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ON THE PARAMETER IN AUGMENTED LAGRANGIAN PRECONDITIONING FOR ISOGEOMETRIC DISCRETIZATIONS OF THE NAVIER-STOKES EQUATIONS

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Abstract. In this paper, we deal with the optimal choice of the parameter γ for augmented Lagrangian preconditioning of GMRES method for efficient solution of linear systems obtained from discretization of the incompressible Navier-Stokes equations. We consider discretization of the equations using the B-spline based isogeometric analysis approach. We are interested in the dependence of the convergence on the parameter γ for various problem parameters (Reynolds number, mesh refinement) and especially for various isogeometric discretizations (degree and interelement continuity of the B-spline discretization bases). The idea is to be able to determine the optimal value of γ for a problem that is relatively cheap to compute and, based on this value, predict suitable values for other problems, e.g., with finer mesh, different discretization, etc. The influence of inner solvers (direct or iterative based on multigrid method) is also discussed.

Keywords: isogeometric analysis; augmented Lagrangian preconditioner; Navier-Stokes equations

MSC 2020: 35Q30, 65F08, 65M60, 76D05

1. Introduction

Discretization of the linearized stationary and also implicitly discretized time-dependent incompressible Navier-Stokes equations leads to nonsymmetric linear systems of saddle-point type. Solving these linear systems typically takes the majority of the computational effort during the solution process. Therefore, we are interested in efficient iterative solution of these linear systems.

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We consider a particular spatial discretization approach called isogeometric analysis (IgA) [5], [11]. We are interested specifically in the IgA discretization for several reasons. First, it allows exact representation of the computational domain geometry, which is very important in applications, where a good resolution of the solution near the boundaries is essential. Furthermore, it is suitable for the purpose of automatic shape optimization. Isogeometric analysis has many common features with the widely used finite element method: it is based on Galerkin method using basis functions with compact supports, which leads to sparse matrices. On the other hand, there are some important differences that influence properties of the resulting matrices. The isogeometric basis functions (B-spline or NURBS) are generally of higher continuity across the boundaries of individual elements, which makes the IgA matrices denser than those for standard finite elements with basis functions of the same degree.

We choose to solve the linear systems with a preconditioned Krylov subspace method (GMRES). In the recent paper [10], we compared several state-of-the-art block preconditioners for the Navier-Stokes equations and investigated their convergence for IgA discretizations of various degree and interelement continuity as well as different problem parameters such as mesh refinement and Reynolds number. Namely, the pressure convection-diffusion (PCD) preconditioner [12], [15], least-squares commutator (LSC) preconditioner [6], several SIMPLE-type preconditioners (SIMPLE, SIMPLER, MSIMPLER) [18], [19] and augmented Lagrangian preconditioner (AL) [3] and its modified version (MAL) [4] were involved in the comparison. Based on the experiments, we concluded that the block preconditioners can be successfully used for IgA discretizations of the Navier-Stokes equations. The augmented Lagrangian (AL) preconditioner stood out among others with its robustness with respect to all problem parameters. However, the application of this preconditioner is very expensive. Its modified version (MAL), which is cheaper to apply, did not seem that robust, but both AL and MAL depend on a parameter γ, which can influence the convergence significantly and only a fixed value of that parameter was used in all experiments in [10].

In the present paper, we study the dependence of AL and MAL on the parameter γ in more detail. We performed extensive numerical tests for two two-dimensional problems (a backward facing step and a turbine blade profile) and various IgA discretizations and problem parameters. We present the results for the first mentioned problem and comment on the observations that were also verified for the second problem. In [4], Benzi et al. give an empirical rule for the choice of an optimal γ depending on the mesh refinement and present numerical results for several FEM discretizations of the stationary and time-dependent Navier-Stokes equations. One of our main goals is to assess if this optimal value can be predicted for different IgA

discretizations. We consider ideal versions of the preconditioners, where all subproblems are solved with a direct method, and also MAL with approximate solvers for the subproblems.

The text is organized as follows. In Section 2, we formulate the incompressible Navier-Stokes equations and briefly comment on their Galerkin discretization and the basics of isogeometric analysis. The concept of block triangular preconditioners and the AL-based preconditioners are described in Section 3. The results of the numerical experiments are presented in Section 4 and some concluding remarks are given in Section 5.

2. Problem formulation

In this section, we formulate the incompressible Navier-Stokes equations and introduce the linear system resulting from their discretization. We also briefly comment on isogeometric analysis, the discretization approach considered in this work.

2.1. The Navier-Stokes equations. The incompressible Navier-Stokes equations represent a mathematical model describing motion of an incompressible viscous Newtonian fluid. The stationary boundary value Navier-Stokes problem is given as follows: for a bounded domain $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ with the boundary $\partial\Omega$ consisting of two disjoint parts, Dirichlet $\partial\Omega_D$ and Neumann $\partial\Omega_N$, find the velocity field $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{x})$ and pressure field $p = p(\boldsymbol{x})$ such that

$$
\begin{aligned}
-\nu\Delta\boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} + \nabla p &= \boldsymbol{0} && \text{in } \Omega,\\
\nabla\cdot\boldsymbol{u} &= 0 && \text{in } \Omega,\\
\boldsymbol{u} &= \boldsymbol{g}_D && \text{on } \partial\Omega_D,\\
\nu\frac{\partial\boldsymbol{u}}{\partial\boldsymbol{n}} - \boldsymbol{n}p &= \boldsymbol{0} && \text{on } \partial\Omega_N,
\end{aligned}
\tag{2.1}
$$

where ν is the kinematic viscosity and $\boldsymbol{g}_D$ is a given function. We note that the equations are nonlinear due to the convective term $\boldsymbol{u}\cdot\nabla\boldsymbol{u}$.

The character of the flow depends on the ratio of inertial forces to viscous forces, which is characterized by the so-called Reynolds number, a dimensionless quantity defined as $\mathrm{Re} = UL/\nu$, where L is a characteristic length scale of the computational domain and U is a reference velocity.

2.2. Discretization. We consider discretizations of problem (2.1) based on Galerkin method with inf-sup stable pairs of discretization spaces together with Picard linearization of the convective term. The Galerkin method is based on a weak

formulation of the problem and solving the problem projected onto finite dimensional subspaces of the solution and test spaces. Particular Galerkin-based methods are defined by the choice of these subspaces and their bases. The discretization leads to nonsymmetric saddle-point type linear systems of the form

$$\begin{bmatrix} F & B^\top \\ B & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}, \tag{2.2}$$

where F is block diagonal with d diagonal blocks consisting of the discretization of the viscous term and the linearized convective term, $B^\top$ and B are discrete gradient and negative divergence operators, respectively. Nonzero elements in the right-hand side vectors f and g arise due to Dirichlet boundary conditions.

In the case of a time-dependent problem, the first equation of (2.1) contains time derivative of the velocity. We discretize the time derivative first, using an implicit time-stepping procedure, which leads to a sequence of spatial problems that can be discretized similarly to the stationary case. The discretization of the time-dependent problem leads to linear systems of the same block structure as (2.2), the only difference is that the terms arising from the discretized time derivative appear in the block F and in the right-hand side vector f. The term that is added to the block F is of the form $(\Delta t)^{-1} M_u$, where Δt is the time discretization step and M_u is the velocity mass matrix.

The most popular discretization method based on Galerkin method is the finite element method (FEM), where the domain Ω is first divided into simple subdomains (elements) forming a computational mesh. As a consequence, the domain boundary $\partial\Omega$ has to be approximated in most cases. The basis functions of the finite dimensional solution and test spaces are defined as piecewise polynomials with supports containing only a few elements. Therefore, FEM discretization results in sparse matrices. More details on Galerkin and finite element discretization of fluid flow problems including the Navier-Stokes equations can be found, e.g., in [7].

2.3. Isogeometric analysis. We consider a different Galerkin-based discretization approach called isogeometric analysis (IgA), see [5], [11]. One of its main goals is to avoid the meshing step and work with the exact geometry of the domain Ω. In industrial practice, the computational domain is usually a complex model created using CAD (Computer Aided Design) tools, where the geometry is typically represented by B-spline and NURBS objects. Isogeometric analysis is based on the isoparametric concept, which means that the basis functions used for the geometry representation are also used as a basis of the solution and test spaces. Thus, we work with B-spline or NURBS basis functions in IgA.

