Robust and parallel preconditioners for mechanical problems

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problem from the work floor: material analysis

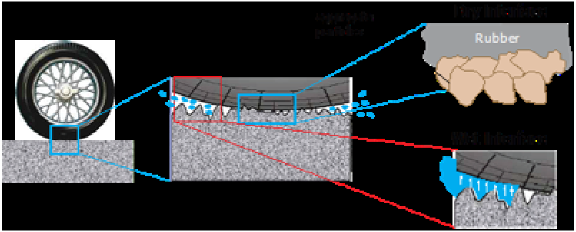


Figure: EU project, SKIDSAFE: asphalt-tire interaction

problem from the work floor: material analysis

20th century science

consider materials to be homogeneous

21th century science

shift from MACRO to MESO/MICRO scale

- Obtain CT scan from material specimen
- Convert CT scan to mesh
- Use finite element method for discretization of governing equations

problem from the work floor: material analysis

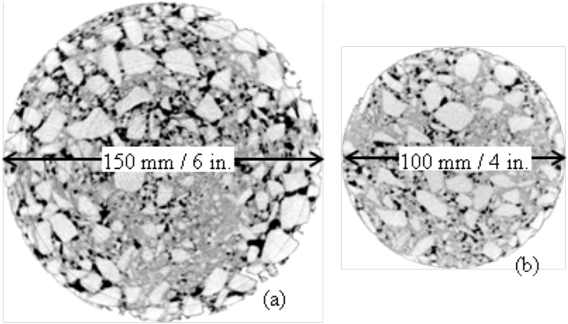


Figure: CT scan of asphalt column

problem from the work floor: material analysis

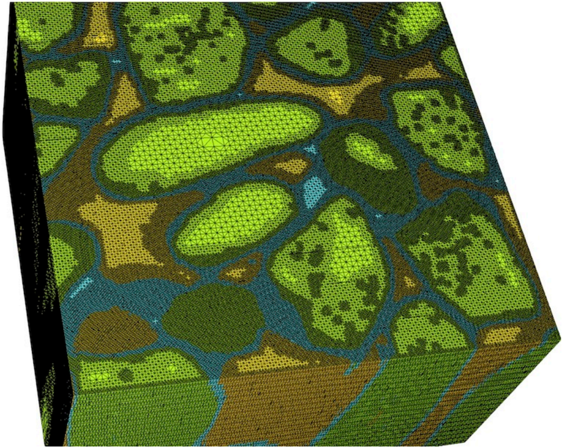


Figure: from CT scan to mesh, approx. 3 mln DOF

problem from the work floor: material analysis

governing equations

$$K \Delta u = \Delta f \quad (1)$$

Stiffness matrix K, change in displacement Δu and change of force Δf. The change of force involves evaluation of non-linear equations that depend on displacement field.

problem from the work floor: material analysis

properties of stiffness matrix K

- symmetric, positive definite: $\forall \Delta u \neq 0,\ \Delta u^T K \Delta u > 0$
- $K \in \mathbb{R}^{n \times n}$, $n >> 10^6$
- discontinuities in values matrix entries $\sim \mathcal{O}\left(10^6\right)$: ill-conditioned

Start of the project

2008

- 2D problems
- Direct solver
- Sequential
- Small grid size

End of the project

2012

- 3D problems
- Iterative solver
- Parallel 128 CPU's
- Huge grid size

End of the project

Tools

- Krylov solver
- Block IC or AMG preconditioner
- Grid partitioning (mesh based)
- Deflation Coarse grid and jumping coefficients
- Deflation for systems
- Deflation for multi-materials
- Automatic generation of Deflation vectors

Existing solvers

just some possible methods and preconditioners

- preconditioned conjugate gradient method (PCG) combined with,
- BIM: Jacobi, SSOR
- Decomposition methods: (Additive-Schwarz) ILU(ϵ)
- direct solvers: MUMPS, PARDISO, SuperLU
- multigrid: geometric multigrid, algebraic multigrid (smoothed aggregation)

Existing solvers

bottom line: no free lunch
no black box solution for large, ill-conditioned systems

