Parallel Space Decomposition Solvers for the Geo-oriented FE System GEM

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Abstract. This paper introduces a 3-D finite-element package called GEM and its aspirations for demanding mathematical simulations arising in geosciences. We deal mainly with GEM's (basic) solvers for linear systems arising from the linear elasticity problems, which are based on the conjugate gradient method and parallelizable preconditioning belonging to a general framework of the DoF space decomposition. In particular, we show that the displacement decomposition and the black-box overlapping domain decomposition techniques fit in this space decomposition framework. Possible application types and some numerical results are presented for illustration.

1 Introduction

The Institute of Geonics of the Czech Academy of Sciences is active in the scientific research related to the Earth's crust. Its main interests include mathematical modelling and simulations of the thermo-hydro-mechanical processes in the rock mass that are associated with the construction, operation and safety of underground structures, e.g. mines or waste deposits. For this purpose, a proprietary software called GEM is being developed and maintained at the Institute.

GEM can be characterized as non-commercial three-dimensional finite-element (FE) package oriented on the solution of problems arising in geosciences. GEM serves both research purposes and practical modelling and its development is mainly problem-driven, reflecting the requirements of the current research and applications on increasing complexity of the models and methods.

The following sections address GEM's solvers, i.e. the modules responsible for numerical processing of the systems of equations arising from the FE analysis, computationally the most demanding phase in the FE method simulation chain preprocessing – assembling the FE system – solution of the system – postprocessing. We shall consider modelling of the mechanical response, which is in the centre of our interest from the very beginning, while the heat and flow phenomena have been taken account of in GEM only recently, see e.g. [8].

We focus on the iterative conjugate gradient method and its parallelizable preconditioners. In particular, we describe our novel idea of the DoF (degrees of freedom) *space decomposition* (SD) as a generalization of the Schwarz type preconditioning framework [16], [17], [6]. This SD framework includes the displacement decomposition [1], [4], leading to a basic parallelization limited in

scalability, and the overlapping domain decomposition, which combines a special 1D decomposition and coarse space created by aggregation and provides more scalability. Moreover, the SD framework can also encompass the local refinement [7] and multiscale hierarchical methods.

2 GEM's building blocks

The solvers operating in GEM can be highlighted as follows:

Finite elements. For the solution of the problem of elastic deformation, see [13] and Section 5, the finite element method (FEM) is employed. The FE discretization of this boundary value problem, based on linear tetrahedral finite elements in GEM, leads to the linear system of the type $Au = b$, $u, b \in R^n$, where A is a symmetric positive definite $n \times n$ stiffness matrix, $b \in R^n$ is the right-hand side given by the loading and $u \in R^n$ is the n-dimensional vector of unknown nodal displacements.

Structured meshes. Since its very beginning, GEM uses structured meshes for the discretization of the modeled domain, which can be viewed as adaptation (deformation) of a regular rectangular (reference) grid of nodes to the solved problem. More on this topic in Section 4.

Conjugate gradients and preconditioning. The symmetry and positive definiteness of the stiffness matrix A permit to solve the linear system above by the standard (iterative) preconditioned conjugate gradient (PCG) method. In the PCG algorithm, the preconditioning should be efficient and parallelizable. We shall address this theme in the context of the general DoF space decomposition and its two instances, see Sections 5 – 7.

Parallel processing. The increasing demands on the size and complexity of the modelling and the growing availability of the multiprocessor systems promote parallel processing in the numerical solution. However, the parallelization of the solution is not straightforward, due to the irreducible global character of the solved systems. In fact, this is the background topic of the whole paper. Nevertheless we skip technical details on the parallel implementation (e.g. the message passing scheme), and refer to [9] instead.

3 Large-scale modelling in focus

GEM's development has always been strongly influenced by difficult real problems coming from geotechnical practice. In this section, we introduce two examples, expressed as linear elasticity problems (see Section 5, eq. (1)). Let us premise that a fairly big number of DoF in both of them is a consequence of the complicated inner structure in the 3D domains. In the first example, the mesh structure reflects a complicated system of the mined-out spaces in complex geological conditions. The second example tries to utilize the entire information gained from the computer tomograph scanning of the microstructure of material.

