Multitrace formulations and Dirichlet-Neumann algorithms

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1 Introduction

Multitrace formulations (MTF) for boundary integral equations (BIE) were developed over the last few years in [4] and [1, 2] for the simulation of electromagnetic problems in piecewise constant media, see also [3] for associated boundary integral methods. The MTFs are naturally adapted to the developments of new block preconditioners, as indicated in [5], but very little is known so far about such associated iterative solvers. The goal of our presentation is to give an elementary introduction to MTFs, and also to establish a natural connection with the more classical Dirichlet-Neumann algorithms that are well understood in the domain decomposition literature, see for example [6, 7]. We present for a model problem a convergence analysis for a naturally arising block iterative method associated with the MTF, and also first numerical results to illustrate what performance one can expect from such an iterative solver.

2 One-dimensional example

In this section we introduce the Calderon projectors and the multitrace formulation for the one dimensional model problem

$$Au := u''(x) - a^2 u(x) = 0, \quad a > 0. \tag{1}$$

The family of bounded solutions of (1) on the domains $\Omega^\pm = \mathbb{R}^\pm$ is given by $u(x) = Ce^{\mp ax}$, where $C = u(0)$. We say that the solution spaces of the operator A on $\mathbb{R}^\pm$ are given by

$$Z^\pm = \{u \in L^2(\Omega) | u(x) = Ce^{\mp ax},\, C \in \mathbb{R}\} = \mathbb{R}e^{\mp ax}.$$

Note that any $u_\pm \in Z^\pm$ satisfies the relation $u'_\pm(0) = \pm a u_\pm(0)$ and thus the space of all possible Cauchy data of the solutions of (1) on $\mathbb{R}^\pm$ is given by

$$V^\pm = \{(g_0, g_1) = C(1, \pm a),\, C \in \mathbb{R}\} = \mathbb{R}\begin{pmatrix} 1 \\ \pm a \end{pmatrix}.$$

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Definition 1 (Calderon projectors). Let $\rho^\pm : Z^\pm \to V^\pm$ be the operator that associates to any solution of $Au = 0$ on $\mathbb{R}^\pm$ its pair of traces $(u(0), u'(0))$. Let $K^\pm : \mathbb{R}^2 \to Z^\pm$ be the operator that associates to any pair $(h_0, h_1) \in \mathbb{R}^2$ the quantity $K^\pm(h_0, h_1) = c_\mp e^{\mp ax}$, where $u(x) = c_+ e^{ax} + c_- e^{-ax}$ is the unique solution of (1) with Cauchy data (h_0, h_1),

$$Au = 0,\ u(0) = h_0 \text{ and } u'(0) = h_1. \tag{2}$$

Calderon projectors are defined as the projections $P^\pm : \mathbb{R}^2 \to V^\pm$, such that

$$P^\pm = \rho^\pm \circ K^\pm.$$

The expressions of $P^\pm$ for our model problem can be computed explicitly. The solution of (2) is

$$u(x) = \frac{1}{2a}(ah_0 + h_1)e^{ax} + \frac{1}{2a}(ah_0 - h_1)e^{-ax},$$

and thus $K^\pm(h_0, h_1) = \frac{1}{2a}(ah_0 \mp h_1)e^{\mp ax}$ and

$$P^\pm(h_0, h_1) := (\rho^\pm \circ K^\pm)(h_0, h_1) = \begin{pmatrix} \frac{1}{2a}(ah_0 \mp h_1) \\ \mp\frac{1}{2}(ah_0 \mp h_1) \end{pmatrix} \Rightarrow P^\pm = \begin{bmatrix} \frac{1}{2} & \mp\frac{1}{2a} \\ \mp\frac{a}{2} & \frac{1}{2} \end{bmatrix}.$$

Remark 1. From the previous construction we see that the Calderon projector is unique. When working with subdomains, it is however more convenient to introduce normal derivatives at interfaces, instead of $u'(0)$, and we thus define the Calderon projectors for normal derivatives with the modified sign

$$\mathbb{P}^\pm(h_0, h_1) := P^\pm(h_0, \mp h_1) \Rightarrow \mathbb{P}^+ = \mathbb{P}^- = \begin{bmatrix} \frac{1}{2} & \frac{1}{2a} \\ \frac{a}{2} & \frac{1}{2} \end{bmatrix}, \tag{3}$$

and we will use $\mathbb{P}^\pm$ in what follows.