- performance of PCG depends on spectrum of K, large jumps induce small eigenvalues, hence performance degrades when number of jumps (different materials) increases
- direct solvers (may) become expensive for large meshes
- AMG can be insensitive to jumps, however to achieve this one has to define the coarse grid specifically

Use deflation

Deflation based operator is not a classical preconditioner, i.e. it is not an approximation of K. The deflation operator is a projection which, by the right choice of the projection vectors, removes eigenvalues from the spectrum of the projected system.

definition

split displacement vector u,

$$u = \left(I - P^T\right) u + P^T u, \tag{2}$$

and let us define the projection P by,

$$P = I - KZ(Z^T KZ)^{-1} Z^T, \quad Z \in \mathbb{R}^{n \times m} \tag{3}$$

the DPCG method

We use deflation based operator in conjunction with preconditioning (e.g. diagonal scaling) to remove those small eigenvalues that correspond to the jumps (discontinuities) in the values of the stiffness matrix.

Deflated Preconditioned Conjugate Gradient (DPCG) method

Solve for $M^{-1}PK\Delta u = M^{-1}P\Delta f$

How to choose the deflation vectors?

- We have observed in [2][1] that the rigid body modes of the regions corresponding to the different materials coincide with the eigenvectors of the 'jump' eigenvalues.
- By removing those rigid body modes (RBM) using deflation, we remove the corresponding 'jump' eigenvalues from the system.
- The rigid body modes of sets of finite elements can be easily computed.

[1] Jonsthovel et al., CMES, 2009

How do RBM relate to stiffness matrix K?

The kernel of the element matrix of an arbitrary unconstrained finite element is spanned by the rigid body modes of the element. In 3D six rigid body modes: three translations, three rotations.

How do RBM relate to stiffness matrix K?

Theorem

We assume a splitting $K = C + R$ such that C and R are symmetric positive semi-definite with $\mathcal{N}(C) = span\{Z\}$ the null space of C [1][2]. Then

$$\lambda_i(C) \leq \lambda_i(PK) \leq \lambda_i(C) + \lambda_{max}(PR). \quad (4)$$

Moreover, the effective condition number of PK is bounded by,

$$\kappa_{eff}(PK) \leq \frac{\lambda_n(K)}{\lambda_{m+1}(C)}. \quad (5)$$

[2] Vuik, Frank, SIAM, 2001

How do RBM relate to stiffness matrix K?

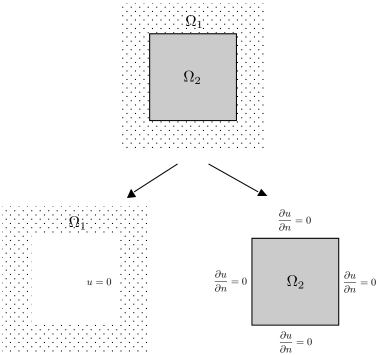


Figure: Principle of rigid body mode deflation

How do RBM relate to stiffness matrix K?

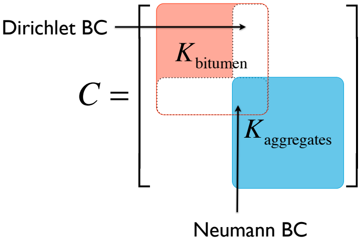


Figure: Principle of rigid body mode deflation: construction of C

How do RBM relate to stiffness matrix K?

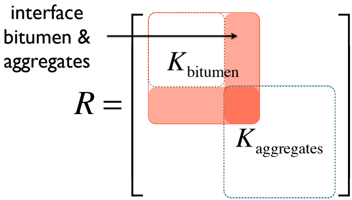


Figure: Principle of rigid body mode deflation: construction of R

Recursive deflation

However, the definition of P given by first theorem does not provide insight in the effect of individual deflation vectors on the spectrum of PK. Introduce a recursive deflation operator which can be used for more extensive eigenvalue analysis of PK.

