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An analysis of one regularization
approach for solution of pure
Neumann problem

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Vorwort

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Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.



Prof. Dr. Dieter Prätzel-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

An analysis of one regularization approach for solution of pure Neumann problem

E. Savenkov H. Andrä O. Iliev*

Abstract

In this paper, the analysis of one approach for the regularization of pure Neumann problems for second order elliptical equations, e.g., Poisson's equation and linear elasticity equations, is presented. The main topic under consideration is the behavior of the condition number of the regularized problem. A general framework for the analysis is presented. This allows to determine a form of regularization term which leads to the "natural" asymptotic of the condition number of the regularized problem with respect to mesh parameter. Some numerical results, which support theoretical analysis are presented as well.

The main motivation for the presented research is to develop theoretical background for an efficient and robust implementation of the solver for pure Neumann problems for the linear elasticity equations. Such solvers usually are needed in a number of domain decomposition methods, e.g. FETI. Developed approaches are planned to be used in software, developing in ITWM, e.g. `KneeMech` simulation software.

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1 Introduction

Pure Neumann problems often arise in a number of important applications, e.g. in Neumann-Neumann domain decomposition methods [1], construction of free-free flexibility matrices in elasticity [3] and others.

The motivation of this study comes from FETI domain decomposition method, where pure Neumann problems for subdomains have to be solved at each iteration and for each subdomain. Lets consider this briefly, focussing the algebraic structure of the method. For comprehensive consideration we refer to [1, 2].

Consider computational domain Ω , decomposed into a number N_Ω of non-overlapping subdomains Ω_i . We assume that Ω is decomposed into finite elements in such a way, that each subdomain Ω_i is a set of elements of such triangulation. Then the approximate solution of the problem can be obtained from minimization of the following (finite-dimensional) functional:

$$\mathcal{L}(u) = \frac{1}{2}u^T Au - f^T u \rightarrow \min$$

with equality-type constraints $Bu = 0$, which describe continuity conditions at subdomains' boundaries. Here the stiffness matrix A and the matrix B are block matrices given by

$$A = \text{diag}(A_1, A_2, \dots, A_{N_\Omega}), \quad B = [B_1, B_2, \dots, B_{N_\Omega}]. \quad (1)$$

The block vectors

$$f = [f_1, f_2, \dots, f_{N_\Omega}]^T, \quad u = [u_1, u_2, \dots, u_{N_\Omega}]^T$$

denote right-hand side and problem's solution. Each block with number i corresponds to subdomain Ω_i . Local stiffness matrices K_i are usually symmetric and positive semi-definite, as well as global stiffness matrix A . Nevertheless,

the full problem is well-posed if $\ker A \cap \ker B = \{0\}$, which usually holds as soon as some Dirichlet boundary conditions are prescribed on $\partial\Omega$.

A kernel of A can be described via some matrix R , such that $\text{range } R = \ker A$, $\text{range } R_i = \ker A_i$,

$$R = \text{diag}(R_1, R_2, \dots, R_{N_\Omega}),$$

which is assumed to be known.

Let λ be the vector of Lagrangian multipliers for the constraint $Bu = 0$. Then the minimization problem, stated above, is equivalent to:

$$\begin{aligned} Au + B^T \lambda &= f, \\ Bu &= 0. \end{aligned}$$

Solving first equation for u , one obtains

$$u = A^+(f - B^T \lambda) + R\alpha, \quad (2)$$

where the non-nodal degrees of freedom α have to be determined. Here A^+ denotes pseudo-inverse for A ,

$$A^+ = \text{diag}(A_1^+, A_2^+, \dots, A_{N_\Omega}^+).$$

Substitution of u into the second equation leads to

$$BA^+(f - B^T \lambda) + BR\alpha = 0,$$

which is equivalent to the following equation for the Lagrangian multipliers λ :

$$\begin{aligned} P(F\lambda - d) &= 0, \\ G^T \lambda &= e, \end{aligned}$$

with $G = BR$, $F = BA^+B^T$, $d = BA^+f$, $e = R^T f$ and $P = I - G(G^T G)^{-1}G^T$.

The solution of the last equation with projected preconditioned conjugate gradient (projected PCG) method is called FETI method.

After λ is computed, the vector $\alpha = -(GG^T)^{-1}G^T(d - F\lambda)$ and the solution in a particular subdomain can be obtained from (2). Pseudo-inverses of matrices A^+ have to be computed for that. In practice, pseudo-inverse matrices A_i^+ are not explicitly computed. Instead, a linear system of the form

$$A_i u_i = f_i$$

with several right-hand sides f_i is solved to obtain the subdomain solution u_i . This system is singular, symmetric and positive semi-definite and has to be solved in each subdomain for each projected PCG iteration. Hence, it is a crucial point for the efficient implementation of FETI methods to have an efficient and robust solver for such a kind of linear systems.

Finite element stiffness matrices A_i (see (1)), which arise in the latter case along with many other cases, are sparse, symmetric, semi-definite, and have non-trivial kernel, — i.e., the matrices are singular.

A number of approaches were suggested to deal with such problems — iterative as well as direct ones. The most comprehensive overview is presented in [5], where a number of approaches are considered from the unified point of view. This paper also contains analysis of the most “sparse” way of regularization of the singular stiffness matrix, which utilize Dirac’s δ -s as regularization functionals. It was shown, that for this case and Poisson’s equation the condition number growth faster, than $1/h^2$ for 2d and 3d cases. Here, h is mesh parameter. Details will be discussed later.

This paper focuses only on one of such methods, where the original, singular stiffness matrix A for a certain problem is regularized via addition of some matrix B_ω to it. The matrix B_ω has to be defined in such a way, that the regularized matrix

$$A_\omega = A + B_\omega$$

is non-singular. Then the resulting system of equation can be solved by conventional direct or iterative approaches for non-singular problems. The solution of the regularized problem is some particular solution of the original, singular, problem — if B_ω is chosen properly.

Generally, matrix B_ω should be chosen in a way such that A_ω is non-singular, positive-definite and provides A_ω with “nice” properties of A , namely, sparsity and symmetry.

Usually, it is easy to chose B_ω in a way, such that A_ω is non-singular, symmetric and positive-definite. But a certain problems are arise to keep A_ω sparse and well conditioned: How to choose regularization term B_ω to (i) keep the resulting, regularized, problem to be sparse; (ii) keep condition number of A_ω as close as possible to the natural condition number (which is defined, for positive semi-definite matrices as ratio between maximal and minimal positive eigenvalues) of A (at least, to keep condition number reasonably “good” in terms of its asymptotic in mesh parameter h , e.g., of the order $1/h^2$ for the case of 2-nd order elliptic problems)?

An answer to the first question is known: It is possible to have only diagonal non-zero entities in B_ω . The number of such non-zero diagonal elements is equal to dimension of $\ker A$ [3]. In the variational approach,

which is used in the current paper and in [5], this corresponds to usage of Dirac's δ -s as regularization functionals. Paper [5] contains comprehensive analysis of this case, including the condition number asymptotic, etc. This analysis shows, that in the case under consideration, the regularized problem is very badly conditioned (although, non-singular) — asymptotic of condition number of the regularized problem is worse then $1/h^2$ for 2d and 3d cases.