Definition 2 (Cauchy traces). Following the notations in [4], we denote by

$$\mathbb{T}^\pm u := \begin{pmatrix} u(0) \\ \mp u'(0) \end{pmatrix} \tag{4}$$

the Cauchy trace (Dirichlet and Neumann) on the boundary $\{x = 0\}$ of a solution u of the equation $Au = 0$ posed on the half space $\mathbb{R}^\pm$.

Suppose now we have a decomposition of $\mathbb{R}$ into two subdomains $\Omega_1 = \Omega^-$ and $\Omega_2 = \Omega^+$ and we want to solve equation (1) by an iterative algorithm involving Dirichlet and Neumann traces on the interface $\{x = 0\}$. Let $\mathbb{T}_{1,2}$ be the trace operators as defined in (4) ($\mathbb{T}_1 = \mathbb{T}^-$ and $\mathbb{T}_2 = \mathbb{T}^+$) for the subdomains $\Omega_{1,2}$, and $\mathbb{P}_{1,2}$ the corresponding Calderon projectors as defined in (3) ($\mathbb{P}_1 = \mathbb{P}^-$ and $\mathbb{P}_2 = \mathbb{P}^+$) .

Definition 3 (Multitrace formulation). The *multitrace formulation* from [4] states that the pairs $(\mathbb{T}_i u_i)_{i=1,2}$ are traces of the solution defined on Ω_i if they verify the relations

$$\begin{cases} (\mathbb{P}_1 - I)\mathbb{T}_1 u_1 - \sigma_1 \left(\mathbb{T}_1 u_1 - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathbb{T}_2 u_2 \right) = 0, \\ (\mathbb{P}_2 - I)\mathbb{T}_2 u_2 - \sigma_2 \left(\mathbb{T}_2 u_2 - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathbb{T}_1 u_1 \right) = 0, \end{cases} \tag{5}$$

where $\sigma_{1,2}$ are some relaxation parameters.

We see that a natural iterative method (also introduced in [5]) for (5) starts with some initial guesses $(u_i^0, v_i^0)_{i=1,2}$ for the traces, and computes for $n = 1, 2, \ldots$ the new trace pairs from the relations

$$\begin{cases} (\mathbb{P}_1 - I)\begin{pmatrix} u_1^n \\ v_1^n \end{pmatrix} - \sigma_1 \begin{pmatrix} u_1^n \\ v_1^n \end{pmatrix} = -\sigma_1 \begin{pmatrix} u_2^{n-1} \\ -v_2^{n-1} \end{pmatrix}, \\ (\mathbb{P}_2 - I)\begin{pmatrix} u_2^n \\ v_2^n \end{pmatrix} - \sigma_2 \begin{pmatrix} u_2^n \\ v_2^n \end{pmatrix} = -\sigma_2 \begin{pmatrix} u_1^{n-1} \\ -v_1^{n-1} \end{pmatrix}. \end{cases} \tag{6}$$

By introducing the expressions of $\mathbb{P}_i$, we can rewrite the iteration in the form

$$\begin{bmatrix} -(\sigma_1 + \frac{1}{2}) & \frac{1}{2a} & & \\ \frac{a}{2} & -(\sigma_1 + \frac{1}{2}) & & \\ & & -(\sigma_2 + \frac{1}{2}) & \frac{1}{2a} \\ & & \frac{1}{2} & -(\sigma_2 + \frac{1}{2}) \end{bmatrix} \begin{pmatrix} u_1^n \\ v_1^n \\ u_2^n \\ v_2^n \end{pmatrix} = \begin{pmatrix} -\sigma_1 u_2^{n-1} \\ \sigma_1 v_2^{n-1} \\ -\sigma_2 u_1^{n-1} \\ \sigma_2 v_1^{n-1} \end{pmatrix}, \tag{7}$$

or when solving for the new iterates

$$\begin{pmatrix} u_1^n \\ v_1^n \\ u_2^n \\ v_2^n \end{pmatrix} = \begin{bmatrix} 0 & A_1 \\ A_2 & 0 \end{bmatrix} \begin{pmatrix} u_1^{n-1} \\ v_1^{n-1} \\ u_2^{n-1} \\ v_2^{n-1} \end{pmatrix} =: A \begin{pmatrix} u_1^{n-1} \\ v_1^{n-1} \\ u_2^{n-1} \\ v_2^{n-1} \end{pmatrix}, \tag{8}$$

where

$$A_i = \frac{1}{2(\sigma_i + 1)} \begin{bmatrix} 2\sigma_i + 1 & -\frac{1}{a} \\ a & -(1 + 2\sigma_i) \end{bmatrix}, \quad i = 1, 2.$$

