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## Iterative solution of singular systems with applications

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Dedicated to Professor Ivo Marek on the occasion of his 80th birthday.

# 1 Introduction

This contribution concerns the iterative solution of singular systems which arise in many applications. Let us mention the following

- solution of PDE problems with pure Neumann boundary conditions (which is our main aim), see [7], [8], [20]. Such problems have a specific role in numerical upscaling, see [6],
- solution of Neumann type subproblems in domain decomposition techniques as FETI, Neumann-Neumann, BDDC methods, see [22], [16],
- analysis of Markov chain problems, computation of stochastic vector, see e.g. [18], [19],
- computer tomography [15], [14] and inverse problems [4], [21].

### 2 Iterative solution of singular symmetric semidefinite systems

Let us focus on iterative solution of linear systems of the form

$$Au = b, \tag{1}$$

where A is a singular, symmetric, positive semidefinite  $n \times n$  matrix,  $b \in \mathbb{R}^n$ . For  $u, v \in \mathbb{R}^n$  denote  $\langle u, v \rangle = u^T v$  and ||u|| the Eucledian inner product and norm. Due to symmetry of A, the range R(A) and the null space N(A) are mutually orthogonal with respect to the Eucledian inner product and the vectors  $u \in \mathbb{R}^n$  can be uniquely decomposed as

$$u = u_N + u_R$$
, where  $u_N \in N(A)$  and  $u_R \in R(A)$ .

Let  $b = b_N + b_R$ , then the system (1) has infinitely many generalized (least squares) solutions u,

$$||Au - b|| = \min\{||Av - b||, v \in \mathbb{R}^n\}$$
(2)

among which there is a unique least squares solution  $u^*$  with the minimal Eucledian norm. Note that  $u^* = A^+ b$ , where  $A^+$  is the Moore-Penrose pseudoinverse of A, see [10], [16]. If  $b \in R(A)$ , i.e. the system (1) is consistent, then the generalized solutions are standard solutions of (1).

Let us assume that (1) is solved iteratively with denoting the i-th iteration  $u^i$ ,

$$u^{i} \in u^{0} + K_{i}(A, r^{0}) = u^{0} + \operatorname{span}\{r^{0}, Ar^{0}, \dots, A^{i-1}r^{0}\}, r^{0} = b - Au^{0},$$
 (3)

where  $K_i(A, r^0) = \operatorname{span}\{r^0, Ar^0, \dots, A^{i-1}r^0\}$  is a Krylov space. Then

$$u^{i} = u^{0} + q_{i-1}(A)r^{0}$$
, where  $q_{i-1}$  is a polynomial of order  $\leq i - 1$ . (4)

The convergence can be investigated through behaviour of  $e^i = u^i - u^*$ . If  $e^i \to 0$  then the iterations converge to the minimal least squares solution  $u^*$ . If  $e^i \to w$ , where  $w \in N(A)$ , then the iterations converge to a (generalized) solution of A.

From (4), it follows that

$$e^{i} = u^{0} - u^{*} + q_{i-1}(A)(b_{N} + Au^{*} - Au^{0}) = p_{i}(A)e^{0} + q_{i-1}(0)b_{N},$$
(5)

where  $p_i(\lambda) = 1 - \lambda q_{i-1}(\lambda)$ .

If  $e^0 = e_N^0 + e_R^0$  then  $p_i(A)e_N^0 = u_N^0$  and  $p_i(A)e_R^0$  depends on values  $p_i(\lambda)$  on  $\lambda \in \sigma(A) \setminus \{0\}$ . The second term is zero for consistent problems, but otherwise can be convergent if  $q_{i-1}(0) = -p'_i(0) \neq 0$ .

The simplest Richardson's iteration  $u^{i+1} = u^i + \omega A(b - u^i)$  fulfill (3), (4), (5) with

$$p_i(\lambda) = (1 - \omega \lambda)^i, \quad p_i(0) = 1, \quad q_{i-1}(0) = -p'_i(0) = (i+1)\omega.$$

Thus, the method converges  $(e^0 \rightarrow u_N^0)$  for the consistent problems, but diverges (the second terms gradually dominates) for the inconsistent case  $(b_N \neq 0)$ .

To get convergence even for inconsistent case, the method needs a modification. For example, we can use extrapolation of Richardson's iterations [17]. For

$$\bar{u}^{i+1} = u^{i+1} - (i+1)(u^{i+1} - u^i),$$

we get

$$\bar{u}^{i+1} - u^* = u^{i+1} - u^* - (i+1)(u^{i+1} - u^i) = p_{i+1}(A)e^0 + (i+1)\omega(b_N + A(u^* - u^i))$$
  
$$= p_{i+1}(A)e^0 + (i+1)\omega Ae^i = p_{i+1}(A)e^0 + (i+1)\omega A(p_i(A)e^0 + i\omega b_N))$$
  
$$= p_{i+1}(A)e^0 + (i+1)\omega(p_i(A)Ae^0)).$$

This extrapolated method converges since  $p_i(\lambda) \leq q^i$  for all  $\lambda \in \sigma(A) \setminus \{0\}$ , where q < 1 for a suitable  $\omega$ .

