Total FETI method for sensitivity analysis in contact shape optimization problems

Vít Vondrák
Zdeněk Dostál
David Horák
Dept. of Applied Mathematics
VŠB-Technical University of Ostrava
Czech Republic

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

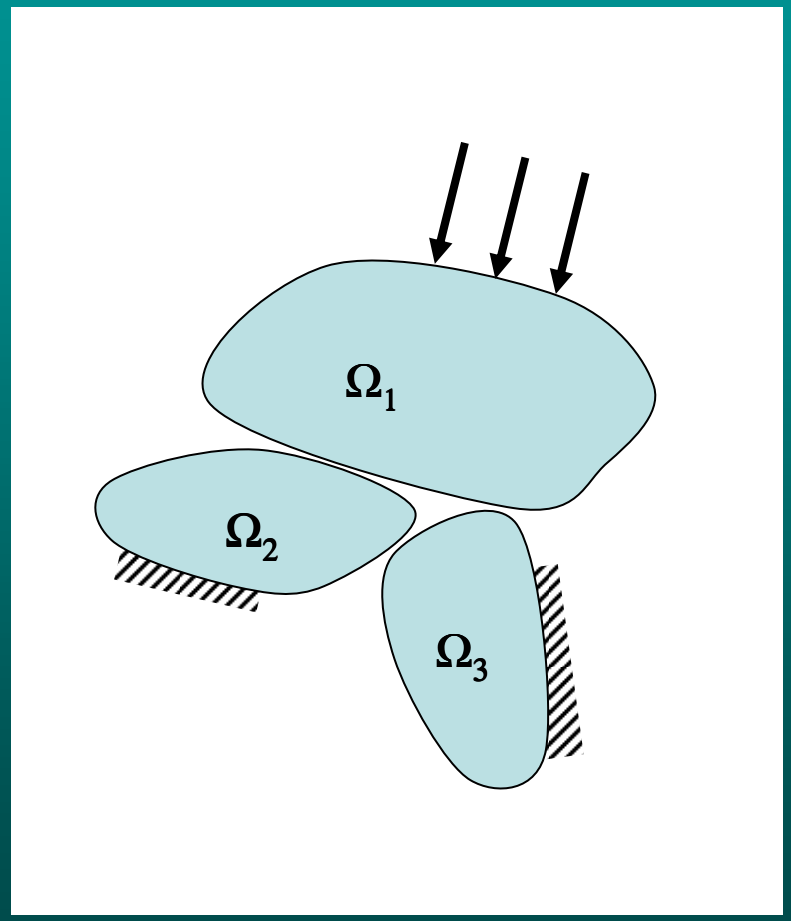
$$a(u, v-u) \geq b(v-u), \quad \forall v \in C$$

$$\downarrow$$

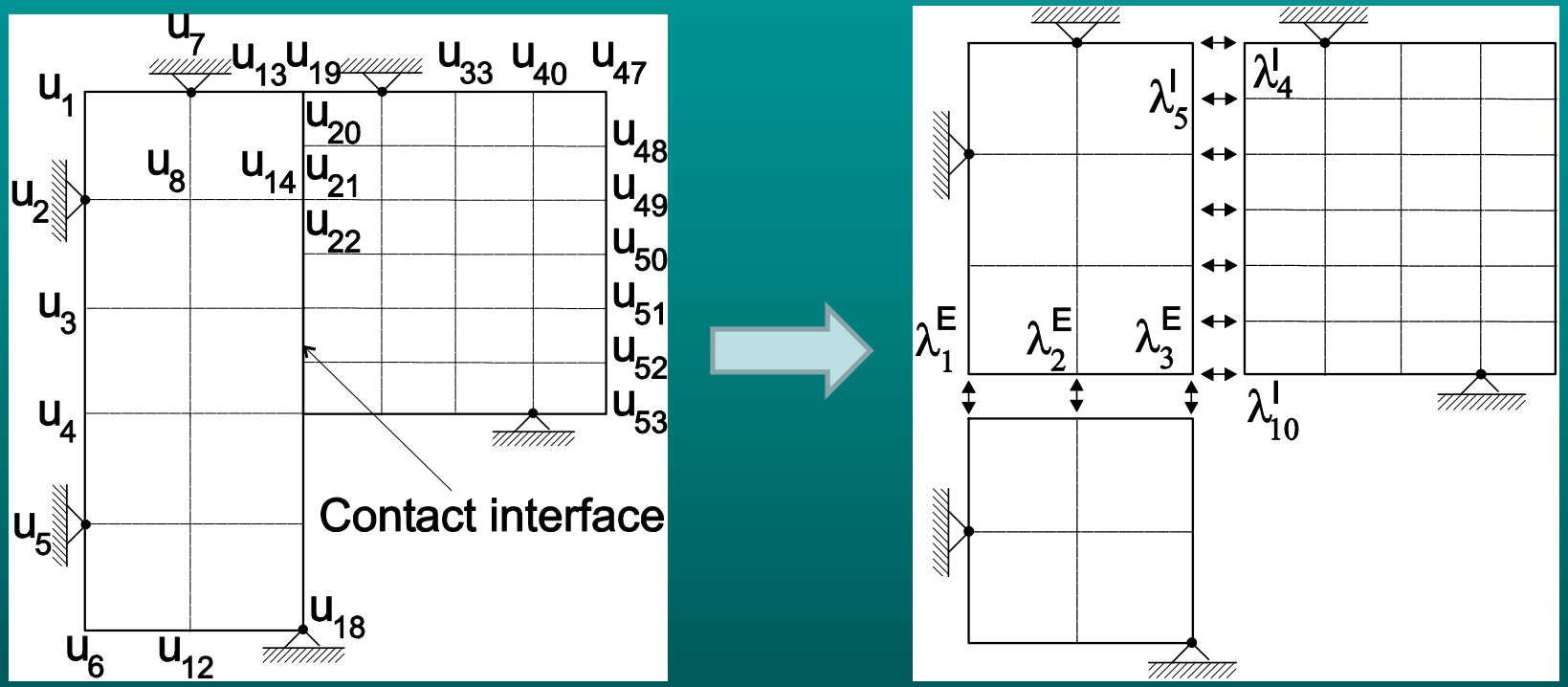
$$\min \tfrac{1}{2} u^T K u - u^T f,$$

$$\text{s.t. } B_I u \leq c_I$$

$$K = \begin{pmatrix} K_1 & & 0 \\ & \ddots & \\ 0 & & K_P \end{pmatrix}$$



FETI domain decomposition method



Primal problem

$$\min \tfrac{1}{2} u^T K u - u^T f \ \text{ subject to } \ B_I u \le c_I, B_E u = 0$$

FETI solution of contact problem

$$\min \tfrac{1}{2}\lambda^T F \lambda - \lambda^T d \text{ subject to } \lambda_I \geq o,\ E\lambda = g$$

$$F = BK^+B^T \quad d = BK^+ f - c$$

$$E = R^T B^T \quad g = R^T f$$

$$K^+ = diag\left(K_1^+, \ldots, K_N^+\right)$$

$$\lambda = \begin{bmatrix} \lambda_E \\ \lambda_I \end{bmatrix},\ B = \begin{bmatrix} B_E \\ B_I \end{bmatrix},\ c = \begin{bmatrix} o \\ c_I \end{bmatrix}$$

