Theoretically supported scalable algorithms for contact problems

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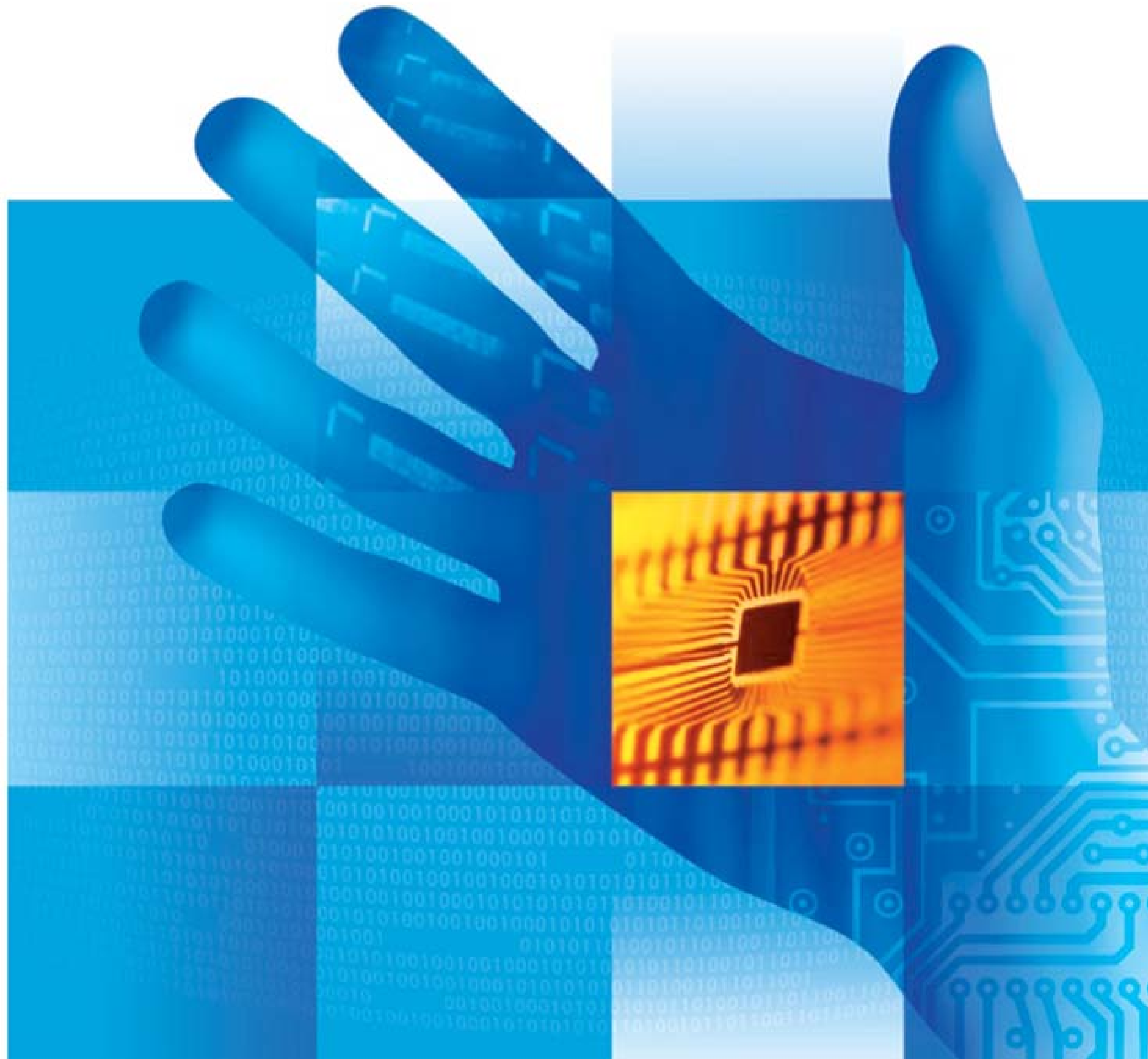
18th June, 2010
UPSA7
Palmanova



With

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Marie Sadowská

Petr Horyl

…

Outline

1. Challenges
2. Frictionless contact problem
3. Total FETI/BETI for frictionless problems
4. Problems with Tresca (given) friction
5. Bounds on the spectrum of the Hessian
6. Optimality results
7. Numerical experiments and MatSol

Challenges

- Identify the active constraints for free
- Get rate of convergence independent of conditioning of constraints
- Use only preconditioners that preserve separable constraints (projection)
- Get an initial approximation which is near the solution, i.e.

$$\left\| \widehat{\mathbf{u}} - \mathbf{u}^0 \right\| \leq C \left\| \mathbf{f} \right\|, \ \mathbf{u}^0 \text{ feasible}$$