It means that there are ways how to damp the divergence of the null space component of the iterations. On the other hand, this divergence in the null space component may not cause a problem in case that we are interested only in quantities, which do not depend on the null space component, like gradients, fluxes, strains and stresses.

A similar analysis can be done for other iterative methods applied to singular systems, see e.g. [10]. For the conjugate gradient (CG) method, the convergence can be proven in the consistent case, see eg. [1]. But the inconsistence influence both N(A) and R(A) components of the iterations, see [13], [7] and the next section.

## **3** Solution of Neumann problems

The solution of boundary value problems with pure Neumann boundary conditions arises in different applications, see the other sections. If the solution of the continuous Neumann problem exists, then global balance (consistency) conditions like (7) are satisfied. On the contrary, these conditions guarantee the existence of the (not unique) solution. For example ([20], [7]), for the Neumann problem,

$$-\operatorname{div}(\nabla u) = f \text{ in } \Omega \quad \text{and} \quad \nabla u \cdot n = g \text{ in } \partial \Omega \tag{6}$$

the solution exits if and only if

$$\int_{\Omega} f \, dx + \int_{\partial \Omega} g \, dx = 0. \tag{7}$$

In the case (6), (7), if u is a solution, then u+v is a solution for all  $v \in \mathcal{N} = \text{span}\{1\}$ , where 1 is a constant function in  $\Omega$ . A finite element discretization then should provide a consistent singular linear system (1) with the nullspace  $N(A) = \mathcal{N}_h$  provided by discretization of  $\mathcal{N}$ . However, the computer arithmetic and numerical integration errors may cause that the FEM system is inconsistent and/or  $N(A) \neq \mathcal{N}_h$ .

Problems with inconsistency and singularity can be treated by using a priori knowledge about  $\mathcal{N}$ and  $\mathcal{N}_h$ . For example, we are able to regularize the problem by fixing some degrees of freedom and solving the problem  $R_{dof}AR_{dof}^T u = R_{dof}b$  instead of (1). Here,  $R_{dof}$  is the restriction opperator omitting the fixed DOF's. Such a technique is frequently used in engineering community, but without a special care [9] the modified system matrix  $R_{dof}AR_{dof}^T$  can be very ill-conditioned which is a serious drawback for the iterative solution.

Using the knowledge of  $\mathcal{N}$ , other techniques use the projection  $P: \mathbb{R}^n \to \mathcal{R}_h$ , where  $\mathcal{R}_h$  is the orthogonal complement of  $\mathcal{N}_h$ . The projector can be constructed as  $P = I - V(V^T V)^{-1} V^T$ , where V is a matrix, whose columns create a basis of  $\mathcal{N}_h$ . Such projector can be applied within any iterative method. In PCGstab1 algorithm, the projection P is used to project the right hand side vectors or all residuals during the PCG iterative process. In PCGstab2, the projection P is applied twice per iteration to project both residuals and computed iterations. Figure shows these stabilizations of the PCG method. PCGstab2 is equivalent to the replacement of A by PAP which also makes the system matrix singular. The fully stabilized PCGstab2 was introduced e.g. in [11]. Note that g = G(r) denotes the action of preconditioner, which can be also nonlinear (variable, flexible).

given 
$$u^0$$
  
compute  $r^0 = P_a(b - Au^0)$ ,  $g^0 = P_bG(r^0)$ ,  $v^0 = g^0$   
for  $i = 0, 1, \dots$  until convergence do  
 $w^i = P_cAP_dv^i$   
 $\alpha_i = \langle r^i, g^i \rangle / \langle w^i, v^i \rangle$   
 $u^{i+1} = u^i + \alpha_i v^i$   
 $r^{i+1} = P_a(r^i - \alpha_i w^i)$   
 $g^{i+1} = P_bG(r^{i+1})$   
 $\beta_{i+1} = \langle g^{i+1}, r^{i+1} \rangle / \langle g^i, r^i \rangle$   
 $v^{i+1} = g^{i+1} + \beta_{i+1}v^i$   
end  
a) Standard PCG:  
 $P_a = P_b = P_c = P_d = I$   
b) *PCGstab1*:  
 $P_a = P_b = P_c$   
 $P_d = P_c = I$   
or equivalently  
 $P_a = P_b = I$   
 $P_c = P_d = I$ 

Figure: PCG algorithms.

Note that an application of PCG to inconsistent system is problematic from two reasons. The inconsistent part of the right hand side enters the N(A)-part of the iterations and can make them divergent, but the inconsistent part also enters the formulas for  $\alpha$  and  $\beta$  and spoils the R(A)-part of the iterations, see [13], [5].

