Total FETI method for sensitivity analysis in contact shape optimization problems

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Outline

• Contact problems
• FETI and Total FETI methods
• Optimality of solution algorithm
• Numerical experiments
• Contact shape optimization
• FETI based sensitivity analysis
• Conclusions
Contact problem

Variational inequality

\[ a(u, v - u) \geq b(v - u), \quad \forall v \in C \]

\[ \Downarrow \]

\[ \min \frac{1}{2} u^T Ku - u^T f, \]

s.t. \( B_I u \leq c_I \)

\[
K = \begin{pmatrix}
K_1 & 0 \\
& \ddots \\
0 & & K_P
\end{pmatrix}
\]
FETI domain decomposition method

Primal problem

$$\min \frac{1}{2} u^T Ku - u^T f \quad \text{subject to} \quad B_I u \leq c_I, \, B_E u = 0$$
FETI solution of contact problem

\[
\min \frac{1}{2} \lambda^T F \lambda - \lambda^T d \quad \text{subject to} \quad \lambda_i \geq 0, \quad E\lambda = g
\]

\[
F = BK^+ B^T \quad d = BK^+ f - c
\]
\[
E = R^T B^T \quad g = R^T f
\]

Reconstruction formula

\[
u = K^+ \left( f - B^T \lambda \right) + R\xi
\]

with appropriate vector \( \xi \in \mathbb{N}_{rhm} \)

Construction of \( R \) is costly and depends on some \( \varepsilon \)!

Total FETI domain decomposition method

Primal problem

$$\min \frac{1}{2} u^T K u - u^T f \quad \text{subject to} \quad B_I u \leq c_I, B_E u = 0, B_B u = 0$$
Total FETI solution of contact problem

\[
\min \frac{1}{2} \lambda^T F \lambda - \lambda^T d \quad \text{subject to } \lambda_i \geq 0, \quad E \lambda = g
\]

\[
F = BK^+ B^T \quad d = BK^+ f - c \\
E = R^T B^T \quad g = R^T f
\]

Reconstruction formula

\[
u = K^+ \left( f - B^T \lambda \right) + R \xi
\]

with appropriate vector \( \xi \in \mathbb{R}^{6N} \)

\[
K^+ = \text{diag} \left( K_1^+, \ldots, K_N^+ \right)
\]

\[
\lambda = \begin{bmatrix}
\lambda_B \\
\lambda_E \\
\lambda_I
\end{bmatrix}, \quad B = \begin{bmatrix}
B_B \\
B_E \\
B_I
\end{bmatrix}, \quad c = \begin{bmatrix}
o \\
o \\
c_i
\end{bmatrix}
\]

\[
\text{span}\{R_{*,i}\} = \text{null}\ K
\]

\[R\] is a-priori known!
MPRGP for bound constrained QP (QPB)

\[
\min \frac{1}{2} \lambda^T F \lambda - \lambda^T d \quad \text{subject to } \lambda \geq 0
\]

- Proportioning
- Conjugate gradient step
- Expansion step (direction of reduced projected gradient)

- **Modified Proportioning Reduced Gradient Projection**
Proportioning

\( \lambda \) proportional: \( \| \beta(\lambda) \|^2 \leq \Gamma^2 \phi^T(\lambda) \phi(\lambda) \)

Reduction of the active set for non-proportional iterations
Proportional iterations

Feasible conjugate gradient step:

Projection step: expansion of the active set
SMALBE for bound and equality constrained QP

(QPBE) \( \min \frac{1}{2} \lambda^T F \lambda - \lambda^T d \) subject to \( \lambda \geq 0 \), \( E \lambda = 0 \)

Augmented Lagrangian with projected gradient

\[ L(\lambda, \mu, \rho) = f(\lambda) + \mu^T E \lambda + \frac{1}{2} \rho \|E \lambda\|^2 \]

- Outer loop: Update of \( \mu \) \( \mu \leftarrow \mu + \rho E \lambda \)
- Inner loop: Inexact MPRGP \( \|g^P(\lambda, \mu, \rho)\| \leq M \|E \lambda\| \)

SemiMonotonic Augmented Lagrangian for Bound and Equality constrained QP
Optimality of SMALBE

• Penalty $\rho$ is uniformly bounded
  \[ \rho \leq \gamma M^2 / \lambda_{\min}(F) \]