The B-spline basis functions form a canonical basis of spline function spaces. A kth degree spline function $s\colon [a,b] \to \mathbb{R}$, over a partition of the interval $[a,b]$ defined by a vector $\mathbf{x} = (x_0, x_1, \ldots, x_\ell)$, where $a = x_0 < x_1 < \ldots < x_{\ell-1} < x_\ell = b$, is defined as a piecewise polynomial function such that

- ▷ s is a polynomial of degree at most k in the intervals $[x_i, x_{i+1})$ for $i = 0, \ldots, \ell-1$,
- ▷ s has r_i continuous derivatives at x_i for $i = 1, \ldots, \ell-1$.

The definition of a B-spline basis of a given degree k is based on a so-called knot vector $\Xi = (\xi_1, \xi_2, \ldots, \xi_{n+k+1})$, where n is the dimension of the spline space. The knot vector is obtained from the vector $\mathbf{x}$ by repeating x_i such that its multiplicity is $m_i = k - r_i$ for $i = 1, \ldots, \ell-1$. The ith B-spline basis function of degree k, $N_{i,k}(\xi)$, is defined recursively as follows:

$$
\begin{aligned}
N_{i,0}(\xi) &= \begin{cases} 1, & \xi_i \leqslant \xi < \xi_{i+1}, \\ 0, & \text{otherwise}, \end{cases} \\
N_{i,k}(\xi) &= \omega_{i,k}(\xi) N_{i,k-1}(\xi) + (1 - \omega_{i+1,k}(\xi)) N_{i+1,k-1}(\xi) \quad \text{for } k > 0,
\end{aligned}
\tag{2.3}
$$

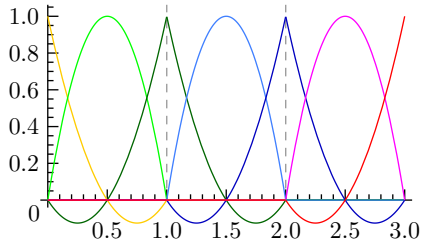
where

$$
\omega_{i,k}(\xi) = \begin{cases} \dfrac{\xi - \xi_i}{\xi_{i+k} - \xi_i}, & \xi_i \neq \xi_{i+k}, \\ 0, & \text{otherwise}. \end{cases}
\tag{2.4}
$$

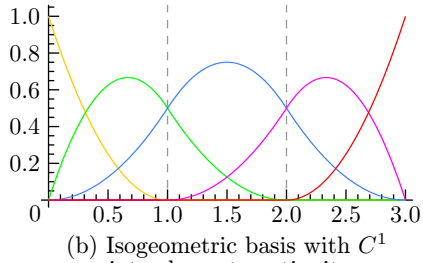
The NURBS basis functions are a rational generalization of B-splines. Both B-spline and NURBS basis functions share some important features, for example, they are all pointwise nonnegative, form a partition of unity and the support of each basis function is $k+1$ knot spans. We limit ourselves to B-spline bases in this work.

In IgA, we usually work with so-called open knot vectors, where the first and the last knot are repeated $k+1$ times, which corresponds to no continuity conditions at the endpoints of the interval $[a,b]$. We refer to the basis as C^r-continuous if the multiplicity of all inner knots is $m_i = k - r$ for all i. The highest possible continuity of a kth degree basis is C^{k-1}.

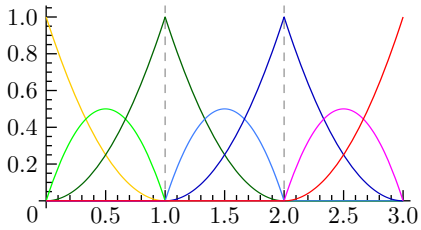
In higher dimensions ($d > 1$), given a degree and a knot vector in each direction, a multivariate B-spline basis is formed by a tensor-product of the univariate B-spline bases. For example, for $d = 2$, degrees k, l and knot vectors Ξ, Ψ, the basis consists of the functions $Q^{k,l}_{i,j}(\xi, \psi) = N_{i,k}(\xi) N_{j,l}(\psi)$, where $N_{i,k}(\xi)$ and $N_{j,l}(\psi)$ are the univariate B-spline basis functions for the knot vectors Ξ and Ψ, respectively. The computational mesh on a domain described as a B-spline surface in $\mathbb{R}^2$ is given by the product of the two knot vectors $\Xi \times \Psi$. Thus, if the subsequent knots are different from each other, i.e., $\xi_i \neq \xi_{i+1}$ and $\psi_j \neq \psi_{j+1}$ for a given i, j, then $[\xi_i, \xi_{i+1}] \times [\psi_j, \psi_{j+1}]$ defines an element.



(a) Finite element basis.



(b) Isogeometric basis with C^1 interelement continuity.



(c) Isogeometric basis with C^0 interelement continuity.

Figure 1. Comparison of 1D quadratic discretization bases on a "mesh" with three elements in standard FEM and IgA.

Figure 1 shows a comparison of univariate quadratic bases on a "mesh" with three equal elements: a standard FEM basis, a C^1- and a C^0-continuous B-spline basis. One of the main differences between FEM and IgA is that the classical FEM basis functions are interpolatory and thus their coefficients obtained from the linear system (2.2) correspond to the nodal values of the finite element solution. This is not true for IgA. Another important difference is that IgA allows various interelement continuity. On the other hand, one of the important common features of the two methods is a compact support of the basis functions, which results in sparse linear systems. However, high-continuity of IgA leads to denser matrices than FEM due to larger overlaps of the basis function supports.

For more details on the IgA discretization of the Navier-Stokes equations, we refer to [2], [1], [10] and the references therein.

3. Solution methods

We consider approximate solution of linear system (2.2) using the preconditioned GMRES method. Some of the state-of-the-art preconditioners for the linear systems resulting from the discretization of the incompressible Navier-Stokes equations are based on the block LU decomposition of the saddle-point matrix

$$\mathcal{A} = \begin{bmatrix} F & B^\top \\ B & 0 \end{bmatrix} = \begin{bmatrix} I & 0 \\ BF^{-1} & I \end{bmatrix} \begin{bmatrix} F & B^\top \\ 0 & S \end{bmatrix}, \tag{3.1}$$

where $S = -BF^{-1}B^\top$ is the Schur complement of F in $\mathcal{A}$. If the system is preconditioned from the right with the matrix

$$\mathcal{P} = \begin{bmatrix} F & B^\top \\ 0 & S \end{bmatrix}, \tag{3.2}$$

then the preconditioned matrix $\mathcal{A}\mathcal{P}^{-1}$ is lower block triangular with identity diagonal blocks, hence with all eigenvalues equal to one. As shown in [14], GMRES would converge in at most two iterations in this case. However, constructing and applying such preconditioner would be impractical, especially the construction of and solving systems with S would be very expensive, since it is typically a dense matrix.

A class of preconditioners based on (3.2) is called block triangular preconditioners. The idea is that the matrix S is replaced by an approximation $\widehat{S} \approx S$. The application of the preconditioner, i.e., solving a linear system with the matrix $\mathcal{P}$, includes solving two smaller linear systems, one with the matrix F and one with $\widehat{S}$. Solving the linear system with $\widehat{S}$ often includes solving subproblems with a Poisson-type matrix. If all these subproblems are solved with a direct method, we talk about an ideal version of the preconditioner. Alternatively, they can be solved approximately, e.g., by a small number of iterations of an iterative method or one or more V-cycles of a suitable multigrid solver. Two main representatives of block triangular preconditioners are pressure convection-diffusion (PCD) preconditioner [12], [15] and least-squares commutator (LSC) preconditioner [6]. Another preconditioning technique which also belongs to the class of block triangular preconditioners is the augmented Lagrangian (AL) preconditioner [3].

