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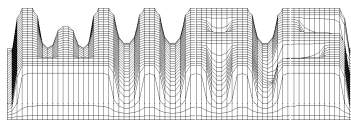
## Multigrid optimization in applications

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## Abstract

Iterative techniques are a key methodology for the numerical solution of optimization problems in differential equations. In two practical application problems with different characteristics, this paper shows, how multigrid methods can be applied efficiently to this problem class. Problem formulations, solution approaches as well as numerical results are presented.

## 1 Introduction

Multigrid methods are known as powerful tools for the fast solution of linear systems arising from discretizations of (typically elliptic) differential equations. However, they can be successfully applied to saddlepoint problems arising from variational principles and even to model based optimization problems, as has been shown recently. The aim of this paper is to present practically important and recently developed formulations of multigrid algorithms for optimization problems and to show their efficacy in real world applications. For theoretical convergence results on these algorithms, we refer to other publications [18,20,16].

Our considerations are based on the iterative nullspace paradigm as introduced in [22] for the solution of linear-quadratic (QP) subproblems within a successive quadratic programming approach for the (directly) discretized optimization problem. There have been other related approaches, e.g. by Hackbusch [8], where it is assumed that the discretized model equation is solved exactly in each optimization step or by Ta' Asan [26], where particularly projected gradient steps are performed in each optimization iteration. For a complete overview over the relevant literature, we refer to [20].

Here we focus on two practically relevant formulations of multigrid methods for optimization problems:

- Reduced SQP with multigrid solution of the linearized model equation
- Simultaneous multigrid methods for the solution of quadratic subproblems in a SQP-algorithm

For both formulations, we present practical implementations and results.

The first application problem is the shape optimization of turbine blades. There, multigrid methods are applied within a partially reduced SQP-approach, where the approximation of the partially reduced Hessian is constructed from update formulas of the Broyden-family. This approach is recommended, when the difference between the number of optimization degrees of freedom and the number of state equations is as big as in this case. By use of this method, it has been possible

for the engineers involved to solve blade design problems which before have taken hours using standard optimization approaches, now in minutes of cpu-time.

The second practical optimization problem is the topology optimization of elastic structures. A nonlinear interior point strategy for the treatment of the arising inequality conditions is profitably coupled with a simultaneous multigrid strategy for the solution of the quadratic subproblems. Thus it is possible for the first time to solve topology optimization problems with optimal complexity.

A further practical application (not discussed in detail here, see [14]) of the new multigrid methods developed is a new approach to the geostatistical inverse modeling in groundwater flow, which has been investigated in cooperation with hydraulic engineers. By using this new approach, the available information is fully exploited. On the other hand the approach depends on the repeated solution of inverse problems. These can be solved with optimal complexity by the simultaneous multigrid methods presented here.

This paper is organized in the following way: in the following section, we introduce the notation and basic facts for the considerations in the succeeding sections. There, we formulate also the basic algorithmic concept under investigation. In section 3 we present a partially reduced SQP approach which uses multigrid methods for the solution of the linearized model equations. This approach is applied to the practical problem of shape optimization for turbine blades. In section 4 we investigate simultaneous multigrid methods within an SQP context, which are applied to topology optimization problems.

## 2 Basics

### 2.1 Multigrid methods briefly sketched

Multigrid methods are typically used as fast solvers for linear equations

$$Lx = b,$$

representing a differential equation in a computational region  $\Omega$ . For an introduction to the concepts of multigrid methods, the reader is referred to [9]. A typical multigrid method uses a sequence of  $m + 1$  nested discretization grids of increasing fineness

$$\Omega_0 \subset \Omega_1 \subset \dots \subset \Omega_m = \Omega_\pi,$$

where  $\Omega_\pi$  denotes the finest grid currently used for the discretization of a differential equation. Associated to the grid sequence is a sequence of finite element

spaces

$$V_0 \subset V_1 \subset \dots \subset V_m = V_\pi.$$

The mesh hierarchy induces linear systems

$$L_l x_l = b_l, \quad l = 0, \dots, m \quad (1)$$

on each grid level  $l$ . The matrix  $L_m$  is obtained from a discretization of the differential operator on the finest grid  $\Omega_m$ . The coarse grid matrices  $L_l$ ,  $l < m$  can be constructed by the Galerkin approach entirely from  $L_m$  or can be computed separately on each grid. In addition to the linear systems on the several grid levels, we need transfer operators between finer and coarser grids in the form of linear mappings

$$R_l : \mathbb{R}^{n_l} \rightarrow \mathbb{R}^{n_{l-1}} \quad (\text{restriction}), \quad (2)$$

$$P_l : \mathbb{R}^{n_{l-1}} \rightarrow \mathbb{R}^{n_l} \quad (\text{prolongation}), \quad (3)$$

where  $n_l$  denotes the number of nodes in grid  $\Omega_l$ . Thus, a two-grid correction iteration is defined by

$$x_l^{\text{new}} = x_l^{\text{old}} - P_l L_{l-1}^{-1} R_l (L_l x_l^{\text{new}} - b_l). \quad (4)$$

A typical multigrid iteration for the iterative improvement of a given vector  $x_l$  can be briefly sketched as

$$\begin{aligned} & \text{mgc} ( l, x_l, b_l ) \\ & \{ \\ & \quad \text{if} ( l == 0 ) x_0 = L_0^{-1} b_0; \\ & \quad \text{else} \{ \\ & \quad \quad \text{Apply } \nu_1 \text{ smoothing iterations to } L_l x_l = b_l; \\ & \quad \quad d_{l-1} = R_l (b_l - L_l x_l); \quad [\text{defect}] \\ & \quad \quad v_{l-1} = 0; \quad [\text{initial guess}] \\ & \quad \quad \text{for} ( g = 1, \dots, \gamma ) \text{mgc} ( l - 1, v_{l-1}, d_{l-1} ); \\ & \quad \quad x_l = x_l + P_l v_{l-1}; \\ & \quad \quad \text{Apply } \nu_2 \text{ smoothing iterations to } L_l x_l = b_l; \\ & \quad \} \\ & \}. \end{aligned}$$

The parameter  $\gamma$  characterizes the cycle type. Typical values are  $\gamma = 1$  (V-cycle) or  $\gamma = 2$  (W-cycle). The so-called smoothing iterations mentioned in the generic algorithm above are defined by using a splitting of the matrix

$$L_l = M_l - N_l$$

into a nonsingular, but comparably cheaply invertible matrix  $M_l$  and a rest matrix  $N_l$ . One step of a (damped) smoothing iteration (of, e.g., Jacobi, Gauss-Seidel oder ILU type) is then given by

$$x_l^{\text{new}} = x_l^{\text{old}} - \omega M_l^{-1} (L_l x_l^{\text{old}} - b_l).$$

A well known intuitive understanding of the multigrid effect is that the smoothing iterations reduce high frequency errors while the coarse grid corrections reduce the complementary low frequency errors.