The answer to the second question is known as well. In a linear algebra context, one can consider regularization of the stiffness matrix of the form

$$A_\omega = A + RR^T, \quad (3)$$

where R is orthonormalized block-row matrix, whose columns spans $\ker A$, i.e.

$$AR = R^T A = 0, \quad R^T R = I,$$

where I is an identity matrix of the certain dimension. Matrix R is usually known *a-priori*. For instance, for linear elasticity problems, matrix R is orthonormalized rigid-body matrix.

This regularization shifts all zero eigenvalues of $A \in \mathbb{R}^{N \times N}$ to one. If minimal and maximal eigenvalues of A satisfies

$$0 \leq \lambda_{\min}(A) < \lambda_{\max}(A)$$

and

$$0 < \min_{i=1, N, \lambda_i > 0} \lambda_i(A) < 1 < \max_{i=1, N} \lambda_i(A),$$

then it holds:

$$\min_{i=1, N} \lambda_i(A_\omega) = \min_{i=1, N} \lambda_i(A), \quad \max_{i=1, N} \lambda_i(A_\omega) = \max_{i=1, N} \lambda_i(A),$$

and, hence,

$$\kappa(A_\omega) = \tilde{\kappa}(A),$$

where $\tilde{\kappa}(A)$ stands for natural condition number of A , which is defined as

$$\tilde{\kappa}(A) = \frac{\max_{i=1, N, \lambda_i > 0} \lambda_i(A)}{\min_{i=1, N} \lambda_i(A)}.$$

But in this approach matrix RR^T is usually dense, and, hence, regularization leads to the dense matrix A_ω .

Another choice of regularization matrix is possible [3], i.e

$$A_\omega = A + HH^T, \quad (4)$$

where H is an arbitrary matrix, which satisfies:

$$\dim H = \dim R, \quad \text{rank } AH = \dim \ker A = \text{rank } R. \quad (5)$$

Generally, it is possible to choose HH^T as a diagonal matrix. In this case the number of its diagonal entries is equal to the dimension of the problem's kernel, $\dim \ker(A)$.

Two questions arise here: (i) How to choose H , which satisfies eq. (5) *a-priorily*? (ii) How to estimate condition number and its dependency on the mesh parameter h for the given matrix H ?

In practice, both approaches (with dense regularization matrix RR^T and with sparse HH^T) are used. Both of them have some advantages and disadvantages.

Let us also note, that the latter approach also allows to solve linear systems with matrix (3). This is done via solving sparse regularized system with the matrix (4) and then projecting the obtained solution to the $(\ker A)^\perp$ using the projector $P = I - R(R^T R)^{-1}R^T$.

In the case of the dense regularization matrix, a resulting system can be solved iteratively. For the methods, that require, at each iteration, an application of A_ω to some vector v , it can be done efficiently without explicitly formed A_ω . Only A and R has to be stored, and terms $z = RR^T x$ can be computed efficiently in two steps: $y = R^T x$ and $z = Ry$. In this case a problem with a storage for A_ω doesn't arise [5]. Nevertheless, iterative methods are not the best choice for some problems — for example, when it is required to solve a number of problems with the same matrix and different right-hand sides (this is a common case for domain decomposition methods).

Direct approaches for solution of regularized system can be based on a certain modification of LU elimination process. In this case, it is often impossible to store LU-factors and the sparse regularization matrix H is necessary.

A common approach is not to form matrix H explicitly, but to obtain it in an implicit manner during some modified LU elimination process, see, e.g. [3] and [4]. But this approach has its own problems, lack of robustness (see [3]), and requires modification of the existent codes.

The discussion above shows that the topic concerning efficient regularization is still of the interest.

The aim of this paper is to analyze some of the issues discussed above. The questions addressed are: (i) How to choose regularization term to obtain condition number of the order $1/h^2$? (ii) What is the “minimal”, in terms of sparsity, regularization term?

For convenience, variational framework is used as opposed to linear algebra framework.

Outline of the paper is the following. A general framework for our analysis is presented. Properties of the regularization term of the general form, that lead to the proper behavior of the condition number, are determined. As the main tool, different versions of Poincaré and Friedrichs inequalities (see cited papers and [10]) are used. As applications, we consider pure Neumann problems for Poisson’s equation and linear elasticity equations.

Some numerical results, which confirm obtained theoretical estimates are presented. For some cases, numerical results are better than those obtained theoretically, i.e., condition number of the regularized system not only has the proper asymptotic, but also the same value as natural condition number for the corresponding singular system, i.e.

$$\kappa(A_\omega) = \tilde{\kappa}(A).$$

2 Problem statement and general analysis framework

We start with quite a general consideration of an abstract problem. A motivation is to show main features of the presented analysis and to decouple problem-independent issues, which hold for a quite general class of problems — and problem-dependent ones, consideration of which have to be more focused and concrete.

Similar analysis, but in a context of solvability of pure Neumann problems for 2-nd order elliptical PDEs was performed in [7, 8, 9]. In [7] general second-order elliptical problems are considered. Papers [8] and [9] cover the particular case of linear elasticity. Although regularized problems aren’t discussed there, a very comprehensive analysis of pure Neumann problem was performed, including conditions of solvability and uniqueness for solution of the problem, different versions of Korn’s inequalities, etc. Here we utilize these results in a way, which is more convenient for analysis of regularized finite elements approximations. The key difference is that we work with modified (regularized) equations and “original” solution spaces — rather than with “original” (not modified) equations and modified, quotient, spaces.

In the sequel we will deal with two kinds of problems. The first one is the “original”, singular problem. The second one is a conventional well-posed variational problem, which is the regularization of the first problem.

We start with the first problem.

Consider linear operator \mathcal{A} which acts on a Hilbert space V , and maps V onto its dual, i.e.

$$\mathcal{A} : V \rightarrow V',$$

and space $H = H'$, such that $V \subset H = H' \subset V'$. Let $(\cdot, \cdot)_H \equiv (\cdot, \cdot)$ denote the inner product in H or duality between H and H' .

Then the following Green's formula is valid under certain circumstances (see [6]):

$$(\mathcal{A}u, v)_H = a(u, v) - \langle \gamma_1 u, \gamma_0 v \rangle,$$

for an arbitrary $u, v \in V$. Here $a(\cdot, \cdot)$ is a bilinear form induced by operator \mathcal{A} ; γ_0 is an abstract "trace" operator, which maps function $u \in V$ to some function $\gamma_0 u \in T$,

$$\gamma_0 : V \rightarrow T,$$

where T stands for certain "trace" space; and

$$\gamma_1 : V \rightarrow T'$$

is the "conormal derivative" operator which corresponds to \mathcal{A} . The duality between T' and T or the corresponding inner product is denoted by $\langle \cdot, \cdot \rangle$.

An abstract pure Neumann problem reads: Find $u \in V$, such that

$$\mathcal{A}u = f, \quad f \in V'; \quad \gamma_1 u = g.$$

Hence, using Green's formula, one can obtain a variational statement of this problem: Find $u \in V$ such that

$$a(u, v) = F(v), \quad v \in V, \tag{6}$$

where $F \in V'$ is defined by

$$F(v) = f(v) + \langle g, \gamma_0 v \rangle. \tag{7}$$

Since our goal is to consider the case of singular operator \mathcal{A} , we assume that $\ker \mathcal{A}$ is non-trivial, $\ker \mathcal{A} \neq \{0\}$. Also we assume that $a(\cdot, \cdot)$ is symmetric and semi-definite.

A kernel of operator \mathcal{A} and bilinear form $a(\cdot, \cdot)$ is defined as

$$\ker \mathcal{A} = \{r \in V : a(r, v) = 0, \quad \forall v \in V\} \neq \{0\}.$$

Hereafter r denotes an arbitrary element from $\ker \mathcal{A}$.