In paper [10], we presented a comparison of the ideal versions of the above-mentioned methods and several SIMPLE-type preconditioners for various IgA discretizations of the incompressible Navier-Stokes equations. Here we are interested in some aspects of the AL preconditioner, which will be described in more detail in the following.

3.1. Augmented Lagrangian preconditioners. In the augmented Lagrangian approach, the original system (2.2) is replaced by an equivalent system

$$\begin{bmatrix} F_\gamma & B^\top \\ B & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f_\gamma \\ g \end{bmatrix}, \tag{3.3}$$

where $F_\gamma = F + \gamma B^\top W^{-1} B$, $f_\gamma = f + \gamma B^\top W^{-1} g$, $\gamma > 0$ is a parameter and W is a positive definite matrix. Denote the coefficient matrix of the augmented system (3.3) as $\mathcal{A}_\gamma$. System (3.3) is then preconditioned with the block triangular preconditioner

$$\mathcal{P}_{\mathrm{AL}} = \begin{bmatrix} F_\gamma & B^\top \\ 0 & \widehat{S}_{\mathrm{AL}} \end{bmatrix}, \tag{3.4}$$

where the inverse of the Schur complement approximation is given by

$$\widehat{S}_{\mathrm{AL}}^{-1} := -\nu \widehat{M}_p^{-1} - \gamma W^{-1} \tag{3.5}$$

and $\widehat{M}_p$ is a pressure mass matrix approximation, usually a diagonal matrix. The matrix W is often chosen to be equal to $\widehat{M}_p$. We set $W = \widehat{M}_p$ and $\widehat{M}_p$ equal to the main diagonal of the pressure mass matrix.

Generally, a large value of the parameter γ would lead to small number of iterations of the preconditioned Krylov subspace method. However, as pointed out in [3], the block F_γ becomes increasingly ill-conditioned for large γ, since $B^\top W^{-1} B$ is obviously a singular matrix. Therefore, it is often set $\gamma \approx 1$. The conditioning of F_γ also influences the conditioning of the whole system matrix $\mathcal{A}_\gamma$ and thus the quality of the obtained approximate solution of (3.3), which will be commented on later.

The main difficulty of this approach is solving the subsystems with the matrix F_γ. The additional term $\gamma B^\top W^{-1} B$ makes the matrix denser than the block F and introduces a coupling between the velocity components, which is not present in the discretization of the Picard linearization of the Navier-Stokes equations. Direct solution of these subsystems becomes very expensive and effective approximate solution requires specialized solvers, see [3], [8].

One way to simplify the solution of the systems with F_γ is the modified AL preconditioner (MAL) [4]. The idea is to replace F_γ by its block triangular part. For example, in two dimensions, if we partition the matrix into blocks corresponding to the velocity components

$$F_\gamma = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \tag{3.6}$$

the modified approach suggests to use the matrix

$$\widetilde{F}_\gamma = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} \tag{3.7}$$

instead. Thus, instead of solving the whole system at once, we solve d smaller systems with the blocks A_{ii}, $i = 1, \ldots, d$. These blocks can be interpreted as discrete anisotropic convection-diffusion operators. Let us denote the resulting preconditioner as $\mathcal{P}_{\mathrm{MAL}}$.

We are interested in the dependence of the behavior of the AL-based preconditioners on the parameter γ for different IgA discretizations. We present numerical experiments mainly for the ideal versions of the preconditioners, but we also involve some experiments for MAL with approximate solution of the subproblems. As an

approximate solver we choose a multigrid method using a standard V-cycle with different smoothers. We are aware that the chosen inner solvers are not the best possible choice for the problems of anisotropic convection-diffusion type, moreover, discretized by isogeometric analysis. However, the main aim of these experiments is not to find an optimal inner solver, but to investigate how the optimal value of the parameter γ changes when replacing the direct inner solvers with approximate solvers.

4. Numerical experiments

We present comparisons of the iterative solution of the linear systems obtained from various IgA discretizations of the incompressible Navier-Stokes equations for a well-known benchmark problem of flow in a simple backward facing step geometry in 2D. The linear systems are solved with the GMRES method preconditioned with the AL and MAL preconditioners described above. The main attention is paid to the influence of the value of the parameter γ. We performed similar experiments also for a more complex two-dimensional domain from industrial practice, a 2D blade row that stems from a simplified problem of flow in a water turbine. However, since the blade shape is described using cubic B-splines, it is not possible to construct discretizations of arbitrary degree and continuity while preserving the exact geometry representation. Therefore, we present only the results for the backward facing step domain which can be described using B-splines of arbitrary degree $k = 1, 2, \ldots$ and all possible continuities from C^0 to C^{k-1}. We verified our observations also for the blade row problem and we comment on these results in the conclusion of this paper.

The linear systems solved in the experiments are obtained after performing several Picard iterations (steady problem) or time steps (time-dependent problem). We solve each system using GMRES with no restarts with AL and MAL preconditioners with different values of the parameter γ. Although it is preferable to start the iteration from the solution computed in the most recent Picard iteration or time step in practical computations, we choose the initial solution equal to the zero vector in all cases for our comparison. From our experience, the number of linear iterations starting from the zero initial vector is almost the same in every Picard iteration (after some initial phase) and every time step. Thus, studying the number of iterations at a particular iteration/time step is reasonable for our purpose. The stopping criterion will be discussed later in this section.

The linear systems are obtained from an in-house isogeometric fluid flow solver which is implemented in C++ in the framework of G+Smo (Geometry and Simulation modules) library (see [13]). We also implemented the tested preconditioners in the framework of G+Smo, exploiting the available linear algebra tools that are

mostly inherited from the Eigen library [9]. Specifically, we use the sparse LU direct solver, the incomplete LU decomposition with a dual threshold strategy (ILUT) and the Jacobi solver available in Eigen.

We compare the convergence of GMRES for a set of values of the parameter γ for discretizations with various degree and continuity, different Reynolds numbers and also different meshes. We consider time-dependent problems with two different values of the time step Δt.

Along with these convergence properties, we also observe their dependence on the problem parameters (discretization, Reynolds number and mesh refinement level) for particular values of γ. Robustness with respect to these parameters is also an important criterion for choosing a suitable value of γ.

In the following we will use the designation k, C^r for the discretization with C^r-continuous basis functions of degree k for pressure and $k+1$ for velocity. Further, we will denote by γ_{opt} an experimentally found "optimal" value of the parameter γ, determined as the value with the least number of GMRES iterations from a set of experiments with different values of γ. These values are chosen from the interval $[0.01, 100000]$ with a variable step between two subsequent values. However, they are plotted equidistantly on the x-axis of the presented graphs.

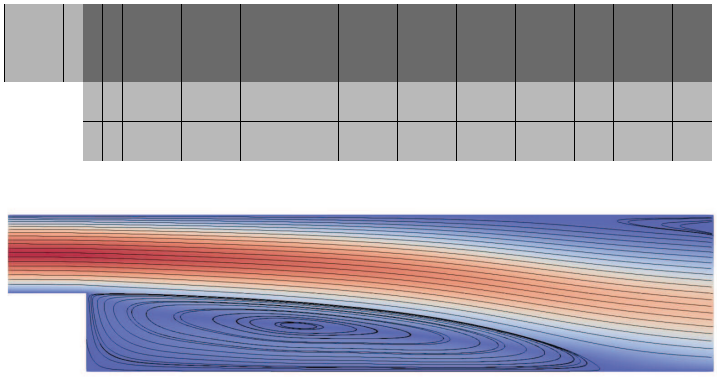


Figure 2. Backward facing step 2D domain: computational mesh M1 (up), illustration of a steady velocity field (down).

Backward facing step. We consider a problem of flow over a 2D backward facing step of height $h = 1$. The computational domain and a velocity field of a steady flow with viscosity $\nu = 0.004$ are shown in Figure 2 for illustration. The rightmost vertical boundary is defined as $\partial\Omega_N$ (the outflow) and the rest of the boundaries form $\partial\Omega_D$. A parabolic inlet velocity profile with maximum of 1 is defined at the leftmost vertical boundary (the inflow) and the rest of $\partial\Omega_D$ is a no-slip wall with zero velocity. The

characteristic length L in the definition of the Reynolds number is chosen equal to the step height. Setting the characteristic velocity U equal to the maximum inlet velocity, the Reynolds number is $\mathrm{Re} = UL/\nu = 1/\nu$.