## 2.2 Optimization conditions

We consider (nonlinear) differential equations with boundary conditions as equations of the type

$$c(x, p) = 0, \quad \text{with } c : X \times P \rightarrow Z$$

for appropriate Hilbert spaces  $X, P$  and Banach space  $Z$ , where we assume non-singularity w.r.t. the states, i.e.

$$\|c_x^{-1}\|_{Z \leftarrow X} \leq M, \quad M < \infty.$$

Indices  $x$  and  $p$  denote corresponding derivatives w.r.t. these variables.

By using a functional  $f : x \times P \rightarrow \mathbb{R}$  representing the optimization criterion, we define the optimization problem

$$\min f(x, p) \tag{5}$$

$$\text{s.t. } c(x, p) = 0. \tag{6}$$

With this optimization problem we associate the Lagrangian

$$\mathfrak{L}(x, p, \lambda) := f(x, p) + \lambda(c(x, p)),$$

where the Lagrange-multiplier  $\lambda(\cdot) \in Z^*$  is a linear functional from the dual space of  $Z$ . The necessary conditions of first order for a local optimum  $(x, p)$  are

$$\begin{aligned} \nabla_{(x,p)} \mathfrak{L}(x, p, \hat{\lambda}) &= 0 \\ c(x, p) &= 0 \end{aligned}$$

for some  $\hat{\lambda} \in Z^*$ . For twice continuously Fréchet-differentiable  $f$  and  $c$  the necessary conditions of second order have to be satisfied, as well:

$$\langle d, \nabla_{(x,p)}^2 \mathfrak{L}(\hat{x}, \hat{p}, \hat{\lambda}) d \rangle \geq 0 \quad \forall d \in \mathfrak{N}(c'(x, p))$$

where  $\langle \cdot, \cdot \rangle$  denotes the scalar product in the Hilbert space  $X \times P$ . A slightly more strict formulation of this condition results in the sufficient conditions of second order:

$$\exists \lambda \in Z^*, \exists m_1 > 0 : \langle d, \nabla_{(x,p)}^2 \mathfrak{L}(\hat{x}, \hat{p}, \hat{\lambda}) \rangle > m_1 \|d\|^2 \forall d \in \mathfrak{N}(c'(x, p)). \quad (7)$$

This condition ensures the well posedness of the optimization problem (5,6), as well. The nullspace  $\mathfrak{N}(c'(x, p))$  can be represented in the simple form

$$\begin{aligned} \mathfrak{N}(c'(x, p)) &= T(x, p)P \\ \text{with } T(x, p) : P &\rightarrow X \times P, ; T(x, p) := \begin{bmatrix} -c_x(x, p)^{-1}c_p(x, p) \\ id_p \end{bmatrix} \end{aligned} \quad (8)$$

so that condition (7) can be rewritten as

$$\exists m_2 > 0 : \langle \Delta p, G(\hat{x}, \hat{p})\Delta p \rangle \geq m_2 \|\Delta p\|^2, \forall \Delta p \in P,$$

where

$$G(x, p) := T(x, p)^* \frac{\partial^2}{\partial(x, p)^2} \mathfrak{L}(x, p, \lambda) T(x, p)$$

denotes the so-called projected Hessian. Thus we see that the reduced Hessian is not only of algorithmic importance, but also characterizes the properties of the optimization problem under investigation.

### 2.3 The simultaneous SQP approach

According to the topic of this special issue we employ the direct discretization approach in order to arrive from the infinite dimensional problem at a computationally tractable nonlinear programming problem which is then solved in a simultaneous solution approach—here SQP-type methods. For ease of presentation we use the same symbols as above, in order to denote the discretized quantities.

We use the following conceptual iteration for  $x^i, p^i$  starting at  $i = 0$ .

*Algorithm 1: basic multigrid SQP algorithm*

```

repeat
{
(1)  determine approximation:  $H \approx \frac{\partial^2}{\partial(x,p)^2} \mathcal{L}(x^i, p^i, \lambda^i)$ ;
(2)  compute defects:
       $g_x := \nabla_x f(x^i, p^i), g_p := \nabla_p f(x^i, p^i), c := c(x^i, p^i)$ ;
(3)  solve the QP approximatively by a multigrid method:
      
$$\min_{(\Delta x, \Delta p)} \begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix}^\top H \begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix} + \begin{pmatrix} g_x \\ g_p \end{pmatrix}^\top \begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix} ;$$

      s. t.  $c_x(x^i, p^i)\Delta x + c_p(x^i, p^i)\Delta p + c = 0$ 
      ( $\lambda^{QP}$  denotes the adjoint variable of the QP)
(4)  add increments:  $x^{i+1} = x^i + \Delta x; p^{i+1} = p^i + \Delta p; \lambda^{i+1} = \lambda^{QP}$ ;
}
until convergence

```

The matrix  $H$  approximating the Hessian of the Lagrangian determines, which SQP variant is performed (Newton-, generalized Gauss-Newton-, partially reduced, etc.). Since we will use multigrid methods for the solution of the linear-quadratic subproblems, this solution will not be exact. Therefore we actually use a more robust variant of the SQP algorithm above, which is only stationary, if the solution of the optimization problem is reached—also in the case of inexact QP solution.

*Algorithm 2: robust MG SQP algorithm*

```

repeat
{
(1)  determine approximation:  $H \approx \frac{\partial^2}{\partial(x,p)^2} \mathcal{L}(x^i, p^i, \lambda^i)$ ;
(2)  compute defects:
 $g_x := \nabla_x f(x^i, p^i) + c_x(x^i, p^i)^\top \lambda^i, g_p := \nabla_p f(x^i, p^i) + c_p(x^i, p^i)^\top \lambda^i, c := c(x^i, p^i)$ ;
(3)  solve the QP approximatively by a multigrid method:

$$\min_{(\Delta x, \Delta p)} \begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix}^\top H \begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix} + \begin{pmatrix} g_x \\ g_p \end{pmatrix}^\top \begin{pmatrix} \Delta x \\ \Delta p \end{pmatrix} ;$$

s.t.  $c_x(x^i, p^i) \Delta x + c_p(x^i, p^i) \Delta p + c = 0$ 
( $\Delta \lambda$  denotes the adjoint variable of the QP)
(4)  add increments:  $x^{i+1} = x^i + \Delta x; p^{i+1} = p^i + \Delta p; \lambda^{i+1} = \lambda^i + \Delta \lambda$ ;
}
until convergence