Some previous work

Multigrid

Hackbusch, Mittelman 1981 experiments,

Mandel 1983 proof of convergence,

Kornhuber (monotone multigrid, book 1996),

Vassilevski, Iontcheva 2005, Krause 2008, …

DDM

Schoeberl 1998, 2000 (proof of optimality),

Z.D., Friedlander, Santos 1998, experiments,

Duresseix, Farhat 2000,

Z.D., Gomes, Santos 2000

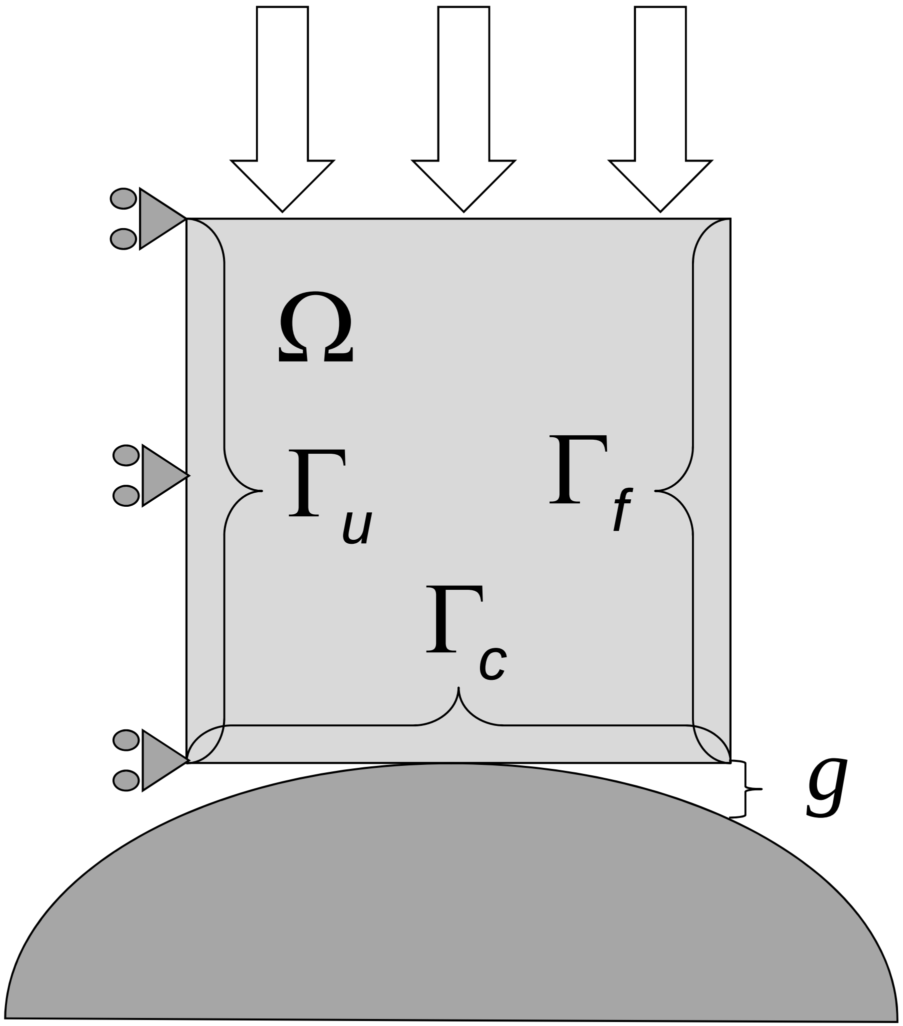
Avery, Farhat 2009, …

Key observation and results

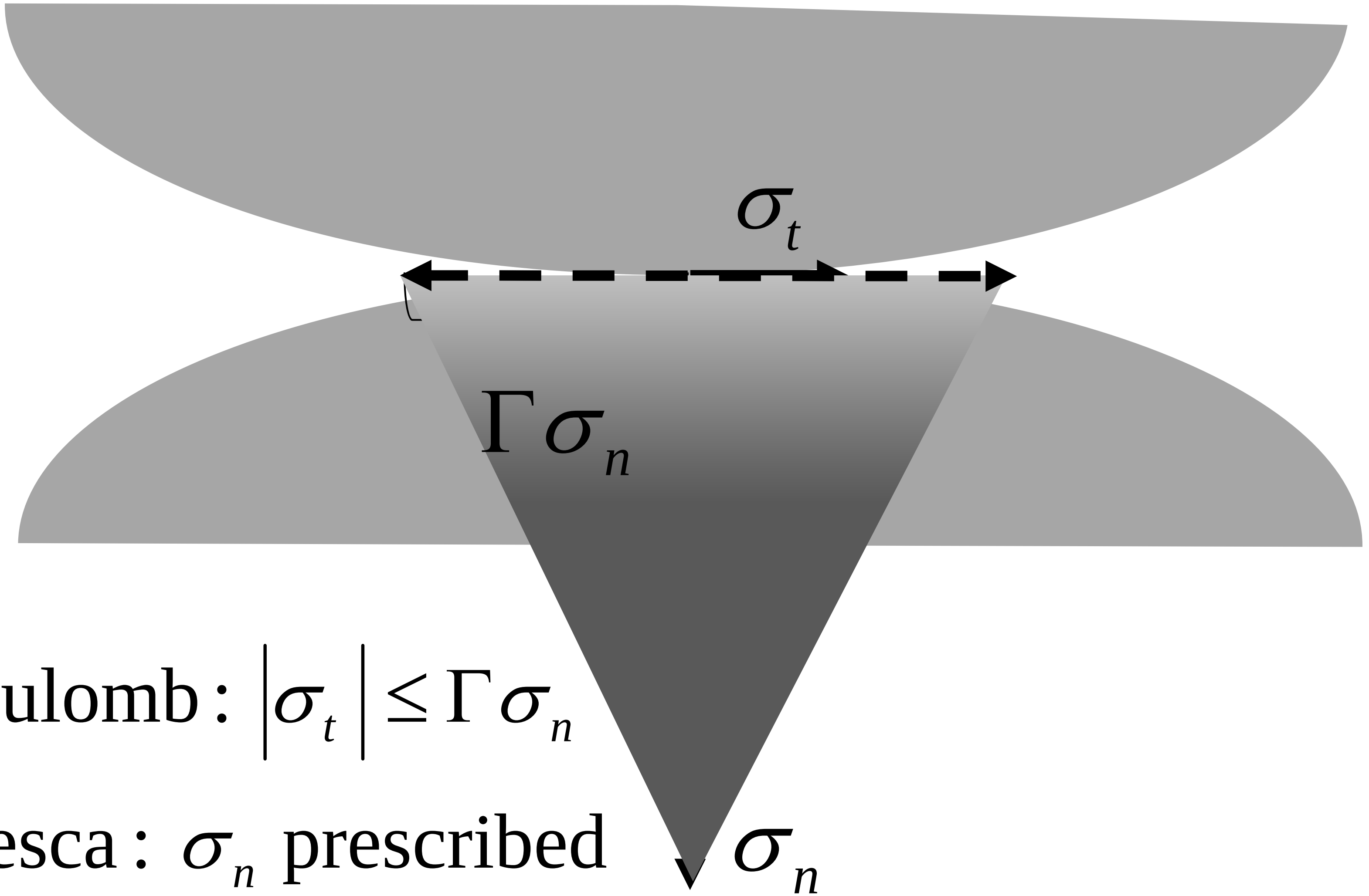
- In dual, there is a well defined subspace with the solution that can be used as an effective coarse grid

- There are algorithms for mininimization of quadratic function *f* subject to separable and linear constraints with error bounds in the extreme eigenvalues of the Hessian of *f*