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

Reconstruction formula

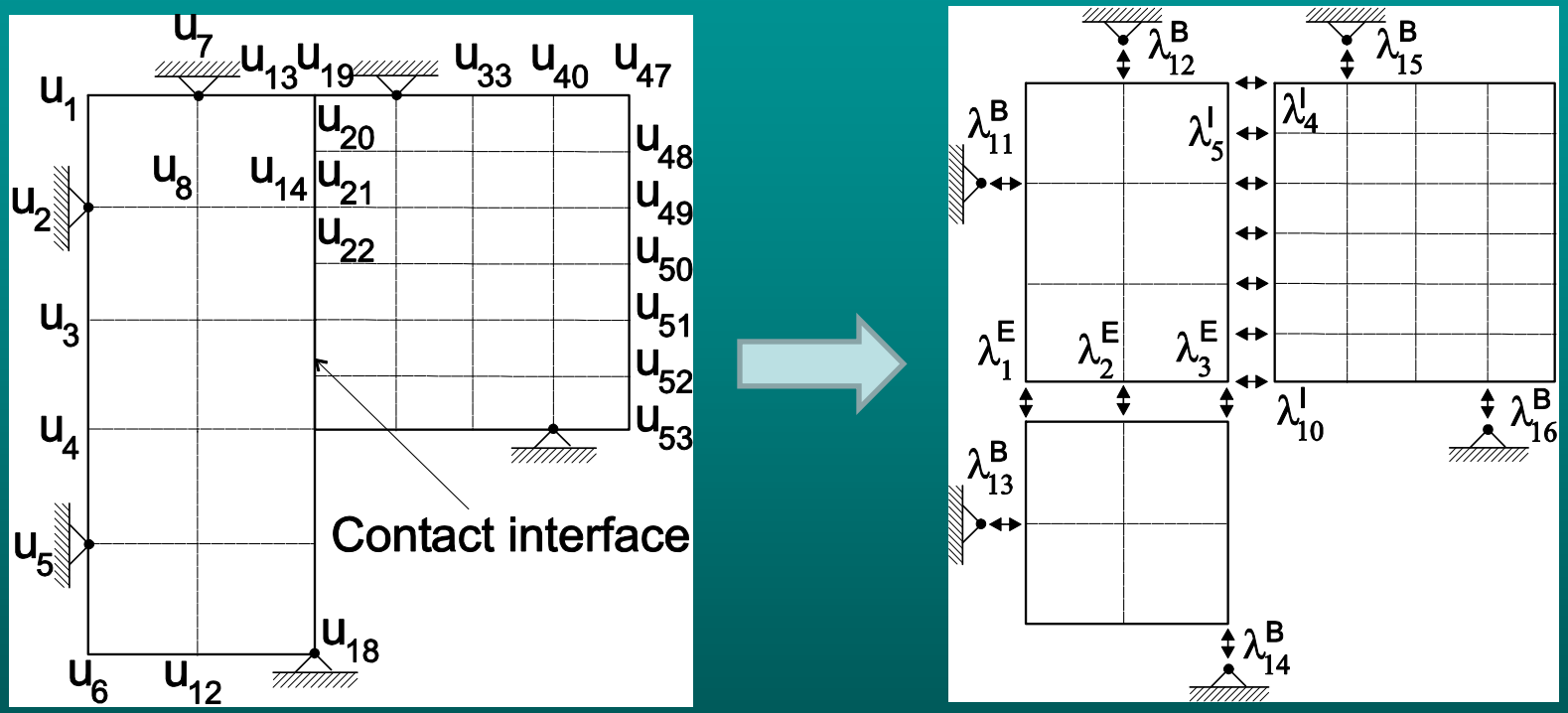
$$u = K^+\left(f - B^T\lambda\right) + R\xi$$

with appropriate vector $\xi \in \mathbb{R}^{N_{rbm}}$

Construction of R is costly and depends on some ε!

FARHAT, C., GERARDIN, M., On the general solution by a direct method for a large scale singular system of linear equation. Int. Journal for Num. Meth. in Engng., 1998, vol. 41, p. 675-696.

Total FETI domain decomposition method



Primal problem

$$\min \tfrac{1}{2} u^T K u - u^T f \;\text{ subject to }\; B_I u \le c_I, B_E u = 0, B_B u = 0$$

Total FETI solution of contact problem

$$\min \tfrac{1}{2}\lambda^T F \lambda - \lambda^T d \text{ subject to } \lambda_I \geq o,\ E\lambda = g$$

$$F = BK^+B^T \quad d = BK^+ f - c$$

$$E = R^T B^T \quad g = R^T f$$

Reconstruction formula

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

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

$$K^+ = diag\left(K_1^+, \ldots, K_N^+\right)$$

$$\lambda = \begin{bmatrix} \lambda_B \\ \lambda_E \\ \lambda_I \end{bmatrix},\ B = \begin{bmatrix} B_B \\ B_E \\ B_I \end{bmatrix},\ c = \begin{bmatrix} o \\ o \\ c_I \end{bmatrix}$$

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

R is a-priori known!

MPRGP for bound constrained QP

(QPB) $\min \frac{1}{2}\lambda^T F \lambda - \lambda^T d \quad \text{subject to } \lambda \geq o$

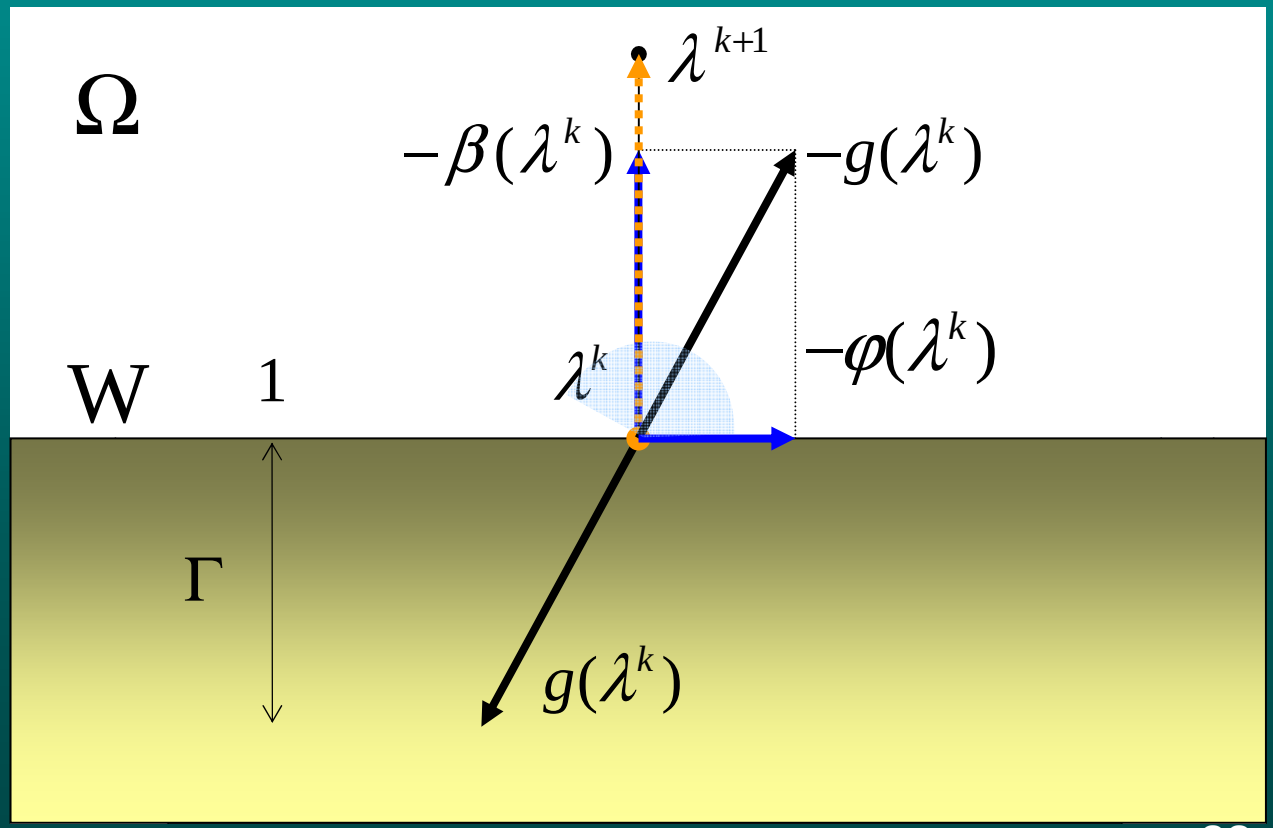
- Proportioning
- Conjugate gradient step
- Expansion step (direction of reduced projected gradient)