Definition

$P^{(k)} = I - KZ_k(Z_k^{\mathrm{T}} KZ_k)^{-1} Z_k^{\mathrm{T}}$ with $Z_k = [\tilde{Z}_1, \tilde{Z}_2, ..., \tilde{Z}_k]$, where $\tilde{Z}_j \in \mathbb{R}^{n \times l_j}$ and has rank l_j.

Recursive deflation

Theorem

Let $P^{(k)}$ and Z_k as in Definition 2, then

$$P^{(k)}K = P_k P_{k-1} \cdots P_1 K$$

where $P_{i+1} = I - \tilde{K}_i \tilde{Z}_{i+1} (\tilde{Z}_{i+1}^{\mathrm{T}} \tilde{K}_i \tilde{Z}_{i+1})^{-1} \tilde{Z}_{i+1}^{\mathrm{T}}$, $\tilde{K}_i = P_i \tilde{K}_{i-1}$, $\tilde{K}_0 = K$,

$\tilde{Z}_i^{\mathrm{T}} \tilde{K}_{i-1} \tilde{Z}_i^{\mathrm{T}}$ *and* $Z_k^{\mathrm{T}} K Z_k$ *are non-singular because* $\tilde{Z}_i$ *are of full rank and* K *is a symmetric positive definite matrix.*

Numerical experiment: real asphalt core

From playground to real engineering; consider mesh from introduction. Size of system approx. 3 million DOF, material parameters given in table below,

Table:

(a) *E* modulus materials

aggregate	bitumen	air voids
70000	5000	100

Numerical experiment: real asphalt core

We compare PCG and DPCG combined with three different preconditioners,

- diagonal scaling: low cost, weak properties
- AMG smoothed aggregation, default parameters, no specific information on mesh provided: relative low set up and solve cost, designed for solving elastic equations
- AMG smoothed aggregation, approx. null space of operator and dof-to-node mapping provided: expensive set up and solve cost, high memory usage

Numerical experiment: real asphalt core

Iteration count and CPU time.
All algorithms implemented in C++, Trilinos (SANDIA).
Preconditioners insensitive to domain decomposition.

	4 domains		8 domains		64 domains	
	iter	cpu (s)	iter	cpu (s)	iter	cpu (s)
PCG (diag)	n.c.	-	n.c.	-	n.c.	-
DPCG (diag)	9018	9883	9017	5456	9015	680
PCG (SA)	2018	6687	2016	6906	1942	1123
DPCG (SA)	1210	9450	1206	5043	1199	771
PCG (SA+)	o.o.m.	-	376	1118	379	455
SuperLU	o.o.m	-	o.o.m	-	n.a.	3979