Solution of problem (6) is not unique and is defined up to an arbitrary function from $\ker \mathcal{A}$. To define a unique solution, some restrictions have to be imposed on u . The most natural way is to require orthogonality of u to $\ker \mathcal{A}$, i.e.

$$u \perp \ker \mathcal{A},$$

or

$$(u, r) = 0, \quad \forall r \in \ker \mathcal{A}, \quad (8)$$

where orthogonality is considered with respect to inner product in H .

In other words, we are looking for a unique solution of (6) in the quotient space $V/\ker \mathcal{A}$, and problem (6) turns into

$$a(u, v) = F(v), \quad v \in V; \quad (u, r) = 0, \quad \forall r \in \ker \mathcal{A}. \quad (9)$$

Substituting an arbitrary $r \in \ker \mathcal{A}$ into (6), one obtains:

$$F(r) = f(r) + \langle g, \gamma_0 r \rangle = 0, \quad \forall r \in \ker \mathcal{A}, \quad (10)$$

which is a consistency condition for the problem (6).

In what follows we suppose that $\ker \mathcal{A}$ is finite-dimensional,

$$\ker \mathcal{A} = \text{span}\{r_1, r_2, \dots, r_L\}, \quad \dim \ker \mathcal{A} = L$$

with $r_l \in \ker \mathcal{A}$, $l = \overline{1, L}$.

Particularly, this holds for pure Neumann problem for Poisson's equation ($L = 1$) and linear elasticity ($L = 3$ for 2D case and $L = 6$ for 3D case).

We assume, that r_l are orthonormalized r_l with respect to scalar product in H , i.e.

$$(r_l, r_k) = \delta_{kl},$$

where δ_{kl} is Kronecker δ . In the general case it is always possible to orthonormalize r_1, \dots, r_L using Gram-Schmidt procedure.

Then $u \perp \ker \mathcal{A}$ means:

$$(u, r) = 0, \quad \forall r = \sum_{l=1}^L \alpha_l r_l \in \ker \mathcal{A}, \quad \alpha \in \mathbb{R}^L. \quad (11)$$

Since r_l are orthonormalized, an arbitrary $r \in \ker \mathcal{A}$ can be expanded in terms of r_l as:

$$r = \sum_{l=1}^L (r, r_l) r_l = \sum_{l=1}^L \alpha_l r_l; \quad \alpha_l = (r, r_l), \quad \forall l \in \overline{1, L},$$

and $\alpha = \{\alpha_1, \dots, \alpha_L\} \in \mathbb{R}^L$. When v runs over $\ker \mathcal{A}$, then α runs over \mathbb{R}^L and otherwise.

The following holds for arbitrary $v \in V$ and $r \in \ker \mathcal{A}$:

$$(v, r) = \left(v, \sum_{l=1}^L \alpha_l r_l \right) = \sum_{l=1}^L (v, r_l) \alpha_l = \sum_{i=1}^L (v, r_i) (r, r_i).$$

Hence, equation (11) can be written as:

$$\sum_{i=1}^L (r_i, u)(r_i, u) = 0, \quad \forall r \in \ker \mathcal{A}. \quad (12)$$

The next step involves decomposition of space V into direct sum

$$V = V^\perp \oplus \ker \mathcal{A}, \quad V^\perp = (\ker \mathcal{A})^\perp, \quad v^\perp \perp \ker \mathcal{A}. \quad (13)$$

An arbitrary $v \in V$ can now be decomposed as

$$v = v^\perp + v_r, \quad v^\perp \in V^\perp, \quad v_r \in \ker \mathcal{A},$$

where $(v^\perp, v_r) = 0$. Hence, the relation

$$\forall r \in \ker \mathcal{A}: \quad (r, v) = (r, v_r)$$

is valid, and we can see, that equation (12) holds if $r \in \ker \mathcal{A}$ is replaced with an arbitrary $v \in V$, i.e.

$$\sum_{i=1}^L (u, r_i)(v, r_i) = 0, \quad \forall v \in V.$$

All of these lead to the following variational problem for (9): Find $u \in V$, such that

$$\begin{aligned} a(u, v) &= F, \quad \forall v \in V^\perp, \\ \sum_{l=1}^L (r_l, r)(r_l, u) &= 0, \quad \forall r \in \ker \mathcal{A}, \end{aligned}$$

or, since (13) holds: Find $u \in V$, such that

$$a(u, v) + \sum_{l=1}^L (r_l, v)(r_l, u) = F(v), \quad \forall v \in V. \quad (14)$$

Any solution of the original problem (9) satisfies this equation. To show that an inverse result is valid, it is enough to substitute $v \in \ker \mathcal{A}$ in the last equation.

More general conditions, that provide uniqueness of solution of problem (6) can be imposed in the following way.

Consider some functionals $\omega_l \in V'$, $l = \overline{1, L}$, such that matrix $M \in \mathbb{R}^{l \times l}$ with elements

$$M_{kl} = \omega_l(r_k) \quad (15)$$

is non-singular.

Now replace r_l in (14) with functionals $\omega_l \in V'$ to obtain the following regularized problem: Find $u \in V$ such that

$$a_\omega(u, v) = F(v), \quad \forall v \in V, \quad (16)$$

where $a_\omega(\cdot, \cdot)$ is a regularized bilinear form which corresponds to $a(\cdot, \cdot)$,

$$a_\omega(u, v) = a(u, v) + \sum_{l=1}^L \omega_l(u)\omega_l(v),$$

and $F \in V'$ is given by (7).

Substituting $v = r_k$ in (16), one obtains:

$$\sum_{l=1}^L \omega_l(u)\omega_l(r_k) = 0, \quad \forall k = \overline{1, L}.$$

Here a zero right-hand side appears due to the consistency conditions on f and g , see (10).

The last equation can be rewritten as:

$$Mu_\omega = 0,$$

where M is defined by (15) and column vector $u_\omega \in \mathbb{R}^L$ is

$$u_\omega = [\omega_1(u), \omega_2(u), \dots, \omega_L(u)]^T.$$

Since M is non-singular, $u_\omega = 0$. It means that solution of (16) satisfies (6) and is orthogonal to

$$\text{span}(\omega_1, \dots, \omega_L)$$

with respect to duality between V and V' .

Since the goal of such regularization is to obtain a well-posed problem (16), bilinear form $a_\omega(\cdot, \cdot)$ has to satisfy conditions of Lax-Milgram Lemma [6], which states that $a_\omega(\cdot, \cdot)$ has to be coercive and continuous in V :

$$C_1 \|u\|_V^2 \leq a_\omega(u, u), \quad \forall u \in V; \quad a(u, v) \leq C_2 \|u\|_V \|v\|_V, \quad \forall u, v \in V. \quad (17)$$

Let us also note, that when the original bilinear form $a(\cdot, \cdot)$ is symmetric, $a_\omega(\cdot, \cdot)$ is also symmetric.

A proof of regularity of (16) for some particular cases of $a(\cdot, \cdot)$ and ω_l is a main topic for the following sections.