- Modified Proportioning Reduced Gradient Projection

Proportioning

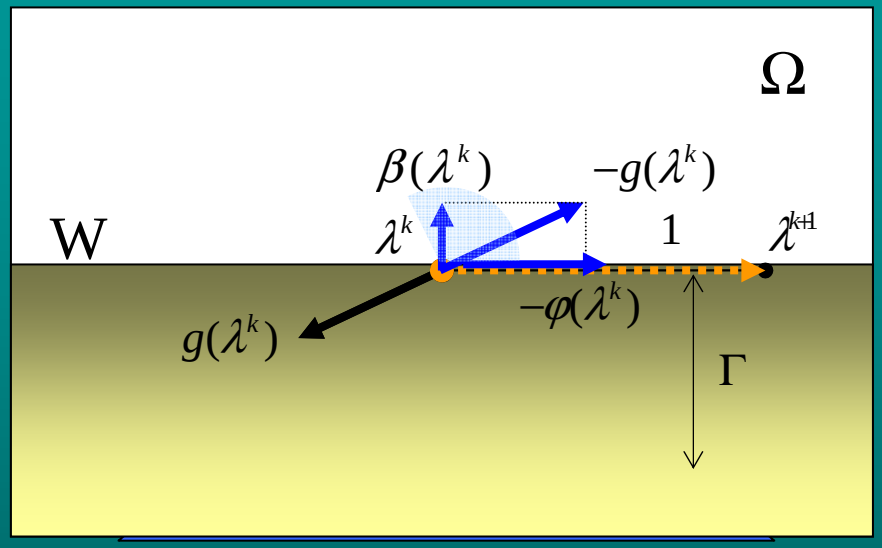
λ proportional: $\|\beta(\lambda)\|^2 \le \Gamma^2 \tilde{\varphi}^T(\lambda)\varphi(\lambda)$

Reduction of the active set for non-proportional iterations

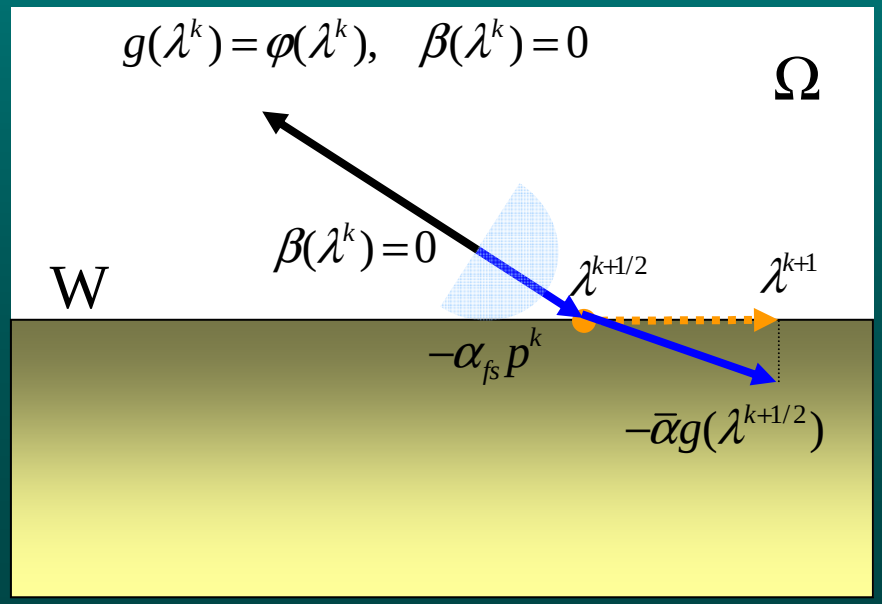


Proportional iterations

Feasible conjugate gradient step:



Projection step: expansion of the active set



SMALBE for bound and equality constrained QP

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

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 μ $\quad \mu \leftarrow \mu + \rho E\lambda$
- Inner loop: Inexact MPRGP $\quad \|g^P(\lambda,\mu,\rho)\| \leq M\|E\lambda\|$

