Scalable FETI based algorithms for numerical solution of variational inequalities

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Multiscale Problems: Modelling
Adaptive Discretization, Stabilization, Solvers
Cortona
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http://www.am.vsb.cz

with

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Outline

1. Motivation, optimal algorithms
2. Contact problems and their FETI/BETI based discretization
3. Optimal quadratic programming algorithms
4. Scalable FETI/BETI based algorithms
5. Numerical experiments

Scalable (optimal) algorithms

Numerical scalability:

cost $\approx$ number of unknowns

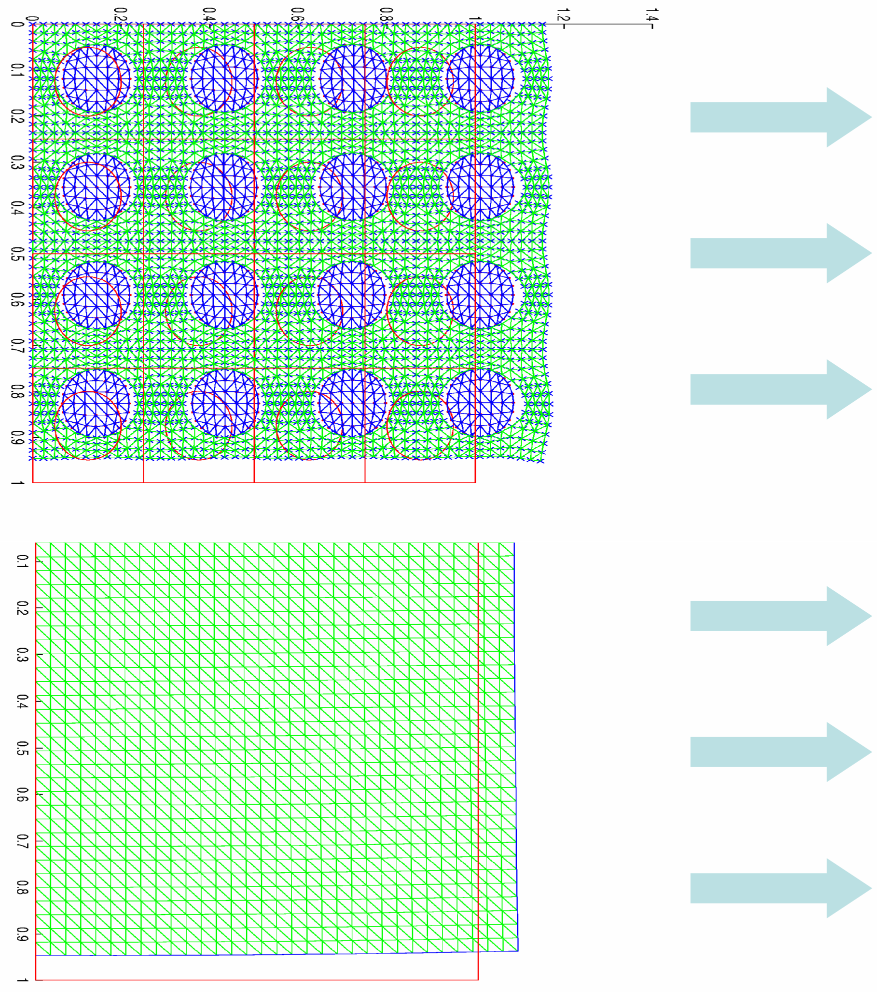
Parallel scalability:

