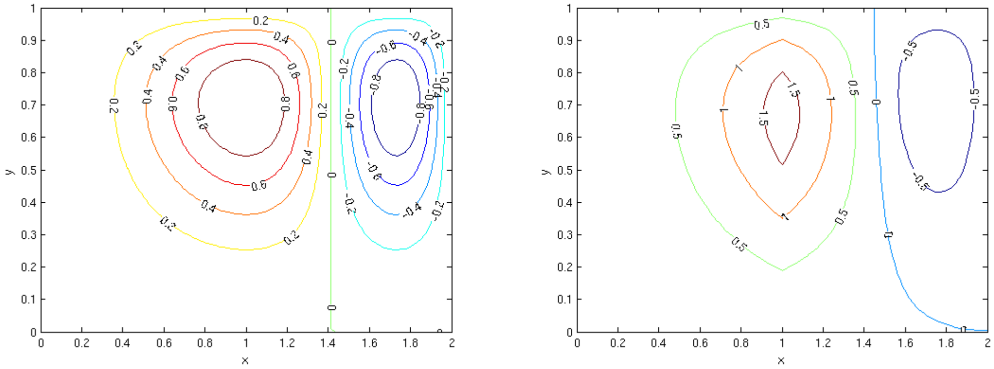

Figure 1: Exact and discrete solution with $\Delta x = 1/40$

We discretize this problem using central differences with a constant mesh width of $\Delta x = \Delta y$. As initial guess for the Dirichlet-Neumann procedure, we employ a vector of all zeros. All linear systems are solved using CG. The exact solution and the discrete solution with $\Delta x = 1/40$ can be seen in figure 1.

We first look at the convergence properties of the fixed point schemes for different mesh widths and different termination criteria. The difference $\|\mathbf{x}_\epsilon - \mathbf{x}^*\|_2$ for a constant tolerance τ in both CG-subsolvers can be seen in table 6 for the relative termination criterion (10) and in table 7 for the absolute termination criterion (11). As can be seen, the schemes behave essentially as if the perturbation were constant and do not converge to the

Δx τ	1/10	1/20	1/40	1/80
1e-1	7.606e-1	4.189e-0	3.440e+149	3.755e+148
1e-2	9.620e-2	2.502e-2	2.621e-1	7.288e-1
1e-3	1.230e-2	2.773e-3	1.192e-1	1.254e-1
1e-4	9.110e-4	1.033e-3	1.074e-2	2.602e-2

Table 6: $\|x_\epsilon - x^*\|_2$ for different values of τ and Δx for the transmission problem (20) with relative termination criterion (10)

Δx τ	1/10	1/20	1/40	1/80
1e-1	6.643e-3	7.308e-3	8.993e-3	7.187e-3
1e-2	7.727e-4	6.344e-4	8.048e-4	6.775e-4
1e-3	7.117e-5	8.603e-5	8.354e-5	6.880e-5
1e-4	5.497e-6	7.426e-6	7.685e-6	6.470e-6

Table 7: $\|x_\epsilon - x^*\|_2$ for different values of τ and Δx for the transmission problem (20) with absolute termination criterion (11)

exact solution. In particular, for the relative termination criterion (10), the error becomes large for smaller mesh widths and is up to a 100 times larger than the desired tolerance. Not that this criterion is the one implemented in the MATLAB version of CG and that thus, a native implementation of the Dirichlet-Neumann iteration in MATLAB will not produce a correct solution.

Otherwise, there is again a proportionality to τ, though it's not as clear this time. We attribute this to the fact that a relative tolerance in CG is only an upper bound on the perturbation, which can in fact be much smaller than τ if CG oversolves. Furthermore, the perturbed solutions become in general less accurate when the mesh is refined. This can be explained by the dependence on the norms of $\mathbf{A}^{-1}$ and $\mathbf{B}^{-1}$, which increase with decreasing mesh width.

In the case of the termination criterion (9), we recover the exact solution, as predicted by the theory.