SemiMonotonic Augmented Lagrangian for Bound and Equality constrained QP

Optimality of SMALBE

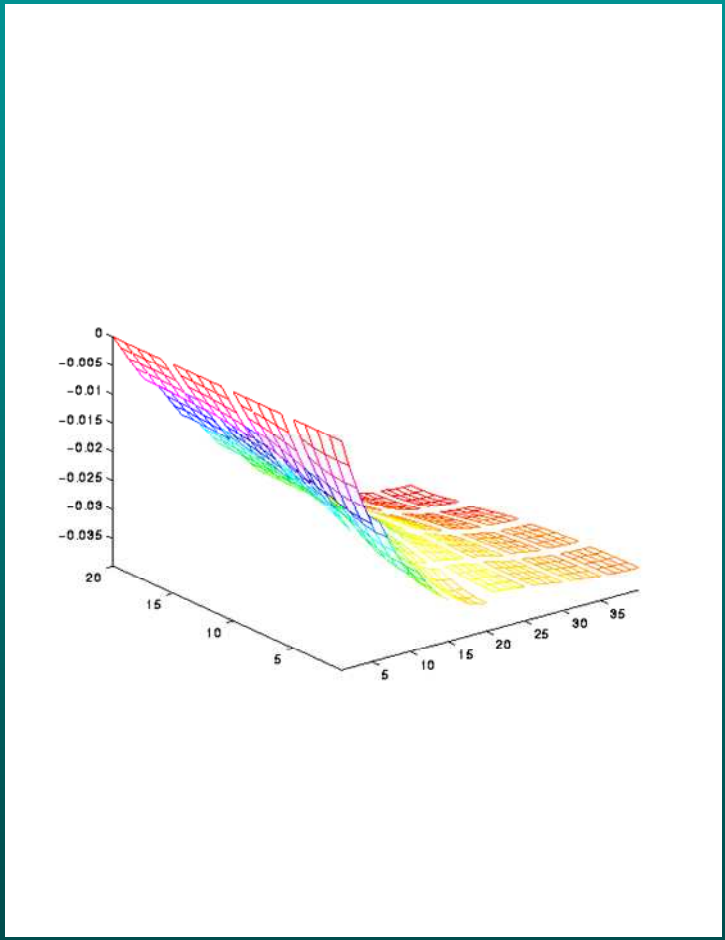
- Penalty ρ is uniformly bounded

$$\rho \le \gamma M^2 / \lambda_{\min}(F)$$

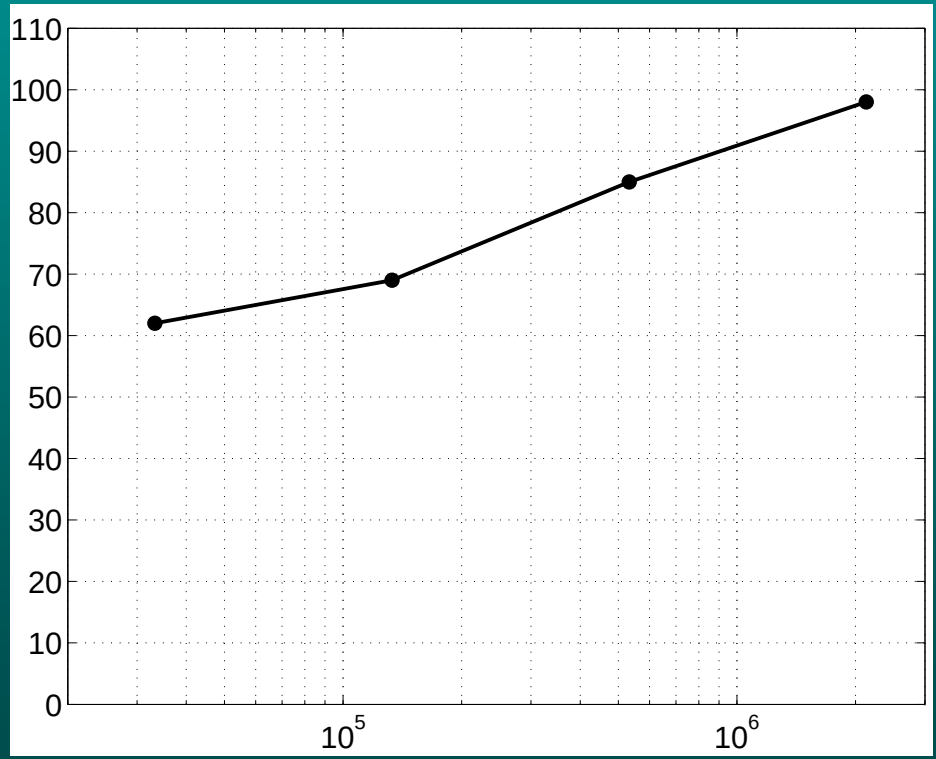
- SMALBE generates λ at O(1) outer iterations
- SMALBE with MPRGP generates λ at O(1) matrix-vector multiplications

DOSTÁL, Z. Inexact semi-monotonic augmented Lagrangians with optimal feasibility convergence for convex bound and equality constrained quadratic programming. SIAM Journal on Numerical Analysis, 2005, vol. 43, 1, s. 96-115.