The computational domain consists of three rectangular patches (see Figure 2, top) that can be described as B-spline surfaces of arbitrary degree k. We consider several parametrizations of the domain using B-splines of degree k varying from 1 to 4 and with C^0 to C^{k-1} interelement continuity in the interior of the patches. We use conforming meshes, where the patches are connected by identifying the corresponding basis functions at the interfaces, hence the continuity along the patch interfaces is always C^0.

We investigate four uniform meshes, the coarsest of which (denoted as M1) is shown in Figure 2 (top) and the other meshes are obtained by one (M2), two (M3) and three (M4) additional uniform refinements. Table 1 shows the number of degrees of freedom (DOFs), the number of nonzeros and the density of the system matrix in (2.2) for various IgA discretizations with the mesh M3 for illustration of the matrix properties.

	DOFs	nonzeros	density
$1, C^0$	38769	960292	0.06%
$2, C^0$	95233	3968584	0.04%
$2, C^1$	40378	2346622	0.14%
$3, C^0$	177809	11084516	0.04%
$3, C^1$	97802	8212490	0.09%
$3, C^2$	42005	4394180	0.25%
$4, C^0$	286497	24903928	0.03%
$4, C^1$	181338	20480014	0.06%
$4, C^2$	100389	14075224	0.14%
$4, C^3$	43650	7142158	0.37%

Table 1. Number of degrees of freedom, nonzero elements and density of the matrices for the mesh M3.

As already mentioned, the block F_γ and the augmented system matrix $\mathcal{A}_\gamma$ are increasingly ill-conditioned as γ grows. To see how fast the growth is with respect to γ, we present an example for the matrices obtained for two discretizations of the steady backward facing step problem in Figure 3. The condition numbers were computed using the function `condest` in Matlab. It seems that the condition number of F_γ grows approximately linearly with γ for larger values of γ. The growth of the condition number of $\mathcal{A}_\gamma$ is also linear at first, but rather quadratic for large values of γ. We also show the condition number of the preconditioned matrix $\mathcal{A}_\gamma \mathcal{P}_{\mathrm{AL}}^{-1}$, which is very close to 1 for $\gamma > 100$, especially for the low degree discretization. The

dependence of the condition number of $\mathcal{A}_\gamma \mathcal{P}_{\mathrm{MAL}}^{-1}$ is not so straightforward, but it reaches a minimum for a relatively small value of γ and then grows again.

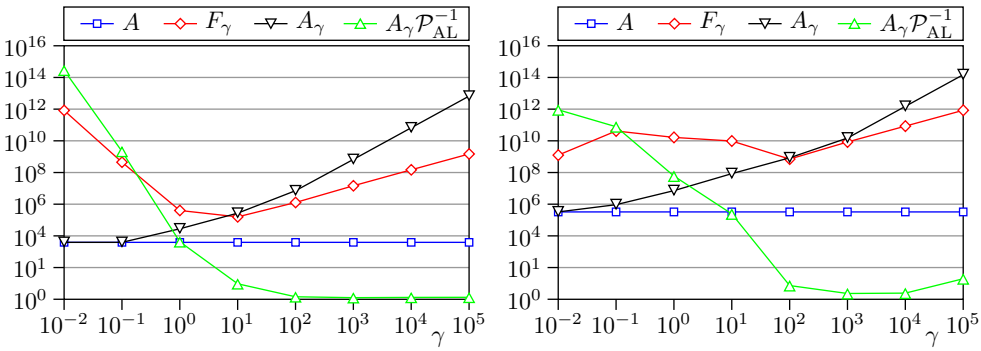


Figure 3. Condition numbers of the matrices $\mathcal{A}$, F_γ, $\mathcal{A}_\gamma$ and $\mathcal{A}_\gamma \mathcal{P}_{\mathrm{AL}}^{-1}$ with respect to the value of γ for the steady problem with $\nu = 0.004$ on the mesh M1 for the discretization $1, C^0$ (left) and $4, C^3$ (right).

The stopping criterion for Krylov subspace methods is usually such that the relative residual norm smaller than a given tolerance ε is reached. However, a small residual norm may say nothing about the quality of the approximate solution if the system matrix is ill-conditioned. The solutions obtained with GMRES with AL-based preconditioning with a fixed stopping tolerance ε become very inaccurate for large γ. We define an "error" of the approximate solution ($\mathbf{u}_{\mathrm{GMRES}}$) as

$$\text{error} = \frac{\|\mathbf{u}_{\mathrm{GMRES}} - \mathbf{u}_{\mathrm{direct}}\|_2}{\|\mathbf{u}_{\mathrm{direct}}\|_2}, \tag{4.1}$$

where $\mathbf{u}_{\mathrm{direct}}$ is a solution of the original system (2.2) obtained with the sparse LU direct solver mentioned above. For illustration, we display the error of the solutions obtained with the AL preconditioner with $\varepsilon = 10^{-6}$ for a steady and unsteady problem in Figure 4. We note that the convergence of GMRES is very fast for large γ (only a few iterations), but these solutions are obviously useless, especially in the unsteady case. Therefore, we decided to use a different stopping criterion based on the error (4.1) for the purpose of this paper. Specifically, the GMRES iteration is stopped when the error is smaller than 10^{-6} in all presented experiments. This is not practically applicable, but it can be used here to assess the optimality of the parameter γ. In practice, a residual-based stopping criterion with a tolerance dependent on the value of γ should be probably used to obtain solutions of comparable quality. Our preliminary experiments indicate that the appropriate stopping tolerance for the residual norm could be of the form ε/γ or ε/γ^2 in accordance with the growth of the condition number of $\mathcal{A}_\gamma$, but its proper formulation would require a further research which is beyond the scope of this paper.

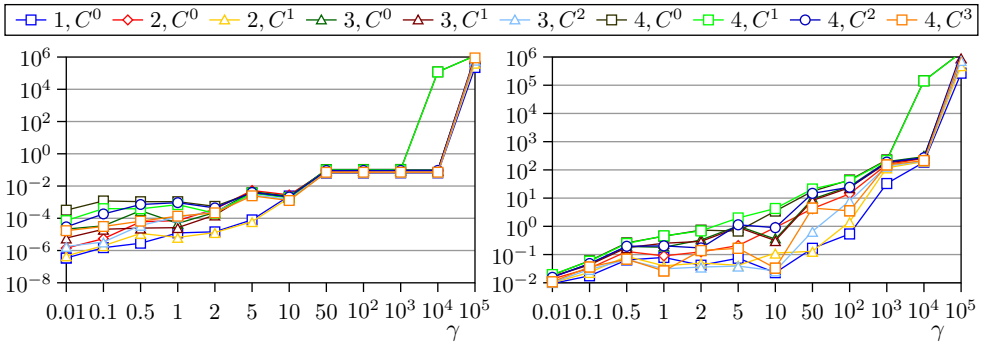


Figure 4. Ideal AL preconditioner, mesh M3, $\nu = 0.004$: solution error for the steady problem (left) and the unsteady problem with $\Delta t = 0.01$ (right), residual-based stopping criterion with $\varepsilon = 10^{-6}$.

4.1. Augmented Lagrangian preconditioner—ideal version. This section is devoted to experiments with the ideal version of the AL preconditioner. It means that all subsystems are solved with direct solver as mentioned before.

4.1.1. Steady case. The number of iterations for the tested values of γ for different IgA discretizations are shown in Table 2 and illustrated in Figure 5 (left). Some entries of the last column of the table are marked with a star *, because the solution error did not converge to the required tolerance even in 1000 iterations in these cases. The error reaches the values $5.7 \cdot 10^{-6}$ $(4, C^0)$, $1.5 \cdot 10^{-6}$ $(4, C^1)$ and $1.2 \cdot 10^{-6}$ $(4, C^3)$ in the third iteration, where the most of the cases converged. For more insight into the convergence, we show the residual and error evolution during 50 GMRES iterations for the discretization $4, C^3$ in Figure 6. We observe that the smallest attainable error increases with increasing γ. The plots also indicate that the residual-based stopping criterion, which would be used in practice, should be chosen carefully for large γ. Both residual and error drop very quickly in the first iterations, but the error may increase significantly in another few iterations.

