Fast iterative methods for mechanical problems with interfaces

C. Vuik, T.B. Jönsthövel, M.B. van Gijzen

Delft University of Technology

IV European Congress on Computational Mechanics: Solids, Structures and Coupled Problems in Engineering 16-21 May 2010

Introduction

what is the use of another Krylov preconditioner?

problem from the work floor: material analysis

Iterative methods

what is in store already?

why and what is deflation?

Conclusions and references

what is the use of another Krylov preconditioner?

i. we have to deliver to the end-user: the engineer, solving real life problems.

what is the use of another Krylov preconditioner?

i. we have to deliver to the end-user: the engineer, solving real life problems.

ii. direct methods are not well suited for large problems

what is the use of another Krylov preconditioner?

i. we have to deliver to the end-user: the engineer, solving real life problems.

ii. direct methods are not well suited for large problems

iii. iterative (Krylov) methods only perform well when combined with a correct preconditioner

what is the use of another Krylov preconditioner?

the catch

any physical problem demands a tailored preconditioner

problem from the work floor: material analysis

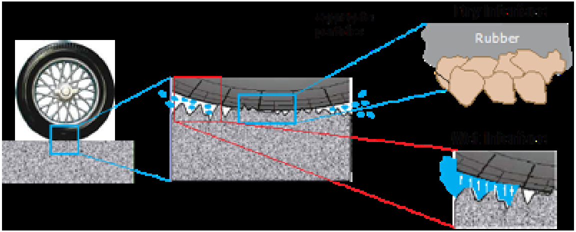

Figure: EU project, SKIDSAFE: asphalt-tire interaction

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

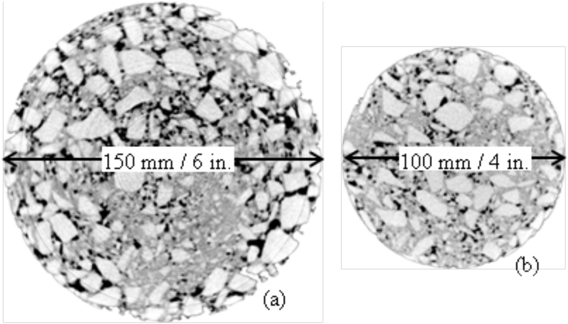

Figure: CT scan of asphalt column

problem from the work floor: material analysis

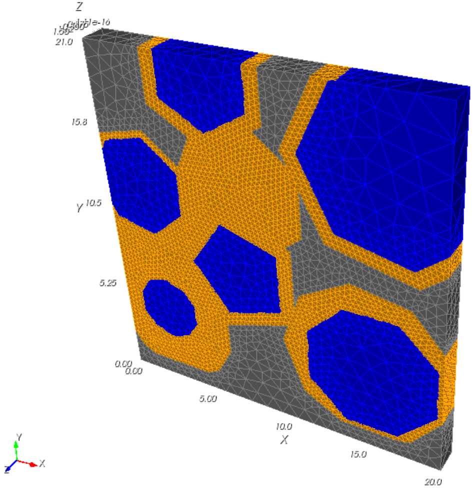

Figure: from CT scan to mesh

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

what is in store already?

just some possible methods and preconditioners

- preconditioned conjugate gradient method (PCG) combined with,
  - BIM: Jacobi, SSOR
  - Incomplete decomposition methods: ILU(ϵ)
- geometric multigrid, algebraic multigrid (AMG)

what is in store already?

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

- AMG can be insensitive to jumps, however to achieve this one has to define the coarse grid specifically

why and what is 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,

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

the DPCG method

We use the 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 Pre conditioned 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 null space 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?

Consider 4 noded finite element in 3D, displacement given by:

$$\left\{ \begin{array}{cccccccccccc} x_1 & y_1 & z_1 & x_2 & y_2 & z_2 & x_3 & y_3 & z_3 & x_4 & y_4 & z_4 \end{array} \right\}^T \tag{4}$$

How do RBM relate to stiffness matrix K?

Translations

$$\left\{\begin{matrix} 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \end{matrix}\right\}^T$$
$$\left\{\begin{matrix} 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \end{matrix}\right\}^T$$
$$\left\{\begin{matrix} 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \end{matrix}\right\}^T$$

How do RBM relate to stiffness matrix K?

Rotations: x-y plane

$$\theta_j = \tan^{-1}\left(\frac{y_j}{x_j}\right) \phi_j = \cos^{-1}\left(\frac{z_j}{r_j}\right) \quad \left\{\begin{array}{c} -r_1 \sin(\theta_1)\sin(\phi_1) \\ r_1 \cos(\theta_1)\sin(\phi_1) \\ 0 \\ -r_2 \sin(\theta_2)\sin(\phi_2) \\ r_2 \cos(\theta_2)\sin(\phi_2) \\ 0 \\ -r_3 \sin(\theta_3)\sin(\phi_3) \\ r_3 \cos(\theta_3)\sin(\phi_3) \\ 0 \\ -r_4 \sin(\theta_4)\sin(\phi_4) \\ r_4 \cos(\theta_4)\sin(\phi_4) \\ 0 \end{array}\right\},$$

How do RBM relate to stiffness matrix K?