3 Approximations and condition number estimates

Approximations of problem (16) are obtained in a conventional way. The space V is approximated by a finite-dimensional space $V_h \subset V$ to obtain a finite dimensional problem: Find $u_h \in V_h$ such that

$$a_\omega(u_h, v_h) = F(v_h), \quad \forall v \in V_h.$$

Let

$$V_h = \text{span}(\varphi_1, \varphi_2, \dots, \varphi_N),$$

where N is the total number of unknowns (degrees of freedom, DOFs). The corresponding stiffness matrix

$$A_\omega = A + B_\omega, \tag{18}$$

is given by

$$A_{ij} = a(\varphi_i, \varphi_j), \quad (B_\omega)_{ij} = \sum_{l=1}^L \omega_l(\varphi_i) \omega_l(\varphi_j), \quad i, j = \overline{1, N}.$$

Matrix A_ω is the stiffness matrix for the regularized problem. Matrix A is the stiffness matrix of the original (singular) problem and B_ω approximates the regularization term and can be written as

$$B_\omega = C_\omega C_\omega^T,$$

where matrix $C \in \mathbb{R}^{N \times L}$ is defined by

$$C = \begin{pmatrix} \omega_1(\varphi_1) & \omega_2(\varphi_1) & \cdots & \omega_L(\varphi_1) \\ \omega_1(\varphi_2) & \omega_2(\varphi_2) & \cdots & \omega_L(\varphi_2) \\ \vdots & \vdots & \ddots & \vdots \\ \omega_1(\varphi_N) & \omega_2(\varphi_N) & \cdots & \omega_L(\varphi_N) \end{pmatrix}.$$

Further, estimation of the condition number, depends on particular problems, choice of regularization terms, basis functions, etc.

Therefor, before we proceed, we briefly discuss how these estimates are usually obtained. For details see, for example, [1].

The first step is to obtain estimates (17) for a particular bilinear form and functional spaces. This step actually does not depend on any mesh-dependent parameter, choice of approximations (i.e., basis functions), etc.

The second step is essentially “finite-dimensional” and uses inverse estimates in Sobolev spaces (see [6] or [1]), and estimates for eigenvalues of the mass or Gram matrix $M_{ij} = (\varphi_i, \varphi_j)_H$.

The latter step does not depend on the particular structure of the form $a_\omega(\cdot, \cdot)$ and depends only on the choice of functional spaces V and H and corresponding finite-dimensional space V_h .

Combination of these estimates provide us with an estimate for the condition number of the form

$$\kappa(A_\omega) \leq Ch^\alpha,$$

with a certain α , which depends on the choice of functional spaces and basis functions.

The main observation here is that once all function spaces and type of approximations are chosen, the last estimate does not depend on particular form of $a(\cdot, \cdot)$ — once (17) holds.

For the case of second order elliptical problems and first order finite elements basis functions on triangular or tetrahedral meshes, the estimate

$$\kappa(A_\omega) \leq Ch^{-2}, \tag{19}$$

is obtained for an arbitrary problem, which satisfies (17).

Discussion, presented above, allows us to choose the following strategy: after fixing type of approximations (piece-wise linear finite elements on triangular or tetrahedral meshes) and an “original”, singular, bilinear form, we consider regularization terms of some form and prove estimates (17).

An analysis of such coercivity and continuity estimates is strongly problem-dependent and is the main topic for the rest of the paper. Once these estimates are obtained for regularized problem, we automatically have its condition number satisfying (19).

Next, we consider, in a sequel, two particular cases: pure Neumann problem for Poisson’s equation and linear elasticity equation. For Poisson’s equation 2d and 3d cases are considered. For elasticity equations only problems in 3d are considered.

As it was mentioned before, we are interested in estimates (17) for the corresponding regularized problems.

4 Poisson’s equation

Consider the following problem in domain $\Omega \subset \mathbb{R}^n$, $n = 2$ or 3 : Find u such that

$$-\Delta u = f \text{ in } \Omega; \quad \frac{\partial u}{\partial \vec{n}} = g \text{ on } \Gamma,$$

where $\Gamma = \partial\Omega$ and g denote the Neumann boundary condition on Γ .

In this case we have $V = H^1(\Omega)$, $V' = H^{-1}(\Omega) = [H_0^1(\Omega)]'$ and $H = H' = L^2(\Omega)$ with conventional norms and semi-norms

$$\|u\|_{L^2(\Omega)}^2 = \int_{\Omega} u^2 d\Omega,$$

$$|u|_{H^1(\Omega)}^2 = \int_{\Omega} \nabla u \cdot \nabla u d\Omega, \quad \|u\|_{H^1(\Omega)}^2 = \|u\|_{L^2(\Omega)}^2 + |u|_{H^1(\Omega)}^2.$$

The variational problem has the form (6), where

$$a(u, v) = \int_{\Omega} \nabla u \cdot \nabla v d\Omega, \quad (20)$$

and

$$F(v) = (f, v)_{L^2(\Omega)} + \langle g, \gamma_0 v \rangle_{\Gamma},$$

where $\langle \cdot, \cdot \rangle_{\Gamma} \equiv \langle \cdot, \cdot \rangle$ denotes conventional inner product in $L^2(\Gamma)$.

A kernel of this problem is one-dimensional ($L = 1$) and spans constant functions. Hence, we can chose $r = \text{const}$. In what follows, we take $r = |\Omega|^{-1}$, where $|\Omega|$ is area of Ω in \mathbb{R}^2 or its volume in \mathbb{R}^3 . Let us note, that in this case operator $P : u \mapsto (u, r) \cdot 1(x)$ (where $1(x) = 1$ for all $x \in \Omega$) defines projector in $L^2(\Omega)$.

Regularization functional ω in (16) can be chosen as an arbitrary element from $H^{-1}(\Omega)$ and the regularized problem is defined by:

$$a(u, v) + \omega(u)\omega(v) = F(v), \quad \forall v \in H^1(\Omega), \quad (21)$$

where $a(\cdot, \cdot)$ is given by (20).

The most simple choice is to take $\omega = \text{const}$ in Ω . In this case the regularization term reads

$$\omega(u) = (\omega, u) = \int_{\Omega} \omega u d\Omega.$$

As in [5], we assume $w(r) > 0$. This implies correctness of the regularized problem and its positive definiteness; refer to (15) for discussion concerning properties of matrix M .

Another possible choice for ω is

$$\omega(u) = \langle \omega_{\Gamma}, u \rangle_{\Gamma} = \int_{\Gamma} \omega_{\Gamma} u d\Gamma.$$

with $\omega_\Gamma \in L^2(\Gamma)$. In this case (21) reads

$$a(u, v) + \langle \omega_\Gamma, u \rangle_\Gamma \langle \omega_\Gamma, v \rangle_\Gamma = f(v), \quad \forall v \in H^1(\Omega), \quad (22)$$

i.e., regularization term “lives” only at the domain’s boundary.

A motivation for such choice of regularization term is that, using FEM approximation for (21) and $\omega = \text{const}$ in Ω , one obtains a dense finite-dimensional problem, due to that fact that regularization term in (21) is non-local, and, hence, matrix B_ω in (18) is dense. Obviously, using boundary regularization term, it is possible to increase sparsity of the matrix B_ω and regularized matrix A_ω . It will be shown later, that this choice for ω , while increasing sparsity of the problem, doesn’t change behavior of condition number of the regularized problem — at least when talking about its asymptotic in mesh parameter h .