#### 4 Application in upscaling

The elastic response of a representative volume  $\Omega$  is characterized by homogenized elasticity C or compliance S tensors  $(S = C^{-1})$ . The compliance tensor can be determined from the relation

$$S\langle\sigma\rangle = S\sigma_0 = \langle\varepsilon\rangle,\tag{8}$$

where  $\langle \sigma \rangle$  and  $\langle \varepsilon \rangle$  are volume averaged stresses and strains computed from the Neumann problem

$$-\operatorname{div}(\sigma) = 0, \quad \sigma = C_m \varepsilon, \quad \varepsilon = (\nabla u + (\nabla u)^T)/2 \quad \text{in } \Omega, \tag{9}$$

$$\sigma n = \sigma_0 n \quad \text{on } \partial \Omega. \tag{10}$$

Above,  $\sigma$  and  $\varepsilon$  denote stress and strain in the microstructure,  $C_m$  is the variable local elasticity tensor, u and n denote the displacement and the unit normal, respectively. The use of Neumann boundary conditions allows us to get a lower bound for the upscaled elasticity tensor [6].

In analysis of geocomposites (see [6]), the domain  $\Omega$  is a cube with a relatively complicated microstructure. The FEM mesh is constructed on the basis of CT scans. Consequently using the GEM software [3], the domain is discretized by linear tetrahedral finite elements. The arising singular system is then solved by stabilized *PCGstab1* method implemented in different software and using various preconditioners:

- **GEM-DD** is a solver fully implemented in GEM software. It uses one-level additive Schwarz domain decomposition preconditioner with subproblems replaced by displacement decomposition incomplete factorization described in [2]. The resulting preconditioner is symmetric positive definite.
- **GEM-DD-CG** solver differs in preconditioning, which is a two-level Schwarz domain decomposition arising from the previous GEM-DD by additive involvement of a coarse problem correction. The coarse problem is created by a regular aggregation of  $6 \times 6 \times 3$  nodes with 3 DOF's per aggregation. In this case, the coarse problem is singular with a smaller null space containing only the rigid shifts. The coarse problem is solved only approximately by inner (not stabilized) CG method with a lower solution accuracy - relative residual accuracy  $\varepsilon_0 \leq 0.01$ .
- **Trilinos ILU** is solver running in Trilinos, where the system from GEM is imported. The preconditioner is similar to GEM-DD, i.e. one-level Schwarz with the minimal overlap and working on the same subdomains as in GEM-DD are used. The subproblems are replaced by ILU without displacement decomposition, using a drop tolerance and a fill limit.
- **Trilinos ML-DD** is again running in TRILINOS and uses multilevel-level V-cycle preconditioner exploiting smoothed aggregations with aggressive coarsening, see [12]. Six DOF's translational plus rotational are used per aggregation. ILU is applied as smoother at the finest level, other smoothing is realised by symmetrized Gauss-Seidel. The coarsest problem is solved by a direct solver.

	GEM						Trilinos					
	DD			DD+CG			ILU			ML-DD		
$\#\operatorname{Sd}$	#It	$T_{prep}$	$T_{iter}$	#It	$T_{prep}$	$T_{iter}$	#It	$T_{prep}$	$T_{iter}$	#It	$T_{prep}$	$T_{iter}$
1							345	224.5	2672.4		×	
2	293	0.3	541.4	137	20.1	256.4	472	135.9	1628.3	43	813.6	804.5
4	302	0.2	302.2	124	20.0	125.9	463	112.5	1022.6	46	445.6	404.9
8	300	0.1	175.3	115	19.9	75.7	441	85.9	517.6	53	302.9	203.8
16	350	0.1	148.5	116	19.9	73.6	387	75.4	443.9	57	335.4	146.9

Table: Solution of the Neumann problem in elasticity, slightly more than 6 million mil DOF's, stopping criterion  $||r||/||rhs|| \leq \varepsilon = 10^{-5}$ . Numbers of iterations (#It), wall-clock time in seconds for solver preparation (T<sub>prep</sub>) and time for performing the iterations (T<sub>iter</sub>) are provided for various numbers of subdomains (#Sd; always corresponding to the number of employed processing units). GEM solvers have not the single processor mode, the ML-DD solver ended on single processor with the message "Not enough space for domain decomposition" (×).

The parallel computing was performed on 32 core NUMA machine at the Institute of Geonics with eight quad-core AMD Opteron 8830/2.5 GHz processors and 128 GB of DDR2 RAM. Because of using stabilized PCG and also because we were interested only on strains and stresses, we concentrate on R(A)-part of the solution and watch in Table only the convergence in the residual norm.

We can see that the stabilized CG works well. On the other hand the unstabilized version converge up to a smaller residual tolerance  $\varepsilon = 0.01 - 0.001$  and then started to blow up, see [5]. It indicates that numerical consistency and numerical singularity are not enough, which was a bit unexpected in our case as we used lowest order linear finite elements and problem with piecewise constant boundary condition, so that the adopted numerical integration should be exact. On the other hand, the systems were assembled in single precision.

# 5 Conclusions

The aim of this contribution was to show techniques for efficient solution of singular symmetric positive semidefinite problems. We can see that the stabilized PCG is a good choice for systems arising from the numerical solution of Neumann problems, or more generally problems with a known small dimensional null space. There are also other possibilities of stabilization as e.g. the use of additive regularization.

The second aim was a comparison of specialized solvers from the in-house finite element software GEM and more general solvers from the Trilinos library. We provided some comparison while this work is still continuing.

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