From the results in Table 2, it turns out that the convergence of the AL preconditioner is quite fast with $\gamma = 1$, which is often used, however, it deteriorates a bit with the degree of the discretization. For larger values of γ, the convergence is even faster and it requires only a few iterations for all tested discretizations.

An example of how the relative residual norm of the converged solution decreases for increasing value of γ independently of particular discretization is shown in Figure 5 (right) for the mesh M3. As the mesh is refined, the numbers of iterations decrease (see Figure 7, right). If γ is sufficiently large, there are almost no differences in convergence for cases with different mesh refinements and discretizations. The convergence is almost independent of viscosity (see Figure 7, left), especially for large values of γ.

num. of iter. \ γ	0.01	0.1	0.5	1	2	5	10	50	10^2	10^3	10^4	10^5
$1, C^0$	103	19	9	7	6	5	5	4	4	4	4	3
$2, C^0$	88	17	9	7	6	5	5	4	4	4	4	3
$2, C^1$	99	18	9	7	6	5	5	4	4	4	4	3
$3, C^0$	124	23	10	7	6	5	5	4	4	4	4	3
$3, C^1$	108	21	10	8	6	5	5	4	4	4	4	3
$3, C^2$	154	24	10	8	7	6	5	4	4	4	4	3
$4, C^0$	323	65	26	19	14	10	8	6	5	4	4	1000*
$4, C^1$	236	43	17	12	9	7	6	5	4	4	4	1000*
$4, C^2$	360	63	24	17	12	8	7	5	5	4	4	3
$4, C^3$	464	76	23	15	10	7	6	4	4	4	4	1000*

Table 2. GMRES iteration count with the ideal AL preconditioner for the steady problem on the mesh M3, $\nu = 0.004$.

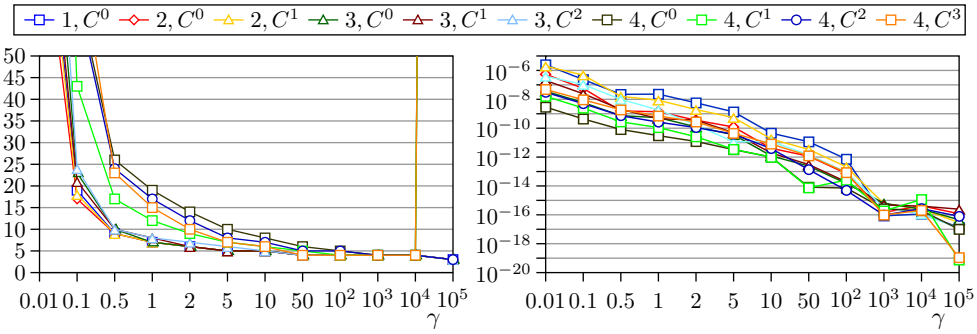


Figure 5. Ideal AL preconditioner, steady problem, $\nu = 0.004$, mesh M3: GMRES iteration count (left) and relative residual norm (right) for different discretizations.

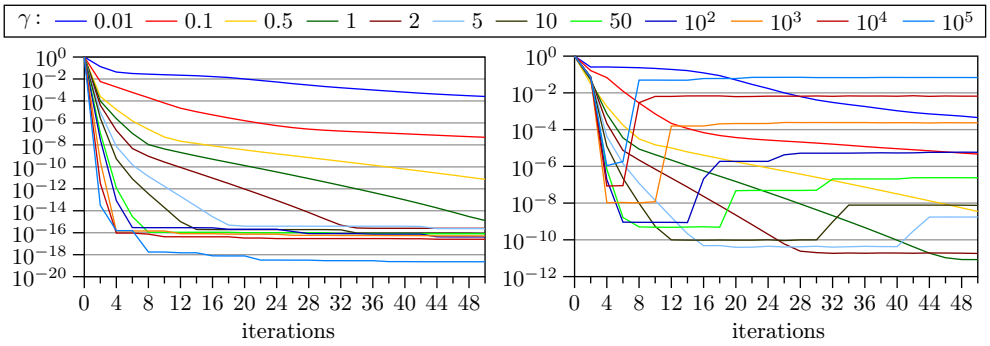


Figure 6. Ideal AL preconditioner, steady problem, $\nu = 0.004$, mesh M3, discretization $4, C^3$: evolution of relative residual norm (left) and corresponding error (right) for different values of γ.

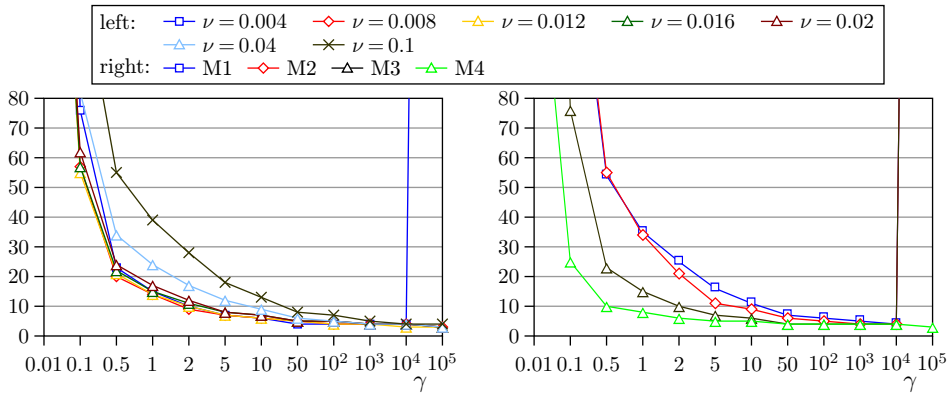


Figure 7. Ideal AL preconditioner, steady problem, discretization $4, C^3$: GMRES iteration count for different viscosity values on the mesh M3 (left) and for different meshes with $\nu = 0.004$ (right).

4.1.2. Unsteady cases. Similarly to the steady case, in the unsteady case with time step $\Delta t = 0.01$, the fastest convergence is achieved for high values of the parameter γ (see Table 3). Although the stopping tolerance is not reached in two cases again (marked by star $*$ in the table) the solutions have errors $5.2 \cdot 10^{-6}$ in the fifth iteration $(4, C^0)$ and $1.4 \cdot 10^{-6}$ in the sixth iteration $(4, C^1)$. The relative residual norms (see Figure 8, left) are significantly smaller than in the steady case in general, thus, a more strict residual-based stopping tolerance might be needed to solve unsteady problems. The number of iterations is dependent on the mesh refinement, but only in the case of small values of γ. If the value of γ is sufficiently large, the number of iterations is almost constant for all meshes (see Figure 8, right for illustration). A similar observation can be done for viscosity dependence—a weak dependence for smaller values of γ, whereas there is no dependence for larger values.

num. of iter. \ γ	0.01	0.1	0.5	1	2	5	10	50	10^2	10^3	10^4	10^5
$1, C^0$	248	156	80	59	43	30	23	14	12	8	6	5
$2, C^0$	323	148	69	50	37	26	20	12	11	7	6	5
$2, C^1$	250	140	68	50	37	26	20	12	11	7	6	5
$3, C^0$	371	138	63	44	33	23	18	12	10	7	6	5
$3, C^1$	318	133	61	44	33	23	18	12	10	7	6	5
$3, C^2$	262	127	61	45	34	23	18	12	10	7	6	5
$4, C^0$	423	147	66	47	34	24	18	11	10	7	6	1000*
$4, C^1$	357	127	57	40	30	21	17	11	10	7	6	1000*
$4, C^2$	335	131	60	43	31	21	17	11	10	7	6	6
$4, C^3$	263	117	55	41	30	22	17	11	10	7	6	5

Table 3. GMRES iteration count with the ideal AL preconditioner for the unsteady ($\Delta t = 0.01$) problem on the mesh M3, $\nu = 0.004$.