A proof of coercivity of both problems (21) and (22) is provided by the following theorem [1]:

Theorem 1. *Let $\Omega \subset \mathbb{R}^n$ be a bounded domain and let $f_i, i = 1, \dots, L, L \geq 1$, be functionals (not necessary linear) in $H^1(\Omega)$, such that, if v is constant in Ω ,*

$$\sum_{i=1}^L |f_i(v)|^2 = 0$$

is equivalent to

$$v = 0.$$

Then, there exist constants, depending only on Ω and functionals f_i , such that,

$$\|v\|_{L^2(\Omega)} \leq C_1 |v|_{H^1(\Omega)} + C_2 \sum_{i=1}^L |f_i(v)|^2, \quad \forall v \in H^1(\Omega).$$

Choosing f_i in a different ways, we can obtain different versions of Poincaré and Friedrichs inequalities.

Coercivity of (21) follows if one choose $L = 1$ and

$$f(v) = \omega(v) = (\omega, v),$$

and coercivity of (22) follows if one choose $L = 1$ and

$$f(v) = \omega(v) = \langle u, \omega_\Gamma \rangle_\Gamma.$$

Continuity of the first problem (21) can be easily proved using Cauchy-Schwartz inequality in $L^2(\Omega)$.

Continuity of the second problem (22) can be proved utilizing Cauchy-Schwartz inequality in $L^2(\Gamma)$ and well known property of continuity of the trace operator: For all v from $H^1(\Omega)$ it holds [6]

$$\|\gamma_0 u\|_{L^2(\Omega)} \leq \|\gamma_0 u\|_{H^{1/2}(\Omega)} \leq C_\Gamma \|u\|_{H^1(\Omega)}, \quad \gamma_0 u = u|_\Gamma. \quad (23)$$

Hence, estimates (17) hold for both problems under consideration.

According to the consideration in section 3, we have the same estimates for the condition number of the regularized problem, i.e. (19). At the same moment the second approach (22) adds to the stiffness matrix a number of nonzero elements of the order $O(N^{2/3})$ for 3d case and $O(N^{1/2})$ for 2d case, while the first one — $O(N)$.

The existence of the trace theorem (23) shows the differences between an arbitrary set of nodes, that can be used for construction of regularization matrix B_ω , and a set of the boundary nodes.

5 Elasticity equations

In this section pure Neumann problem for 3d linear elasticity equations is considered.

For the following section we use notation \vec{x}, \vec{u}, \dots for geometrical vectors and vector fields in $\Omega \subset \mathbb{R}^3$. We do not use vector sign for algebraic vectors. Also, dot sign “.” denotes inner product in \mathbb{R}^3 , and “:” denotes convolution of tensor and vector or convolution of two tensors. Tensors are typesetted in bold typeface ($\boldsymbol{\sigma}, \boldsymbol{\epsilon}, \dots$).

For the case of pure Neumann problem for linear elasticity, we have the following problem statement: Find the displacements $\vec{u} = [u_1, u_2, u_3]^T$ such that

$$-\operatorname{div} \boldsymbol{\sigma}(\vec{u}) = \vec{f} \text{ in } \Omega, \quad \boldsymbol{\sigma} : \vec{n}|_\Gamma = \vec{g}, \quad \Gamma = \partial\Omega,$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor. The Hookean law

$$\boldsymbol{\sigma}(\vec{u}) = \boldsymbol{C} : \boldsymbol{\epsilon}(\vec{u})$$

is the relation between the stress tensor $\boldsymbol{\sigma}$ and the infinitesimal strain tensor, which is defined by

$$\boldsymbol{\epsilon}(\vec{u}) = \frac{1}{2} (\nabla \vec{u} + (\nabla \vec{u})^T),$$

\boldsymbol{C} is 4-th order elastic moduli tensor.

The variational problem has a form of (6) with

$$V = (H^1(\Omega))^3, \quad H = (L^2(\Omega))^3,$$

(equipped with conventional direct product norm, semi-norms and inner products) and

$$a(\vec{u}, \vec{v}) = \int_{\Omega} \boldsymbol{\sigma}(\vec{u}) : \boldsymbol{\epsilon}(\vec{v}) d\Omega = \int_{\Omega} \boldsymbol{\epsilon}(\vec{u}) : \mathbf{C} : \boldsymbol{\epsilon}(\vec{v}) d\Omega,$$

$$\gamma_1 \vec{u} = \boldsymbol{\sigma}(\vec{u}) : \vec{n}.$$

For simplicity, we consider the case of

$$\boldsymbol{\sigma}(\vec{u}) = \mathbf{C} : \boldsymbol{\epsilon}(\vec{u}) = 2\mu\boldsymbol{\epsilon}(\vec{u}) + \lambda \operatorname{div}(\vec{u})\mathbf{I}$$

where \mathbf{I} is identity tensor and λ, μ are Lamé parameters. Generalization to the \mathbf{C} of general form is straightforward.

Then

$$a(\vec{u}, \vec{v}) = \int_{\Omega} (2\mu\boldsymbol{\epsilon}(\vec{u}) : \boldsymbol{\epsilon}(\vec{v}) + \lambda \operatorname{div}(\vec{u}) \operatorname{div}(\vec{v})) d\Omega,$$

or, equivalently,

$$a(\vec{u}, \vec{v}) = 2\mu(\boldsymbol{\epsilon}(\vec{u}), \boldsymbol{\epsilon}(\vec{v}))_{L^2(\Omega)} + \lambda(\operatorname{div}(\vec{u}), \operatorname{div}(\vec{v}))_{L^2(\Omega)},$$

and

$$F(v) = (\vec{f}, \vec{v})_{L^2(\Omega)} = \int_{\Omega} \vec{f} \cdot \vec{v} d\Omega + \int_{\Gamma} \vec{g} \cdot \vec{v} d\Gamma.$$

Here, for arbitrary tensors $\boldsymbol{\epsilon}$ and $\boldsymbol{\sigma}$ we define

$$(\boldsymbol{\epsilon}, \boldsymbol{\sigma})_{L^2(\Omega)} = \int_{\Omega} \boldsymbol{\epsilon} : \boldsymbol{\sigma} d\Omega = \sum_{i,j=1}^n \int_{\Omega} \epsilon_{ij} \sigma_{ij} d\Omega, \quad \|\boldsymbol{\epsilon}\|_{L^2(\Omega)}^2 = (\boldsymbol{\epsilon}, \boldsymbol{\epsilon})_{L^2(\Omega)}.$$

A kernel of elasticity operator $\mathcal{A}\vec{u} = -\operatorname{div} \boldsymbol{\sigma}(\vec{u})$ (also called rigid body modes space, \mathcal{RB}) and the corresponding bilinear form is 6-dimensional, consisting of 3 translation and 3 rotations around 3 non-collinear directions (for 3d case). An arbitrary kernel element is:

$$\vec{r}(\vec{x}) = \vec{a} + \vec{b} \times \vec{x}, \quad \vec{x} = [x_1, x_2, x_3]^T \in \mathbb{R}^3,$$

where $\vec{a} = [a_1, a_2, a_3] \in \mathbb{R}^3$ corresponds to translations and $\vec{b} = [b_1, b_2, b_3] \in \mathbb{R}^3$ corresponds to rotational degrees of freedom. So, rigid body modes space can be defined as

$$\mathcal{RB} \equiv \ker \mathcal{A} = \left\{ \vec{r}(\vec{x}) = \vec{a} + \vec{b} \times \vec{x}, \quad \vec{a}, \vec{b} \in \mathbb{R}^3 \right\}.$$