3.1 Stability of a mine opening – the DR problem

One of the most challenging mathematical models processed in the GEM environment in the past[1] and an example of large-scale modelling in geomechanics was the simulation of mining in the uranium ore deposit at Dolní Rožínka (DR) in the Bohemian-Moravian Highlands. Mathematical modelling aimed at the assessment of the geomechanical effects of mining, e.g. comparison of different mining methods from the point of view of stress changes and possibility of dangerous rockbursts, through a four-stage sequence of computations with changing material distribution. The 3D linear elastic model considered a domain of $1430 \times 550 \times 600$ meters, located about 700 m under the surface, with three longitudinal inclined uranium ore veins, where the mining was concentrated. Its discretization led to a FE system of 3 873 264 DoF. Several variants of boundary conditions have been considered to cope with the uncertainty in the pre-mining stress measurements. This simulation, originally requiring 22 hours of (sequential) computation time on a powerful workstation, motivated experiments in methods, e.g. with composite meshes, and novelties in computer realization, the most important one being the parallelization. For benchmarking purposes in Sections 6, 7, by the DR problem we understand just the solution of the fourth mining stage.

3.2 Microstructure modelling – the CT problem

The second example shows GEM in a new area of interest, totally different in scale: the μFEM analysis, in which FEM is adapted for the derivation of material behaviour from its complex microstructure. This modelling helps in the assessment and optimization of the grouting technology. Its goal may be to find out some physical parameters of materials, which have complicated heterogeneous inner structure, but which can be considered as piecewise homogeneous from a certain scale. In our modelling we are interested in geocomposite materials produced by injection of polyurethane resin into coal environment, e.g. to reinforce coal pillars. Due to permeable and fractured coal, the geocomposites have complex microstructure making their FE analysis difficult.

Our model captures the microstructure of a cubic geocomposite sample 75 mm in size, which has been scanned with a special X-ray computer tomograph (CT) and discretized by a uniform grid of $231 \times 231 \times 37$ grid voxels, resulting in a linear system of 6 135 936 DOF. The model assumes homogeneous material in voxels – it is assigned according to the CT scan values. In GEM we compute the homogenized material properties of the cube making use of numerical upscaling via stress and strain driven tests. The voxel approach (uniform FE grid) has some specific features with impact on the numerical algorithms. A paper with more details is under preparation. In the numerical experiments in Sections 6,

[1] A resumption of the modelling with even more demanding discretization is expected in a near future, motivated by the plans to continue the extraction of ore in greater depths.

7, the CT problem is computed with the Dirichlet boundary conditions (strain driven test).

4 Structured FE meshes

Structured meshes, employed for discretization in GEM, originate from a regular rectangular (reference) mesh by its adaptation to the domain geometry and inner structure. The adaptation is finished by a division into tetrahedra. They bring in the following advantages:

- relatively simple construction of a mesh generator, which can be based on successive refinement of the mesh and interpolation of the data;
- efficient storage of the stiffness matrix, which takes advantage of the regular stencil and/or diagonal format, and allows fast matrix handling routines;
- possibility of simple balanced mesh partitioning as well as construction of the coarse approximation and transfer operators for one-level and two-level Schwarz methods;
- simplification of the visualization techniques.

Of course, structured meshes may be inconvenient when complex geometries are to be covered or local refinement is needed. In such cases, structured meshes may imply too many DoF and/or distorted FE shapes. But in the geotechnical problems such as investigation of processes in the near/far field of various underground constructions (mines, repositories, reservoirs, tunnels, etc.), the benefits outweigh the disadvantages and they are commonly used for this type of problems. Moreover, the flexibility can be increased e.g. by the use of the composite meshes, which also fit into the DoF space decomposition framework, while preserving the advantages of the structured grids [7].

5 Space decomposition preconditioning

We consider elasticity problems which can be formulated in terms of displacement $u(x)$ of points x of the body $\Omega \subset R^3$. The weak formulation is: Find $u\colon \Omega \to R^3$,

$$u - u_0 \in \mathcal{V} \quad \text{and} \quad a(u,v) \,=\, b(v) \quad \forall v \in \mathcal{V}\,, \tag{1}$$

where

$$\mathcal{V} = \{v = (v_1, v_2, v_3)\colon v_i \in H^1(\Omega),\ v_i = 0 \text{ on } \Gamma_D^{(i)} \subset \partial\Omega \text{ for } i = 1,2,3\},$$

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

$$\varepsilon_{ij}(u) = \tfrac{1}{2}\left(\tfrac{\partial u_i}{\partial x_j} + \tfrac{\partial u_j}{\partial x_i}\right), \quad \varepsilon_{kl}(v) = \tfrac{1}{2}\left(\tfrac{\partial v_k}{\partial x_l} + \tfrac{\partial v_l}{\partial x_k}\right).$$

Above, $H^1(\Omega)$ is the Sobolev space, $u_0 \in [H^1(\Omega)]^3$ is the function that prescribes nonzero Dirichlet boundary conditions, c_{ijkl} are elastic moduli, $\Gamma_D^{(i)}$ are parts of

the boundary $\partial\Omega$ and b is a linear functional determined by the applied forces. For more details see e.g. [13].