time $\approx$ 1/number of processors

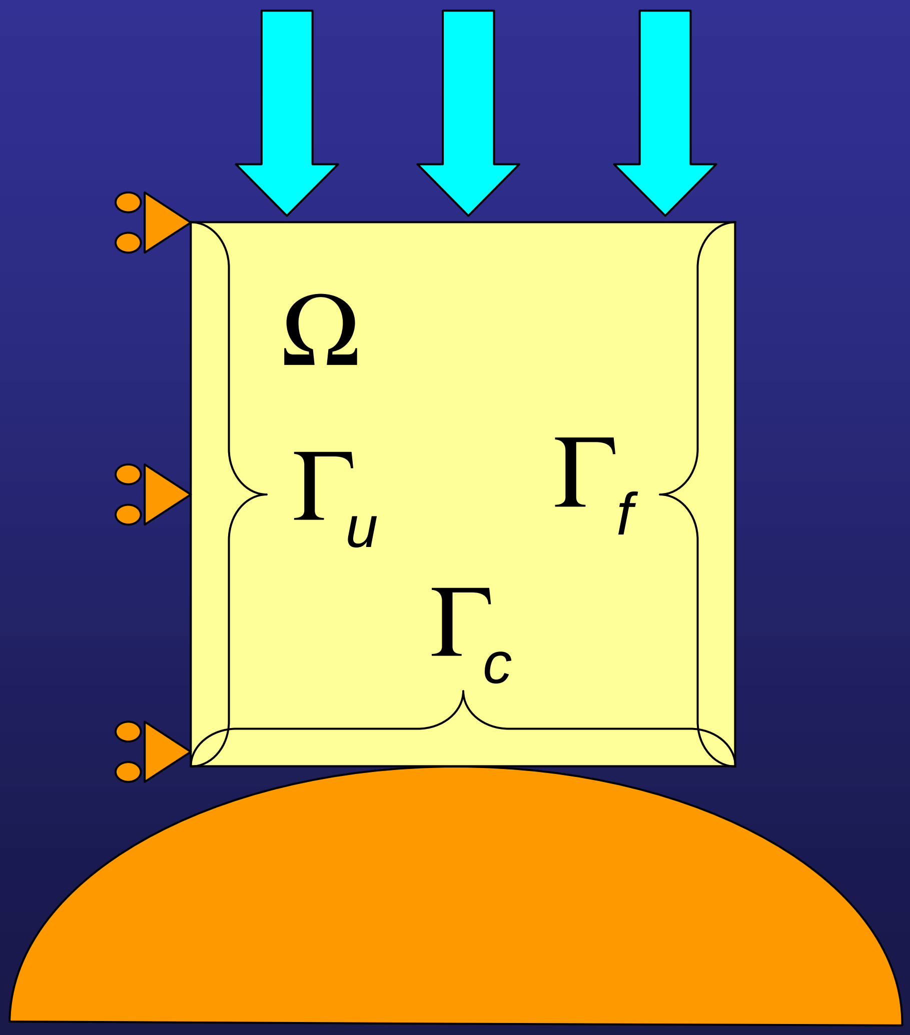
Challenges

- Identify the active constraints for free
- Get rate of convergence independent of conditioning of constraints
- Marry preconditioning with constraints