```

### 3 Multigrid techniques for reduced SQP approaches

In many application problems the degrees of freedom  $p$  for the optimization constitute a rather low dimensional space. Thus it does not make sense to build up an own multigrid structure for them as the formulation of algorithm 1 seems to suggest. For this type of problems it is much more practicable to use an approximation of the Hessian of the type

$$H = \begin{bmatrix} H_{xx} & H_{xp} \\ H_{px} & H_{pp} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & B \end{bmatrix} \quad (9)$$

where

$$B \approx T(x, p)^\top \frac{\partial^2}{\partial(x, p)^2} \mathcal{L}(x, p, \lambda) T(x, p)$$



with  $T(x, p)$  corresponding to (8) is an approximation of the so-called reduced Hessian of the Lagrangian. These lower dimensional reduced Hessian matrices can be efficiently approximated by corresponding update techniques analogously to quasi-Newton methods. The full system of the form  $B\Delta p = (\text{r.h.s.})$  can be solved with negligible effort due to the low dimension. Because of the special choice (9) the whole KKT-system is decoupled appropriately. The resulting method is of the reduced SQP-type and possesses superlinear convergence properties. It can be formulated in the following way.

*Algorithm 3: reduced SQP-algorithm*

```

repeat
{
(1)  compute reduced gradients  $\gamma_k := T(x_k, p_k)^\top \nabla_y f(x_k, p_k)$ ,
      determine an approximation  $B_k$  of  $T(x_k, p_k)^\top \frac{\partial^2}{\partial y^2} \mathcal{L}(x_k, p_k, \lambda_k) T(x_k, p_k)$ ;
(2)  solve  $B_k \Delta p_k = -\gamma_k$ ;
(3)  determine step  $(\Delta x_k, \Delta p_k) := T(x_k, p_k) \Delta p_k - c_x(x_k, p_k)^{-1} c(x_k, p_k)$ ;
(4)  add increments:  $(x_{k+1}, p_{k+1}) := (x_k, p_k) + (\Delta x_k, \Delta p_k)$ ,  $k := k + 1$ ;
}
until convergence

```

The application of the operators  $T(x_k, p_k)$  and  $T(x_k, p_k)^\top$  in steps 1 and 3 involves the solution of systems of equations with the matrix  $c_x(x_k, p_k)$  and  $c_x(x_k, p_k)^\top$ . These solutions are achieved by using appropriate multigrid methods. Since these systems of equations are not solved exactly we have to be careful with the construction of the adjoint solver in order to guarantee a decrease direction in the step. The approximate inverses  $\tilde{C}_x^{-1} \approx c_x^{-1}$  and  $\tilde{C}_x^{-\top} \approx c_x^{-\top}$  have to satisfy the following consistency condition.

$$\bar{\gamma}(x, p) := \nabla_p f(x, p) - \tilde{C}_x^{-\top} \nabla_x f(x, p) = \left. \frac{\partial}{\partial \Delta p} \right|_{\Delta p=0} f(x - \tilde{C}_x^{-1} c_p \Delta p, p + \Delta p)^\top =: \tilde{\gamma}(x, p)$$

According to [18, Theorem 3.5] both multigrid methods have to be exactly symmetric. In particular the restriction ( $R$ ) and prolongation ( $P$ ) operators should satisfy the following correspondence:

$$R_{\tilde{C}_x^{-1}} = P_{\tilde{C}_x^{-\top}}^\top, \quad R_{\tilde{C}_x^{-\top}} = P_{\tilde{C}_x^{-1}}^\top.$$

In many cases there are additional inequalities of the type

$$g(x, p) \geq 0$$

in the problem formulation which have to be satisfied by the solution of the optimization problem. For those application oriented problem formulations in [18] there have been introduced so-called partially reduced SQP methods. The essential idea is to formulate the reduced SQP methods only for those constraints which permit a global parameterization and to treat the remaining constraints in the same manner as in usual SQP methods—only reduced to the kernel of the latter constraints. Step (2) of algorithm 3 is substituted essentially by

( $\tilde{2}$ ) solve QP:

$$\begin{aligned} & \min_{\Delta p_k} \Delta p_k^\top B_k \Delta p_k + \gamma_{1,k}^\top \Delta p_k \\ \text{s. t. } & G_k T_k \Delta p_k + g_k + G_k C_{x,k}^{-1} c_{1,k} \geq 0 \\ & \text{and determine } \lambda_G \text{ (i.e. adjoints to } G); \end{aligned}$$

Thus a combination of the advantages of reduced SQP methods (small quadratic subproblems) with those of full SQP methods (flexible treatment of equalities and inequalities without global parameterization) is achieved. The local convergence properties of the resulting methods are determined by the choice of the approximation of the reduced Hessian. Here we use the BFGS update formula where the necessary differences of the  $p$ -variables and the reduced gradients are evaluated at intermediate points. A thorough discussion of this method and further variants and the corresponding convergence theory especially in the case of further substructures in the optimization problem can be found in [18,19].

In the sequel we apply the method described above to a practical shape optimization problem in turbine blade design. This research has been the subject of a joint project together with MTU Munich and ABB Baden, Switzerland, supported by the German ministry for education, science, research and technology (BMBF).

During the design of a turbomachinery the optimal cross sectional shape of a turbine blade is searched for in order to reproduce a given velocity distribution at the blade profile as well as possible. This can be considered a subtask on the way to an optimization of the whole turbine.

We consider the steady flow between two turbine blades (blade to blade computation). Using the results of Wu [28], we focus on the two-dimensional flow along a representative stream surface which is a manifold  $S := \{(r, \phi, z) : r = r(z)\}$  (cylindrical coordinates,  $z$  coincides with the engine axis). An orthogonal local coordinate system  $(\phi, m)$  exists on  $S$  with meridional coordinate  $m$ . The inter-

section of the blade with the stream surface, i.e., the profile, is represented as a twice continuously differentiable closed B-spline-curve,

$$\Gamma(t, p) = (\phi(t, p), m(t, p)) = \left( \sum_{i=1}^n p_i^\phi N_i(t), \sum_{i=1}^n p_i^m N_i(t) \right),$$

with fixed knot vector and fixed order. We look for an optimal vector  $p$  of control points, the design parameters.