We shall solve the above problem by the FE method using the FE space (in our case the space of continuous piecewise linear functions) $V \subset \mathcal{V}$. Selected FE basis $\{\phi_i\}_{i=1}^n$ of V then defines an isomorphism of V and the space of DoF $\mathbf{V} \equiv R^n$. The FE approximation of the solution has the form

$$u_V = \sum_{i=1}^{n} u_i \phi_i. \tag{2}$$

where the components (DoF) u_i form the vector $u \in \mathbf{V}$ can be obtained from the solution of the linear system

$$Au = b\,, \quad u, b \in R^n. \tag{3}$$

Here $A = (a(\phi_i,\, \phi_j))$ is the stiffness matrix, which is supposed to be symmetric, positive definite, sparse and large[2]. The system (3) can be solved by the standard preconditioned conjugate gradient (PCG) method.

In the PCG algorithm, let $g = G(r)$ be the preconditioning operation, which computes the pseudoresidual g from the residual r. Then the construction of the preconditioner G, which aims at providing g approximating the error $A^{-1}r$, can be based on the decomposition of the FE and correspondingly the DoF space

$$V = V_1 + \ldots + V_p, \quad \mathbf{V} = \mathbf{V}_1 + \ldots + \mathbf{V}_p, \tag{4}$$

where V_k, $\mathbf{V}_k$ are subspaces of V, $\mathbf{V}$, respectively. The subspaces are not necessarily linearly independent.

Let V_k be isomorphic to R^{n_k}. We construct transfer matrices I_k, representing the prolongation $I_k : R^{n_k} \to R^n$ given by the inclusion $V_k \subset V$, and R_k representing the restriction $R_k : R^n \to R^{n_k}$ given by $R_k = I_k^T$. The transfer matrices allow to introduce matrices $A_k = R_k A I_k$ corresponding to the subproblems on the subspaces. The matrices A_k will also be symmetric and positive definite.

Now, we can introduce a class of *space decomposition preconditioners* through the algorithm shown in Fig. 1.

$g^0 = 0$
for $k = 1, \ldots, p$ **do**
    $g^k = g^{k-1} + I_k A_k^{-1} R_k\, z^k$
end
$g = g^p$

Fig. 1. The SD algorithm.

The simplest choice $z^k = r$ gives the so called *additive preconditioner*

$$G(r) = G_A r\,, \; G_A = \sum_{k=1}^{p} I_k A_k^{-1} R_k. \tag{5}$$

[2] Typically in the range from 10^5 to 10^7 for the considered geomechanical models.

It is easily parallelizable and directly applicable to the PCG method since G_A is symmetric positive definite.

The updated residuals $z^k = r - Ag^{k-1}$ provide the so called *multiplicative preconditioner*, which is represented by a nonsymmetric linear mapping G_M. To get a symmetric positive definite preconditioner, we can repeat the corrections in the SD algorithm (Fig. 1) in the reverse order, i.e. the loop should be performed for $k = 1, \ldots p, p-1, \ldots, 1$. This modification defines the *symmetrized multiplicative preconditioner*. More about general SD methods, including hybrid additive/multiplicative variant, can be found e.g. in [6], [17].

The operations $w_k = A_k^{-1} v_k$, which appear in all the space decomposition preconditioners, can be replaced by inexact solutions of the systems $A_k w_k = v_k$ by inner iterations. The inner iterations can be stopped to get an approximation $S_k(v_k)$ to $A_k^{-1} v_k$ with accuracy $\| v_k - A_k S_k(v_k) \| \leq \varepsilon_0 \| v_k \|$.

For the nonsymmetric multiplicative preconditioner or inexact solution of the subproblems, the space decomposition preconditioner cannot be represented by a linear symmetric positive definite mapping. In this case, the standard PCG method may be not efficient or can even fail. Therefore, it can be appropriate to employ the generalized PCG method with an explicit orthogonalization of the new search direction to m previous search directions. This GPCG[m] algorithm is described and analyzed in [14], [5], a similar GCR method can be found in [2].

The use of inner-outer iterations can be very favourable for parallelization since it also allows to balance the load of the processors as well as to tune the ratio between computations and communications, as we shall see in the next section (variants DiD-IF, DiD-II).

SD serves for data distribution and parallelization of the solution of the FE systems (3). The additive space decomposition preconditioners are ready for parallelization, p processors are employed to process p subspace computations in parallel. The multiplicative preconditioners are parallelizable only in the case that some groups of subproblems are independent and the computation is suitably ordered. The subspace decomposition of the data allows to parallelize not only preconditioners, but also the matrix-vector multiplication and other operations involved in the PCG algorithm.