Contact problem



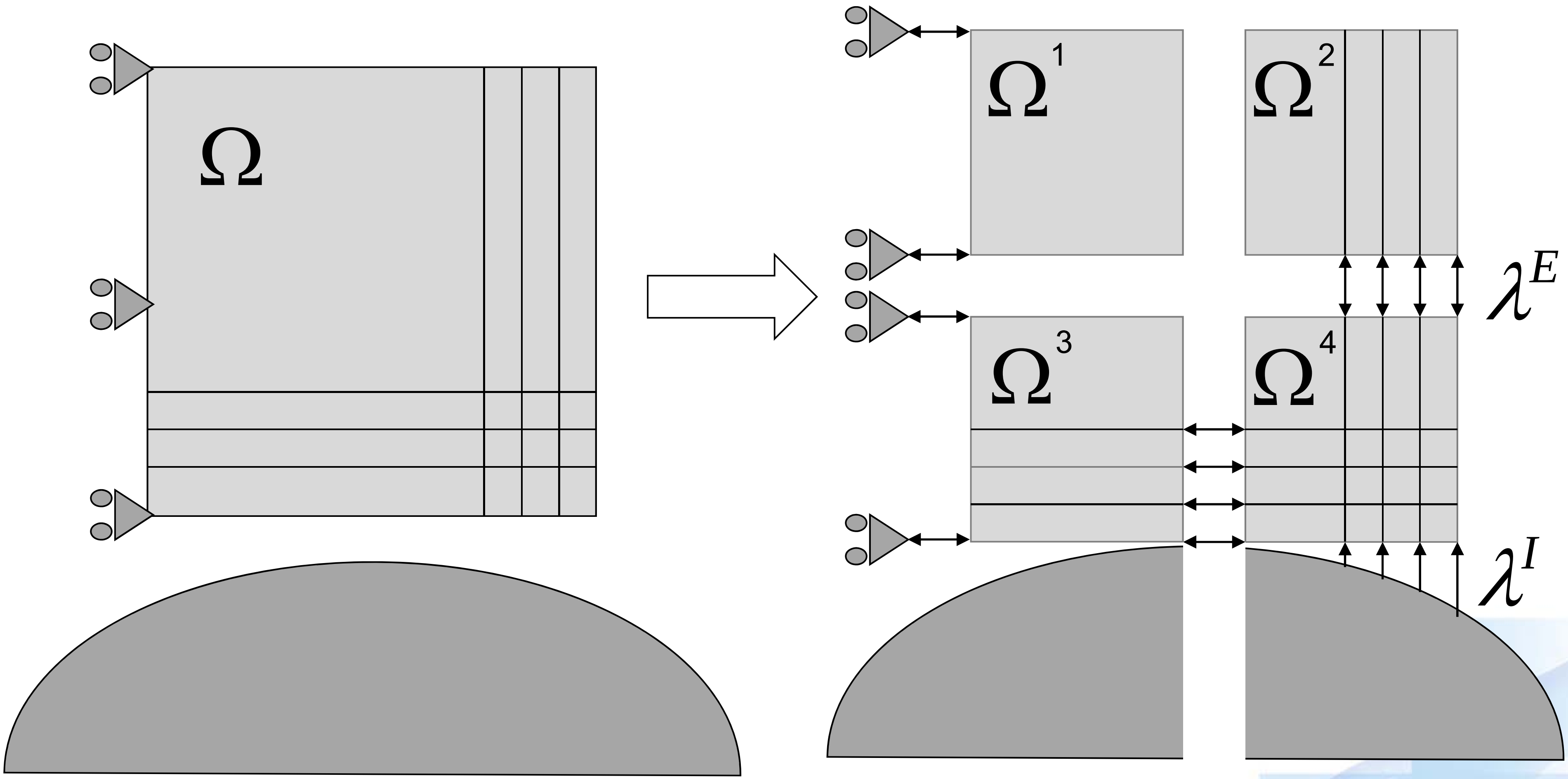
Coulomb and Tresca (given) friction



$$\text{Coulomb}: \left|\sigma_t\right| \leq \Gamma\sigma_n$$

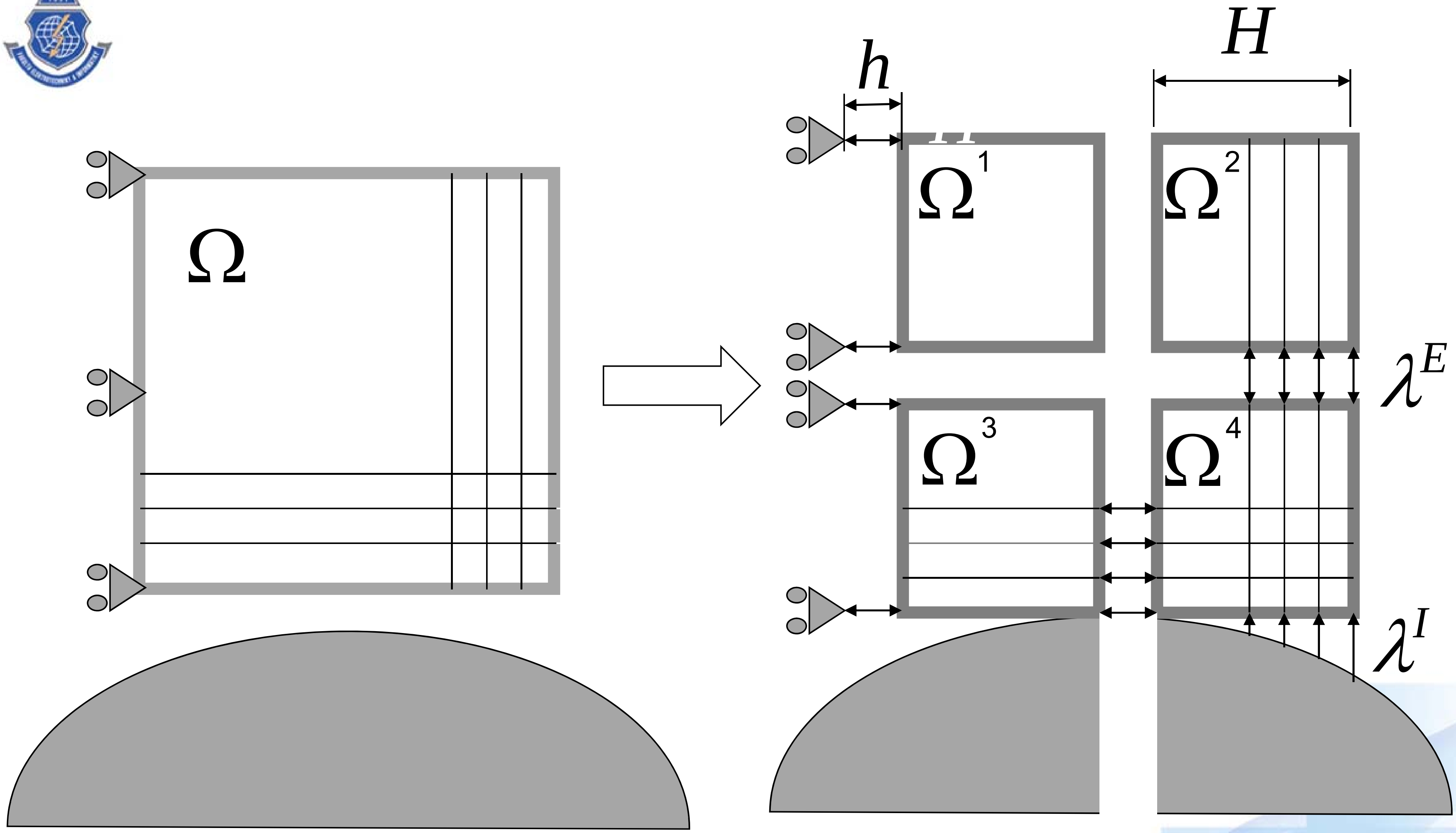
$$\text{Tresca}: \ \sigma_n \ \text{prescribed}$$

TFETI (AF FETI) domain decomposition



Z.D., Horák, Kučera CNME 2006, Of Thesis 2006, Park et al. 1996

TBETI (AF BETI) domain decomposition



Linear problems Langer and Steinbach Computing 2003
Variational inequalities Bouchala, Z.D., Sadowská Computing 2008, 2009

Discretized frictionless problem

$$J(\mathbf{u}) = \frac{1}{2}\mathbf{u}^T\mathbf{K}\mathbf{u} - \mathbf{f}^T\mathbf{u} \quad \text{(convex)}$$

$$\text{gluing}: \ \mathbf{B}^E\mathbf{u} = \mathbf{o}$$

$$\text{non-penetration}: \ \mathbf{B}^I\mathbf{u} \le \mathbf{g}$$

$$\mathcal{K}_h = \left\{\mathbf{u}: \ \mathbf{B}^E\mathbf{u} = \mathbf{o} \quad \text{and} \quad \mathbf{B}^I\mathbf{u} \le \mathbf{g}\right\}$$

$$(\mathrm{P}_h) \quad \text{Find} \qquad \min J_h(\mathbf{u}) \qquad \text{s.t.} \quad \mathbf{u} \in \mathcal{K}_h$$

Stiffness matrices TFETI

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}^1 & & \\ & \ddots & \\ & & \mathbf{K}^s \end{bmatrix} \quad \text{(positive semidefinite)} \qquad \mathbf{f} = \begin{bmatrix} \mathbf{f}^1 \\ \vdots \\ \mathbf{f}^s \end{bmatrix}$$

$$\operatorname{Ker} \mathbf{K}^j = \begin{bmatrix} y_i & 1 & 0 \\ -x_i & 0 & 1 \end{bmatrix} \quad \text{(in 2D)}$$

$$\operatorname{Ker} \mathbf{K}^j = \begin{bmatrix} 0 & -z_i & y_i & 1 & 0 & 0 \\ z_i & 0 & -x_i & 0 & 1 & 0 \\ -y_i & x_i & 0 & 0 & 0 & 1 \end{bmatrix} \quad \text{(in 3D)}$$

FETI notation and homogenization

Notation :

$\mathbf{F} = \mathbf{B}\mathbf{K}^{+}\mathbf{B}^{T}$ $\qquad$ $\mathbf{G} = \mathbf{R}^{T}\mathbf{B}^{T}$

$\hat{\mathbf{d}} = \mathbf{B}\mathbf{K}^{+}\mathbf{f} - \mathbf{c}$ $\qquad$ $\mathbf{e} = \mathbf{R}^{T}\mathbf{f}$

$$\frac{1}{2}\lambda^{T}\mathbf{F}\lambda - \lambda^{T}\hat{\mathbf{d}} \rightarrow \min$$

$$\text{s.t.} \quad \lambda^{I} \geq \mathbf{o} \quad \text{and} \quad \mathbf{G}\lambda = \mathbf{e}$$

Homogenization :

$\mathbf{G}\overline{\lambda} = \mathbf{e}$ $\qquad$ $\lambda = \mu + \overline{\lambda}$

$\mathbf{G}\lambda = \mathbf{e} \quad \Leftrightarrow \quad \mathbf{G}\mu = \mathbf{o}$

$\lambda^{I} \geq \mathbf{o} \quad \Leftrightarrow \quad \mu^{I} \geq -\overline{\lambda}^{I}$

$$(\text{FETI}_{h}) \qquad \frac{1}{2}\lambda^{T}\mathbf{F}\lambda - \lambda^{T}\mathbf{d} \rightarrow \min$$

$$\text{s.t.} \quad \lambda^{I} \geq -\overline{\lambda}^{I} \quad \text{and} \quad \mathbf{G}\lambda = \mathbf{o}$$

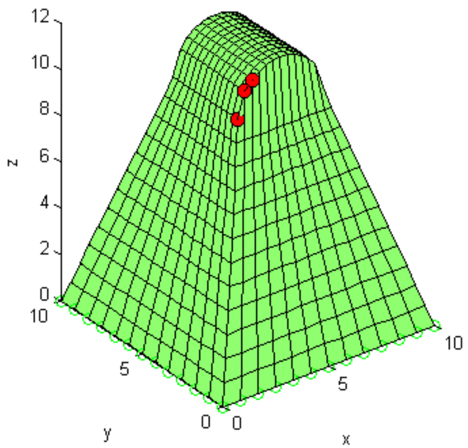
Generalized inverse with fixing points

$$\mathbf{PKP}^T = \begin{bmatrix} \mathbf{K}_{rr} & \mathbf{K}_{rs} \\ \mathbf{K}_{sr} & \mathbf{K}_{ss} \end{bmatrix} = \begin{bmatrix} \mathbf{L}_{rr} & \mathbf{O} \\ \mathbf{L}_{sr} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{L}_{rr}^T & L_{sr}^T \\ \mathbf{O} & \mathbf{S} \end{bmatrix}$$

$$\mathbf{K}^+ = \mathbf{P} \begin{bmatrix} \mathbf{L}_{rr}^{-T} & -\mathbf{L}_{rr}^{-T}\mathbf{L}_{sr}^T\mathbf{S}^+ \\ \mathbf{O} & \mathbf{S}^+ \end{bmatrix} \begin{bmatrix} \mathbf{L}_{rr}^{-1} & \mathbf{O} \\ -\mathbf{L}_{sr}\mathbf{L}_{rr}^{-T} & \mathbf{I} \end{bmatrix} \mathbf{P}^T$$

$$\overline{\lambda}_{\min}(\mathbf{K}) \le \overline{\lambda}_{\min}(\mathbf{S}), \qquad \text{(interlacing Smith LAA 1992)}$$