There is another, more convenient way for describing of an arbitrary $\vec{r} \in \mathcal{RB}$. Direct computations show that

$$\vec{r}(\vec{x}) = \vec{a} + \vec{b} \times \vec{x} = \vec{a} + Q\vec{x}, \quad (24)$$

with

$$Q = \begin{pmatrix} 0 & -b_3 & b_2 \\ b_3 & 0 & -b_1 \\ -b_2 & b_1 & 0 \end{pmatrix}.$$

Another, equivalent, form of (24) is

$$\vec{r}(\vec{x}) = R(\vec{x})\alpha,$$

where

$$\alpha = [a_1, a_2, a_3, b_1, b_2, b_3] \in \mathbb{R}^6,$$

and matrix $R \in \mathbb{R}^{3 \times 6}$ reads:

$$R(\vec{x}) = \begin{pmatrix} 1 & 0 & 0 & 0 & +x_3 & -x_2 \\ 0 & 1 & 0 & -x_3 & 0 & x_1 \\ 0 & 0 & 1 & x_2 & -x_1 & 0 \end{pmatrix}. \quad (25)$$

Columns of the matrix R form a basis in the rigid-body modes space, i.e., one can chose:

$$\vec{r}_1 = [1, 0, 0]^T, \quad \vec{r}_2 = [0, 1, 0]^T, \quad \vec{r}_3 = [0, 0, 1]^T, \quad (26)$$

$$\vec{r}_4 = [0, -x_3, x_2]^T, \quad \vec{r}_5 = [x_3, 0, -x_1]^T, \quad \vec{r}_6 = [-x_2, x_1, 0]^T. \quad (27)$$

Compatibility conditions (10) reads:

$$\int_{\Omega} \vec{f} \cdot \vec{r} d\Omega + \int_{\Gamma} \vec{g} \cdot \vec{r} = 0, \quad \forall \vec{r} \in \ker \mathcal{A},$$

and poses self-equilibrium conditions for the applied boundary and volume forces.

Regularized problem is formulated in the form (16) with

$$a_{\omega}(\vec{u}, \vec{v}) = a(\vec{u}, \vec{v}) + \sum_{l=1}^6 \omega_l(\vec{u})\omega_l(\vec{v}).$$

Since $\mu_0 > 0$ exists, such that

$$2\mu\epsilon(\vec{u}) : \epsilon(u) + \lambda \operatorname{div}^2(\vec{u}) \geq \mu_0\epsilon(\vec{u}) : \epsilon(\vec{u}),$$

almost everywhere [9], an estimate

$$a(\vec{u}, \vec{u}) \geq C \|\boldsymbol{\epsilon}(\vec{u})\|_{L^2(\Omega)}^2$$

holds, and hence, for regularized form one has

$$a_\omega(\vec{u}, \vec{u}) \geq C \|\boldsymbol{\epsilon}(\vec{u})\|_{L^2(\Omega)}^2 + \sum_{l=1}^6 \omega_l(\vec{u}) \omega_l(\vec{u}). \quad (28)$$

Now we have to obtain corresponding coercivity estimates of the form

$$\|\boldsymbol{\epsilon}(\vec{u})\|_{L^2(\Omega)}^2 + \sum_{l=1}^6 \omega_l(\vec{u}) \omega_l(\vec{u}) \geq \|\vec{u}\|_V^2. \quad (29)$$

These estimates are known for some particular cases.

Consider a system of linear functionals $\omega_l \in V'$, such that from

$$\vec{v} \in \mathcal{RB} : \sum_{l=1}^6 \omega_l^2(\vec{v}) = 0$$

it follows that

$$\vec{v} = 0,$$

then Korn's inequality (29) holds [7, 8, 9].

This condition is equivalent to the condition of non-degeneracy of the matrix M , presented above, see (15).

Different choices of ω_l can be considered; see, again [7, 8, 9] for examples. An interesting to us case is

$$\omega_l(\vec{v}) = \int_X v_l dX, \quad l = \overline{1, 3}; \quad \omega_l(\vec{v}) = \int_X (\vec{x} \times \vec{v})_{l-3} dX, \quad l = \overline{4, 6}, \quad (30)$$

where X is either a set of positive volume measure, $X = \tilde{\Omega} \subset \Omega$, or an arbitrary open part Γ' of the boundary $\tilde{\Gamma} = \partial\tilde{\Omega}$. This is also valid for $\tilde{\Omega} = \Omega$, $\tilde{\Gamma} = \Gamma = \partial\Omega$ and, so, as particular case, for $X = \Gamma' \subset \Gamma$ being a part of the domain's boundary Γ . Thus, the same result as obtained for Poisson's equation holds for this case too, i.e. $\kappa(A_\omega) \leq Ch^{-2}$, when ω_l are chosen according to (30).

Now coercivity estimates for $a_\omega(\cdot, \cdot)$ are direct implication of (28) and (29). Continuity estimates for regularized problem can be easily obtained, taking into account, that ω_l is continuous, i.e. $\omega_l \in V'$.

The choice $X = \Omega$ leads to regularized problem, solution of which is orthogonal to \mathcal{RB} with respect to $L^2(\Omega)$ inner product. The case $X = \Gamma$ leads to the case of the boundary regularization.

6 Implementation

This section covers only the case of boundary regularization term. Since the topic of our interest is to consider only the properties of the problem's stiffness matrix, boundary conditions and its approximations, right-hand side, etc., are not considered below.

Consider at first the case of Poisson's equation. Let us remind, that finite dimensional problem under consideration is: Find $u_h \in V_h$ such that

$$a(u_h, v_h) + \langle \omega, u_h \rangle_\Gamma \langle \omega, v_h \rangle_\Gamma = f(v_h), \quad \forall v_h \in V_h. \quad (31)$$

Finite element approximation u_h to the solution u of the problem, reads

$$u_h = \sum_{i=1}^N u_i \varphi_i,$$

where N is a number of finite-element nodes in Ω and $\varphi_i \in V_h$ are basis functions, $V_h = \text{span}(\varphi_i)$.

The stiffness matrix of the problem is

$$A_\omega = A + B_\omega,$$

where A corresponds to the first term in the left hand side of the equation (31), and B_ω corresponds to the second one.

Matrix A corresponds to the approximation of the pure Neumann problem with zero Neumann boundary conditions and reads:

$$A_{ij} = a(\varphi_i, \varphi_j), \quad i, j = \overline{1, N}.$$

Consider now representation for the second term. Since it depends only on values at the boundary, it is enough to consider $u_{h,\Gamma} = u_h|_\Gamma$ and $v_{h,\Gamma} = v_h|_\Gamma$,

$$u_{h,\Gamma} = \sum_{i \in \Gamma} u_i \varphi_i, \quad v_{h,\Gamma} = \sum_{i \in \Gamma} v_i \varphi_i, \quad \omega_h = \sum_{i \in \Gamma} \omega_i \varphi_i,$$

where $i \in \Gamma$ implies that the summation above is performed only over the set of boundary nodes. For some v_h , denote as v_Γ a set of its boundary components, i.e. $v_\Gamma = \{v_i, i \in \Gamma\}$. Then, for an arbitrary v_h one has:

$$\langle v_{h,\Gamma}, \omega_h \rangle_\Gamma = \omega^T M_\Gamma v_\Gamma,$$

where $M_\Gamma \in \mathbb{R}^{N_\Gamma \times N_\Gamma}$ is "boundary" Gram's or mass matrix,

$$(M_\Gamma)_{ij} = \langle \varphi_i, \varphi_j \rangle_\Gamma, \quad i, j \in \Gamma;$$

vectors $v_\Gamma, \omega_\Gamma \in \mathbb{R}^{N_\Gamma}$ corresponds to the boundary degrees of freedom, and N_Γ is a number of boundary nodes at Γ .