As the problem is symmetric with respect to rotation by the angle  $\alpha = 2\pi/N$ , where  $N$  is the number of blades, the flow is computed between two neighboring blades including the upstream and downstream regions of this passage. Following [7], an inviscid potential flow is assumed. The unit square  $D$  of the computational  $(\xi, \eta)$ -plane is mapped onto the physical flow region by the transformation

$$f : (\xi, \eta) \mapsto (\phi(\xi, \eta; p), m(\xi, \eta; p)) \quad (10)$$

The unknown states describing the flow are a dimensionless normalized stream function  $u$  and the density  $\rho$ . For details of the flow model and its discretization see [21,4].

The engineering optimization problem to be solved is to find design parameters  $p$  for which the flow around the profile approximates a prescribed velocity distribution,  $|\hat{w}|$ . This is stated as

$$\min_{(u, \rho, p)} \int_{\Gamma} W(t) (|w| - |\hat{w}|)^2 dt + \varepsilon \|p - p_0\|_2^2$$

Therein,  $W$  is a weighting function and  $w$  depends on  $u$  and  $\rho$ .

Additionally, three geometric constraints appear which implement the conditions that the leading edge of the blade has to be at a specified position  $(x_{LE}, y_{LE})$  and that the blade has to have a prescribed length. We obtain a large-scale finite dimensional nonlinear optimization problem structured now as

$$\begin{aligned} & \min \psi(x, p) \\ & \text{s.t. } c(x, p) = 0, \quad \frac{\partial c}{\partial x} \text{ nonsingular,} \\ & \quad g(p) = 0, \end{aligned} \quad (11)$$

where  $x \in \mathbb{R}^{20705}$  denotes the discretized stream function and density variables,  $\psi$  the discretized objective criterion,  $c$  the discretized PDAE and  $g$  the geometric constraints for the spline parameters  $p \in \mathbb{R}^{24}$ .

The geometric constraints do not allow for a global parameterization of the resulting manifold in the spline parameters. Therefore that is the point where the par-

tial reduction idea comes into play. We identify the discretized PDE constraints  $c$  with the constraints defining the reduction aspect and leave the geometric constraints  $g$  essentially as they are—but reduced in the QP. The inexact variant of the generic PRSQP algorithm is employed. The approximations  $\tilde{C}^{-1}$  and  $\tilde{C}^{-\top}$  are formed by single multigrid V-cycles. As mentioned above we use as the restriction operator for the adjoint system the adjoint of the prolongation operator of the forward system and vice versa. Typically this is satisfied in the interior of the computational domain [9], but requires special measures to be taken at the boundary (cf. [21,17,4] for details).

The numerical results displayed below represent results with artificial problem data, which intentionally do not correspond to realistic conditions. In this manner it is possible to demonstrate the efficacy of the methods developed without revealing internal details of the industrial partners involved.

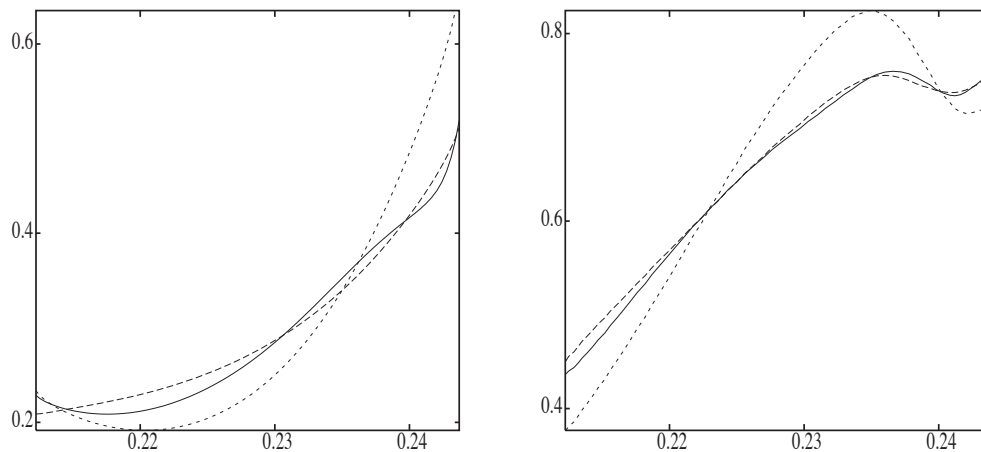


Fig. 1. *Velocity profiles on pressure (left) and suction (right) side*

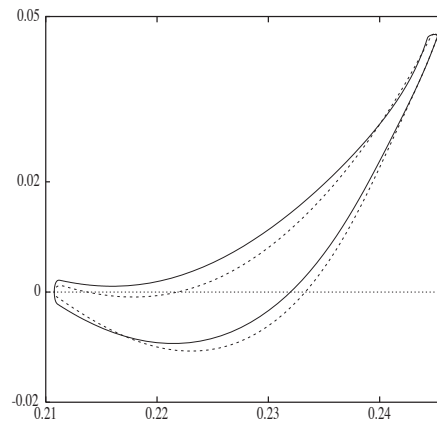


Fig. 2. *Optimized blade profile*

Figure 1 shows velocity (laval number) profiles on the pressure side and on the suction side of the turbine blade to be optimized. The solid lines show the optimized

velocity profiles. The dashed lines near the solid lines represent the objective reference profile  $\hat{w}$ . The dotted lines show the velocity profile of the blade at the start of the optimization process. The horizontal axis in these figures corresponds to the meridional coordinate. The vertical axis in figure corresponds to the Laval number. Figure 2 shows shows the initial (dashed) and optimal profile (solid).

One should note that the partially reduced techniques described above have been successfully applied also to optimal control problems in differential-algebraic equations from robotics and chemical engineering [18,19,11,3,15]. The investigations on turbine and compressor blade design have been pursued further also with another flow model, but involving partially reduced SQP methods in [6,5], as well.