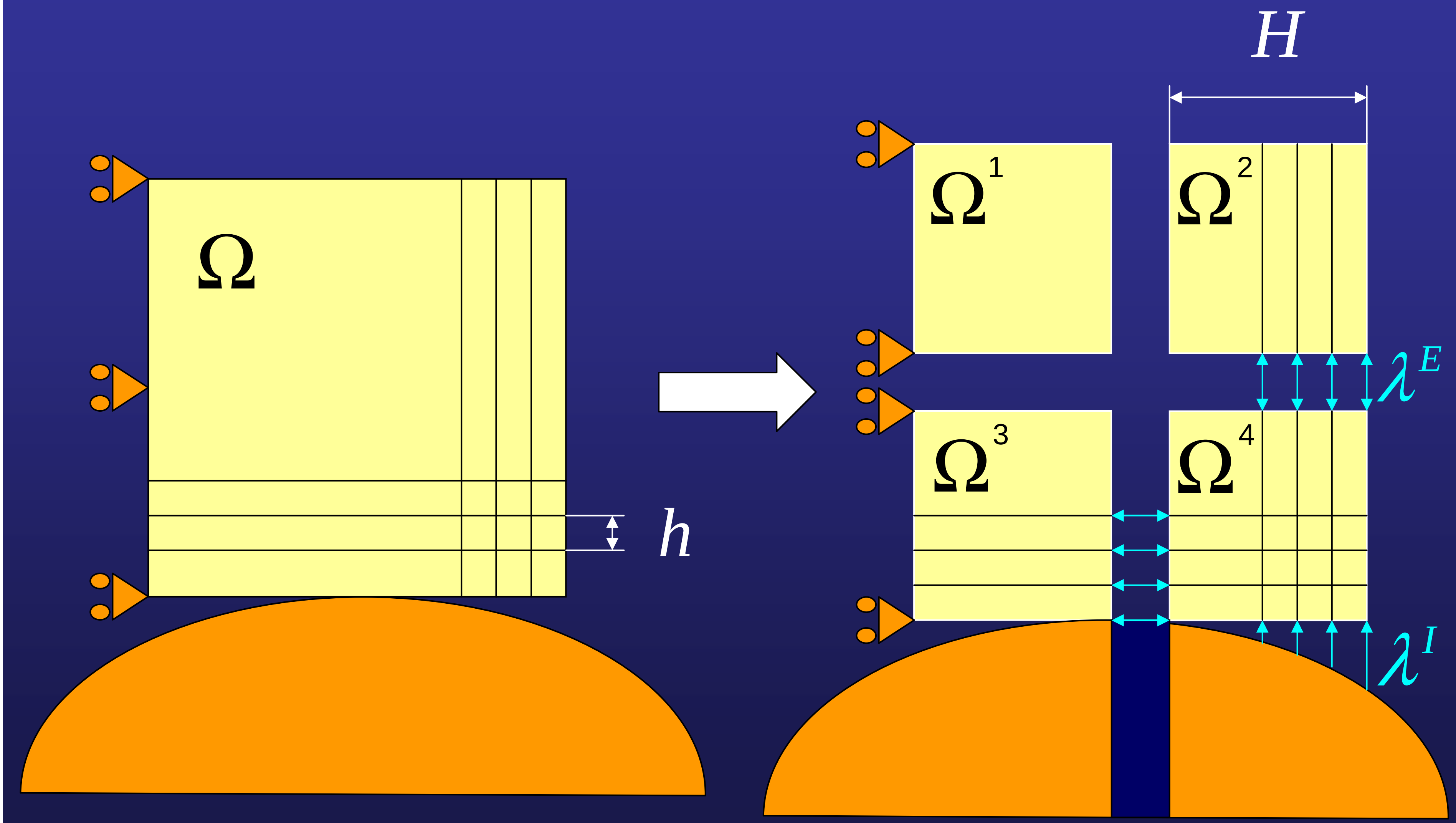
Composite with inserted inclusions



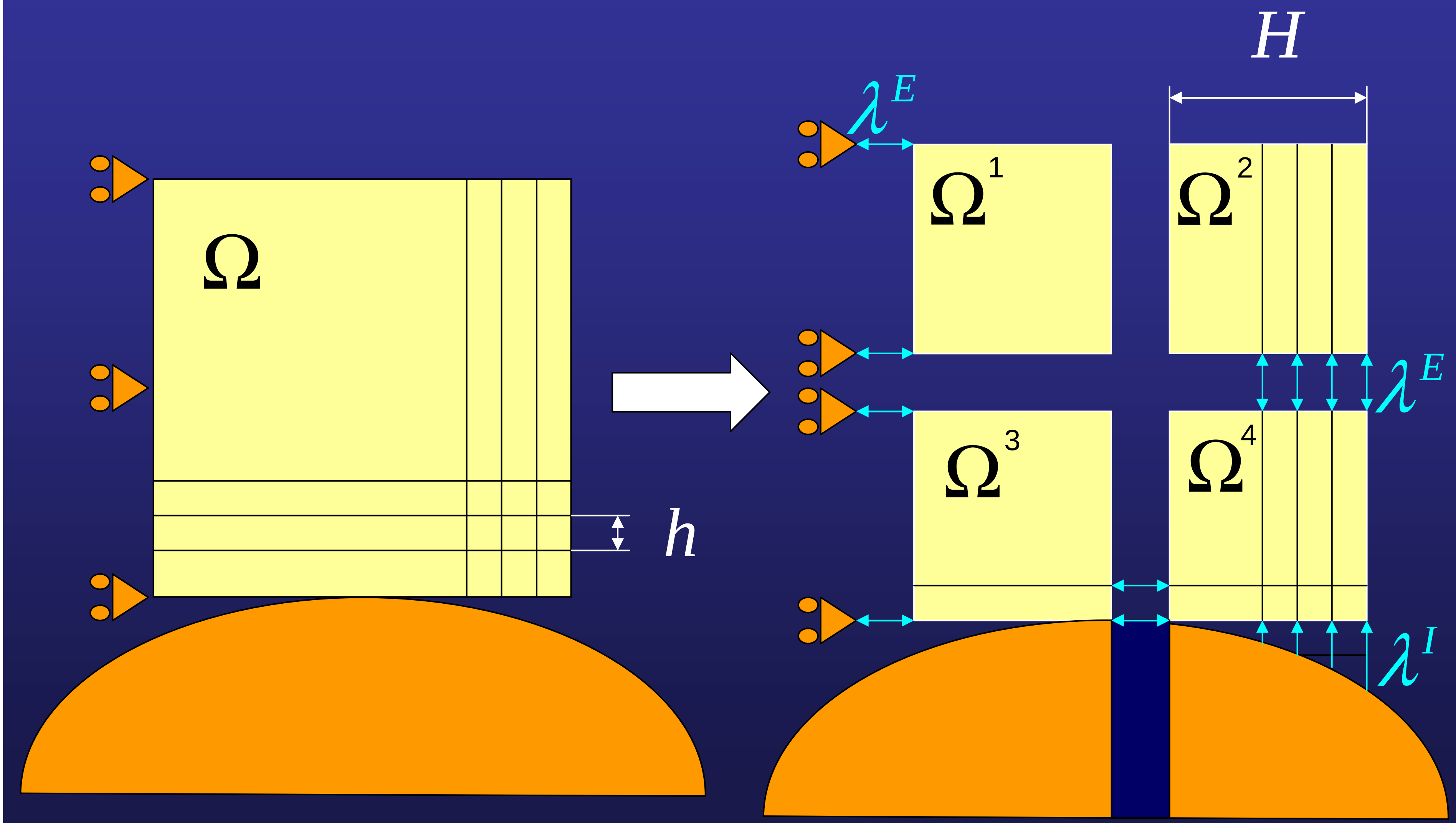
Contact problem of elasticity



FETI domain decomposition

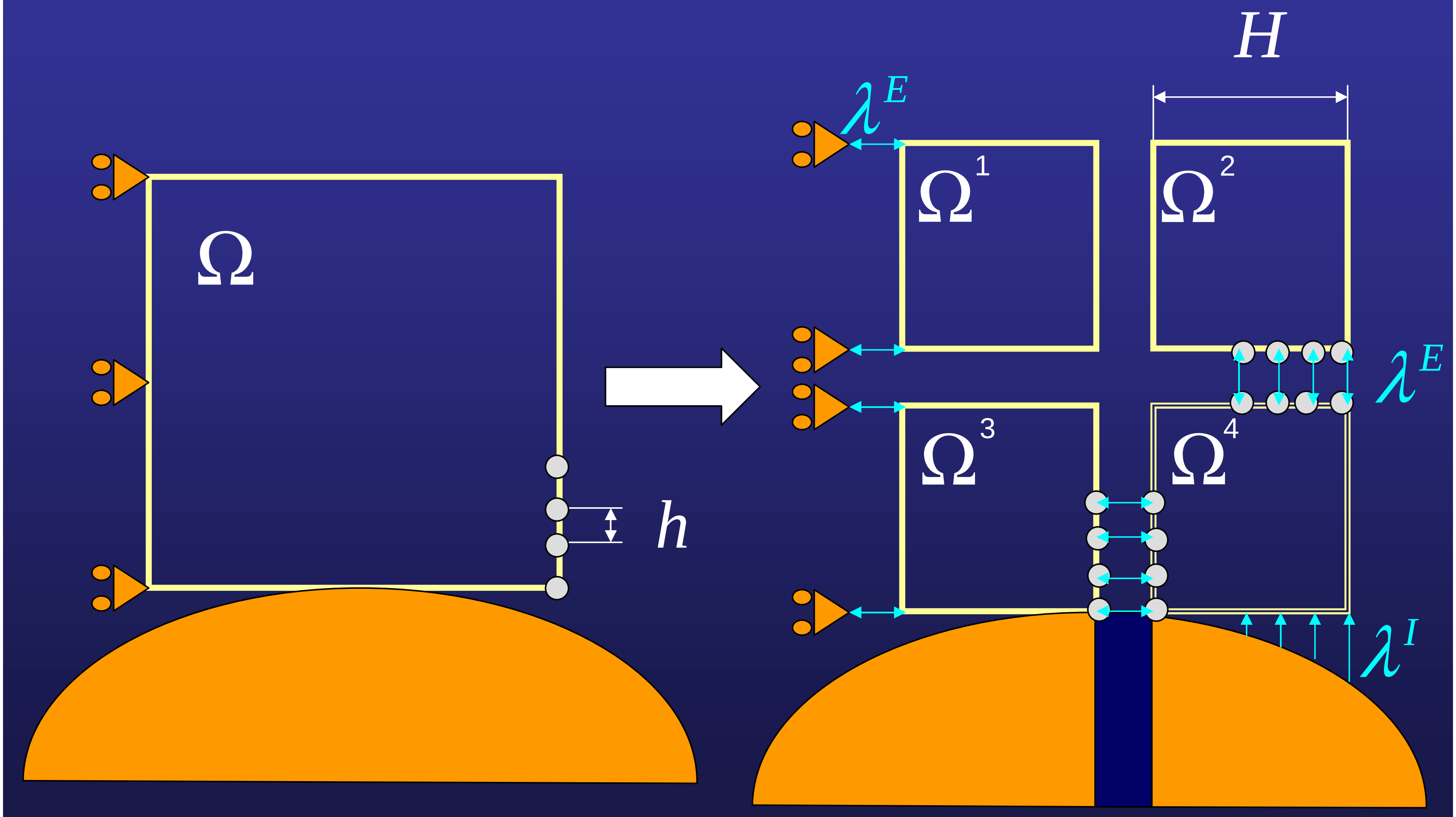


Total FETI domain decomposition

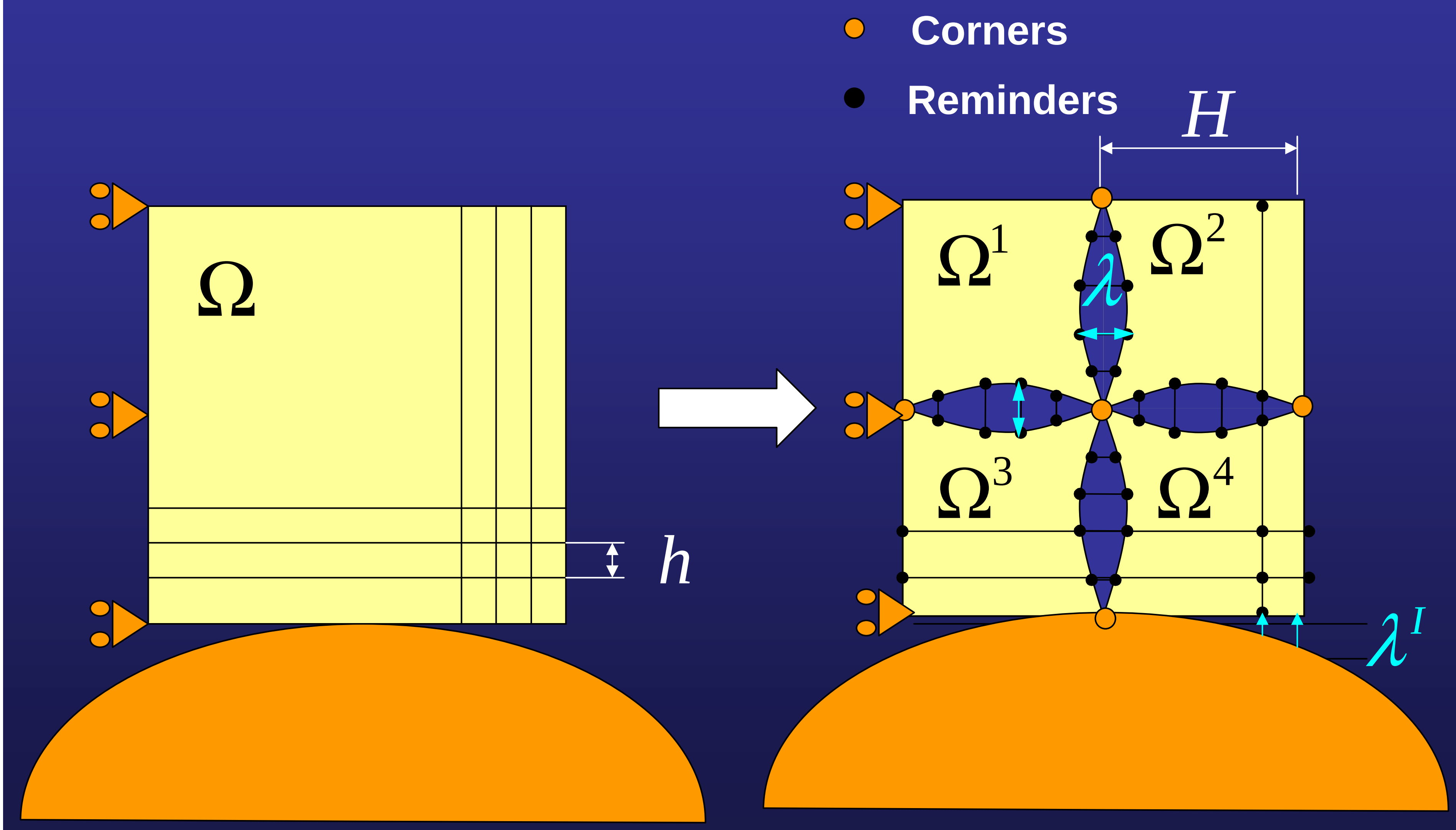