LU-SVD with active choice of regular part



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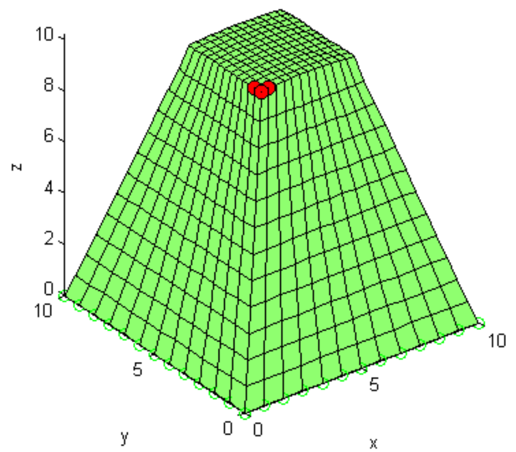

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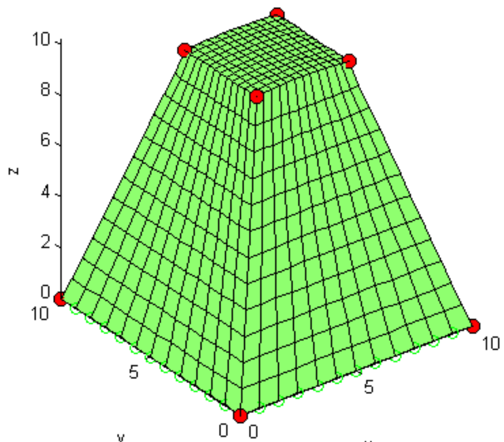

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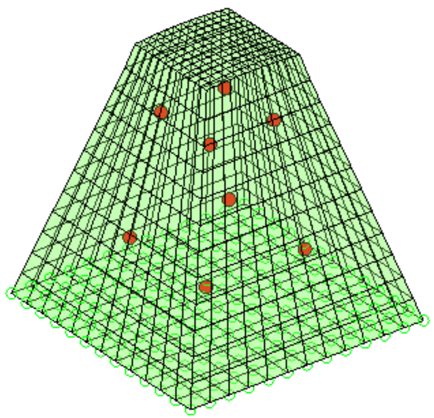

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LU-SVD Farhat, Girardon IJNME1998,
Fixing nodes Brzobohaty, Z.D., Kovar, Kozubek, Markopoulos 2010

More on homogenization

How to choose $\overline{\lambda}$ so that we are able to find $\lambda^0 \geq \overline{\lambda}$ so that

$$\left\|\lambda^0 - \hat{\lambda}\right\| \leq C\|\mathbf{d}\|, \quad C \text{ independent of } h \text{ and } H \text{ ?}$$

(i) Lemma: If the problem is coercive, then there is $\overline{\lambda}$ such that $\lambda = \mathbf{o}$ satisfies $\lambda^I \geq -\overline{\lambda}^I$

(ii) Use $\overline{\lambda}$ which solves $\min \frac{1}{2}\|\lambda\|^2$ s.t. $\lambda^I \geq \mathbf{o}$ and $\mathbf{G}\lambda = \mathbf{e}$

In our experiments $\overline{\lambda} = \mathbf{G}^T(\mathbf{GG})^{-1}\mathbf{e}$

Natural coarse grid projectors and regularization

$$\mathbf{Q} = \mathbf{G}^T \left(\mathbf{G}\mathbf{G}^T\right)^{-1} \mathbf{G} \qquad \mathbf{P} = \mathbf{I} - \mathbf{Q}$$

$$\operatorname{Im} \mathbf{Q} = \operatorname{Im} \mathbf{G}^T \qquad \operatorname{Im} \mathbf{P} = \operatorname{Ker} \mathbf{G}$$

$$(\text{FETI-NCG}_h) \quad \frac{1}{2}\lambda^T \mathbf{PFP}\lambda - \lambda^T \mathbf{Pd} + \rho \left\| \mathbf{Q}\lambda \right\|^2 \quad \to \quad \min$$

$$\text{s.t. } \lambda^I \geq -\overline{\lambda}^I \quad \text{and} \quad \mathbf{G}\lambda = \mathbf{o}$$

$$(\rho \approx \left\| \mathbf{F} \right\|)$$

Discretized Tresca problem

$$J_h(\mathbf{u}) = \frac{1}{2}\mathbf{u}^T\mathbf{K}\mathbf{u} - \mathbf{f}^T\mathbf{u} + j_h(\mathbf{u}) \quad \text{(convex)}$$

$$j_h(\mathbf{u}) = \sum_{i=1}^{m} \psi_i \left\| \mathbf{T}_i \mathbf{u} \right\| \quad \text{(non-differentiable)}$$

$$\text{gluing}: \ \mathbf{B}^E\mathbf{u} = \mathbf{o}$$

$$\text{non-penetration}: \ \mathbf{B}^I\mathbf{u} \le \mathbf{g}$$

$$\mathcal{K}_h = \left\{ \mathbf{u} : \ \mathbf{B}^E\mathbf{u} = \mathbf{o} \quad \text{and} \quad \mathbf{B}^I\mathbf{u} \le \mathbf{g} \right\}$$

$$(\mathrm{P}_h) \quad \text{Find} \quad \min J_h(\mathbf{u}) \quad \text{s.t.} \quad \mathbf{u} \in \mathcal{K}_h$$

Dissipative terms in 2D and 3D

2D :

$$j_h(u) = \sum_1^m \psi_i \left|\mathbf{T}_i\mathbf{u}\right| = \sum_1^m \max_{|\tau_\mathrm{i}|\le\psi_i} \tau_\mathrm{i}\mathbf{T}_i\mathbf{u}$$

3D :

$$j_h(u) = \sum_1^m \psi_i \left\|\mathbf{T}_i\mathbf{u}\right\| = \sum_1^m \max_{\|\tau_\mathrm{i}\|\le\psi_i} \tau_\mathrm{i}\mathbf{T}_i\mathbf{u}$$

Duality and natural coarse grid projectors

$$\mathbf{Q} = \mathbf{G}^T\left(\mathbf{G}\mathbf{G}^T\right)^{-1}\mathbf{G} \qquad \mathbf{P} = \mathbf{I} - \mathbf{Q}$$

$$\operatorname{Im}\mathbf{Q} = \operatorname{Im}\mathbf{G}^T \qquad \operatorname{Im}\mathbf{P} = \operatorname{Ker}\mathbf{G}$$

$$\mathbf{B} = \begin{bmatrix} \mathbf{B}^N \\ \mathbf{T} \\ \mathbf{B}^E \end{bmatrix}, \quad \lambda = \begin{bmatrix} \lambda_N \\ \tau \\ \lambda_E \end{bmatrix}, \quad \Lambda = \Lambda(\psi) = \left\{\lambda : \lambda_N \geq \mathbf{o} \quad \text{and } |\tau_i| \leq \psi_i\right\}$$

$$(\text{TFETI-NCG}_h) \quad \frac{1}{2}\lambda^T\mathbf{PFP} + \rho\|\mathbf{Q}\lambda\|^2 - \lambda^T\mathbf{Pd} \quad \rightarrow \quad \min$$

$$\text{s.t. } \lambda \in \Lambda \quad \text{and} \quad \mathbf{G}\lambda = \mathbf{o}$$

Optimal estimates

Theorem : Let there be positive constants B_1, B_2 such that for any discretization parameter h and H