#### 4 Multigrid Schur complement methods for optimization saddlepoint problems

In this section we investigate multigrid methods based on the nullspace iteration concept as considered in [20] for saddle point problems of the form

$$\begin{bmatrix} H_{xx} & C_x^\top & H_{xp} \\ C_x & 0 & C_p \\ H_{xp}^\top & C_p^\top & H_{pp} \end{bmatrix} \begin{pmatrix} x \\ \lambda \\ p \end{pmatrix} = \begin{pmatrix} f \\ c \\ g \end{pmatrix}. \quad (12)$$

With the definitions

$$A := \begin{bmatrix} H_{xx} & C_x^\top \\ C_x & 0 \end{bmatrix}, \quad B^\top := \begin{bmatrix} H_{xp} \\ C_p \end{bmatrix}, \quad y := \begin{pmatrix} x \\ \lambda \end{pmatrix}, \quad r := \begin{pmatrix} f \\ c \end{pmatrix}, \quad D := H_{pp}$$

we rewrite the linear system as

$$\begin{bmatrix} A & B^\top \\ B & D \end{bmatrix} \begin{pmatrix} y \\ p \end{pmatrix} = \begin{pmatrix} r \\ g \end{pmatrix}.$$

The nullspace iteration concept possesses the advantages over iterative range space concepts that on the one hand well known iterative techniques for the model problem with system matrix  $C_x$  can be transferred to the QP, and on the other hand that the Schur complement we are dealing with is related to the reduced Hessian, which we may assume to be well conditioned. Furthermore we do not have to assume positive definiteness of the Hessian of the Lagrangian. The conceptual basis of the nullspace multigrid methods proposed here are so-called transforming iterations, as established in [27] for variational saddlepoint problems ( $A$  pos. def., i.e. iterative range space method). There, right transforming systems

with block-triangular structure are considered. The aim of our considerations here is first the right-transformation of  $K$  with the matrix

$$\bar{K} := \begin{bmatrix} I - \bar{A}^{-1}B^\top \\ 0 & I \end{bmatrix}$$

and afterwards a splitting of the form

$$K\bar{K} = \begin{bmatrix} A (I - A\bar{A}^{-1})B^\top \\ B & \tilde{S} \end{bmatrix} \quad (13)$$

$$= \begin{bmatrix} \tilde{A} & 0 \\ B & \tilde{S} \end{bmatrix} - \begin{bmatrix} \tilde{A} - A & 0 \\ 0 & \tilde{S} - \bar{S} \end{bmatrix} - \begin{bmatrix} 0 & (I - A\bar{A}^{-1})B^\top \\ 0 & 0 \end{bmatrix} \quad (14)$$

$$=: M - N_1 - N_2 \quad (15)$$

$$=: M - N. \quad (16)$$

Here  $\bar{A}$  is an approximation to  $A$  and  $\tilde{A}$  is a matrix to be used in a smoothing iteration for systems with  $A$ . In particular we use

$$\tilde{A} := \begin{bmatrix} \ell\tilde{C}_x & 0 \\ \ell H_{xx} & \ell\tilde{C}_x^\top \end{bmatrix}, \quad \bar{A} := \begin{bmatrix} \ell\bar{C}_x & 0 \\ \ell H_{xx} & \ell\bar{C}_x^\top \end{bmatrix},$$

Analogously,  $\tilde{S}$  is defined as a smoothing approximation to  $\bar{S} := D - B\bar{A}^{-1}B^\top$ . Then the transforming iteration is defined by

$$y^{i+1} = y^i - \bar{K}M^{-1}(Ky - f). \quad (17)$$

This iteration is to be used as a smoothing iteration in a simultaneous multigrid approach to quadratic problems. For the sake of clarity we rewrite it in a more algorithmic form. The iteration is represented as

$$z^{i+1} = z^i + \Delta z^i$$

with

$$\Delta z^i = \begin{pmatrix} \Delta x^i \\ \Delta \lambda^i \\ \Delta p^i \end{pmatrix}$$

from algorithm 4.

*Algorithm 4: Transforming smoother: Computation of increments*

$$\begin{aligned}
(0) \quad \text{Defects: } & \begin{pmatrix} d_c \\ d_f \\ d_g \end{pmatrix} = \begin{pmatrix} c \\ f \\ g \end{pmatrix} - K \begin{pmatrix} x^i \\ \lambda^i \\ p^i \end{pmatrix} \\
(1) \quad & \tilde{d}_c = \tilde{C}^{-1} d_c \\
(2) \quad & \tilde{d}_f = \tilde{C}^{-\top} (d_f - H_{xx} \tilde{d}_c) \\
(3) \quad & \Delta p^i = -\tilde{S}^{-1} (d_g + H_{xp}^\top \tilde{d}_c + C_p^\top \tilde{d}_f) \\
(4) \quad & \Delta x^i = \tilde{d}_c + \tilde{C}^{-1} C_p \Delta p^i \\
(5) \quad & \Delta \lambda^i = \tilde{d}_f + \tilde{C}^{-\top} (H_{xp} \Delta p^i - H_{xx} \Delta x^i)
\end{aligned}$$

For this smoothing iteration and appropriately chosen canonical grid transfer operators mesh-independent convergence of multigrid W-cycles is shown in [20].

Now we apply this simultaneous multigrid approach to topology optimization in the homogenization formulation. The goal of this optimization problem is to find an elastic structure with minimal compliance supporting exterior or interior force acting on a body, whose shape is searched for. We consider a body occupying a domain  $\Omega \subset \mathbb{R}^d$ , where  $d = 2, 3$ . This body is supposed to be subjected to body forces  $f : \Omega \rightarrow \mathbb{R}^d$  and boundary tractions  $t : \Omega \rightarrow \mathbb{R}^d$ . The goal of finding the optimal shape of the body is reformulated as finding the optimal elasticity tensor

$$E_{ijkl} : \Omega \rightarrow \mathbb{R}, \quad (i, j, k, l) \in \{1, \dots, d\}^4$$

in some given set of admissible elasticity tensors  $U_{ad}$ . For ease of presentation, we restrict the admissible tensors to be of the form

$$E_{ijkl}(x) = \chi(x)^\alpha \bar{E}_{ijkl}, \quad x \in \mathbb{R}^d, \quad \alpha > 0 \quad (18)$$

with an a priori given constant elasticity tensor  $\bar{E}_{ijkl}$ , a “density” function  $\chi : \Omega \rightarrow \mathbb{R}$  and upper and lower limits for  $\chi$ ,

$$\chi(x) \in [a, b], \quad \forall x \in \Omega. \quad (19)$$

However, more general parameterizations of more complicated admissible sets are not excluded for the numerical methods presented in this paper. The optimization criterion is to minimize the compliance subject to the constraint that the volume

of the optimal body,  $V(\rho)$  has to be of a fixed apriori given value. Using the energy bilinear form

$$a(u, v) := \int_{\Omega} E_{ijkl} \varepsilon_{kl}(u) \varepsilon_{ij}(v) dx$$

for linearized strains

$$\varepsilon_{ij}(u) := \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

and the load linear form

$$L(v) := \int_{\Omega} f \cdot v dx + \int_{\partial\Omega} t \cdot v ds,$$

we consider the following problem in variational formulation

$$\min_{\chi, u} L(u) \quad (\text{surface traction}) \quad (20)$$

$$\text{s.t. } a(u, v) = L(v) \quad \forall v \in V \quad (\text{linear elasticity}) \quad (21)$$

$$\int_{\Omega} \chi dx = V_0 \quad (\text{volume constraint}) \quad (22)$$

$$a \leq \chi \leq b \quad (23)$$

Unlike with truss topology design, where a variety of several numerical methods have been developed in recent years, the numerical approaches to the homogenization method are dominated in principal by a black-box type optimization approach (see for instance [2, p. 32]) in connection with some iterative method (e.g., the method of moving asymptotes [24,29,25]) for the optimization part of the algorithm. The elasticity analysis equation (21) is formally solved for the displacements  $u$  which are thus considered as functions of  $\chi$ . Therefore there results an optimization problem which formally only depends on the density  $\chi$ , and the space of unknowns is reduced considerably.