6 Displacement decomposition

Let us introduce the first SD example. If we consider the solution of 3D elasticity problems by the FE method with linear tetrahedral or more generally Lagrangian finite elements, the degrees of freedom u_i in (2) represent nodal displacements in the coordinate directions. Then it is easy to define the *displacement decomposition* (DiD) $V = V_1 + V_2 + V_3$, where V_k corresponds to the vectors, which have nonzero DoF only in the k-th coordinate direction.

In GEM, the DiD method was originally introduced for the construction of incomplete factorizations in the solution of systems arising from the FE analysis of elasticity problems, see [1] and [4], and only later taken advantage of in parallel computations. The parallelization was uncomplicated: Each of the three

displacement direction is processed in parallel by one worker process. Thanks to the block diagonal structure of the preconditioner, the preconditioning operation does not involve any communication. The most demanding data exchange is hidden in the repeated matrix by vector multiplication.

Such parallelization made possible "comfortable" solution of demanding models of several millions DoF such as DR (see Section 3.1) ten years ago already. It perfectly fits small parallel environments, at that time consisting of 3 – 4 workstations, usually with low-speed interconnecting network. But also nowadays parallel computations based on DiD can match e.g. PC's with four-core processors.

To get an idea about practical behaviour of the (additive) DiD preconditioner, let us see Table 1.

DiD solver	# Subdom.	DR problem	CT problem
PCG-DiD-IF (seq.)	1	94 / 892	75 / 1130
PCG-DiD-II ($\varepsilon_0 = 10^{-1}$) (seq.)	1	11 / 1523	9 / 2075
PCG-DiD-IF	3	94 / 527	75 / 677
PCG-DiD-II ($\varepsilon_0 = 10^{-1}$)	3	11 / 319	9 / 484
GPCG[1]-DiD-II ($\varepsilon_0 = 10^{-1}$)	3	9 / 310	8 / 453

Table 1. Iterations/timings [s] of the DR and CT solution using the DiD solvers.

Here, DiD-IF denotes the variant when the subproblem matrices are replaced by their MIC(0)* incomplete factorizations (see [4] for details) and DiD-II(ε_0) is another variant with approximate solution of the subproblems by an inner PCG method with relative (low) accuracy ε_0 and the same MIC(0)* incomplete factorization as the preconditioner. Both the standard PCG and the generalized GPCG[1] methods were considered. The numbers in Table 1 arise from the solution of the DR and CT problems (see Section 3) with the relative residual accuracy $\varepsilon = 10^{-4}$ on a rather outdated Linux cluster (THEA), employing one or three of its eight computational nodes with AMD Athlon/1400 MHz processors and Fast Ethernet interconnect.

For both DiD-IF and DiD-II variants, we can observe parallel speedup. But in the case of a slower network and/or small operational memory (which is the case of the THEA cluster), the inner-outer iteration technique DiD-II clearly outperforms DiD-IF, because it reduces the number of outer iterations, where the matrix-vector multiplications are responsible for the high communication overhead. Moreover, the parallelization, implying the decomposition to smaller subproblems, leads to a superlinear speedup here, thanks to the improved temporal and spatial data locality in the inner iterations. Note that GPCG[1] further decreased the number of iterations and brought some minor performance advantage.

7 Domain decomposition

To achieve more scalability of the parallel computations in GEM, another type of the SD methods, based on the overlapping *domain decomposition* (DD) [16], has been realized.

Let us consider the FE solution of a boundary value problem in a domain Ω divided into finite elements $\mathcal{T}_h$. DD is initialized by the decomposition of Ω into p non-overlapping subdomains $\tilde{\Omega}_k$, which are subsequently extended into overlapping subdomains $\Omega_k, \Omega = \bigcup_{k=1}^{p} \Omega_k$. We assume that each $\tilde{\Omega}_k$, Ω_k can be represented as a union of some elements from the global division $\mathcal{T}_h$. Then the division of Ω induces a decomposition of the FE space V into the subspaces V_k,

$$V_k = \{v \in V : v = 0 \text{ in } \Omega \setminus \Omega_k\}.$$

For this DD, the prolongation is represented by very simple coincidence matrices,

$$I_k = [c_{ij}],\ 1 \le i \le n,\ 1 \le j \le n_k,$$

where $c_{ij} = 1$ if i and j refer to identical DoF, otherwise $c_{ij} = 0$.