Numerical experiment: real asphalt core

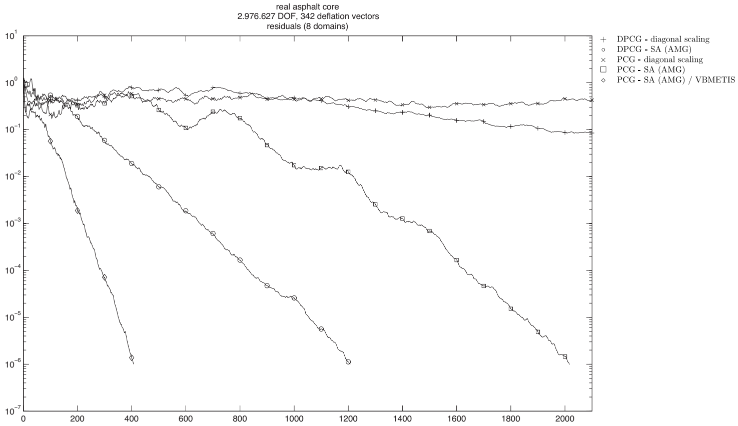


Figure: numerical results: residuals

Numerical experiment: real asphalt core

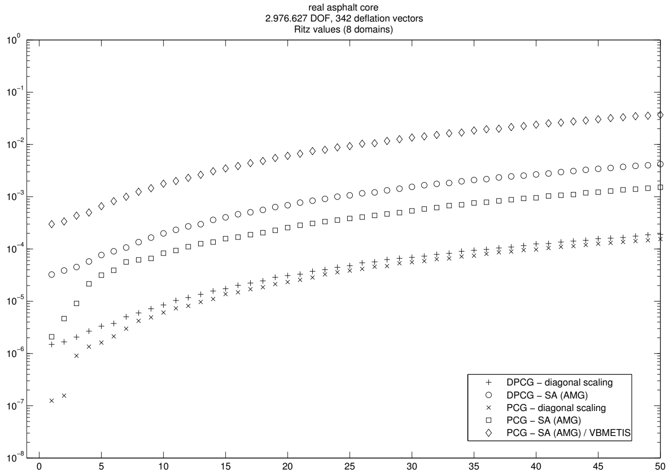


Figure: numerical results: Ritz values derived from (D)PCG

Geomechanical application

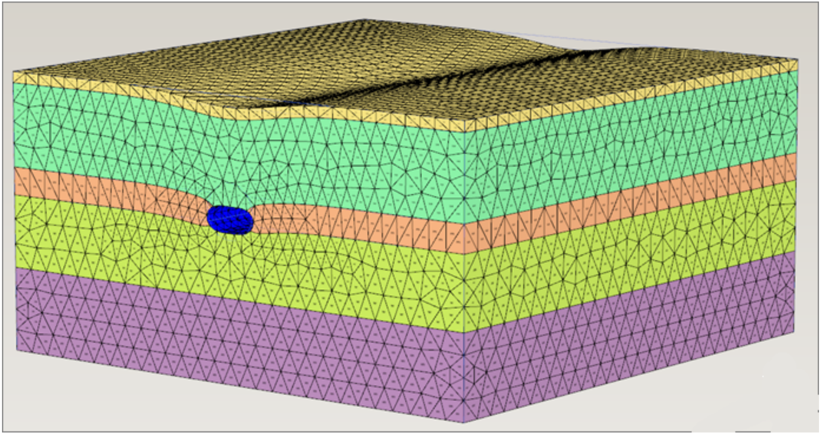
Plaxis software

F.J. Lingen, P. Bonnier, R. Brinkgreve, and M.B. van Gijzen

- Industrial problem
- Good sequential solver available
- Multi-core
- Robust and black box
- Grid partitioning (matrix based)

Typical application

A tunnel of which the walls have been modelled by shell elements, on top of several soil layers with a varying stiffness.

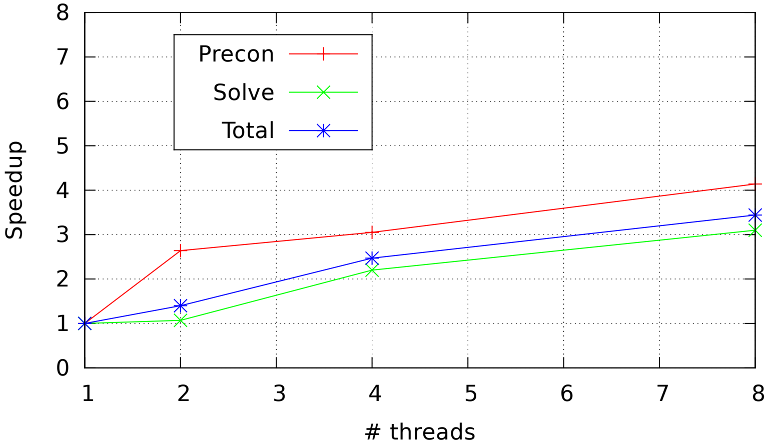


Typical application

Solver	# threads	Precon [s]	Solve [s]	# iter
Original	1	170	140	32
New	1	58	90	62
	2	22	84	74
	4	19	41	39
	8	14	29	45

Typical application

Speedup



Lessons learned

- Mechanical problems can be hard to solve
- Deflation helps for jumping coefficients and parallelization
- Be carefull by partitioning stiff objects
- Rigid body modes lead to good deflation vectors
- Interfaces are important
- Good speedups are achieved both on clusters and multi-core machines

Questions and references

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