In contrast to that, here a new *simultaneous interior point multigrid* approach to shape optimization problems of the type (20-23) is proposed, where no apriori elimination of variables is performed as in the black-box approach outlined above. In an interior point approach, the inequality constraints (23) are reformulated adding corresponding logarithmic barrier terms to the objective functional and the resulting equality constrained optimization problem is solved by an SQP approach, where each quadratic programming subproblem is solved by a simultaneous multigrid algorithm of optimal (i.e., linear) complexity. Thus the elasticity equation (21) is simultaneously solved only once together with the overall optimization problem, which leads to a tremendous reduction of computational complexity.



Following the direct discretization approach we choose a discretization for the influence variables  $\chi$  as well as for the state equations (21) and solve a resulting finite dimensional nonlinear programming problem of the form

$$\begin{aligned} \min_{\chi_h, u_h} \ell_h^\top u_h & \quad (24) \\ \text{s.t. } A_h(\chi_h)u_h &= \ell_h & (25) \\ \mathbb{I}_h(\chi_h) &= V_0 & (26) \\ a &\leq (\chi_h)_i \leq b, \quad \forall \text{ mesh nodes } i. & (27) \end{aligned}$$

Here  $A_h(\chi_h)$  denotes a finite element stiffness matrix for the elasticity equation,  $\ell_h$  the corresponding discretization of the load linear form and  $\mathbb{I}_h$  is a discretization of the integral linear form  $f_\Omega$ . The index  $h$  on all symbols indicates that all these magnitudes are derived from a discretization.

In a primal nonlinear interior point formulation for problem (24-27) we substitute the box constraints (27) by corresponding logarithmic barrier terms in the objective function. That means we consider the one parameter ( $\rho > 0$ ) family of optimization problems

$$\begin{aligned} \min_{\chi_h, u_h} \ell_h^\top u_h - \rho \sum_i (\log(\chi_i - a_i) + \log(b_i - \chi_i)) & \quad (28) \\ \text{s.t. } A_h(\chi_h)u_h &= \ell_h & (29) \\ \mathbb{I}_h(\chi_h) &= V_0, & (30) \end{aligned}$$

whose solution  $(\chi_h(\rho), u_h(\rho))$  converges to the solution of (24-27) for  $\rho \rightarrow 0$ .

The Lagrangian of problem (28-30) is

$$\begin{aligned} \mathfrak{L}_\rho(\chi_h, u_h, \lambda, \mu) &= \ell_h^\top u_h - \rho \sum_i (\log(\chi_i - a_i) + \log(b_i - \chi_i)) \\ &\quad + \lambda^\top (A_h(\chi_h)u_h - \ell_h) + \mu(\mathbb{I}_h(\chi_h) - V_0) \end{aligned}$$

so that its Karush-Kuhn-Tucker (KKT) conditions

$$\begin{aligned} \nabla_{\chi_h} \mathfrak{L}_\rho(\chi_h, u_h, \lambda, \mu) &= 0, & \nabla_{u_h} \mathfrak{L}_\rho(\chi_h, u_h, \lambda, \mu) &= 0 \\ \nabla_\lambda \mathfrak{L}_\rho(\chi_h, u_h, \lambda, \mu) &= 0, & \nabla_\mu \mathfrak{L}_\rho(\chi_h, u_h, \lambda, \mu) &= 0 \end{aligned}$$

can be written with the definition  $\phi := (\chi_h, u_h, \lambda, \mu)$  as

$$\mathfrak{F}_\rho(\phi) := \begin{pmatrix} A_h(\chi_h)^\top \lambda + \ell_h \\ -\rho \cdot \text{diag} \left( \frac{1}{\chi_i - a_i} - \frac{1}{b_i - \chi_i} \right) + \frac{\partial}{\partial \chi_h} \left( \lambda^\top (A_h(\chi_h)u_h + \mu \mathbb{I}_h(\chi_h)) \right) \\ A_h(\chi_h)u_h - \ell_h \\ \mathbb{I}_h(\chi_h) - V_0 \end{pmatrix} = 0. \quad (31)$$

The basic idea of interior point methods is now to apply a Newton method to equation (31), where in each iteration the parameter  $\rho$  is decreased by a certain amount. Thus each iterate  $\phi^{k+1} = \phi^k + \Delta\phi$  is determined by the increment  $\Delta\phi$  to be computed from the equation

$$K_{\rho^k} \Delta\phi = -\mathfrak{F}_{\rho^k}(\phi), \quad (32)$$

where

$$K_{\rho} = \begin{bmatrix} 0 & \mathfrak{L}_{u\chi} & \mathfrak{L}_{u\lambda} & 0 \\ \mathfrak{L}_{\chi u} & \mathfrak{L}_{\chi\chi} & \mathfrak{L}_{\chi\lambda} & \mathfrak{L}_{\chi\mu} \\ \mathfrak{L}_{\lambda u} & \mathfrak{L}_{\lambda\chi} & 0 & 0 \\ 0 & \mathfrak{L}_{\mu\chi} & 0 & 0 \end{bmatrix} \\ := \begin{bmatrix} 0 & (\partial_{\chi_h} \lambda^\top A_h(\chi_h))^\top & A_h(\chi_h)^\top & 0 \\ \partial_{\chi_h} \lambda^\top A_h(\chi_h) & \rho \cdot \text{diag} \left( \frac{1}{(\chi_i - a_i)^2} + \frac{1}{(b_i - \chi_i)^2} \right) & (\partial_{\chi_h} A_h(\chi_h) u_h)^\top & \mathbb{I}^\top \\ A_h(\chi_h) & \partial_{\chi_h} A_h(\chi_h) u_h & 0 & 0 \\ 0 & \mathbb{I} & 0 & 0 \end{bmatrix}.$$

Here it is important to note that  $\mathfrak{L}_{\chi\chi}$  is an easily invertible positive definite diagonal matrix, as long as  $\chi_h$  is in the interior away from the boundary of the box constraints—which is the whole point of interior point methods—and  $\rho$  is nonzero. This observation is important for the multigrid solution of the linear system (32). A primal-dual interior point formulation can be found in [12].