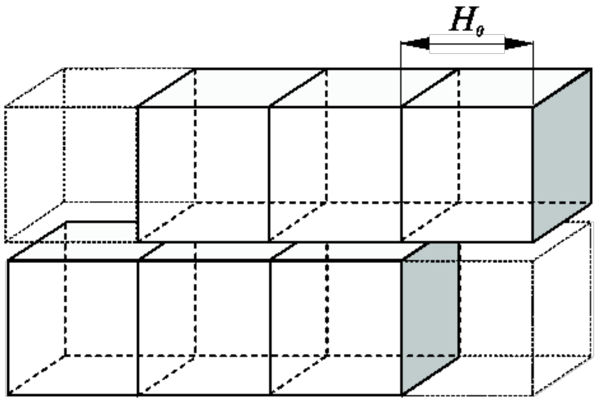
$$B_1 \leq \lambda_{\min}\left(\mathbf{BB}^T\right) \leq \lambda_{\min}\left(\mathbf{BB}^T\right) \leq B_2$$

Let the elements and subdomains have regular shape and size. Then

$$C_1 \leq \lambda_{\min}(\mathbf{F}|\mathrm{Im}\mathbf{F})$$

$$\|\mathbf{F}\| \leq C_2 \frac{H}{h}$$

$$\kappa(\mathbf{F}|\mathrm{Im}\mathbf{F}) \leq C_2 \frac{H}{h}$$



ETI: Farhat, Mandel, Roux 1994

ETI: Bouchala, Z.D., Sadowská 2009, based on Langer and Steinbach 2003

Separable and equality constrained problems

For $i \in \mathcal{T}$ let

$$f_i(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{A}_i\mathbf{x} - \mathbf{b}_i^T\mathbf{x}$$

$$\Omega_i = \{\mathbf{x} : \mathbf{x} \in \Lambda_i \text{ and } \mathbf{B}_i\mathbf{x} = \mathbf{o}\}, \quad \|\mathbf{B}_i\| \le C_0$$

$$\mathbf{A}_i = \mathbf{A}_i^T$$

$$C_1\|\mathbf{x}\|^2 \le \mathbf{x}^T\mathbf{A}_i\mathbf{x}_i \le C_1\|\mathbf{x}\|^2, \quad \mathbf{o} \in \Omega_i$$

$$(\text{QPSE}_i) \qquad \text{Find} \qquad \min_{\Omega_i} f_i(\mathbf{x})$$

Challenge: Find an approximate solution in O(1) iterations!!!

Computational engin I: SMALSE-M

Augmented Lagrangians for separable and equality constraints

- Outer loop for multipliers for equality constraints
- Problem with separable constraits in inner loop
- Adaptive precision control (by feasibility error)
- No update of regularization parameter

$$\text{Important feature : a bound on number of iterations independent of representation of the equality constraints}$$

Z.D. SINUM 2007, book 2009, Z.D. ,Kučera 2010, Z.D., Kozubek 2010

Algorithm SMALSE-M

$Step\ 0$ $\beta < 1, \rho > 0, M_0 > 0, \eta > 0, \mu^0$

$\{\text{Approximate solution of separably constrained problem}\}$

$Step\ 1$ Find $\mathbf{x}^k$ such that $\left\| \mathbf{g}^P\left(\mathbf{x}^k, \mu^k, \rho\right) \right\| \leq \min\left\{ M_k \left\| \mathbf{Bx}^k \right\|, \eta \right\}$

$\{\text{Test}\}$

$Step\ 2$ if $\left\| \mathbf{g}^P\left(\mathbf{x}^k, \mu^k, \rho\right) \right\|$ and $\left\| \mathbf{Bx}^k \right\|$ are small then $\mathbf{x}^k$ is solution

$\{\text{Update Lagrange multipliers}\}$

$Step\ 3$ $\mu^{k+1} = \mu^k + \rho \mathbf{Bx}^k$

$\{\text{Update } M_k\}$

$Step\ 4$ If $L\left(\mathbf{x}^k, \mu^k, \rho\right) \leq L\left(\mathbf{x}^{k-1}, \mu^{k-1}, \rho\right) + \frac{\rho}{2} \left\| \mathbf{Bx}^k \right\|$

then $M_{k+1} = \beta M_k$

else $M_{k+1} = M_k$

$Step\ 5$ $k = k + 1$ and return to $Step\ 1$

Computational engin II: MPGP

- active set strategy
- adaptive precision control
- change of the active set by fixed step gradient projection
- conjugate gradients for auxiliary linear problems
- MPRGP for bound constraints

Important features: R-linear rate of convergence of the norm of the projected gradient in the bounds on the spectrum

(Z.D., Schoeberl COA 2005, Z.D. book 2009, Z.D., Kozubek 2010)
Gradient projection Schoeberl 2008, KPRGP Kučera 2007, 2009

Optimality of TFETI with SMALSE/MPGP

heorem (Z.D., Kozubek): Let $\hat{\mathbf{x}}_i$ be the solution of (QPSE$_i$) and $\varepsilon > 0$.

hen $\mathbf{x}_i^k$ that satisfies

$$\left\|\mathbf{B}_i \mathbf{x}_i^k\right\| \le \varepsilon \left\|\mathbf{b}_i\right\| \quad \text{and} \quad \left\|\mathbf{g}^P\left(\mathbf{x}_i^k\right)\right\| \le \varepsilon \left\|\mathbf{b}_i\right\|$$