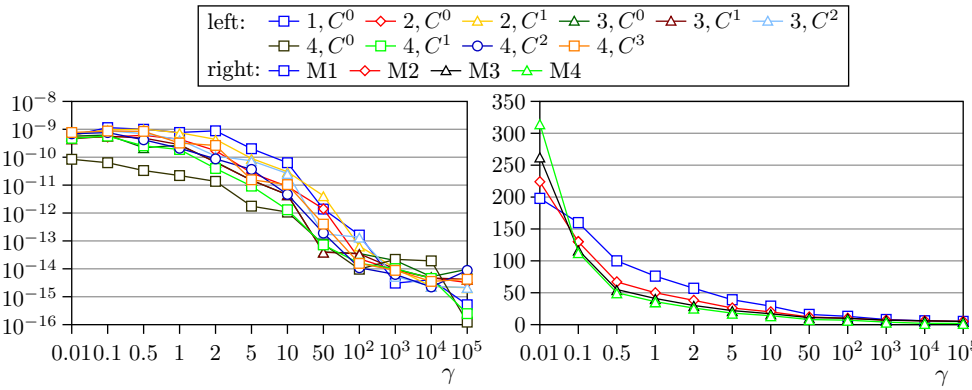


Figure 8. Ideal AL preconditioner, unsteady ($\Delta t = 0.01$) problem, $\nu = 0.004$: relative residual norm for different discretizations on the mesh M3 (left), GMRES iteration count for the discretization $4, C^3$ on different meshes (right).

All observations made for $\Delta t = 0.01$ are also valid in the case of a smaller time step $\Delta t = 0.001$.

4.2. Modified augmented Lagrangian preconditioner—ideal version. This section is devoted to experiments with the ideal version of the MAL preconditioner. The modified version has different properties (with respect to changing values of the parameter γ) than the original AL preconditioner.

4.2.1. Steady case. In the steady case, the optimal value of the parameter γ is around the value 0.1 for all considered discretizations (see Figure 9, left for illustration). The values of relative residual norm are shown in Figure 9 (right). In contrast with AL case, these values are dependent on the discretization—when the value of γ is near γ_{opt}, relative residual norms decrease when the degree of basis function increases.

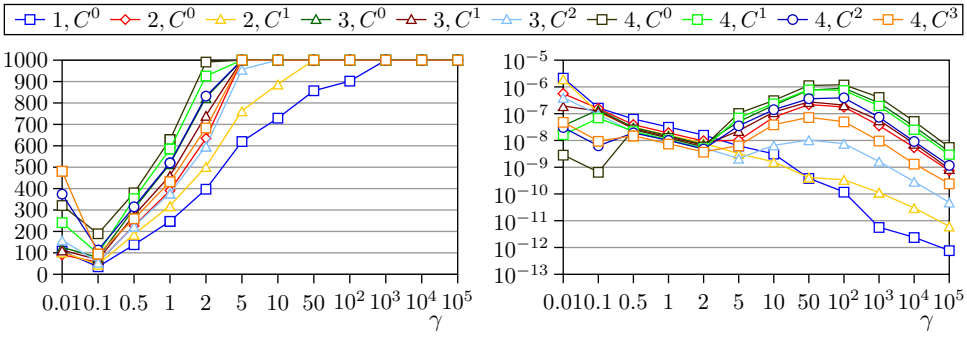


Figure 9. Ideal MAL preconditioner, steady problem, $\nu = 0.004$, mesh M3: GMRES iteration count (left) and error (right) for different discretizations.

The values of γ_{opt} and the corresponding numbers of iterations for individual discretizations are given in Table 4 in detail. The iteration counts increase when the degree of basis functions increases, while they decrease when the mesh is refined. The convergence is less dependent on particular discretization when the computational mesh is finer. Experiments also show that the convergence accelerates with the mesh refinement for values close to γ_{opt}, whereas the convergence slows down for other values of γ (see Figure 10, right). Numbers of iterations increase when the value of viscosity decreases, however, for values of γ close to γ_{opt}, there is almost no dependence on the viscosity value (see Figure 10, left).

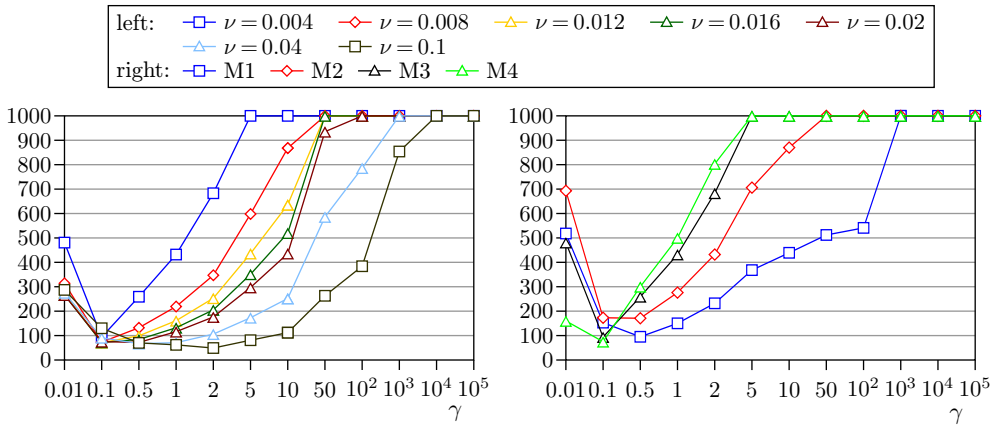


Figure 10. Ideal MAL preconditioner, steady problem, discretization $4, C^3$: GMRES iteration count for different viscosity values on the mesh M3 (left) and for different meshes with $\nu = 0.004$ (right).

	M1		M2		M3		M4		common
	γ_{opt}	iter.	γ_{opt}	iter.	γ_{opt}	iter.	γ_{opt}	iter.	ratio
$1, C^0$	0.12	29	0.08	31	0.065	31	0.055	31	1.3
$2, C^0$	0.11	48	0.065	37	0.04	32	0.03	33	1.6
$2, C^1$	0.145	34	0.09	38	0.055	33	0.04	32	1.5
$3, C^0$	0.14	84	0.07	54	0.055	50	0.05	48	1.5
$3, C^1$	0.175	79	0.085	55	0.045	39	0.04	38	1.7
$3, C^2$	0.23	56	0.14	59	0.055	39	0.035	32	1.9
$4, C^0$	0.295	219	0.185	161	0.165	157	0.155	160	1.3
$4, C^1$	0.285	177	0.145	118	0.1	96	0.095	94	1.5
$4, C^2$	0.38	150	0.2	130	0.125	102	0.05	86	2
$4, C^3$	0.365	97	0.275	114	0.125	86	0.04	53	2.2

Table 4. Ideal MAL preconditioner, steady problem, $\nu = 0.004$: values of γ_{opt}, corresponding GMRES iteration counts and approximate common ratios.

It can also be seen that there are shifts in the optimal value of γ for different meshes. In paper [4], Benzi et al. stated a so-called "$\sqrt{2}$ rule" for a FEM discretization that is analogous to our $1, C^0$ case. This rule says that the value of γ_{opt} decreases by a factor of $\sqrt{2}$ with uniform refinement, i.e., that the optimal values of the parameter γ form an approximate geometric sequence with respect to uniform mesh refinement. Our experiments confirm the approximate validity of this rule for the $1, C^0$ discretization. It turns out that the values of γ_{opt} behave similarly also for other IgA discretizations, although the corresponding geometric sequences have different common ratios that are generally higher for discretizations of higher degree and continuity (see Table 4).