Based on the considerations above we consider equation (32) and rewrite it in null space formulation.

$$K \Delta\phi := \left[ \begin{array}{cc|cc} 0 & \mathfrak{L}_{\lambda u}^\top & \mathfrak{L}_{\chi u}^\top & 0 \\ \mathfrak{L}_{\lambda u} & 0 & \mathfrak{L}_{\lambda\chi} & 0 \\ \hline \mathfrak{L}_{\chi u} & \mathfrak{L}_{\lambda\chi}^\top & \mathfrak{L}_{\chi\chi} & \mathfrak{L}_{\mu\chi}^\top \\ 0 & 0 & \mathfrak{L}_{\mu\chi} & 0 \end{array} \right] \begin{pmatrix} \Delta u \\ \Delta \lambda \\ \Delta \chi \\ \Delta \mu \end{pmatrix} = \begin{pmatrix} -\nabla_{u_h} \mathfrak{L} \\ -\nabla_{\lambda} \mathfrak{L} \\ -\nabla_{\chi_h} \mathfrak{L} \\ -\nabla_{\mu} \mathfrak{L} \end{pmatrix} =: \begin{pmatrix} -\mathfrak{F}^u \\ -\mathfrak{F}^\lambda \\ -\mathfrak{F}^\chi \\ -\mathfrak{F}^\mu \end{pmatrix}. \quad (33)$$

The matrix  $\mathfrak{L}_{\lambda u} = A_h(\chi_h)$  is the stiffness matrix of the elasticity equation. We may with due justice assume that there is an approximate matrix  $\tilde{\mathfrak{L}}_{\lambda u} = \tilde{A}_h(\chi_h)$  available, which can be used in smoothing iterations for the elasticity equations ( $\tilde{\mathfrak{L}}_{\lambda u}$  may be, e.g., defined by a blockwise ILU decomposition or a Jacobi or

Gauss-Seidel iteration). We use a right transformation only with the matrix

$$K^R = \left[ \begin{array}{c|cc} I & - \begin{bmatrix} 0 & \tilde{\mathfrak{L}}_{\lambda u}^{-1} \\ \tilde{\mathfrak{L}}_{\lambda u}^{-\top} & 0 \end{bmatrix} & \begin{bmatrix} \mathfrak{L}_{xu}^\top & 0 \\ \mathfrak{L}_{\lambda x} & 0 \end{bmatrix} \\ \hline 0 & I & \end{array} \right] = \left[ \begin{array}{c|cc} I & 0 & -\tilde{\mathfrak{L}}_{\lambda u}^{-1} \mathfrak{L}_{\lambda x} & 0 \\ 0 & I & -\tilde{\mathfrak{L}}_{\lambda u}^{-\top} \mathfrak{L}_{xu}^\top & 0 \\ \hline 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{array} \right]$$

Thus we obtain the regular splitting

$$\begin{aligned} KK^R &= \left[ \begin{array}{c|cc} 0 & \mathfrak{L}_{\lambda u}^\top & 0 & 0 \\ \mathfrak{L}_{\lambda u} & 0 & 0 & 0 \\ \hline \mathfrak{L}_{xu} & \mathfrak{L}_{\lambda x}^\top & \tilde{S} & \mathfrak{L}_{\mu x}^\top \\ 0 & 0 & \mathfrak{L}_{\mu x} & 0 \end{array} \right] + \left[ \begin{array}{c|cc} 0 & \left( \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} - \begin{bmatrix} 0 & \mathfrak{L}_{\lambda u}^\top \\ \mathfrak{L}_{\lambda u} & 0 \end{bmatrix} \begin{bmatrix} 0 & \tilde{\mathfrak{L}}_{\lambda u}^{-1} \\ \tilde{\mathfrak{L}}_{\lambda u}^{-\top} & 0 \end{bmatrix} \right) & \begin{bmatrix} \mathfrak{L}_{xu}^\top & 0 \\ \mathfrak{L}_{\lambda x} & 0 \end{bmatrix} \\ \hline 0 & 0 & \end{array} \right] \\ &=: M + N \end{aligned}$$

with

$$\tilde{S} = \mathfrak{L}_{xx} - \begin{bmatrix} \mathfrak{L}_{xu} & \mathfrak{L}_{\lambda x}^\top \\ \tilde{\mathfrak{L}}_{\lambda u}^{-\top} & 0 \end{bmatrix} \begin{bmatrix} 0 & \tilde{\mathfrak{L}}_{\lambda u}^{-1} \\ \tilde{\mathfrak{L}}_{\lambda u}^{-\top} & 0 \end{bmatrix} \begin{bmatrix} \mathfrak{L}_{xu}^\top \\ \mathfrak{L}_{\lambda x} \end{bmatrix} = \mathfrak{L}_{xx} - \mathfrak{L}_{xu} \tilde{\mathfrak{L}}_{\lambda u}^{-1} \mathfrak{L}_{\lambda x} - \mathfrak{L}_{\lambda x}^\top \tilde{\mathfrak{L}}_{\lambda u}^{-\top} \mathfrak{L}_{xu}^\top.$$

For approximate inversion of  $M$  we use as approximations for the respective blocks of the block triangular matrix

$$\begin{bmatrix} 0 & \tilde{\mathfrak{L}}_{\lambda u}^\top \\ \tilde{\mathfrak{L}}_{\lambda u} & 0 \end{bmatrix} \approx \begin{bmatrix} 0 & \mathfrak{L}_{\lambda u}^\top \\ \mathfrak{L}_{\lambda u} & 0 \end{bmatrix}, \quad \begin{bmatrix} \mathfrak{L}_{xx} & \mathfrak{L}_{\mu x}^\top \\ \mathfrak{L}_{\mu x} & 0 \end{bmatrix} \approx \begin{bmatrix} \tilde{S} & \mathfrak{L}_{\mu x}^\top \\ \mathfrak{L}_{\mu x} & 0 \end{bmatrix}$$

Note that here we profit heavily from the fact that  $\mathfrak{L}_{xx}$  is a diagonal matrix and therefore cheaply invertible and that  $\mathfrak{L}_{\mu x}$  is just one row vector so that we can efficiently use the decomposition

$$\begin{bmatrix} \mathfrak{L}_{xx} & \mathfrak{L}_{\mu x}^\top \\ \mathfrak{L}_{\mu x} & 0 \end{bmatrix} = \begin{bmatrix} \mathfrak{L}_{xx} & 0 \\ \mathfrak{L}_{\mu x} & -\mathfrak{L}_{\mu x} \mathfrak{L}_{xx}^{-1} \mathfrak{L}_{\mu x}^\top \end{bmatrix} \begin{bmatrix} I & \mathfrak{L}_{xx}^{-1} \mathfrak{L}_{\mu x}^\top \\ 0 & I \end{bmatrix} \quad (34)$$

The resulting multigrid method is implemented within the PDE-toolbox *ug*[1]. For the numerical investigations we use a problem setting as depicted in figure 3. We are looking for an optimal cantilever, which is connected with a wall on the left hand side and should withstand a force pulling downward at the right bottom corner. The volume constraint is defined by  $V_0 = 1/2 |\Omega|$ . This problem is related to the ‘‘airbus’’-problem investigated in [13].