Rotations: y-z plane

$$\theta_j = \tan^{-1}\left(\frac{z_j}{x_j}\right) \phi_j = \cos^{-1}\left(\frac{y_j}{r_j}\right) \quad \left\{ \begin{array}{c} -r_1 \sin(\theta_1)\sin(\phi_1) \\ 0 \\ r_1 \cos(\theta_1)\sin(\phi_1) \\ -r_2 \sin(\theta_2)\sin(\phi_2) \\ 0 \\ r_2 \cos(\theta_2)\sin(\phi_2) \\ -r_3 \sin(\theta_3)\sin(\phi_3) \\ 0 \\ r_3 \cos(\theta_3)\sin(\phi_3) \\ -r_4 \sin(\theta_4)\sin(\phi_4) \\ 0 \\ r_4 \cos(\theta_4)\sin(\phi_4) \end{array} \right\},$$

How do RBM relate to stiffness matrix K?

Rotations: x-z plane

$$\theta_j = \tan^{-1}\left(\frac{z_j}{y_j}\right) \phi_j = \cos^{-1}\left(\frac{x_j}{r_j}\right) \quad \left\{\begin{array}{c} 0 \\ r_1 \cos(\theta_1)\sin(\phi_1) \\ -r_1 \sin(\theta_1)\sin(\phi_1) \\ 0 \\ r_2 \cos(\theta_2)\sin(\phi_2) \\ -r_2 \sin(\theta_2)\sin(\phi_2) \\ 0 \\ r_3 \cos(\theta_3)\sin(\phi_3) \\ -r_3 \sin(\theta_3)\sin(\phi_3) \\ 0 \\ r_4 \cos(\theta_4)\sin(\phi_4) \\ -r_4 \sin(\theta_4)\sin(\phi_4) \end{array}\right\}.$$

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

$$\lambda_i(C) \leq \lambda_i(PK) \leq \lambda_i(C) + \lambda_{max}(PR) \text{ for all } i. \qquad (5)$$

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

$$\kappa_{eff}(PK) \leq \frac{\lambda_n(K)}{\lambda_{m+1}(C)}. \qquad (6)$$

[2] Vuik, Frank, SIAM, 2001

How do RBM relate to stiffness matrix K?

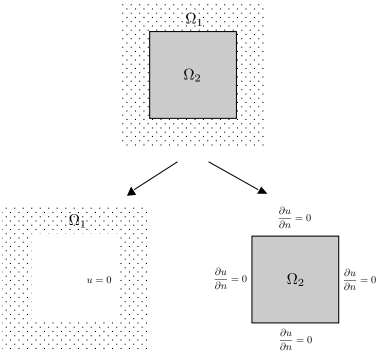

Figure: Principle of rigid body mode deflation

How do RBM relate to stiffness matrix K?

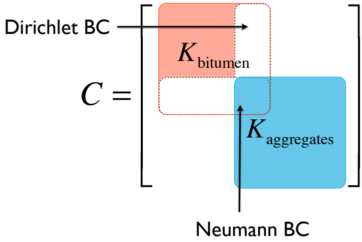

Figure: Principle of rigid body mode deflation: construction of C

How do RBM relate to stiffness matrix K?

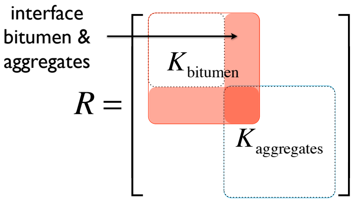

Figure: Principle of rigid body mode deflation: construction of R

Does DPCG work?

The performance of the DPCG method depends on the choice of the regions, hence the choice of deflation vectors. In [2][3] we describe several deflation strategies. Choosing nested regions works best. The method is robust for any choice of material stiffness.

[3] Jonsthovel et al., CMES, 2009

Does DPCG work: numerical experiment

Consider picture from introduction. We have run several variations in material stiffness, hence the size of the jumps.

Table:

(a) *E* modulus materials

	aggregate	bitumen	air voids
standard	70000	5000	100
(a)	**700000**	5000	100
(b)	70000	**50000**	100

Does DPCG work: numerical experiment

Two deflation strategies,

- DPCG I, Nested regions
- DPCG II, Independent regions, no overlap

Does DPCG work: numerical experiment

Table: CPU wall clock time(s) PCG and DPCG (parallel implementation, MPI, 8 CPUs Intel Xeon E5450 running at 3.00GHz), $\sim$ 100.000 DOF

	PCG		DPCG I		DPCG II	
	iter	cpu (s)	iter	cpu(s)	iter	cpu(s)
std	5195	30	1107	9	1469	10
(a)	8670	50	1077	8	1864	11
(b)	5201	28	1414	10	2046	13

Does DPCG work?