• SMALBE generates $\lambda$ at $O(1)$ outer iterations

• SMALBE with MPRGP generates $\lambda$ at $O(1)$ matrix-vector multiplications

Scalability of Total FETI

Model problem up to 2 130 048 dofs
2D semi-coercive problem

<table>
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<tr>
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<th>FETI</th>
<th>Total FETI</th>
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<td>Primal/Dual var.</td>
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<td>CG steps</td>
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In cooperation with C. Farhat, P. Avery, Stanford University

SNA’08
3D semi-coercive problem

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In cooperation with C. Farhat, P. Avery, Stanford University
**3D Hertz problem**

In cooperation with J. Dobiáš, S. Pták, Academy of Sciences of Czech Rep.

**Table:**

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SNA’08 28.1-1.2. 2008
Contact shape optimization

\[
\begin{cases}
\min \mathcal{J}(\alpha, u(\alpha)) \\
\alpha \in U_{ad}
\end{cases}
\]

\(\mathcal{J}(\alpha, u(\alpha))\) ... objective function

\(u(\alpha)\) solves contact problem:

\[
\min \frac{1}{2} u^T K(\alpha) u - u^T f(\alpha)
\]

subject to \(B(\alpha)u \leq c(\alpha)\)

Variational inequality

\[
a_\alpha(u, v - u) \geq b_\alpha(v - u), \quad \forall v \in C_\alpha
\]

\[
\min \frac{1}{2} u^T K(\alpha) u - u^T f(\alpha),
\]

s.t. \(B(\alpha)u \leq c(\alpha)\)
General solution scheme

Start

Analysis

Optimality test

Sensitivity analysis

Optimization step

Stop

Optimal

not optimal

Initial design $\alpha_0$

Solution of state problem $u(\alpha)$ with given $\alpha$
e.g. in linear elasticity $K(\alpha)u(\alpha)=f(\alpha)$

Stopping criterion for optimal design
e.g. $\|\alpha_{new}-\alpha_{old}\|<\epsilon$

Design update controlled by optimization algorithm
$\alpha_{new}=\alpha_{old}+\Delta\alpha$

Figure out $\nabla u(\alpha)$
e.g. for evaluation of objective function $\mathcal{F}(\alpha,u(\alpha))$
Finite difference sensitivity analysis

- Advantage
  - Simple implementation

- Disadvantages
  - \( m+1 \) assemblies of stiffness matrix
  - \( m+1 \) solution of contact problem (\( m+1 \) decompositions of \( K \))
  - \( m+1 \) constructions of \( R \)
  - Numerically unstable

- Does “semi-analytical” method exist?

\[
\frac{\partial u(\alpha)}{\partial \alpha_i} \approx \frac{u(\alpha + he_i) - u(\alpha)}{h}
\]

where \( u(\alpha + he_i) \) solves
\[
\min \frac{1}{2} u^T K(\alpha + he_i)u - u^T f(\alpha + he_i)
\]
subject to \( B(\alpha + he_i)u \leq c(\alpha + he_i) \)

and \( e_i = (0, \ldots, 0, 1, 0, \ldots, 0) \), \( i = 1, \ldots, m \)
Semi-analytical sensitivity analysis

\[ I_C = \{ i : B_{i^*}(\alpha)u(\alpha) = c_i(\alpha) \} \] ... indices of nodal variables in contact

\[ I_S = \{ i : i \in I_C \land \lambda_i(\alpha) > 0 \} \] ... indices of nodal variables in strong contact

\[ I_W = \{ i : i \in I_C \land \lambda_i(\alpha) = 0 \} \] ... indices of nodal variables in weak contact

\[ u'(\alpha, \beta) = \lim_{h \to 0} \frac{1}{h} (u(\alpha + h\beta) - u(\alpha)) \]

solves

\[ \min \frac{1}{2} z^T K(\alpha) z - z^T \bar{f}(\alpha, \beta) \]

s.t. \[ B_W(\alpha) z \leq c_W(\alpha, \beta), \quad B_S(\alpha) z = c_S(\alpha, \beta) \]

\[ \bar{f}(\alpha, \beta) = f'(\alpha, \beta) - K'(\alpha, \beta)u(\alpha) + B'^T(\alpha, \beta)\lambda(\alpha) \]