Then

$$\langle u_h, \omega \rangle_\Gamma \langle v_h, \omega \rangle_\Gamma = v_\Gamma^T (M_\Gamma \omega) (M_\Gamma \omega)^T u_\Gamma = v_\Gamma^T R_\Gamma R_\Gamma^T u_\Gamma = v^T B_\omega u$$

with $R_\Gamma = M_\Gamma \omega$ and

$$B_\omega = \begin{pmatrix} 0 & 0 \\ 0 & R_\Gamma R_\Gamma^T \end{pmatrix}. \quad (32)$$

Resulting system of equations for u_h is

$$A_\omega u_h = F_h,$$

or, in a block form (corresponding to internal $(u_{h,I})$ and boundary $(u_{h,\Gamma})$ degrees of freedom, $u_h = [u_{h,I}, u_{h,\Gamma}]^T$):

$$\left(\begin{pmatrix} A_{II} & A_{I\Gamma} \\ A_{\Gamma I} & A_{\Gamma\Gamma} \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & R_\Gamma R_\Gamma^T \end{pmatrix} \right) \begin{pmatrix} u_{h,I} \\ u_{h,\Gamma} \end{pmatrix} = \begin{pmatrix} F_I \\ F_\Gamma \end{pmatrix}.$$

This equation shows that an additional ‘‘boundary’’ term $R_\Gamma R_\Gamma^T$ regularizes the Schur complement system. Indeed, since A_{II} is non-singular, by direct elimination of internal degrees of freedom, one has

$$S + R_\Gamma R_\Gamma^T = G,$$

where

$$S = A_{\Gamma\Gamma} - A_{\Gamma I} A_{II}^{-1} A_{I\Gamma}$$

is a Schur complement matrix, which is singular.

Thus, we can state, that regularization of the entire singular stiffness matrix using boundary regularization is exactly the same as regularization of the corresponding singular Schur complement matrix.

We now consider a particular case, where $\omega_\Gamma = \text{const}$ ($\omega_{\Gamma,i} = \omega = \text{const}$ for $i = \overline{1, N_\Gamma}$.) In this case

$$(R_\Gamma)_i = (M_\Gamma \omega)_i = \sum_{j \in \Gamma} M_{\Gamma,ij} \omega_j = \sum_{j \in \Gamma} \langle \varphi_i, \varphi_j \rangle_\Gamma \omega = \omega \left\langle \varphi_i \sum_{j \in \Gamma} \varphi_j \right\rangle_\Gamma = \omega \langle \varphi_i, 1 \rangle_\Gamma.$$

This is valid for both the 2d and 3d case.

Now, for simplicity, we consider only the 2d case. If the boundary mesh on Γ , induced from triangulation of Ω , is uniform with mesh parameter h (this is what holds in our numerical experiments), then $\langle \varphi_i, 1 \rangle_\Gamma = h$ and

$$(R_\Gamma)_i = (M_\Gamma \omega)_i = \omega h, \quad i = \overline{1, N_\Gamma}$$

and

$$B_\omega = \omega^2 h^2 J J_\Gamma, \quad (33)$$

where vector $J_\Gamma \in \mathbb{R}^N$ has zero entries at the internal nodes and ones at the boundary nodes. Hence, elements of regularization matrix are

For 3d case, using similar procedure, one has $\langle \varphi_i, 1 \rangle_\Gamma \sim h^2$ to obtain

$$(R_\Gamma)_i = (M_\Gamma \omega)_i \sim \omega h^2, \quad i = \overline{1, N_\Gamma}$$

and

$$B_\omega \sim \omega^2 h^4 J_\Gamma J_\Gamma^T, \quad (34)$$

with J_Γ of the same structure as for 2d case.

The same procedure can be performed for elasticity equations. In the latter case the regularization matrix B_ω , corresponding to the regularization functionals (30) has the form

$$B_\omega = (M_X R)(M_X R)^T \quad (35)$$

with a $(3N) \times 6$ block-column matrix

$$R = \begin{pmatrix} R(\vec{x}_1) \\ R(\vec{x}_2) \\ \vdots \\ R(\vec{x}_N) \end{pmatrix}$$

with $R(\vec{x})$ from (25) and $\vec{x}_i, i = \overline{1, N}$ being finite elements nodal coordinates;

$$M_X = \int_X \Phi^T \Phi dX, \quad M_X \in \mathbb{R}^{3N}$$

where $3 \times 3N$ matrix Φ reads

$$\Phi = (\Phi_1, \Phi_2, \dots, \Phi_N), \quad \Phi_i = \text{diag}(\varphi_i, \varphi_i, \varphi_i).$$

For the matrix $C = M_X R$ another form can be obtained:

$$C = \begin{pmatrix} C_1 \\ C_2 \\ \vdots \\ C_N \end{pmatrix},$$

where $3N \times 6$ matrix C_i reads

$$C_i = \int_X \begin{pmatrix} \varphi_i & 0 & 0 \\ 0 & \varphi_i & 0 \\ 0 & 0 & \varphi_i \end{pmatrix} \begin{pmatrix} (\vec{x} \times \vec{e}_1)\varphi_i & (\vec{x} \times \vec{e}_2)\varphi_i & (\vec{x} \times \vec{e}_3)\varphi_i \end{pmatrix} dX.$$

Here $\vec{x} = x_1\vec{e}_1 + x_2\vec{e}_2 + x_3\vec{e}_3$ and $\vec{e}_1, \vec{e}_2, \vec{e}_3$ are basis vectors. The last three columns of this matrix are components of the corresponding cross products.

Integration in the entries of the matrix C_i over subset X , can be reduced to the integration over $\text{supp } \varpi_i \cap X$.

For the particular case under consideration, X is the domain boundary, $X = \Gamma = \partial\Omega$ and, hence,

$$C_i \sim h^2 R(\vec{x}_i),$$

for all non-zero entries of C . Here h is an ‘‘average’’ mesh step size, i.e.

$$c_1 h \leq h_{min} \leq h_{max} \leq c_2 h,$$

for every h and c_1, c_2 constants, independent on h . Here h_{min} and h_{max} stand for minimal and maximal values of the mesh parameter for the particular mesh.

Hence, for the 3d elasticity problem, that is considered here, one gets

$$B_\omega \sim h^4 R_\Gamma R_\Gamma^T, \quad (36)$$

where matrix R_Γ is obtained from matrix R by setting zero values to those blocks of R which correspond to the internal degrees of freedom.

7 Numerical results

All numerical tests for Poisson’s equation are performed in `Matlab`. Computational domain Ω was chosen to be a unit square $\Omega = [0, 1]^2 \subset \mathbb{R}^2$ or a cube $\Omega = [0, 1]^3 \subset \mathbb{R}^3$. Piece-wise linear first-order, finite elements on a triangular or tetrahedral meshes are used.

All meshes are triangular (for 2d) or tetrahedral (for 3d case), with mesh nodes arranged in 2d (3d) uniform rectangular array. In this case number N of degrees of freedom is equal to $N = N_x \times N_y$ (for 2d) or $N = N_x \times N_y \times N_z$ (for 3d) with $N_x = N_y = N_z$. For 2d case numerical tests were done for values of N from 10 to 300. For 3d case N varies from 5 to 25.

Boundary regularization functional corresponds to the case $\omega_\Gamma = \omega = 1$.