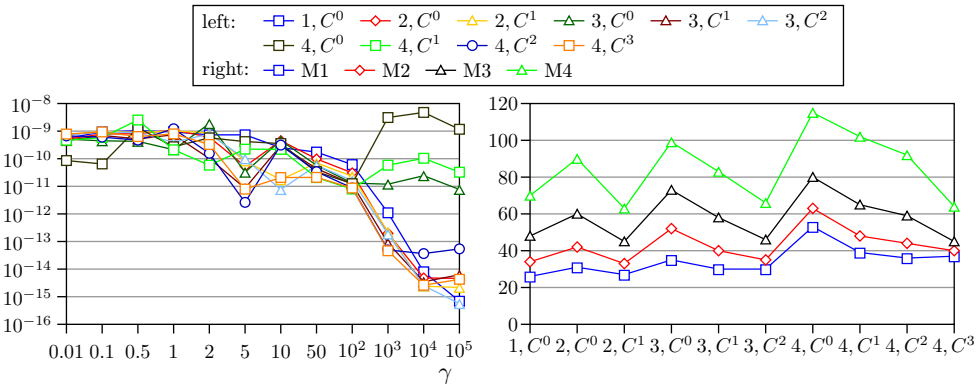


Figure 11. Ideal MAL preconditioner, unsteady ($\Delta t = 0.01$) problem, $\nu = 0.004$: relative residual norm for different discretizations on the mesh M3 (left), GMRES iteration count for different meshes with $\gamma = \gamma_{\text{opt}}$ (right).

num. of iter. \ γ	0.01	0.1	0.5	1	2	5	10	50	10^2	10^3	10^4	10^5
$1, C^0$	285	350	309	164	83	62	**48**	50	62	111	160	293
$2, C^0$	434	511	380	148	75	**60**	65	93	98	225	333	678
$2, C^1$	302	360	299	144	71	53	**45**	55	75	131	190	347
$3, C^0$	617	655	411	141	**73**	78	78	129	146	359	547	1000
$3, C^1$	445	507	364	134	66	**58**	70	105	107	257	379	771
$3, C^2$	337	383	302	130	63	49	**46**	60	85	151	218	405
$4, C^0$	832	796	455	152	**80**	93	109	152	212	537	791	1000
$4, C^1$	617	634	389	128	**65**	78	99	120	165	412	603	1000
$4, C^2$	496	542	371	134	63	**59**	72	122	121	291	433	932
$4, C^3$	366	400	294	119	58	**45**	49	74	87	178	253	504

Table 5. GMRES iteration count (minimal values written in bold) with the MAL preconditioner for the unsteady ($\Delta t = 0.01$) problem on the mesh M3, $\nu = 0.004$.

4.2.2. Unsteady cases. In the unsteady case (with the time step $\Delta t = 0.01$), the optimal value of the parameter γ depends on the particular discretization, but a relatively large range of values of γ give similar convergence. For the considered discretizations, the values of γ_{opt} lie in the interval $(2, 10)$ (see Table 5). For values of γ outside this interval, the number of iterations increases. Thus, like the MAL preconditioner for the steady problems, the convergence is slow for large values of γ. The relative residual norms are dependent on the discretization near values of γ_{opt} as well (see Figure 11, left). The convergence slows down with mesh refinement, but accelerates with increasing interelement continuity of the discretization bases (see Figure 11, right), where it can also be seen that the number of iterations for γ_{opt} is almost the same for different degrees of basis functions with maximum interelement continuity.

Experiments also show that the convergence slows down with mesh refinement for large values of γ, whereas for smaller values there is almost no dependence on mesh refinement for all discretizations (see Figure 12, right, for illustration). Numbers of iterations increase when the value of viscosity decreases. Again, the dependence is weaker for smaller values of γ (see Figure 12, left).

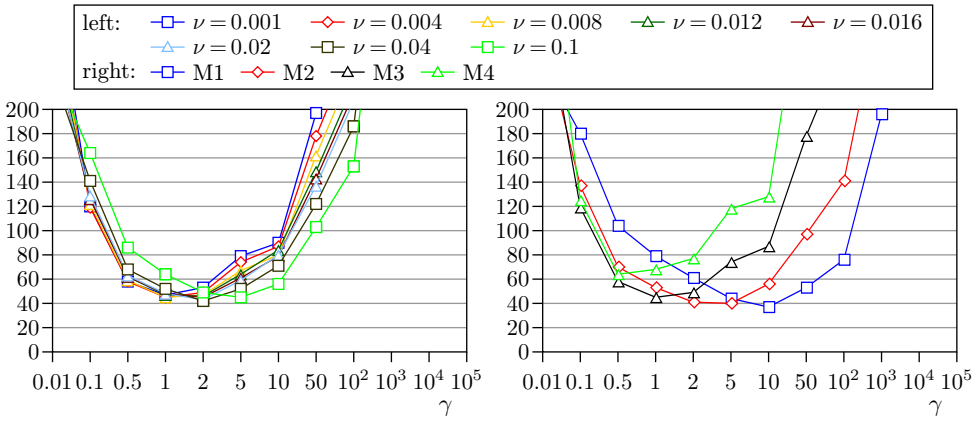


Figure 12. Ideal MAL preconditioner, unsteady ($\Delta t = 0.01$) problem, discretization $4, C^3$: GMRES iteration count for different viscosity values on the mesh M3 (left) and for different meshes with $\nu = 0.004$ (right).

We observe very similar properties for $\Delta t = 0.001$ as well. The optimal values of γ increase, they lie in the interval $(5, 50)$ in this case. The number of iterations is generally a bit higher for all discretizations.

4.3. Approximate solution of subproblems. The results presented in this section were obtained using an approximate solver of the subproblems in the MAL preconditioner. The main goal here is not to find an ideal approximate solver but to examine the influence of approximate solvers on the optimal value of γ.

The approximate solution is realized using V-cycles of a geometric multigrid method [17]. We use one of the simplest smoothers, the relaxed Jacobi method, for part of the experiments. Of course, the GMRES convergence depends on the value of the relaxation parameter τ of the Jacobi smoother. We performed a set of experiments for the steady and unsteady backward facing step problem with various values of the parameter τ for different IgA discretizations, meshes and viscosity values. The same value of τ is set for a given group of problems (steady, unsteady with $\Delta t = 0.01$ and $\Delta t = 0.001$). The value of τ was chosen such that the number of GMRES iterations with the MAL preconditioner using multigrid with the Jacobi smoother was relatively low for most of the tested problems in the given group. Thus, we set $\tau = 0.2$ for the steady and unsteady problems with $\Delta t = 0.01$ and $\tau = 0.3$ for the unsteady problems with $\Delta t = 0.001$.

It has been observed by many authors that the performance of classical multigrid methods (with standard smoothers such as Jacobi or Gauss-Seidel) applied to IgA linear systems is highly dependent on the B-spline degree and the spatial dimension. Inspired by [16], where ILUT(1) is successfully used as a smoother for a multigrid solver for IgA linear systems, we involve ILUT smoothers into our comparison. We set the drop tolerance to 10^{-12} and the fill factors to 0, 1, 2 and 3. In our experiments, the variant with ILUT(0) did not converge in any of the tested cases and therefore, we do not present these results. However, the variants with higher fill factors can give similar numbers of iterations and solution errors as the ideal MAL and, of course, much cheaper.

In all cases, a 3-level V-cycle was used, but the numbers of smoothing steps and number of cycles differ (the number of presmoothing and postsmoothing steps were chosen equal). We tested all smoothers with different numbers of smoothing steps (1, 3, 5) and different numbers of cycles (1, 3, 5) for different problems and different values of γ. In the case of Jacobi smoother, the fastest convergence was usually achieved using three smoothing steps and three cycles. In the case of ILUT, one smoothing step and one V-cycle seemed to be the best choice. Therefore, these settings are used in all following experiments with Jacobi and ILUT smoothers.

We present results for the backward facing step problem with $\nu = 0.004$ on the mesh M3 with all discretizations considered in the previous sections.

4.3.1. Steady case. In this case the convergence of GMRES with MAL using multigrid with ILUT(2) and ILUT(3) smoother differs significantly from the ideal MAL for large values of the parameter γ, while in the neighborhood of the optimal values the numbers of iterations are almost identical to the ideal version. The values of γ_{opt} thus coincide with the optimal values obtained with the direct inner solver. In contrast, when ILUT(1) is used, the values of γ_{opt} shift for some discretizations and

when the Jacobi method is used, they shift in all cases. See Figures 13 for illustration and Table 6 for details.