s found at

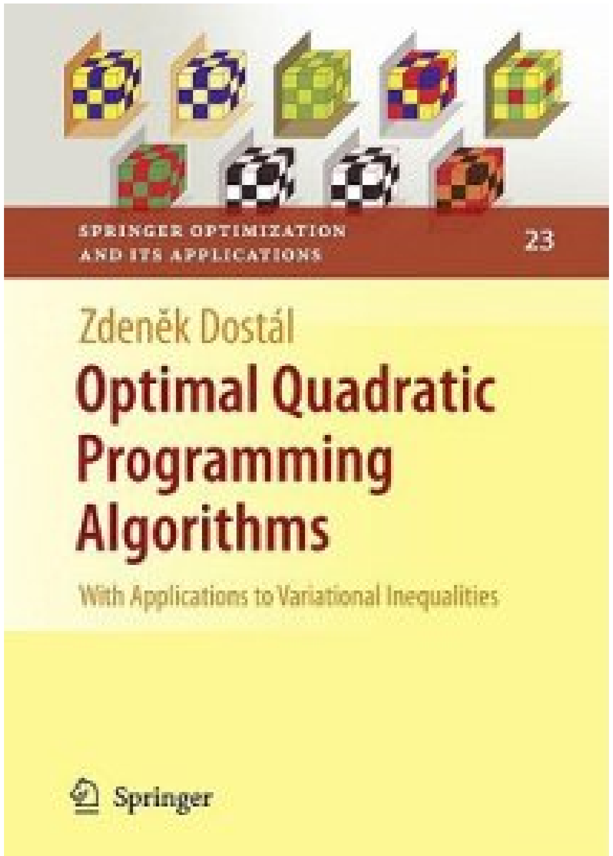
O(1) matrix - vector multiplications

BETI Bouchala, Z.D., Sadowská *Computing* 2008, 2009, *EABE* 2010

rictionless Z.D., Kozubek, Vondrák, Brzobohatý, Markopoulos, Horyl *IJNME* 2010

D friction Z.D., Kozubek, Brzobohatý, Markopoupos, Horyl *JCAM* 2010,

D friction Z.D., Kozubek, Brzobohatý, Markopoupos, Horyl 2010



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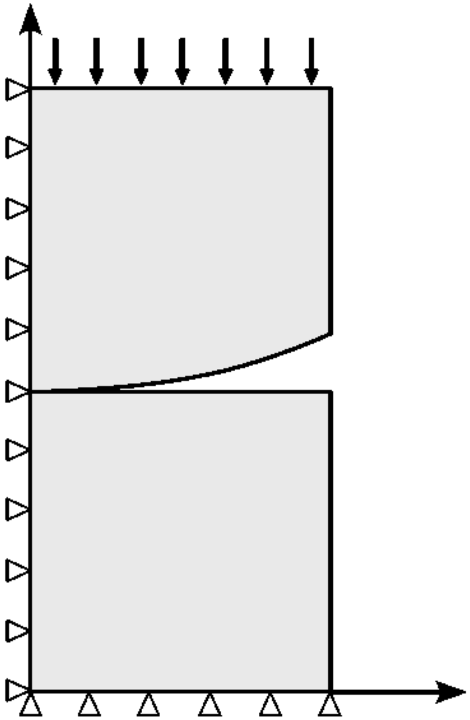
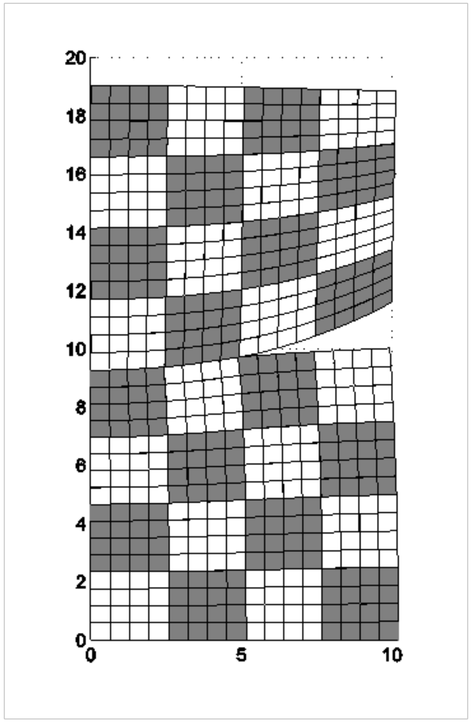
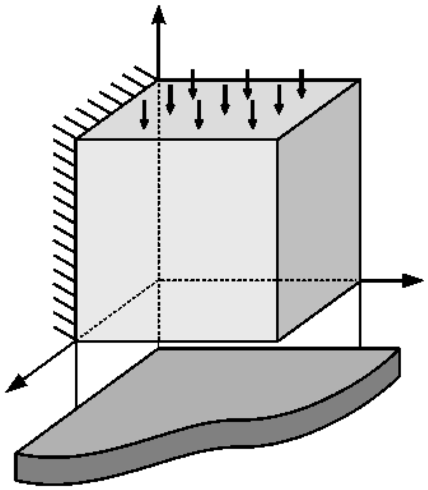
Scalability TFETI – Hertz 2D

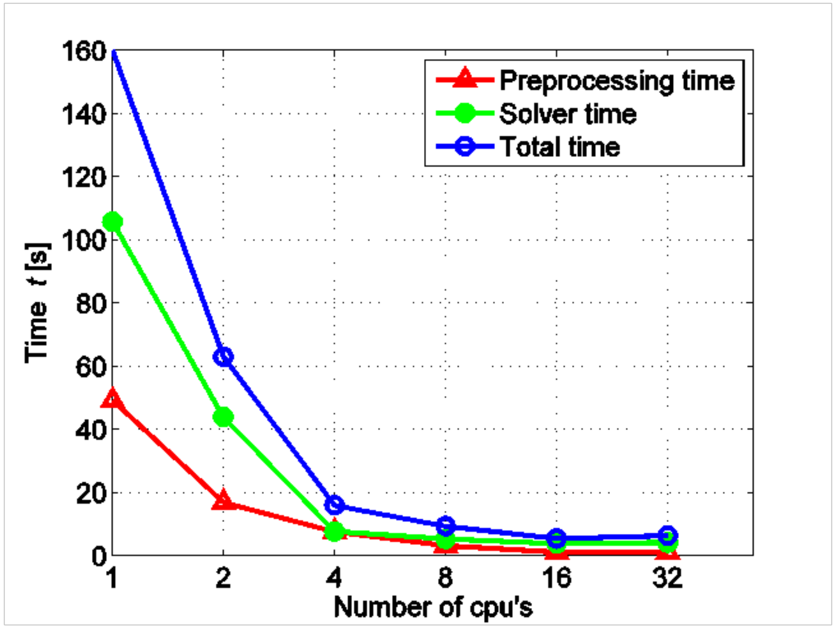




Primal dimension	Dual dimension	Subdomais	Null space	Matrix-vector	Time (sec)
40000	6000	2	6	45	10
640000	11200	32	96	88	78
10240000	198400	512	1536	134	1300

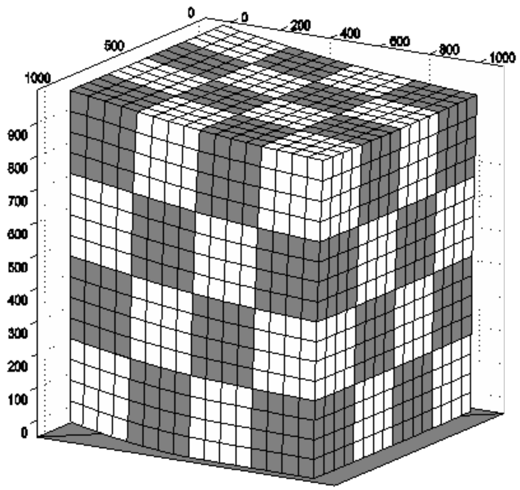
Scalability TFETI – no friction 3D

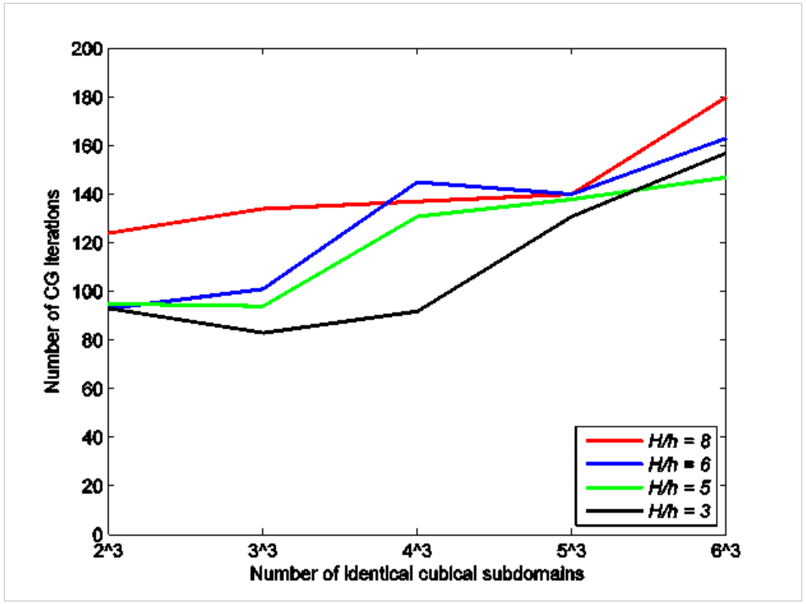




Primal dimension	Dual dimension	Subdomais	Null space	Matrix-vector	Time (sec)
31944	6052	8	48	74	13
255552	59051	64	192	100	51
2044416	514981	512	3072	154	760

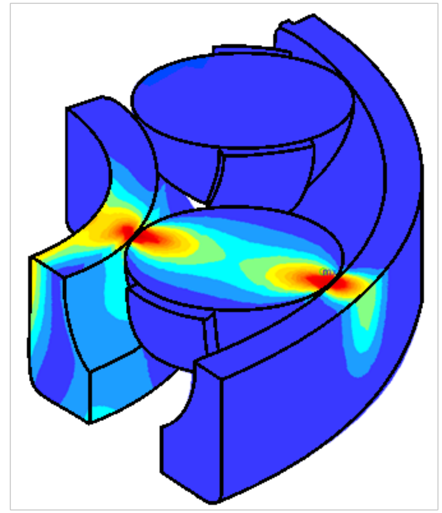
Scalability TBETI – no friction 3D



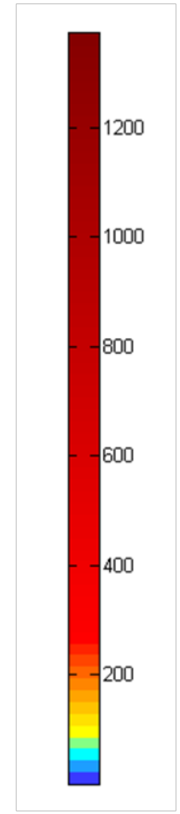


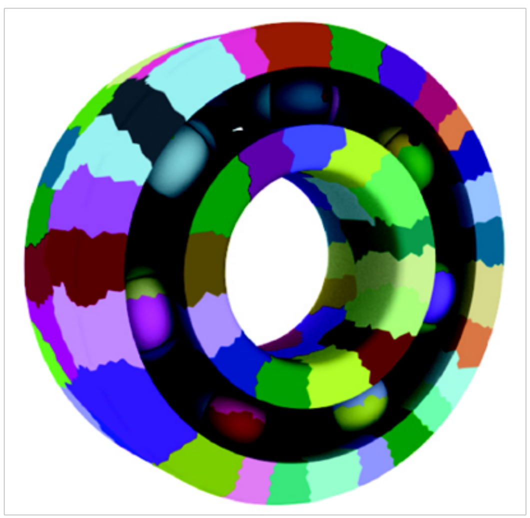
Primal dimension	Dual dimension	Subdomais	Null space	Matrix-vector
11712	5023	8	48	130
93696	43441	64	192	137
316224	63275	396	1068	133