Z.D., D. Horak, R. Kucera, Comm. Num. Meth. Engng. 2006, G. Of 2006

Total BETI domain decomposition



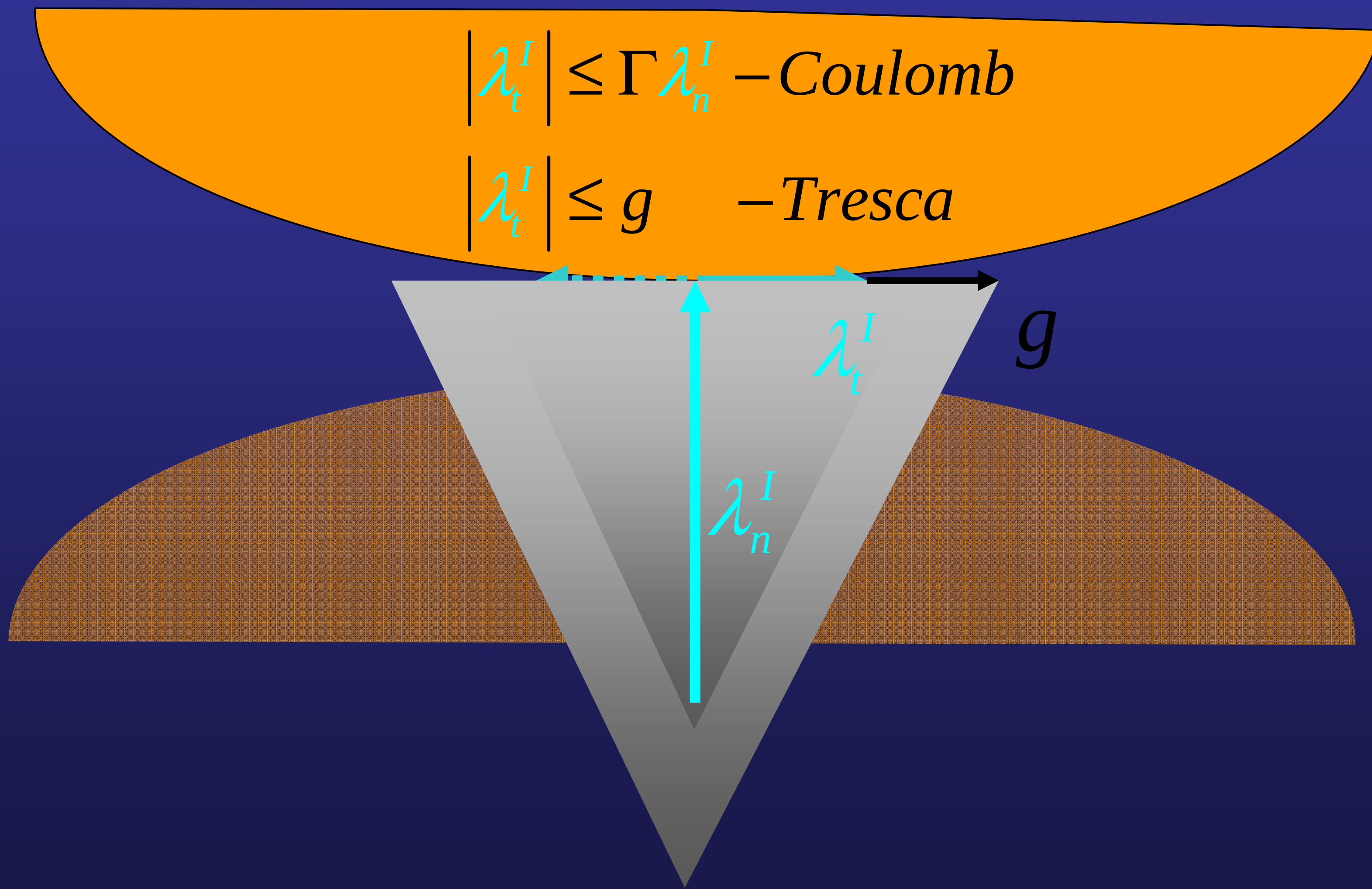
FETI-DP domain decomposition



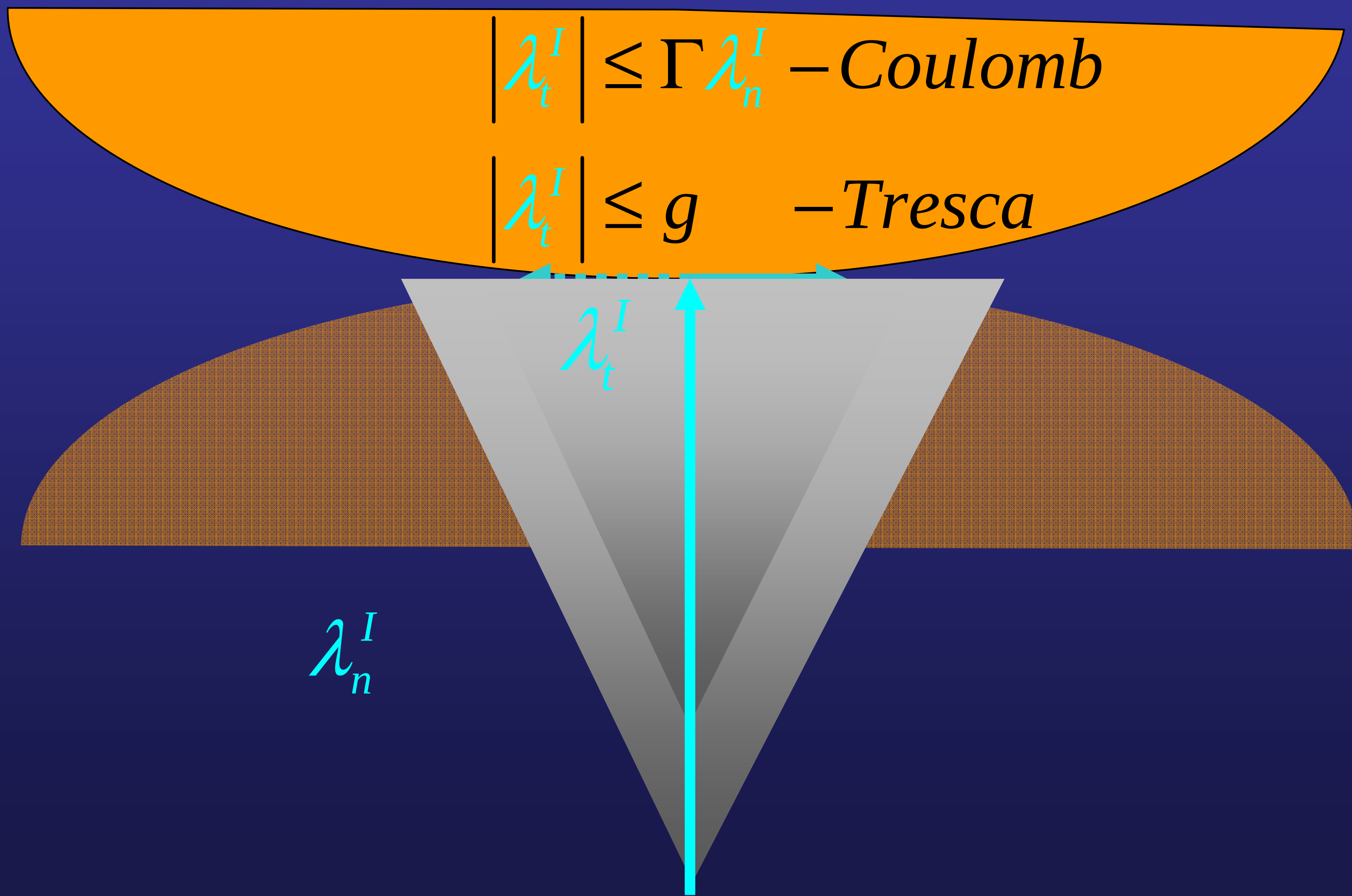
Coulomb and given (Tresca) friction

$$\left|\lambda_t^I\right| \le \Gamma \lambda_n^I \quad -Coulomb$$