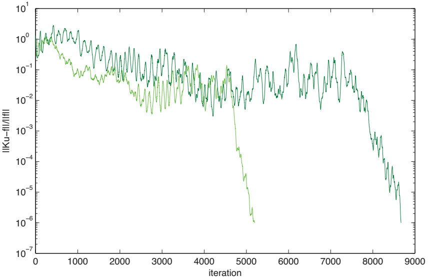

Figure: numerical results: std and (a)

pcg, ●	pcg, ●
dpcg, strategy I, ●	dpcg, strategy I, ●
dpcg, strategy II, ●	dpcg, strategy II, ●

Does DPCG work?

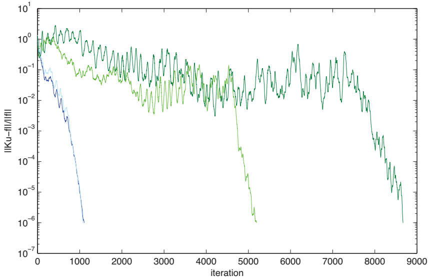

Figure: numerical results: std and (a)

pcg, ●	pcg, ●
dpcg, strategy I, ●	dpcg, strategy I, ●
dpcg, strategy II, ●	dpcg, strategy II, ●

Does DPCG work?

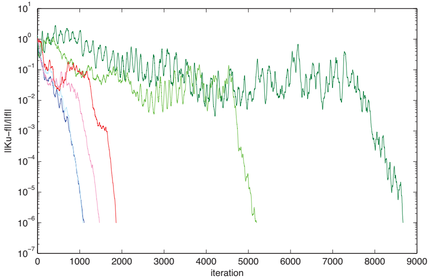

Figure: numerical results: std and (a)

pcg, ● (light green)	pcg, ● (dark green)
dpcg, strategy I, ● (light blue)	dpcg, strategy I, ● (blue)
dpcg, strategy II, ● (pink)	dpcg, strategy II, ● (red)

Does DPCG work?

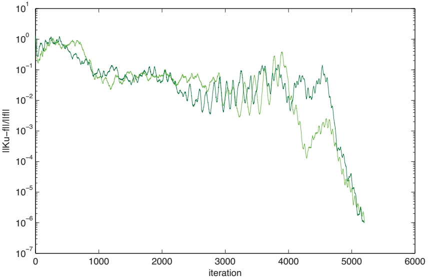

Figure: numerical results: std and (b)

pcg, ●	pcg, ●
dpcg, strategy I, ●	dpcg, strategy I, ●
dpcg, strategy II, ●	dpcg, strategy II, ●

Does DPCG work?

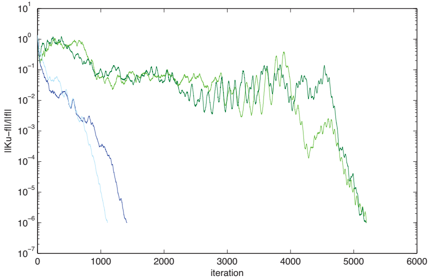

Figure: numerical results: std and (b)

pcg, ●	pcg, ●
dpcg, strategy I, ●	dpcg, strategy I, ●
dpcg, strategy II, ●	dpcg, strategy II, ●

Does DPCG work?

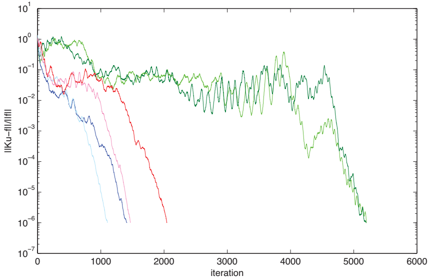

Figure: numerical results: std and (b)

pcg, ●	pcg, ●
dpcg, strategy I, ●	dpcg, strategy I, ●
dpcg, strategy II, ●	dpcg, strategy II, ●

Conclusions and references

- Deflated Preconditioned CG is a fast and robust method
- For problems with interfaces (jumps in properties) the physics should be taken into account
- Rigid Body Modes are suitable as deflation vectors and cheap to construct
- Nested regions strategy is better than the independent region strategy

Conclusions and references

J. Frank and C. Vuik.

On the construction of deflation-based preconditioners.

SIAM J. Sci. Comput., 23(2):442–462, 2001.

T.B. Jönsthövel, M.B. van Gijzen, C.Vuik, C. Kasbergen, and A. Scarpas.

Preconditioned conjugate gradient method enhanced by deflation of rigid body modes applied to composite materials.

Computer Modeling in Engineering and Sciences, 47:97–118, 2009.