Recursively Deflated PCG for mechanical problems

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Introduction

problem from the work floor: material analysis

Iterative methods

overview existing solvers
deflation method
recursive deflation

Numerical experiment: real asphalt core

Questions and references
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

\[ K\Delta u = \Delta f \]  \hspace{1cm} (1)

Stiffness matrix \( K \), change in displacement \( \Delta u \) and change of force \( \Delta f \). 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 $\sim \mathcal{O}(10^6)$: ill-conditioned
Existing solvers

just some possible methods and pre conditioners

• 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 pre conditioner, 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 $u$,

$$u = \left( I - P^T \right) u + P^T u,$$  \hspace{1cm} (2)

And let us define the projection $P$ by,

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

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\(^1\)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 $\mathcal{N}(C) = \text{span}\{Z\}$ the null space of $C$ \cite{1}. Then

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

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

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

\cite{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**

$$P^{(k)} = I - KZ_k(Z_k^T KZ_k)^{-1}Z_k^T$$ 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 $P_{i+1} = I - \tilde{K}_i \tilde{Z}_{i+1}(\tilde{Z}^T_{i+1} \tilde{K}_i \tilde{Z}_{i+1})^{-1} \tilde{Z}_{i+1}^T$, $\tilde{K}_i = P_i \tilde{K}_{i-1}$, $\tilde{K}_1 = P_1 K$, $\tilde{K}_0 = K$, $\tilde{Z}^T_i \tilde{K}_{i-1} \tilde{Z}_i^T$ and $Z_i^T K Z_i$ are non-singular because $Z_i$ are of full rank and $K$ is a symmetric positive definite matrix.
Recursive deflation

Proof.
by induction,

i. show $P_1K = P^{(1)}K$ where $Z_1 = \tilde{Z}_1 \in \mathbb{R}^{n \times l_1}$,

ii. assume $P_{i-1}\tilde{K}_{i-2} = \tilde{K}_{i-1} = P^{(i-1)}K$ where $Z_{i-1} = [\tilde{Z}_{i-1}, \tilde{Z}_{i-2}, \cdots, \tilde{Z}_1]$, show that $P_i\tilde{K}_{i-1} = P^{(i)}K$ where $Z_i = [\tilde{Z}_i, Z_{i-1}]$, $Z_{i-1} \in \mathbb{R}^{n \times l(i-1)}$, $\tilde{Z}_i \in \mathbb{R}^{n \times l_i}$ and $l = \sum_{r=i}^i l_i$.  

☐
Recursive deflation: 1D example

Poisson equation,

\[- \frac{d}{dx} \left( c(x) \frac{du(x)}{dx} \right) = f(x), \quad x \in [0, l] \]

\[u(0) = 0, \quad \frac{du}{dx}(l) = 0\]
Recursive deflation: 1D example

Introduce a FE mesh for the line $[0, l]$ including 3 domains $\Omega_1 = \{x_1, \ldots, x_4\}$, $\Omega_2 = \{x_5, \ldots, x_8\}$ and $\Omega_3 = \{x_9, \ldots, x_{13}\}$. For sake of simplicity we will write $c_i = c(x_i)$ where $i = 1, \ldots, 13$, $x_1 = h$ and $x_{13} = l$. Furthermore because $c_i$ is constant on each material domain we will use $c_i = c_1$, $c_i = c_2$ and $c_i = c_3$ on $\Omega_1$, $\Omega_2$ and $\Omega_3$ respectively.
Recursive deflation: 1D example

After discretization,

\[
K = \frac{1}{h} \begin{bmatrix}
2c_1 & -c_1 & & & \\
& \ddots & \ddots & \ddots & \\
& & 2c_1 & -c_1 & -c_2 \\
& & & \ddots & \ddots \\
& & & & 2c_2 & -c_2 & -c_3 \\
& & & & & \ddots & \ddots \\
& & & & & & 2c_3 & -c_3 & -c_3 \\
\emptyset & & & & & & & \emptyset
\end{bmatrix}
\]
Recursive deflation: 1D example

Figure: sparsity pattern $C_0$, $C_1$ and $C_2$. Nonzero elements represented by symbols; corresponding to deflated material, interface elements and remaining elements pictured by bold crosses, circles and non bold crosses respectively.
Recursive deflation: 1D example

Figure: spectrum of $M^{-1}C_i$ (⋆ correct, + wrong choice deflation vectors) compared to spectrum of $M^{-1}K$ (+)
Numerical experiment: real asphalt core

Consider picture from introduction. Size of system approx. 3 million DOF, material parameters given in table below,

Table:

<table>
<thead>
<tr>
<th></th>
<th>aggregate</th>
<th>bitumen</th>
<th>air voids</th>
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<td>(a) $E$ modulus materials</td>
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<td>5000</td>
<td>100</td>
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</table>
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

<table>
<thead>
<tr>
<th>Method</th>
<th>4 CPUs</th>
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<th>Iterations</th>
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<td>nc</td>
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</tbody>
</table>
Numerical experiment: real asphalt core

Figure: numerical results: residuals
Numerical experiment: real asphalt core

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

J. Frank and C. Vuik.
On the construction of deflation-based preconditioners.

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