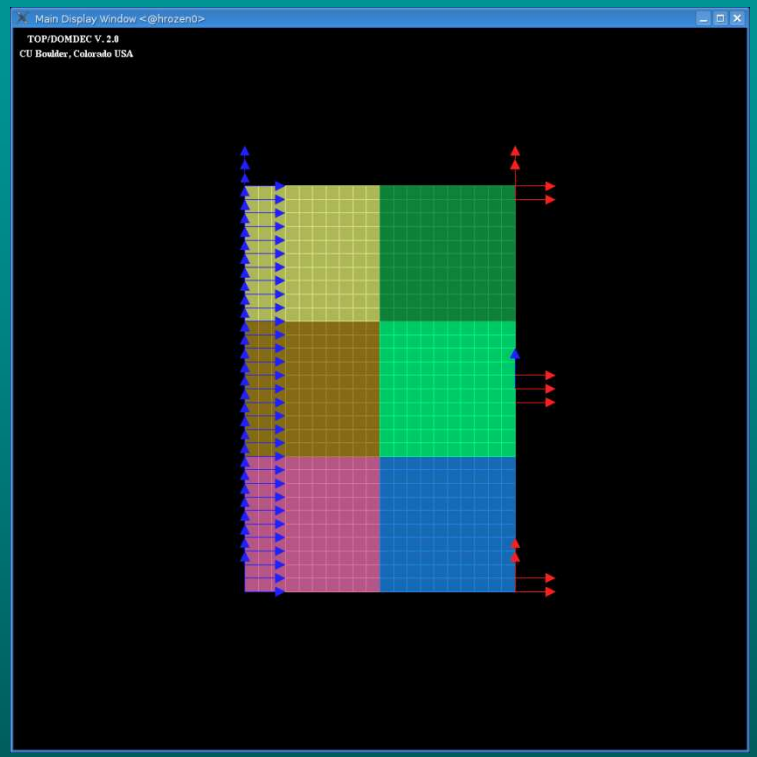
Scalability of Total FETI

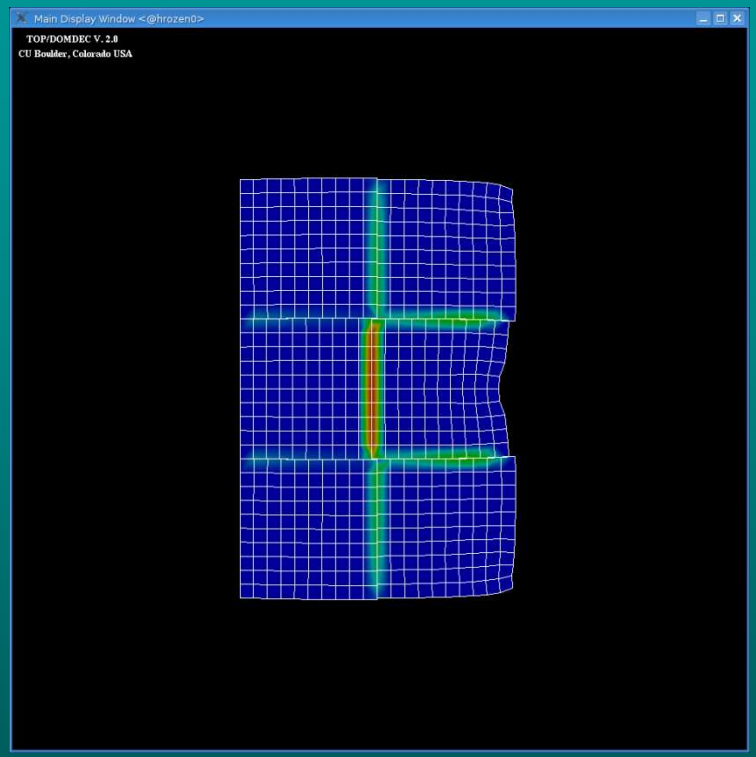


Model problem up to 2 130 048 dofs



2D semi-coercive problem



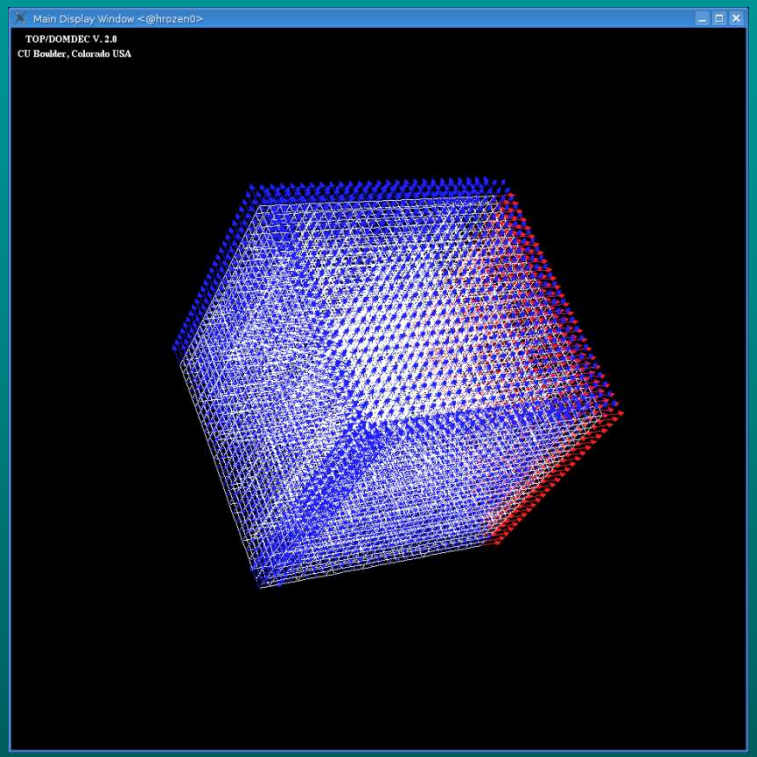


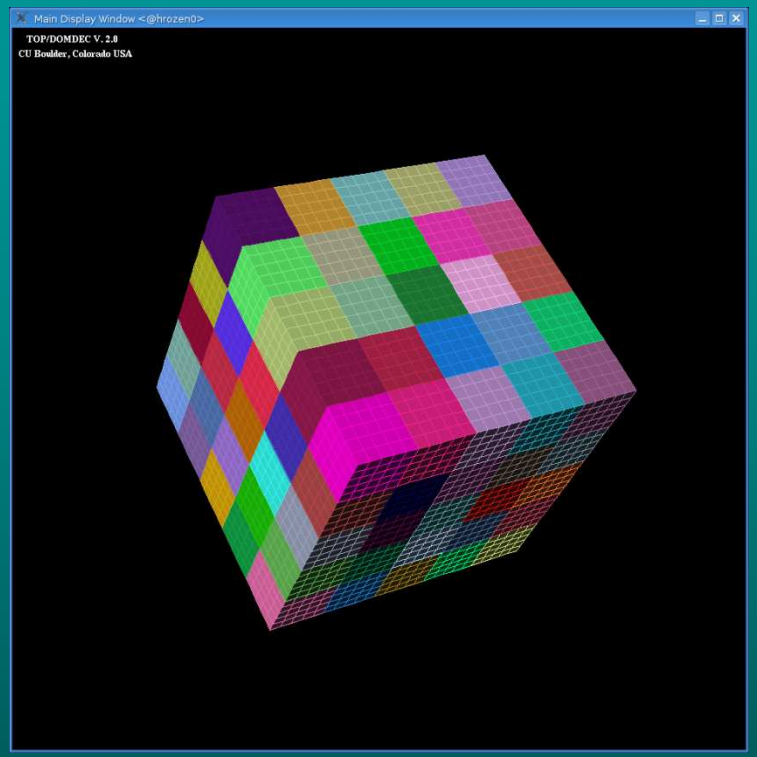
	FETI	Total FETI
Primal/Dual var.	726/77	726/134
CG steps	18	34

Ratio
1.74
1.89

In cooperation with C. Farhat, P. Avery, Stanford University

3D semi-coercive problem

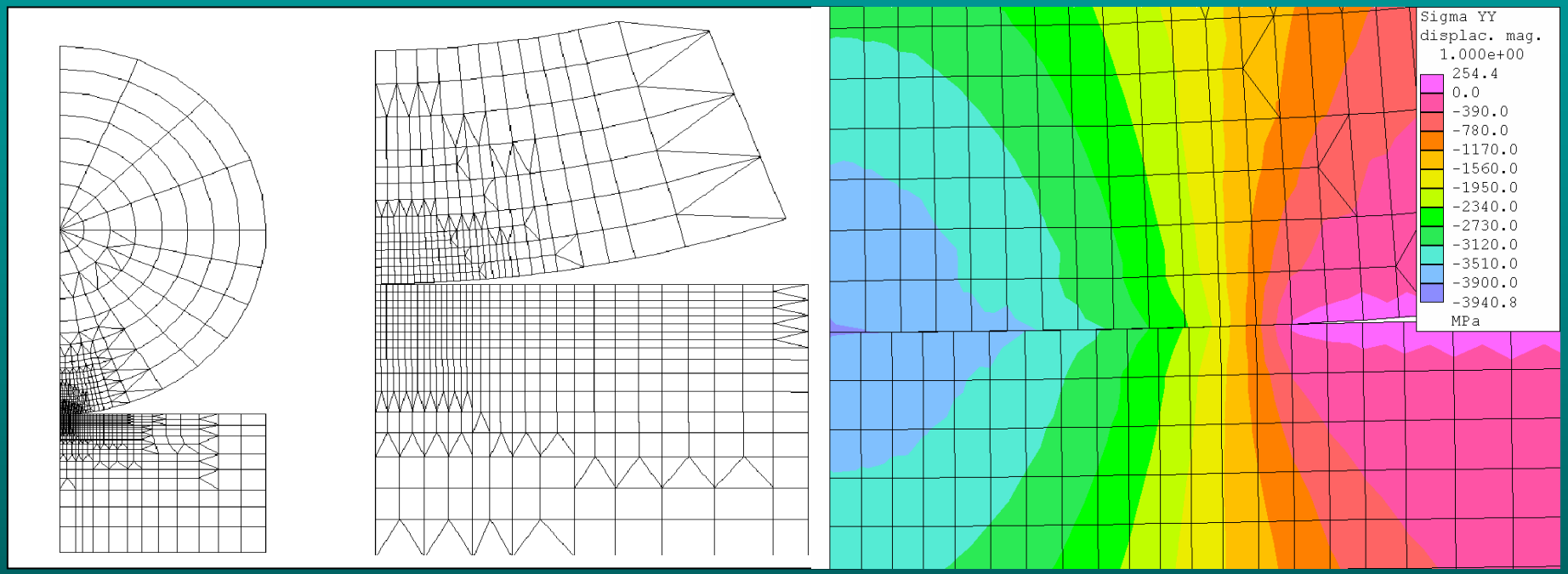




	FETI	Total FETI	Ratio
Primal/Dual var.	27000/4500	27000/7200	1.6
CG steps	28	21	0.75