The convergence factor of (6) is therefore given by the spectral radius of the iteration matrix A, whose eigenvalues are

$$\lambda(A) := \left\{ -\sqrt{\frac{\sigma_1}{\sigma_1 + 1}}, \sqrt{\frac{\sigma_1}{\sigma_1 + 1}}, -\sqrt{\frac{\sigma_2}{\sigma_2 + 1}}, \sqrt{\frac{\sigma_2}{\sigma_2 + 1}} \right\}. \tag{9}$$

We see that the convergence factor is independent of a and thus only depends on the relaxation parameters σ_i. If we suppose by symmetry that $\sigma_1 = \sigma_2 =: \sigma$, the convergence factor becomes $\rho(A) = \sqrt{\frac{\sigma}{\sigma+1}}$, and we show a plot of

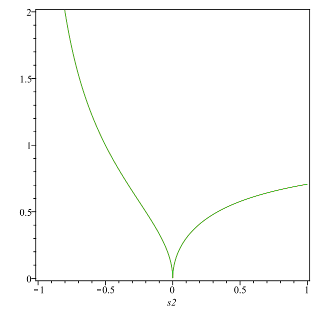

Fig. 1 Convergence factor of the iterative multitrace formulation in 1d as function of the relaxation parameter σ

$\rho(A)$ as a function of σ in Figure 1. We see that the algorithm diverges for $\sigma < -\frac{1}{2}$, stagnates for $\sigma = -\frac{1}{2}$ and converges for $\sigma > -\frac{1}{2}$. For $\sigma = 0$, the convergence factor vanishes, but a closer look at the iteration formula (7) shows that the matrix is then singular and thus the algorithm is no longer well defined for this value. On the other hand, the associated iteration (8) is still well defined, the latter being equivalent to (7) only for $\sigma \neq 0$. Overall, we see that algorithm (7) converges rapidly when the relaxation parameter is chosen close to 0.

3 Two-dimensional example

Suppose we want to solve the Laplace equation

$$u_{xx} + u_{yy} = 0, \quad \text{in } \Omega = \mathbb{R}^2, \tag{10}$$

using the two subdomains $\Omega_1 := \mathbb{R}^- \times \mathbb{R}$ and $\Omega_2 := \mathbb{R}^+ \times \mathbb{R}$ and a multitrace formulation. To use our results from the previous section we take a Fourier transform in the y variable,

$$\hat{u}_{xx} - k^2 \hat{u} = 0.$$

We can now follow the reasoning of the previous section in Fourier space, replacing a by $|k|$. Thus any given pair of boundary functions $(\hat{h}_0(k), \hat{h}_1(k))$ can be projected to become compatible boundary traces using the symbol of the the *Calderon projectors*

$$\widehat{\mathbb{P}}_i \begin{pmatrix} \hat{h}_0 \\ \hat{h}_1 \end{pmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2|k|} \\ \frac{|k|}{2} & \frac{1}{2} \end{bmatrix} \begin{pmatrix} \hat{h}_0 \\ \hat{h}_1 \end{pmatrix}, \quad i = 1, 2.$$

We next express the Calderon projectors in terms of Dirichlet-to-Neumann (DtN) and Neumann-to-Dirichlet (NtD) operators.

Lemma 1 (Calderon projectors and DtN operators). *Calderon projectors can be written in terms of the local DtN and NtD operators as*

$$\widehat{\mathbb{P}}_i = \frac{1}{2}\begin{bmatrix} 1 & \widehat{NtD_i} \\ \widehat{DtN_i} & 1 \end{bmatrix}, \quad i = 1, 2, \tag{11}$$

where DtN_i associates to given Dirichlet data $\hat{g}_0$ on the interface $x = 0$ the normal derivative $\frac{\partial u_i}{\partial n_i}$ of the solution u_i in Ω_i and the NtD_i associates to given Neumann data $\hat{g}_1$ on the interface $x = 0$ the trace of the solution $\hat{u}_i(0, k)$ on the same boundary.