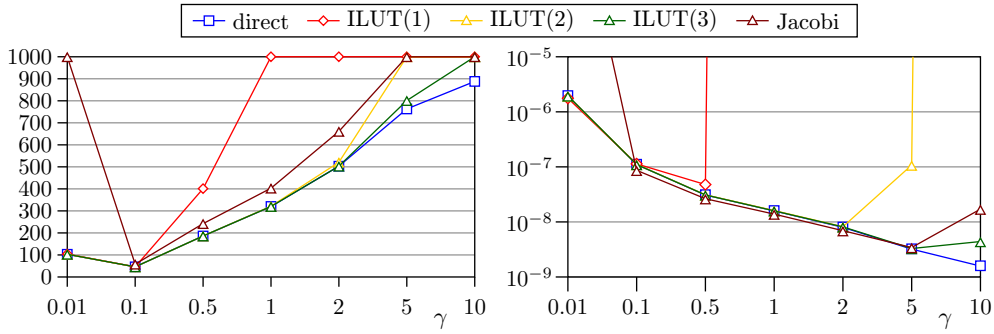


Figure 13. MAL preconditioner, steady problem, $\nu = 0.004$, mesh M3, discretization $2, C^1$: GMRES iteration count (left) and relative residual norm (right) for different inner solvers.

Our experiments indicate that the ILUT smoothers give very similar convergence to the ideal version of MAL preconditioner for values of the parameter $\gamma \in \langle 0, \alpha \rangle$, where α depends on the fill factor and discretization. The values of α are larger for larger ILUT fill factor and also in the cases with maximum continuity of the discretization basis. For $\gamma > \alpha$, the convergence rapidly worsens. This behavior is fundamental for the value of γ_{opt}. This value coincides with the optimal value determined with direct inner solver only in the cases when this value is smaller than the corresponding α. In the opposite case, we can get a significantly worse convergence if we use the same value of γ as for the ideal version of MAL. It is obvious that the optimal value of γ depends on the used approximate solver.

	direct		ILUT(1)		ILUT(2)		ILUT(3)		Jacobi	
	γ_{opt}	iter.	γ_{opt}	iter.	γ_{opt}	iter.	γ_{opt}	iter.	γ_{opt}	iter.
$1, C^0$	0.065	31	0.065	31	0.065	31	0.065	31	0.1	48
$2, C^0$	0.04	32	0.04	33	0.04	32	0.04	32	0.03	46
$2, C^1$	0.055	33	0.055	33	0.055	33	0.055	33	0.085	53
$3, C^0$	0.055	50	0.035	61	0.055	50	0.055	50	0.02	100
$3, C^1$	0.045	39	0.025	63	0.045	39	0.045	39	0.03	97
$3, C^2$	0.055	39	0.055	39	0.055	39	0.055	39	0.09	152
$4, C^0$	0.165	157	0.015	277	0.155	172	0.165	157	0.015	321
$4, C^1$	0.1	96	0.005	568	0.05	103	0.1	96	0.02	297
$4, C^2$	0.125	102	0.08	109	0.125	102	0.125	102	0.03	305
$4, C^3$	0.125	86	0.12	85	0.125	86	0.125	86	0.1	378

Table 6. MAL preconditioner, steady problem, $\nu = 0.004$, mesh M3: values of γ_{opt} and corresponding GMRES iteration counts for different inner solvers.

4.3.2. Unsteady cases. In the unsteady cases, the values of γ_{opt} were from the intervals $(2, 10)$ (for $\Delta t = 0.01$) and $(5, 50)$ (for $\Delta t = 0.001$) for the ideal version of MAL preconditioner. If a multigrid with the Jacobi smoother is used as the inner solver, we get different optimal values of γ that are close to γ_{opt} for the ideal version. In the case of ILUT smoothers, we observe similar behavior as in the steady case—the convergence is very similar to the ideal version for small values of γ, but for values higher than a critical value, the number of iterations rapidly increases. Figure 14 shows how these critical values depend on the discretization and fill factor of the ILUT smoother.

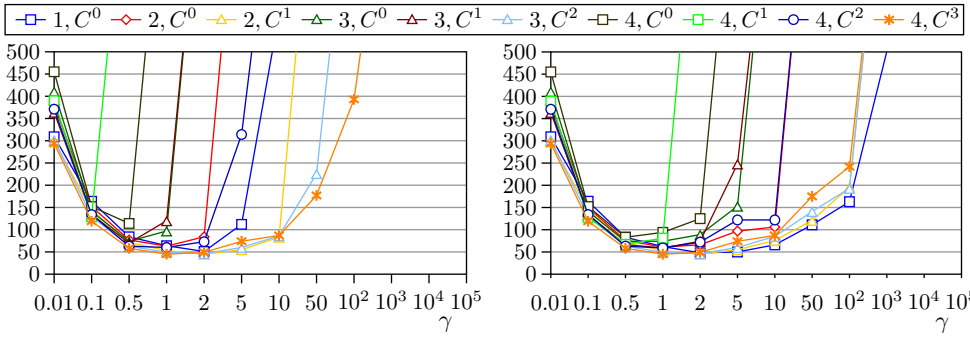


Figure 14. MAL preconditioner, unsteady ($\Delta t = 0.01$) problem, $\nu = 0.004$, mesh M3: multigrid inner solver with ILUT(2) (left) and ILUT(3) (right) smoother.

5. Conclusions

The aim of this paper was to get insight into the choice of the parameter γ for augmented Lagrangian based preconditioners for the incompressible Navier-Stokes equations in the context of isogeometric analysis discretizations. We presented results of extensive experiments for the original augmented Lagrangian (AL) preconditioner and its modified variant (MAL) applied to linear systems obtained from various IgA discretizations of the two-dimensional backward facing step problem. We considered both steady and unsteady problems. We note that we have used an alternative stopping criterion for GMRES in the presented experiments. It is based on the relative norm of the solution "error" which is computed considering a direct solution as exact. Of course, this is not applicable in practical computations, but it is used to assess the optimality of γ with respect to the number of iterations to obtain a solution of comparable quality.

The dependence of convergence of the AL preconditioner on the parameter γ is straightforward in all cases. The iteration count decreases monotonically with increasing value of γ. The iteration counts are similar for different discretizations.

In the unsteady case, the iteration count is generally higher than in the steady case. The convergence of AL is generally independent of the problem parameters for large enough values of γ.

The dependence on the parameter γ is different for the MAL preconditioner. For the steady problems, small values of γ (usually between 0.01 and 0.1) seem to be optimal for all discretizations. In our experiments, the optimal value increased for increasing continuity of the discretization bases on a given mesh and it decreased with mesh refinement, forming an approximate geometric sequence. The common ratio of this geometric sequence is approximately $\sqrt{2}$ for degree $k = 1$ as observed in [4] and increases with the degree and also with the continuity of the basis functions. With these optimal values of γ, the convergence is only weakly dependent on the problem parameters. For unsteady problems for a relatively large time step, the optimal values of γ lie in the interval $(2, 10)$ and the number of iterations does not change much within this interval for all discretizations. Outside this interval, the convergence slows down significantly. For a smaller time step, we observed similar behavior, but γ_{opt} lies in the interval $(5, 50)$ and the convergence is a bit slower.

If approximate solvers are used to solve the subsystems in the MAL preconditioner, the optimal value of γ depends on the particular inner solver. However, our experiments indicate that if we use a good inner solver, we can get very similar iteration counts and errors as for the ideal version, at least in some neighborhood of the optimal value of γ.

We performed similar experiments with the ideal versions of AL and MAL for several IgA discretizations of a problem that stems from an industrial application—flow in a two-dimensional blade row. The meshes on this domain are generally curvilinear and not exactly uniform. We observed similar behavior of AL and MAL convergence for the steady problems as in the case of backward facing step. Also, the dependence on viscosity and mesh refinement is similar. In the MAL case, the optimal values of γ are close to 0.1 in accordance with the observations in Section 4.2.1 and they also decrease with mesh refinement in a similar way. Unsteady cases are not easy to compare due to a different character of the flow and thus a different interplay between the time step size and other problem parameters. However, even in these cases, we observe similar properties presented in this article and therefore, it is possible to determine or estimate optimal values of parameter γ as well.

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