The parallel DD solver of GEM takes up with a simple 1D partition of the domain Ω into p "horizontal" subdomains (layers) along the Z dimension (i.e. each subdomain has at most two neighbours) with minimal overlaps and assigns them to p concurrent processes. Note that 1D partition can be generated also for nonstructured meshes, e.g. by the algorithm described in [12].

According e.g. [6], [17], the convergence rate of PCG with the DD preconditioner improves with the increasing overlap, but deteriorates with growing number of subdomains. The dependence on the number of subdomains can be removed and the overall efficiency can be improved when employing a two-level decomposition with an additional subspace V_0, which can be a FE space corresponding to discretization of the global problem on a coarser mesh $\mathcal{T}_H$. If $\mathcal{T}_H$ and $\mathcal{T}_h$ are nested, then the prolongation $I_0 : V_0 \to V$ is simply defined by the inclusion $V_0 \subset V$. If $\mathcal{T}_H$ and $\mathcal{T}_h$ are not nested, then we have to use a rather complicated interpolation I_0, see [10], which may be expensive to create.

For this reason, we have another option in GEM: The space V_0 constructed from V by the *aggregation*, which means that DoF are divided into disjoint groups (aggregates) and sums of the basis functions corresponding to aggregates create the basis of V_0. Originally, this construction was introduced for the multigrid methods in [3], its use for the overlapping Schwarz method was analyzed e.g. in [6] and [11]. Our aggregation on structured grids uses also regular groupings into $3 \times 3 \times 3$ or similar aggregates (with some exceptions along boundaries). Again, the aggregation can made use of on unstructured grids, too, e.g. by the pairwise aggregation algorithm described in [15]. It uses values characterizing the strength of couplings. For elasticity problems, these coupling characteristics can be evaluated upon the stiffness of the adjacent finite elements.

In Table 2, the performance of GEM's DD solver is demonstrated on the same problems and on the same THEA cluster as in the previous section. The results of the one-level DD and two-level DD with several aggregations show

# Sd	DR problem				CT problem			
	One-level method	Two-level method			One-level method	Two-level method		
		3×3×3	5×5×5	6×6×6		3×3×3	6×6×3	9×9×3
2	104 / 447	45 / 288	51 / 231	56 / 253	76 / 553	41 / 448	47 / 360	51 / 388
3	114 / 337	47 / 264	54 / 168	60 / 186	77 / 409	39 / 390	45 / 254	49 / 273
4	123 / 281	48 / 253	57 / 140	62 / 149	80 / 338	37 / 357	43 / 196	48 / 214
5	129 / 243	51 / 249	60 / 123	65 / 130	82 / 292	37 / 348	43 / 165	46 / 172
6	134 / 221	52 / 252	62 / 112	67 / 117	82 / 258	36 / 343	42 / 147	46 / 154
7	137 / 209	53 / 260	64 / 103	70 / 111	86 / 246	35 / 329	42 / 133	46 / 140

Table 2. Iterations/timings [s] of the DR and CT solution using the DD solver with different aggregations.

higher efficiency than in the DiD case. Moreover, one can observe fairly good scalability.[3]

With the two-level methods, more care has to be devoted to the global communication and load balancing [9]: The choice of the aggregation must match the size of other subproblems, otherwise the processing of the coarse problem would become to a bottleneck of the additive scheme, see Table 2. Note that the DD solution utilized the standard PCG method, the additive SD preconditioner with the subproblems solved approximately by direct use of incomplete factorizations and the aggregated problem solved approximately by an inner PCG algorithm with accuracy $\varepsilon_0 = 10^{-1}$.

8 Conclusions and Comments

To summarize, we presented our geo-oriented FEM software based on structured grids, linear tetrahedral finite elements and parallel solvers, with a novel general DoF space decomposition view on the preconditioning operation. Both the DiD and DD parallel solvers described in the paper fit this SD framework. They could be simply implemented within the already existing sequential FEM package. We illustrated the efficiency of the solvers by solving two large geomechanical problems on a small PC cluster.

This article concerned just (geo-)mechanical modelling in GEM. Recent enhancement of GEM's repertoire is connected with another type of underground constructions, the deep geological repositories of the spent nuclear fuel, which lead to T-H-M (thermo–hydro–mechanical) problems involving heat transfer, water flows and mechanical behaviour and their interactions in a long period of time. In our initial approach we chose the thermal and mechanical phenomena (thermo-elasticity with a one-directional coupling), nowadays we are considering also the hydrogeological phenomena. More about this topic in [8].

[3] With the DR problem, the speedup (decrease in the solution time) was observed up to 30 processors on a large SMP machine. This limit is a consequence of the 1D decomposition of the domain – the layers cannot be thiner.

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