In cooperation with C. Farhat, P. Avery, Stanford University

3D Hertz problem



	FETI	Total FETI
Primal/Dual var.	11430/84	11430/2911
CG steps	12	447

Ratio
34.66
37.25

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

Contact shape optimization

$$\begin{cases} \min \Im(\alpha, u(\alpha)) \\ \alpha \in U_{ad} \end{cases}$$

$\Im(\alpha, u(\alpha))$... objective function

$u(\alpha)$ solves contact problem:

$$\min \tfrac{1}{2} u^T K(\alpha) u - u^T f(\alpha)$$

subject to $B(\alpha)u \le c(\alpha)$

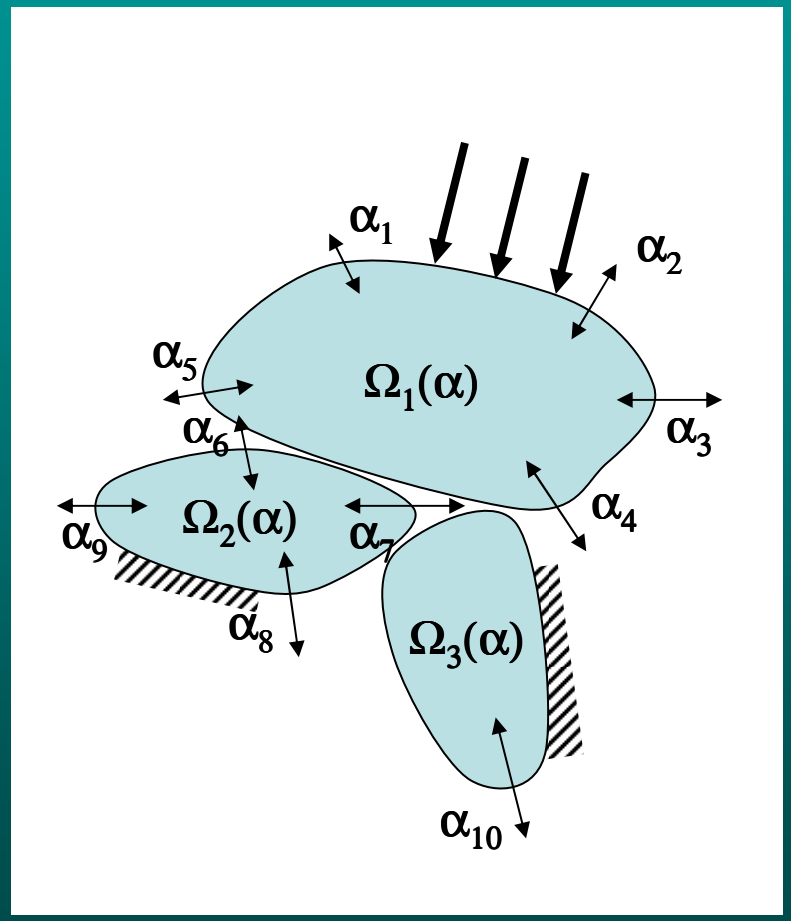
Variational inequality

$$a_\alpha(u, v-u) \ge b_\alpha(v-u), \quad \forall v \in C_\alpha$$

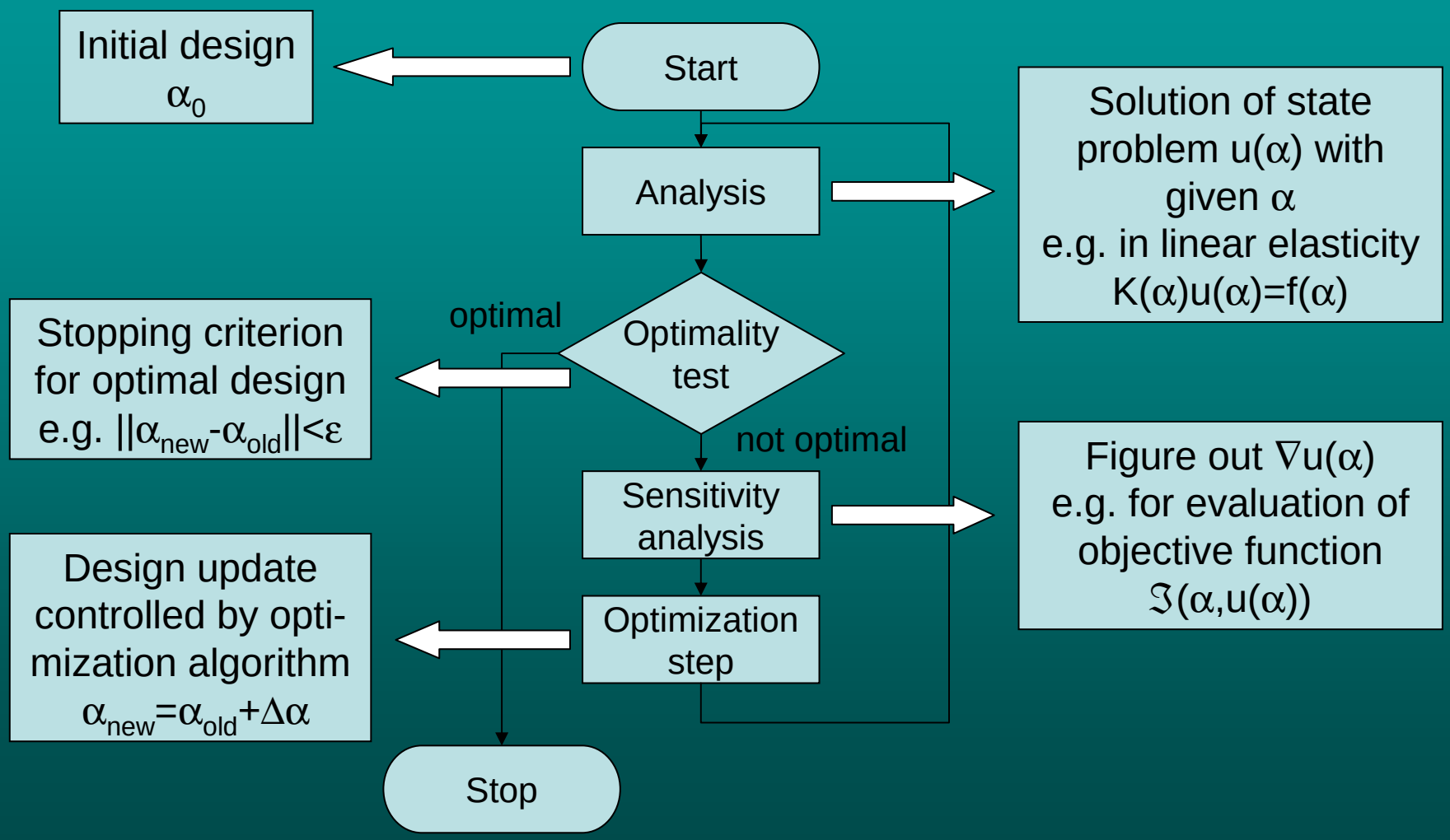
$$\downarrow$$

$$\min \tfrac{1}{2} u^T K(\alpha) u - u^T f(\alpha),$$

s.t. $B(\alpha)u \le c(\alpha)$



General solution scheme



Finite difference sensitivity analysis

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

where

$u(\alpha + he_i)$ solves

$$\min \tfrac{1}{2} u^T K(\alpha + he_i) u - u^T f(\alpha + he_i)$$

subject to $B(\alpha + he_i) u \le c(\alpha + he_i)$

and $e_i = (0, \ldots, 0, \underset{i}{1}, 0, \ldots, 0),\ i = 1, \ldots, m$

- 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?