We now consider the total number of CG and fixed point iterations when using the termination criterion (9) for different tolerances τ and different mesh widths Δx. As can be seen in table 8, the number of CG iterations increases with decreasing mesh width, which is well known behavior due to the spectrum getting more widely distributed on the real line. Furthermore, the number of fixed point iterations is almost independent of τ_r. Thus, the most efficient variant is to solve the systems only up to $\tau_r = 1e - 1$.

Δx τ_r	1/10		1/20	
	#FP	#CG	#FP	#CG
1e-1	106	2220	205	8298
1e-2	105	2903	205	11537
1e-3	105	3121	205	12585
1e-4	105	3369	208	13765
Δx τ_r	1/40		1/80	
	#FP	#CG	#FP	#CG
1e-1	401	29224	379	40556
1e-2	401	44321	803	156774
1e-3	399	48341	759	181789
1e-4	402	53478	835	222359

Table 8: Total CG iterations for the transmission problem (20) for different numbers of τ_r and Δx when using termination criterion (9) and $TOL = 10e - 14$.

Finally, we compare the different termination criteria for values of TOL more relevant in practice. Hereby, we assume that the user wants to have a solution that is TOL close to the exact one. Based on the theory discussed here, there are three choices: Using (9) with $\tau_r = 1e - 1$ independent of TOL, using (11) with $\tau_a = TOL$ or (10) with $\tau_r = TOL$, meaning that for the latter ones, we have to solve the inner iteration more accurately the more accurate we want the outer one. Hereby, we choose the largest problem with $\Delta x = 1/80$.

The results are depicted in table 9. For the computation with a - divergence was observed. Otherwise, the schemes roughly obey the desired behavior that the error is proportional to TOL, although all are above the desired accuracy. Otherwise, the scheme corresponding to (9) is about a factor of five faster than that corresponding to (11) and up to a factor of two faster than that corresponding to (11) while providing more accurate results.

4 Summary and Conclusions

We considered perturbed fixed point iterations where the perturbation results from inexact solves of equation systems by iterative solvers. Thereby, we extended a perturbation result for fixed point equations to the case of a nested fixed point equation. Applying these results to the Picard- and the

	Relative crit. (9)				Relative crit. (10)			
TOL	τ_r	#FP	#CG	$\lVert \mathbf{x}-\mathbf{x}^* \rVert$	τ_r	#FP	#CG	$\lVert \mathbf{x}-\mathbf{x}^* \rVert$
1e-1	1e-1	22	2905	8.215e-1	1e-1	-	-	-
1e-2	1e-1	43	5258	1.203e-1	1e-2	95	10666	3.225e-0
1e-3	1e-1	70	8256	1.397e-2	1e-3	64	10227	5.588e-1
1e-4	1e-1	106	12204	9.919e-4	1e-4	116	22769	2.602e-2
	Absolute crit. (11)							
TOL	τ_a	#FP	#CG	$\lVert \mathbf{x}-\mathbf{x}^* \rVert$				
1e-1	1e-1	35	11459	2.476e-0				
1e-2	1e-2	94	30550	2.454e-1				
1e-3	1e-3	153	50242	2.441e-2				
1e-4	1e-4	212	70848	2.428e-3				

Table 9: Total CG iterations for the transmission problem (20) for different numbers of TOL, τ_r and τ_a when using different termination critera.

Dirichlet-Neumann iteration for steady states, we showed that these converge to the exact solution indepently of the tolerance in the subsolver, if a specific relative termination criterion is employed. This justifies extremely coarse solves in the inner solvers and suggests the use of GMRES as Krylov subspace solver for unsymmetric systems.

If an absolute or standard relative criterion is used, the theory indicates that we will not converge to the exact solution. Numerical results demonstrate this behavior.

Thus, to obtain a certain accuracy in the fixed point solution when using a standard relative or absolute criterion, we have to solve the inner systems more accurate the tighter the tolerance, whereas for the nonstandard relative criterion we can solve the inner systems very coarsely independent of desired accuracy. Numerical results show that this is the most efficient way to treat these systems.

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