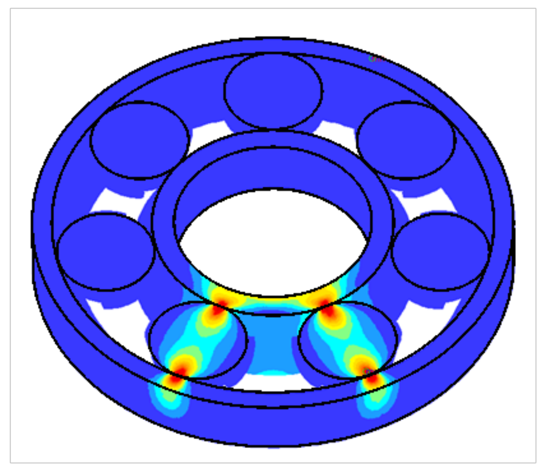
Applications – ball bearings



Von Mises (Mpa)

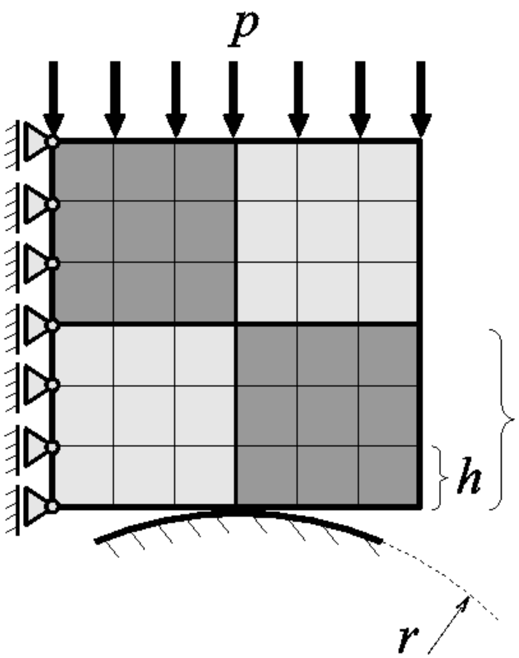


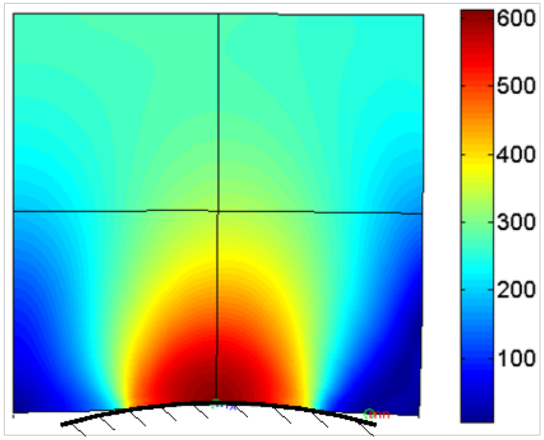




1688 190 primal, 408196 dual, 700 subdomains (Metis)
2364 matrix-vector multiplications, 20843 active constraints, 5383 sec

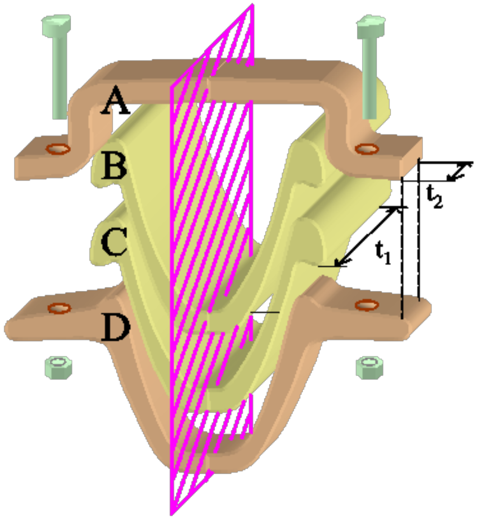
Scalabilty TFETI – 2D Tresca

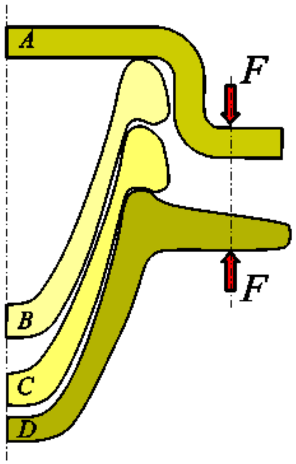


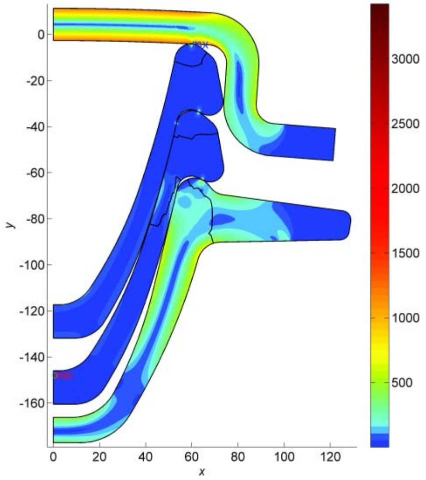


Primal dimension	Dual dimension	Subdomains	Null space	Matrix-vector	Outer iterations
5202	153	1	3	66	4
83232	3033	16	48	130	8
1331712	50913	256	768	208	23

Application TFETI – 2D Tresca



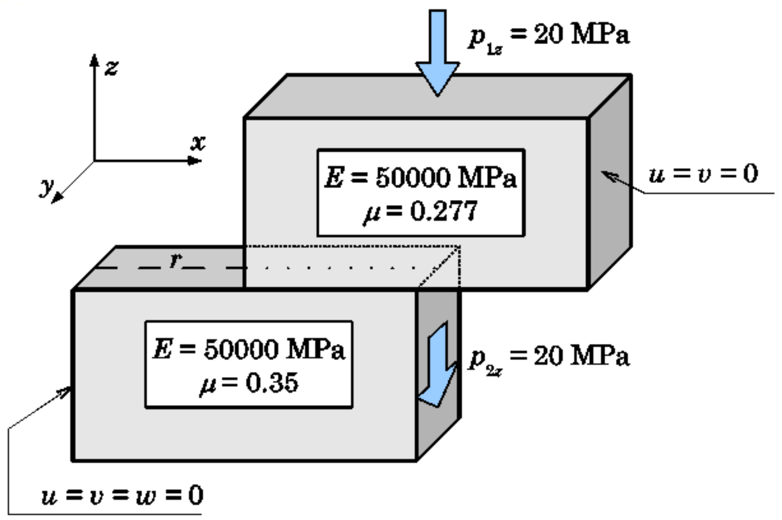


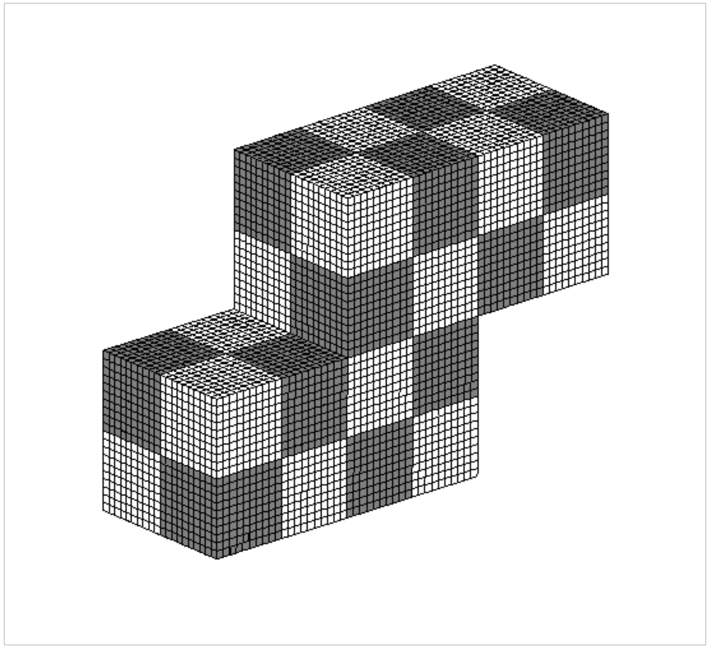


67330 primal, 1786 dual, 8 subdomains
4 bodies, 1287 active constraints
420 sec, 3836 Hessian multiplications