Semi-analytical sensitivity analysis

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

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

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

$$u'(\alpha, \beta) = \lim_{h \to 0} \tfrac{1}{h} \big(u(\alpha + h\beta) - u(\alpha) \big)$$

solves

$$\min \tfrac{1}{2} z^T K(\alpha) z - z^T \overline{f}(\alpha, \beta)$$

$$\text{s.t. } B_W(\alpha) z \le c_W(\alpha, \beta),\ B_S(\alpha) z = c_S(\alpha, \beta)$$

$$\overline{f}(\alpha, \beta) = f'(\alpha, \beta) - K'(\alpha, \beta) u(\alpha) + B'^T(\alpha, \beta) \lambda(\alpha)$$

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

$$B_W(\alpha) = [B_i(\alpha)]_{i \in I_W},\ c_W(\alpha, \beta) = \left[f_i'(\alpha, \beta) - B_{i,*}'(\alpha, \beta) u(\alpha) \right]_{i \in I_W}$$

FETI based sensitivity analysis

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

where

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

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

$$\bar{B}(\alpha) = \begin{bmatrix} B_W(\alpha) \\ B_S(\alpha) \end{bmatrix},\quad \bar{c}(\alpha,\beta) = \begin{bmatrix} c_W(\alpha,\beta) \\ c_S(\alpha,\beta) \end{bmatrix},\quad \bar{\lambda} = \begin{bmatrix} \bar{\lambda}_W \\ \bar{\lambda}_S \end{bmatrix}$$

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

with such appropriate ζ

- 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

SMALE for equality constrained QP

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

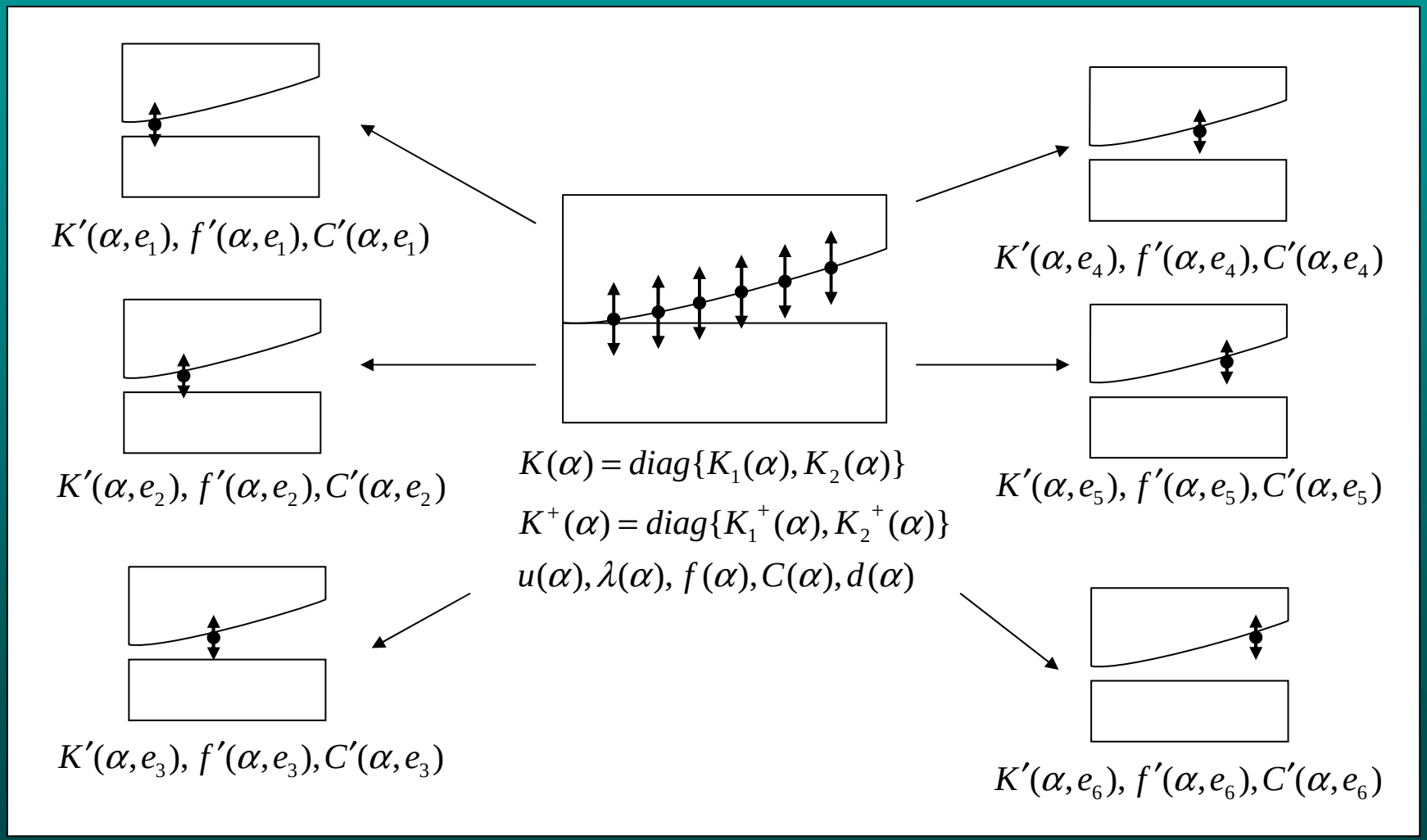
Augmented Lagrangian

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

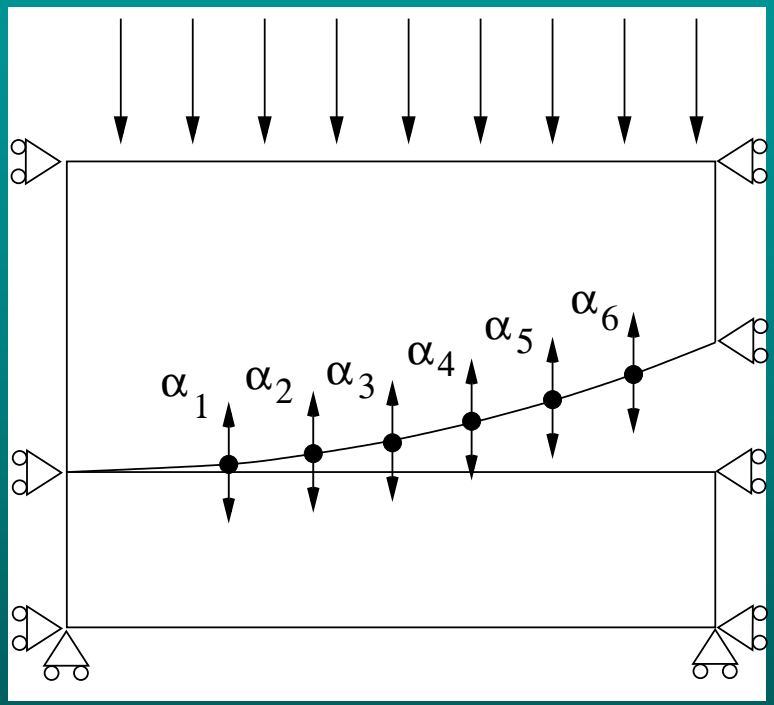
- Outer loop: Update of μ $\quad \mu \leftarrow \mu + \rho\bar{E}(\alpha)\bar{\lambda}$
- Inner loop: Inexact PCG $\quad \left\|g(\bar{\lambda},\mu,\rho)\right\| \le M\left\|\bar{E}(\alpha)\bar{\lambda}\right\|$