Proof. On Ω_1, we obtain explicitly the symbols of these operators from

$$\begin{aligned} &\hat{u}_1(x, k) = \hat{g}_0 e^{|k|x} \Rightarrow \frac{\partial \hat{u}_1}{\partial x}|_{x=0} = |k|\hat{g}_0 \Rightarrow \widehat{DtN_1} = |k|, \\ &\hat{u}_1(x, k) = \hat{u}_1(0, k)e^{|k|x}, \ \frac{\partial \hat{u}_1}{\partial x}|_{x=0} = \hat{g}_1 \Rightarrow \hat{u}_1(0, k)|k| = \hat{g}_1 \Rightarrow \widehat{NtD_1} = \frac{1}{|k|}. \end{aligned}$$

The corresponding symbols for the domain Ω_2 are

$$\widehat{DtN_2} = |k|, \quad \widehat{NtD_2} = \frac{1}{|k|}.$$

Inserting these expressions into (11) concludes the proof.

We are ready now to establish the link between these algorithms and the classical DtN iterations.

Theorem 1 (Link with the DtN iterations). *The iterative multitrace formulation for the special choice $\sigma_1 = \sigma_2 = -\frac{1}{2}$ computes simultaneously a Dirichlet-Neumann iteration (u_1^n, v_2^n) and a Neumann-Dirichlet iteration (v_1^n, u_2^n) without a relaxation parameter.*

Proof. According to the results of Lemma 1, in two dimensions, iteration (6) becomes

$$\begin{aligned} \tfrac{1}{2}\begin{bmatrix} -1 - 2\sigma_1 & \widehat{NtD_1} \\ \widehat{DtN_1} & -1 - 2\sigma_1 \end{bmatrix} \begin{pmatrix} \hat{u}_1^n \\ \hat{v}_1^n \end{pmatrix} &= -\sigma_1 \begin{pmatrix} \hat{u}_2^{n-1} \\ -\hat{v}_2^{n-1} \end{pmatrix}, \\ \tfrac{1}{2}\begin{bmatrix} -1 - 2\sigma_2 & \widehat{NtD_2} \\ \widehat{DtN_2} & -1 - 2\sigma_2 \end{bmatrix} \begin{pmatrix} \hat{u}_2^n \\ \hat{v}_2^n \end{pmatrix} &= -\sigma_2 \begin{pmatrix} \hat{u}_1^{n-1} \\ -\hat{v}_1^{n-1} \end{pmatrix}. \end{aligned} \tag{12}$$

We see that for the special choice $\sigma_1 = \sigma_2 = -\frac{1}{2}$, iteration (12) simplifies to

$$\begin{cases} \widehat{NtD_1}\hat{v}_1^n = \hat{u}_2^{n-1}, \\ \widehat{DtN_1}\hat{u}_1^n = -\hat{v}_2^{n-1}, \end{cases} \begin{cases} \widehat{NtD_2}\hat{v}_2^n = \hat{u}_1^{n-1}, \\ \widehat{DtN_2}\hat{u}_2^n = -\hat{v}_1^{n-1}. \end{cases} \tag{13}$$

From the symbols, we see that $\widehat{NtD_i}^{-1} = \widehat{DtN_i}$, and hence iteration (13) becomes

$$\begin{cases} \hat{v}_1^n = \widehat{DtN_1}\hat{u}_2^{n-1}, \\ \hat{u}_1^n = -\widehat{NtD_1}\hat{v}_2^{n-1}, \end{cases} \quad \begin{cases} \hat{v}_2^n = \widehat{DtN_2}\hat{u}_1^{n-1}, \\ \hat{u}_2^n = -\widehat{NtD_2}\hat{v}_1^{n-1}, \end{cases}$$

which leads to the conclusion.