\[ B_S(\alpha) = [B_i(\alpha)]_{i \in I_S}, \quad c_S(\alpha, \beta) = \left[ f_{i^*}'(\alpha, \beta) - B_{i^*}(\alpha, \beta)u(\alpha) \right]_{i \in I_S} \]

\[ B_W(\alpha) = [B_i(\alpha)]_{i \in I_W}, \quad c_W(\alpha, \beta) = \left[ f_{i^*}'(\alpha, \beta) - B_{i^*}(\alpha, \beta)u(\alpha) \right]_{i \in I_W} \]
FETI based sensitivity analysis

\[
\min \frac{1}{2} \bar{\lambda}^T \bar{F}(\alpha) \bar{\lambda} - \bar{\lambda}^T \bar{d}(\alpha, \beta) \quad \text{s. t.} \quad \bar{\lambda}_w \geq 0, \quad \bar{E}(\alpha) \bar{\lambda} = \bar{g}(\alpha, \beta)
\]

where

\[
\bar{F}(\alpha) = \bar{B}(\alpha) K^+(\alpha) \bar{B}^T(\alpha), \quad \bar{d}(\alpha, \beta) = \bar{B}(\alpha) K^+(\alpha) \bar{f}(\alpha, \beta) - \bar{c}(\alpha, \beta),
\]

\[
\bar{E}(\alpha) = R^T(\alpha) \bar{B}^T(\alpha), \quad \bar{g}(\alpha, \beta) = R^T(\alpha) \bar{f}(\alpha, \beta)
\]

- Only one assembly and one decomposition of stiffness matrix for all \( \beta = e_i, \ i=1,\ldots,m \)
- \( R(\alpha) \) is invariant!
- \( I_W \) is typically empty
  - \( B=B_S \)
  - only equality constraints

\[
u'(\alpha, \beta) = K^+(\alpha) \left( \bar{f}(\alpha, \beta) - \bar{B}(\alpha)^T \bar{\lambda}(\alpha, \beta) \right) + R(\alpha) \zeta
\]

with such appropriate \( \zeta \)
SMALE for equality constrained QP

(QPE) \[ \min \frac{1}{2} \bar{\lambda}^T \bar{F}(\alpha) \bar{\lambda} - \bar{\lambda}^T \bar{d}(\alpha, \beta) \quad \text{subject to } \bar{E}(\alpha) \bar{\lambda} = o \]

Augmented Lagrangian

\[ L(\bar{\lambda}, \mu, \rho) = f(\bar{\lambda}) + \mu^T \bar{E}(\alpha) \bar{\lambda} + \frac{1}{2} \rho \| \bar{E}(\alpha) \bar{\lambda} \|^2 \]

- Outer loop: Update of \( \mu \)
- Inner loop: Inexact PCG

SemiMonotonic Augmented Lagrangian for Equality constrained QP
Parallel implementation

\[ K'(\alpha,e_1), f'(\alpha,e_1), C'(\alpha,e_1) \]

\[ K'(\alpha,e_2), f'(\alpha,e_2), C'(\alpha,e_2) \]

\[ K'(\alpha,e_3), f'(\alpha,e_3), C'(\alpha,e_3) \]

\[ K'(\alpha,e_4), f'(\alpha,e_4), C'(\alpha,e_4) \]

\[ K'(\alpha,e_5), f'(\alpha,e_5), C'(\alpha,e_5) \]

\[ K'(\alpha,e_6), f'(\alpha,e_6), C'(\alpha,e_6) \]

\[ K(\alpha) = \text{diag\{ }K_1(\alpha), K_2(\alpha)\} \]

\[ K^+(\alpha) = \text{diag\{ }K_1^+(\alpha), K_2^+(\alpha)\} \]

\[ u(\alpha), \lambda(\alpha), f(\alpha), C(\alpha), d(\alpha) \]
Model problem “scont”

### Table

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<th>Var.</th>
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<table>
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28.1-1.2. 2008
"scont" optimized design
Conclusions

• Total FETI has a-priori known null spaces of subdomain stiffness matrices
• Solution algorithms have $O(1)$ rate of convergence
• Semi-analytical method significantly speeds up the optimization process
  – In each design step only one stiffness matrix assembly and one decomposition - no null space recomputing
  – No numerical instability caused by perturbation parameters
  – Significant reduction of inequality constraints (if any): typically only SMALE outer loop iterations