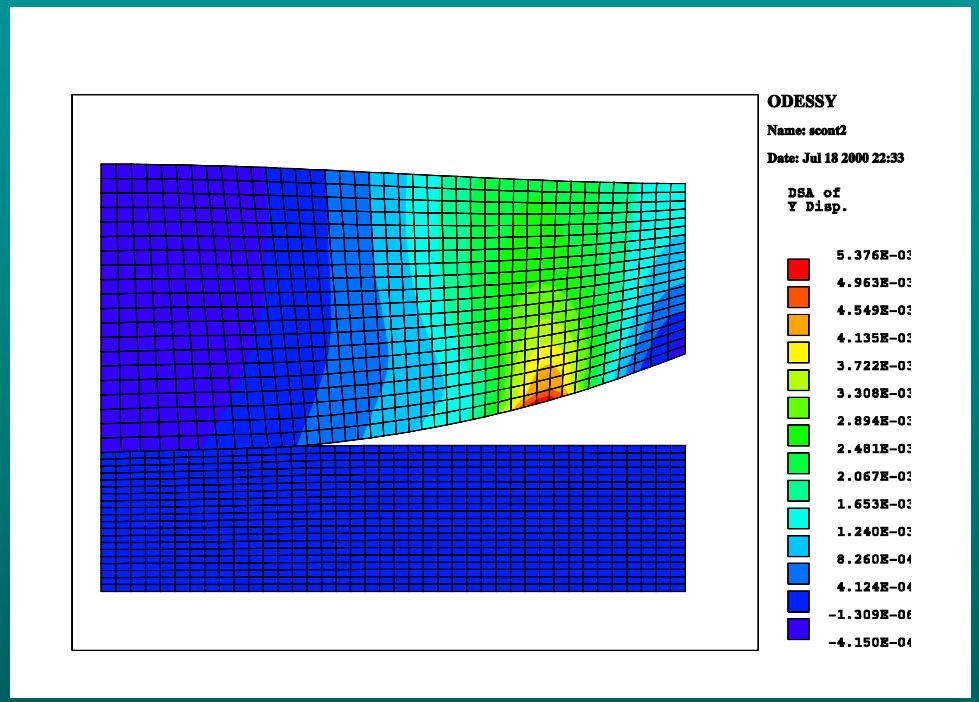
SemiMonotonic Augmented Lagrangian for Equality constrained QP

Parallel implementation



Model problem “scont”

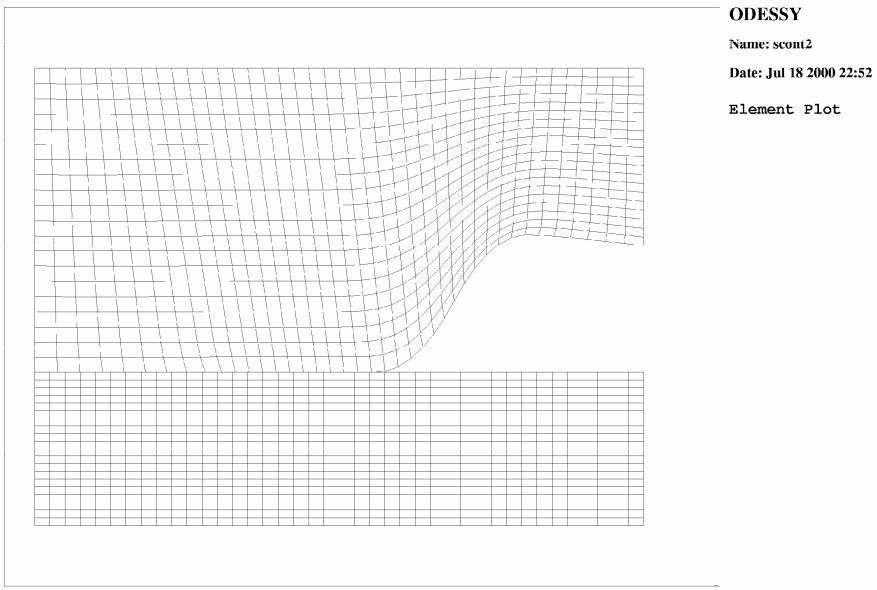


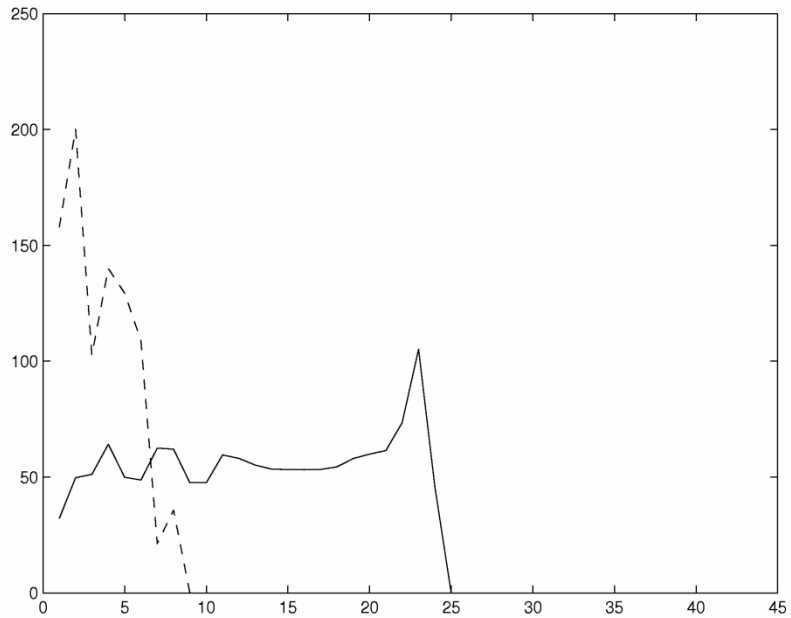


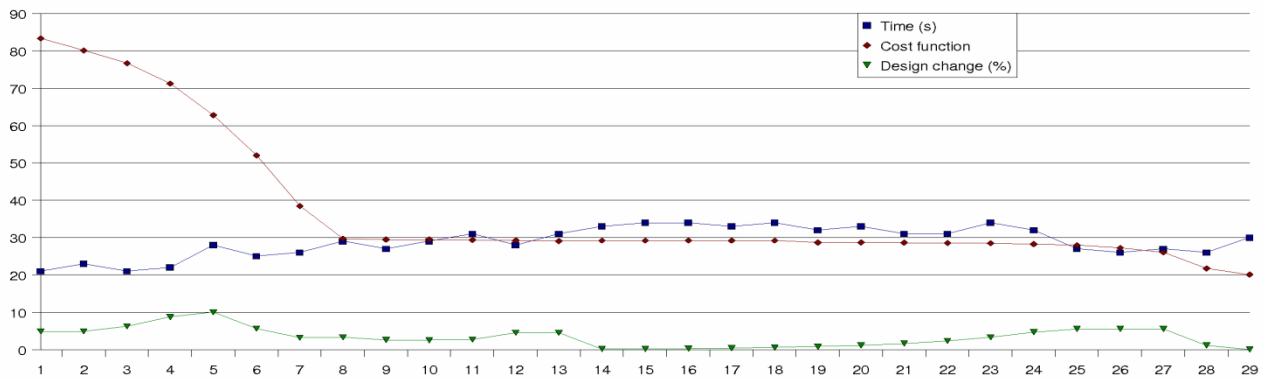
Alg.	Var.	State	DV1	DV2	DV3	DV4	DV5	DV6
FETI	Dual	41	12	12	12	12	12	12
	CG	61	7	8	8	8	8	7
Total FETI	Dual	166	137	137	137	137	137	137
	CG	108	32	32	30	30	30	36

State	DV
4.05	11.42
1.71	4.33

“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**