For simplicity, the ‘‘simplified’’ regularized term of the form (33) and (34) was used. All presented results correspond to this choice of B_ω . Nevertheless,

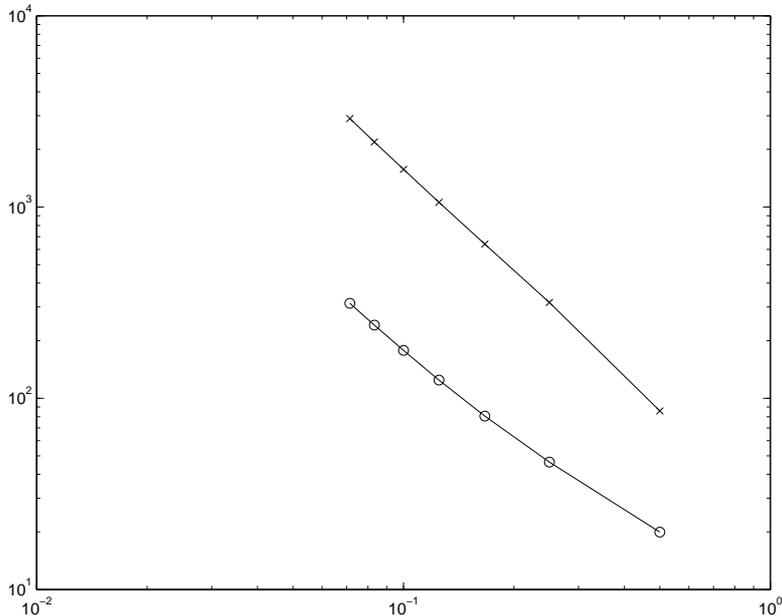


Figure 1: Poisson’s eq., 3d case, $\omega = 1$ (\circ — $\tilde{\kappa}(A)$, (\times — $\kappa(A_\omega)$)

some numerical tests were done for the “full” regularization term (32). They resulted in the same values for condition numbers of the regularized system. This goes to show, that the efficiency of such regularization is due to proper scaling of the rigid body matrix R in mesh parameter h . For example, in 2d case $\omega_\Gamma = 1$ corresponds to $(R_\Gamma)_i = \omega h_\Gamma = h_\Gamma$, where h_Γ is boundary mesh step size, which is set as a constant in our examples.

The numerical results obtained are as follows. For the 2d problem, condition number of the regularized matrix differs only slightly from natural condition number of the original, singular, problem. For example, for $N_x = N_y = 151$ we obtain $\tilde{\kappa}(A) = 18604.3$ and $\kappa(A_\omega) = 20257.0$. Despite the fact that this result is greater, than the one obtained in the previous section, proper asymptotic is also observed.

Results for 3d case and $\omega = 1$ are presented on Fig. 1. In that case we have

$$\kappa(A_\omega) \sim h^{-1.8}$$

which is in compliance with the theoretical results. Let us also note that now the condition numbers are of the same asymptotic, but with different values, when compared to the 2d case.

Now lets turn to the elasticity equations. For this case only 3d experiments were performed. Again, computational domain was chosen to be a cube $\Omega = [0, 2]^3$. All meshes are tetrahedral, with mesh nodes ar-

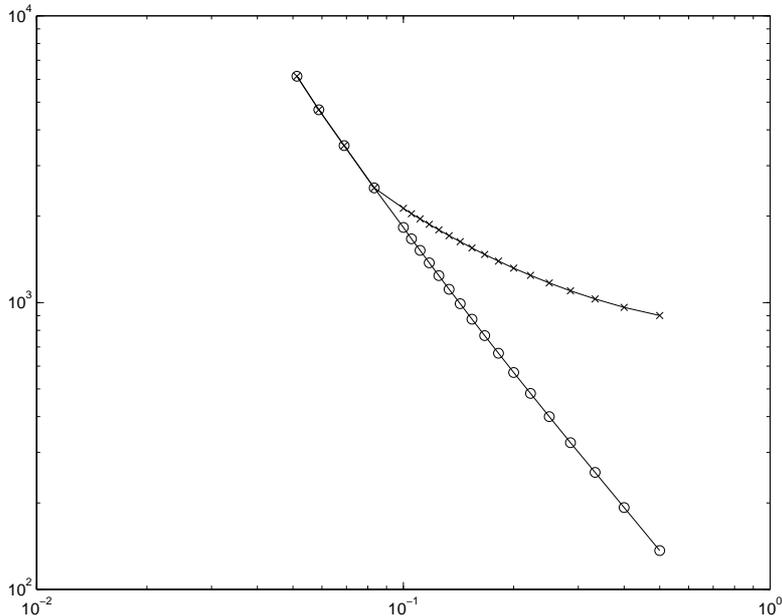


Figure 2: Elasticity equation, 3d case (\circ — $\tilde{\kappa}(A)$, (\times — $\kappa(A_\omega)$)

ranged in 3d uniform rectangular array. Number N of degrees of freedom, $N = 3(N_x \times N_y \times N_z)$, where $N_x = N_y = N_z = 5, \dots, 40$. The boundary regularization matrix was chosen according to (36).

The PRIMME library was used [11, 12] to compute eigenvalues of the matrices.

The results obtained are similar to the case of the Poisson's equation. The resulting plot is presented on Fig. 2. It can be seen, that asymptotics are proper for sufficiently small h . Moreover, values of condition numbers, both for the singular system and the regularized system are the same.

The “ $\sim h$ ” behavior of the condition number of the regularized matrix for large h is also observed. Although we didn't conduct a detailed analysis of this feature, such behavior seems to be natural for such a kind of regularization and is connected with how the orders of minimal and maximal eigenvalues of A in mesh parameter h corresponds with order in h of the entries of regularization matrix B_ω .

For example, consider regularization using orthonormalized rigid body matrix R (3), which shifts all zero eigenvalues of A to 1. Taking into account, that for the 3d case

$$c_1 h^3 \leq \lambda_{\min, >0}(A) < \lambda_{\max}(A) \leq c_2 h,$$

we have

$$\kappa(A_\omega) \leq \frac{\max(1, c_1 h)}{\min(1, c_2 h)}.$$

Hence, we obtain asymptotic $\kappa(A_\omega) \sim h^{-2}$ if $c_1 h^3 < 1 < c_2 h$, $\kappa(A_\omega) \sim h$ if $1 < c_1 h^3 < 1 < c_2 h$ and $\kappa(A_\omega) \sim h^{-3}$ if $h^3 < 1 < c_2 h < 1$.

The above plot displays similar behavior.

This shows, that a proper asymptotic of the condition number can be obtained by appropriate scaling of the regularization term.

8 Conclusions

In this paper, asymptotic behavior of condition number of the regularized problem for solution of pure Neumann problem was investigated. The main result is that the regularization terms should be continuous functionals over corresponding Sobolev space $H^1(\Omega)$ to keep the condition number of the same order in h as the natural condition number for the original singular system. As a particular case, regularization functional can be chosen as a constant function defined on the domain (or its mesh-independent part) or at the boundary of the domain (or its mesh-independent part).

For 2D and 3D Poisson's equations and 3d elasticity equations it was observed that it suffices to consider regularization at the boundary of the domain to keep exactly the same condition number as for the regularization in the entire domain and for the natural condition number of the original singular stiffness matrix.

We conclude with stating that proper scaling of the (boundary) regularization matrix plays a crucial role for the behavior of the condition number.

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