Z.D., Kozubek, Markopoulos, Brzobohatý, Horyl JCAM 2010

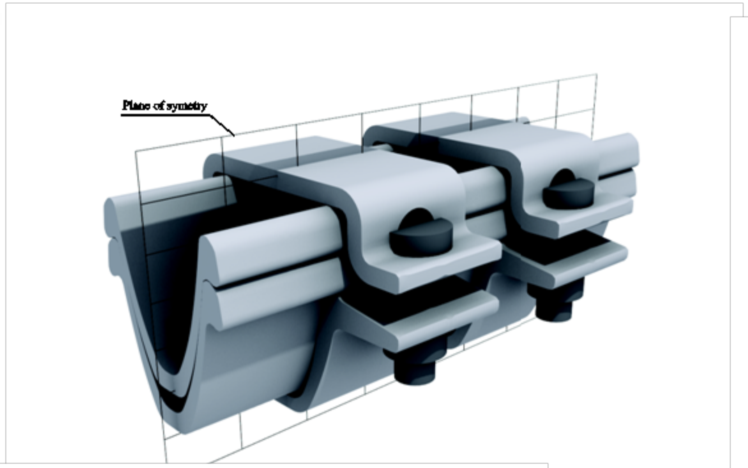
Scalability of TFETI – 3D Tresca

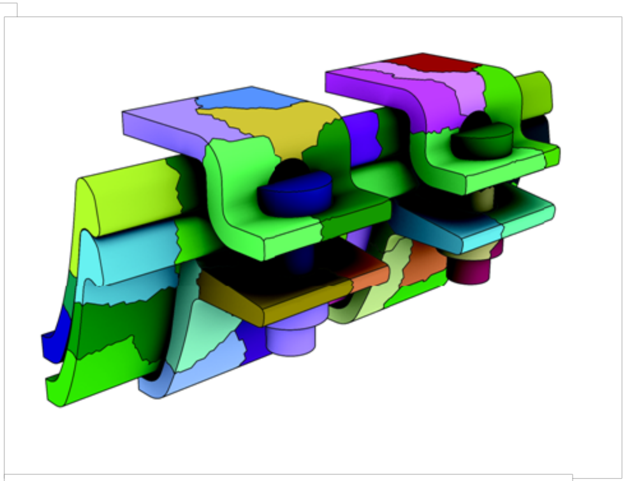


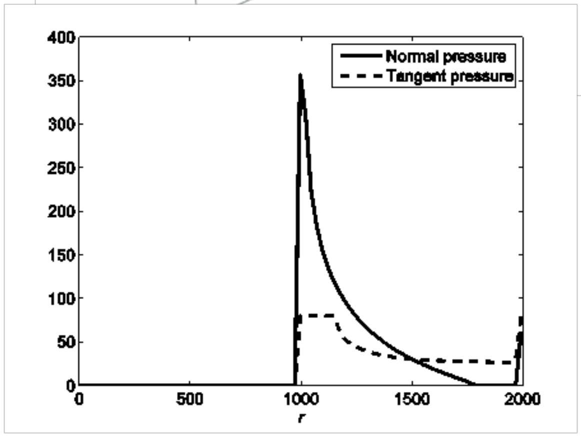


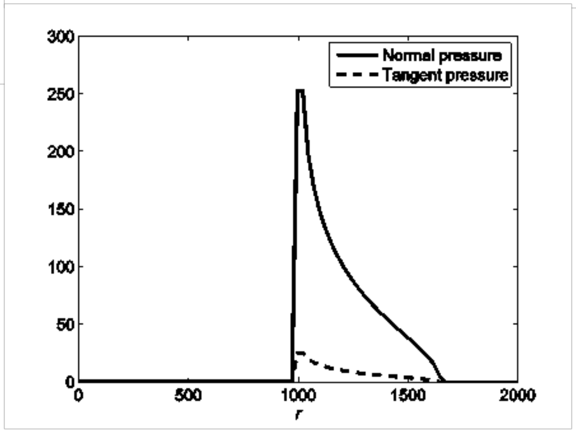
Primal dimension	Dual dimension	Subdomains	Null space	Matrix-vector	Outer iterations
15972	1694	4	24	76	14
255552	50634	64	384	216	6
4088832	942954	1024	6144	325	7

Applications: yielding clamped connection







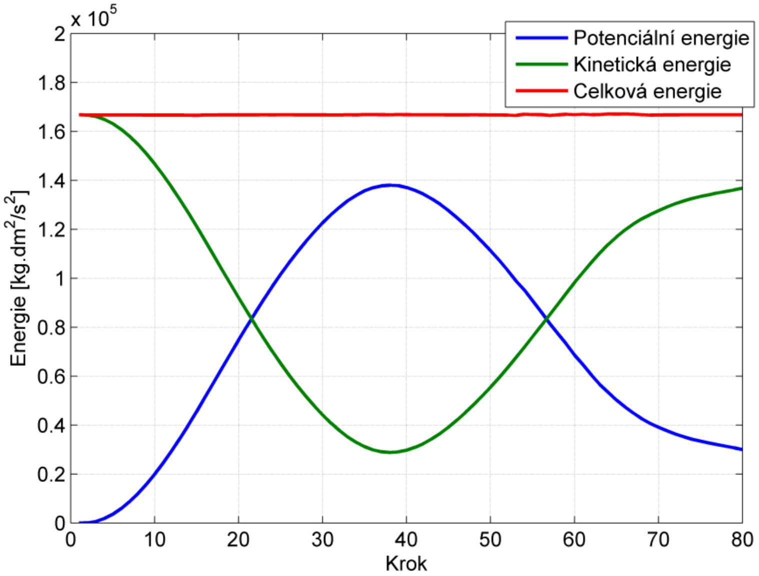


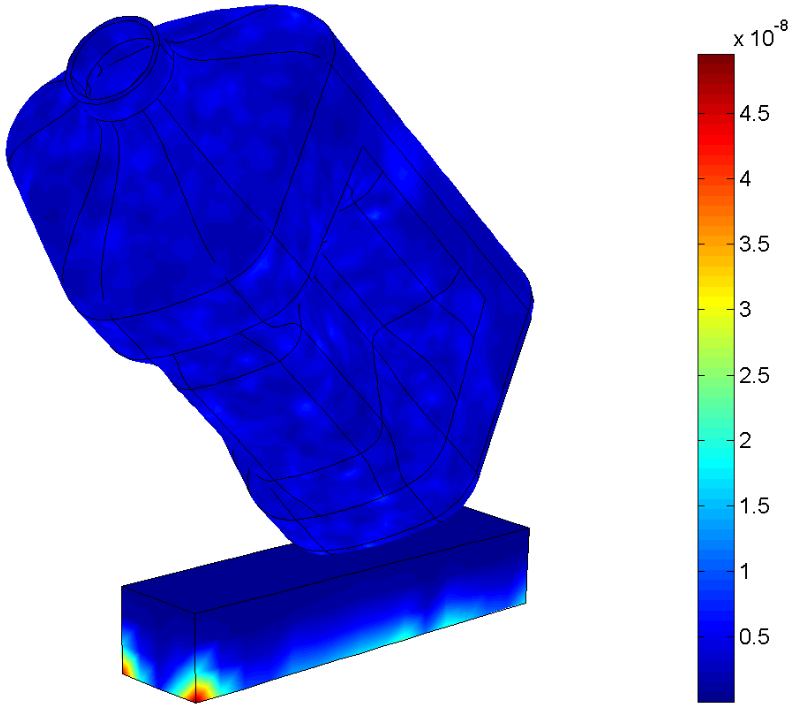
Tresca

Coulomb

1592853 primal, 216604 dual, 250 subdomains,
1922 Hessian multiplications, 5100 sec/24 CPU

Impact (more next time)





Conclusions

- Total FETI/BETI is a powerful tool for the solution of contact problems
- **Natural coarse grid is a nice way how to get coarse grid to the contact interface**
- Theory covers 2D and 3D frictionless contact problems, contact problems with a given (Tresca) friction, and a time step for dynamic frictionless problems
- Easy to extend to quasistatic and orthotropic friction
- Semidefinite matrices with known kernels can be treated as regular ones
- MatSol (Kozubek et al.) is a great tool for the solution of contact problems!
- MatSol often outperforms commercial solvers by orders