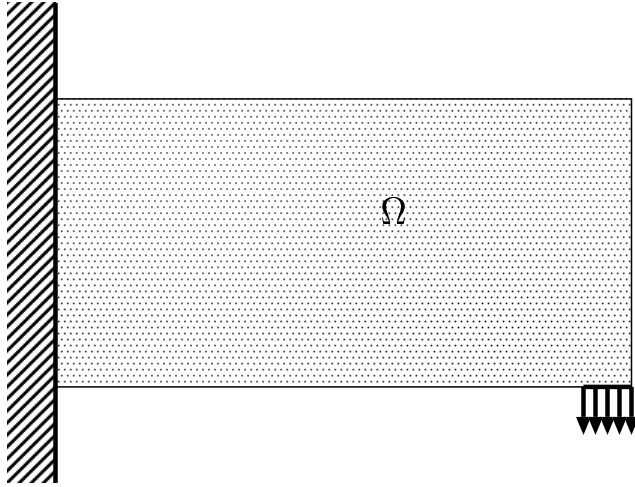


Fig. 3. *Problem setting for the numerical investigations*

For the discretization of the states  $u$  we use 8192 bilinear elements. The density  $\chi$  is evaluated at the center points of the  $u$ -grid. However, in order to avoid well known checker-board structures we use a bilinear continuous approximation for  $\chi$  as well. (For an overview on various strategies for preventing checker-board structures see, e.g., [23]) That makes in total 41725 primal and dual variables in the nonlinear problem. In figure 4 the density distribution for  $\alpha = 2$  (cf., equation (18)) can be seen for  $\rho = 10^{-6}$ . We start the iterations at  $\rho = 10^{-3}$  and get down to  $\rho = 10^{-6}$  in 45 nonlinear iterations, where we need 5 cpu-minutes per nonlinear iteration on a SGI10000. In order to reach a residual tolerance of  $\|\mathfrak{F}_\rho \phi^k\|_2 < 10^{-2}$ , we need another 10 nonlinear iterations. Each nonlinear iteration consists of 7 linear multigrid V-cycles (2 pre- and 2 post-smoothing steps) on 6 grids with a convergence rate of about 0.2. The approximation for  $\tilde{\mathcal{L}}_{\lambda u}$  is performed by an ILU-decomposition.

Here one should note that the toolbox  $ug$  is especially designed for dealing with unstructured grids and is not able to take advantage of the structured grids used here. Therefore great improvements in computing time are to be expected when taking this effect into account.



Fig. 4. *Density distribution for  $\alpha = 2$*

In figure 4 the black color indicates regions, where  $\chi = 1.0$  and the white color indicates regions, where  $\chi = 0.01$ , which has been chosen as a lower bound in order to prevent the stiffness matrix from becoming singular. Different grey shades indicate values in the interval  $(0.01, 1.0)$ . The basic structure of the figure coincides very good with the theoretical results in [10] for similar problems.

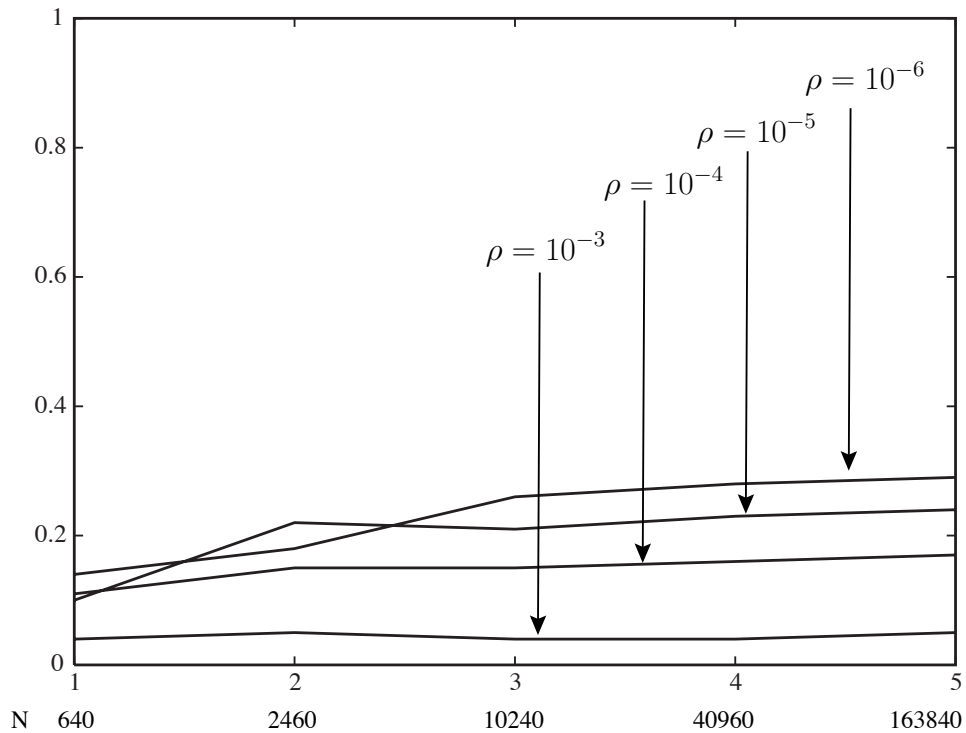


Fig. 5. *Convergence behaviour of the multigrid KKT solver*

The convergence behaviour of the multigrid method is demonstrated in figure 5. It shows average convergence rates of the KKT multigrid method for finer and finer grids and for decreasing barrier parameter  $\rho$ . Below the grid levels, there is indicated the number of all variables in the respective QP. In this figure, we can observe on the one hand an asymptotically mesh independent convergence rate as indicated by the theory and on the other hand a deterioration of this convergence rate for decreasing barrier parameter. However, a convergence rate of 0.3 in the worst case is still acceptable.

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