In order to study the role of the relaxation parameters σ_i, we check first under which conditions iteration (12), written explicitly as

$$\begin{aligned} B_1 \begin{pmatrix} \hat{u}_1^n \\ \hat{v}_1^n \end{pmatrix} &:= \frac{1}{2} \begin{bmatrix} -1-2\sigma_1 & \frac{1}{|k|} \\ |k| & -1-2\sigma_1 \end{bmatrix} \begin{pmatrix} \hat{u}_1^n \\ \hat{v}_1^n \end{pmatrix} = -\sigma_1 \begin{pmatrix} \hat{u}_2^{n-1} \\ -\hat{v}_2^{n-1} \end{pmatrix}, \\ B_2 \begin{pmatrix} \hat{u}_2^n \\ \hat{v}_2^n \end{pmatrix} &:= \frac{1}{2} \begin{bmatrix} -1-2\sigma_2 & \frac{1}{|k|} \\ |k| & -1-2\sigma_2 \end{bmatrix} \begin{pmatrix} \hat{u}_2^n \\ \hat{v}_2^n \end{pmatrix} = -\sigma_2 \begin{pmatrix} \hat{u}_1^{n-1} \\ -\hat{v}_1^{n-1} \end{pmatrix}, \end{aligned} \tag{14}$$

is well defined. This is the case if the matrices B_i are invertible. Since $\det(B_i) = 4\sigma_i(\sigma_i+1)$,the multitrace iteration is well defined if $\sigma_i \neq \{0,-1\}$. In this case (14) is equivalent to

$$\begin{aligned} \begin{pmatrix} \hat{u}_1^n \\ \hat{v}_1^n \end{pmatrix} &= B_1^{-1} \begin{pmatrix} \hat{u}_2^{n-1} \\ \hat{v}_2^{n-1} \end{pmatrix} = \begin{pmatrix} \frac{1+2\sigma_1}{2(\sigma_1+1)}\hat{u}_2^{n-1} - \frac{1}{2(\sigma_1+1)}\widehat{NtD_1}\hat{v}_2^{n-1} \\ \frac{1}{2(\sigma_1+1)}\widehat{DtN_1}\hat{u}_2^{n-1} - \frac{1+2\sigma_1}{2(\sigma_1+1)}\hat{v}_2^{n-1} \end{pmatrix}, \\ \begin{pmatrix} \hat{u}_2^n \\ \hat{v}_2^n \end{pmatrix} &= B_2^{-1} \begin{pmatrix} \hat{u}_1^{n-1} \\ \hat{v}_1^{n-1} \end{pmatrix} = \begin{pmatrix} \frac{1+2\sigma_2}{2(\sigma_2+1)}\hat{u}_1^{n-1} - \frac{1}{2(\sigma_2+1)}\widehat{NtD_2}\hat{v}_1^{n-1} \\ \frac{1}{2(\sigma_2+1)}\widehat{DtN_2}\hat{u}_1^{n-1} - \frac{1+2\sigma_2}{2(\sigma_2+1)}\hat{v}_1^{n-1} \end{pmatrix}. \end{aligned} \tag{15}$$

Algorithm (15) has the same convergence properties as (8), since we obtain the same convergence factor independent of the Fourier variable k, which means convergence is going to be mesh independent.

4 Numerical results

We now show some numerical experiments for illustration purposes on our two-dimensional model problem (10) on the domain $\Omega = (-1,1) \times (0,1)$ decomposed into the two subdomains $\Omega_1 = (-1,0) \times (0,1)$ and $\Omega_2 = (0,1) \times (0,1)$. We use standard five point finite differences for the discretization and simulate directly the error equations corresponding to the algorithm (15) for different values of the parameter σ_i. For $\sigma_i = -0.6$, our analysis shows that the algorithm does not converge, and we see how the error grows in the iteration in Figure 2. For $\sigma_i = -0.5$, our analysis predicts stagnation, and this is also observed in Figure 3. For $\sigma_i = 0.1$, we obtain the predicted rapid convergence seen in Figure 4. We finally show in Figure 5 on the left how the error evolves in the maximum norm as the iteration progresses for different values of σ, and on the right the numerically estimated contraction factor, which looks very similar to the predicted behavior shown in Figure 1.

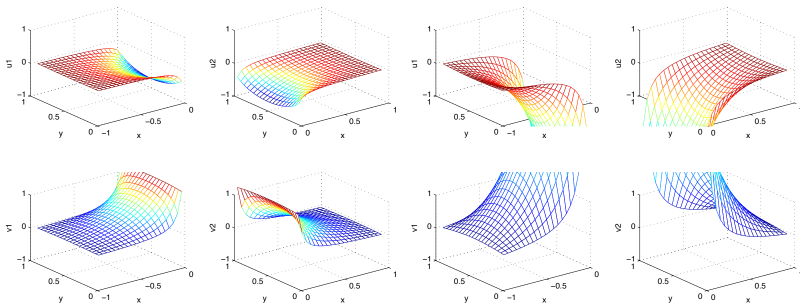

Fig. 2 Evolution of the error for $\sigma = -0.6$ after 2 Iterations (left), 10 iterations (right)

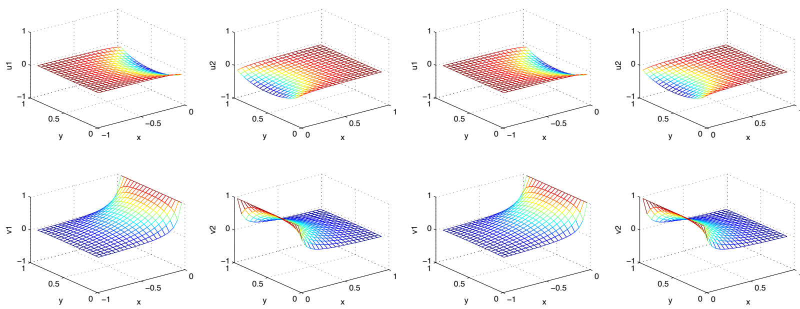

Fig. 3 Evolution of the error for $\sigma = -0.5$ after 2 Iterations (left), 10 iterations (right)

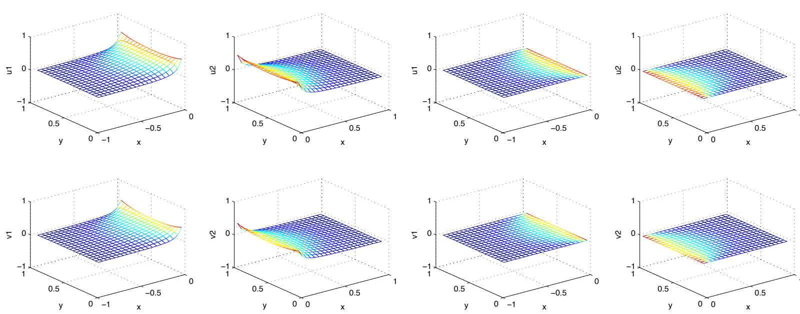

Fig. 4 Evolution of the error for $\sigma = 0.1$ after 2 Iterations (left), 10 iterations (right)

5 Conclusion

Using a simple model problem and two subdomains, we explained multitrace formulations and a naturally associated iterative method of domain decomposition type. Using the formalism of Dirichlet to Neumann operators, we showed that for a particular choice of the relaxation parameter in the multitrace iteration, a combined sequence of an unrelaxed Dirichlet-Neumann and Neumann-Dirichlet algorithm is obtained. Our analysis also indicates good

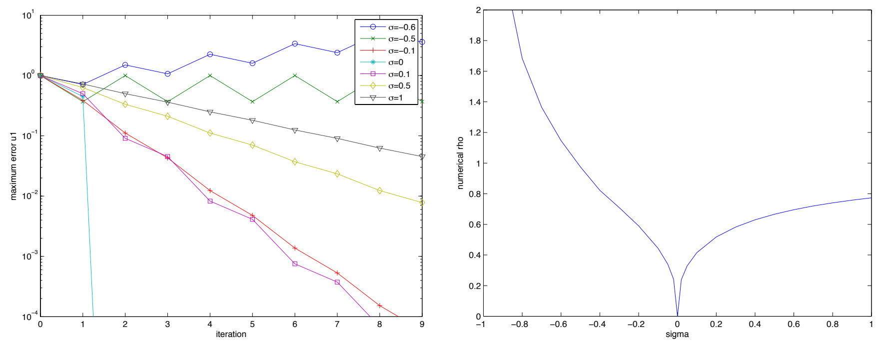

Fig. 5 Error in the maximum norm as a function of the iteration number for different values of σ (left), and numerically measured contraction factor of the multitrace iteration as function of σ (right)

choices for the relaxation parameter in the multitrace iteration, which was confirmed by numerical experiments.

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