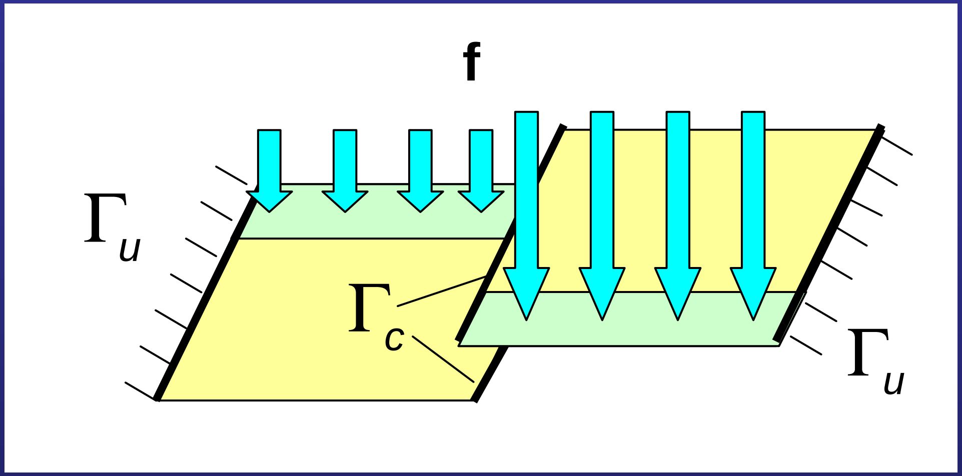
$$\left|\lambda_t^I\right| \le g \quad -Tresca$$

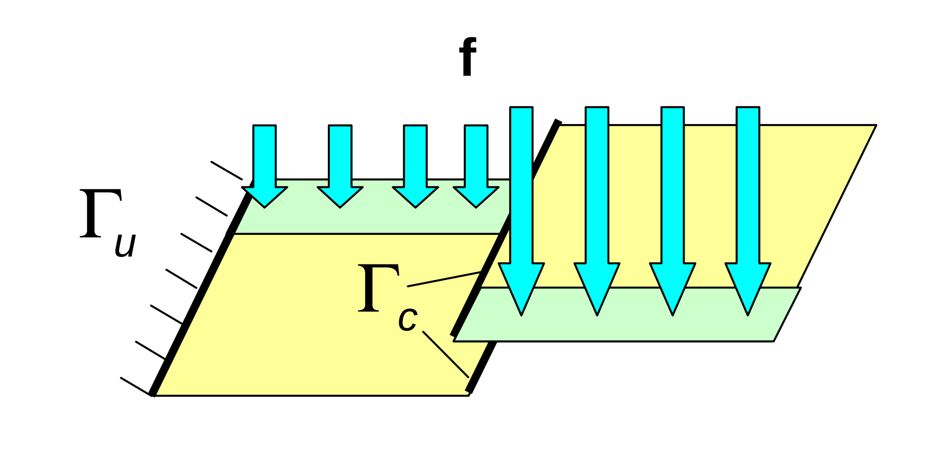


Coulomb and given (Tresca) friction



Model problems





Primal variational formulation

(P) *Find* $\min J(\mathbf{v})$ *for* $\mathbf{v} \in K$

$$J(v) = \tfrac{1}{2} a(\mathbf{v},\mathbf{v}) - l(\mathbf{v})$$ **energy**

$$a : \mathrm{V} \times \mathrm{V} \to \mathbb{R}, \qquad l : \mathrm{V} \to \mathbb{R}$$

$$\mathrm{V} = V^1 \times V^2 \times \ldots \times V^s$$

$$V^i = \left\{ v \in H^1(\Omega^i) : v = 0 \ \ on \ \ \Gamma^i \cap \Gamma_u \right\}$$

$$K^E = \left\{ \mathbf{v} \in \mathrm{V} : v^i = v^k \ \ on \ \ \Gamma^i \cap \Gamma^k \right\}$$ **gluing**

$$K^I = \left\{ \mathbf{v} \in \mathrm{V} : (n^k, v^i - v^k) \le g \ \ on \ \ \Gamma^i \cap \Gamma^k \cap \Gamma_c \right\}$$ **non-penetration**

$K = K^E \cap K^I$ closed convex

Stiffness matrices

FETI1:

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}^1 & & \\ & \ddots & \\ & & \mathbf{K}^s \end{bmatrix}, \quad \mathbf{K}^i \text{ - definite or semidefinite,} \qquad \mathbf{f} = \begin{bmatrix} \mathbf{f}^1 \\ \vdots \\ \mathbf{f}^s \end{bmatrix}$$

Total FETI:

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}^1 & & \\ & \ddots & \\ & & \mathbf{K}^s \end{bmatrix}, \quad \mathbf{K}^i \text{ - semidefinite, same kernels} \qquad \mathbf{f} = \begin{bmatrix} \mathbf{f}^1 \\ \vdots \\ \mathbf{f}^s \end{bmatrix}$$

FETI-DP:

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}^1 & & \mathbf{O} & \mathbf{K}^{1c} \\ & \ddots & & \vdots \\ \mathbf{O} & & \mathbf{K}^s & \mathbf{K}^{sc} \\ \mathbf{K}^{c1} & \cdots & \mathbf{K}^{cs} & \mathbf{K}^{cc} \end{bmatrix}, \quad \mathbf{K}^i \text{ - positive definite,} \qquad \mathbf{f} = \begin{bmatrix} \mathbf{f}^1 \\ \vdots \\ \mathbf{f}^s \\ \mathbf{f}^c \end{bmatrix}$$

(first columns: reminders; last column: corners)

Discretized primal problem

$J_h(\mathbf{u}) = \mathbf{u}^T\mathbf{K}\mathbf{u} - \mathbf{f}^T\mathbf{u}$ convex and coercive

"gluing" $u_i - u_k = 0 \Leftrightarrow [\cdots \overset{i}{1} \cdots -\overset{k}{1} \cdots]\begin{bmatrix} \vdots \\ u_i \\ \vdots \\ u_k \\ \vdots \end{bmatrix} = 0 \Rightarrow \mathbf{B}^E\mathbf{u} = \mathbf{o},$

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

$K_h \equiv \left\{ \mathbf{u} : \mathbf{B}^E\mathbf{u} = \mathbf{o} \ \ and \ \ \mathbf{B}^I\mathbf{u} \le \mathbf{g} \right\}$

(P_h) *Find* $\min \ J_h(\mathbf{v})$ *for* $\mathbf{v} \in K_h$

Mixed (saddle point) formulation

$$L_h(\mathbf{u},\lambda) = \tfrac{1}{2}\mathbf{u}^T\mathbf{K}\mathbf{u} - \mathbf{u}^T\mathbf{f} + \lambda_I^T\mathbf{B}^I\mathbf{u} + \lambda_E^T\mathbf{B}^E\mathbf{u} = J_h(\mathbf{u}) + \mathbf{u}^T\mathbf{B}^T\lambda$$

$$\mathbf{B} = \begin{bmatrix} \mathbf{B}^I \\ \mathbf{B}^E \end{bmatrix}, \quad \lambda = \begin{bmatrix} \lambda^I \\ \lambda^E \end{bmatrix}, \quad \lambda^I \geq 0$$

$$(\mathrm{SP}_h) \quad \textit{Find} \quad \min_{\mathbf{u}} \max_{\lambda^I \geq 0} L_h(\mathbf{u},\lambda) = \max_{\lambda^I \geq 0} \min_{\mathbf{u}} L_h(\mathbf{u},\lambda)$$

Drawback : 2 sets of variables

Dual formulation (1): coercive FETI-DP

Convexity of $L(\,.\,,\lambda)$ and gradient argument:

$$\mathbf{Kx} - \mathbf{f} + \mathbf{B}^T\lambda = \mathbf{o}$$

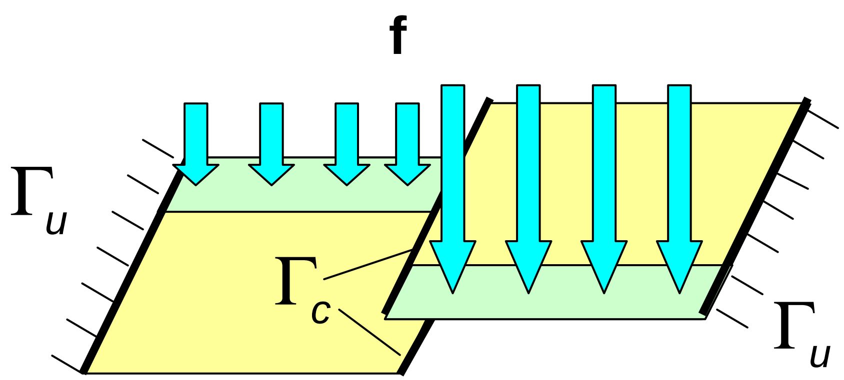
$$\mathbf{x} = \mathbf{K}^{-1}(\mathbf{f} - \mathbf{B}^T\lambda)$$

$(\mathrm{D_C})$ *Find* min $\lambda^T\mathbf{BK}^{-1}\mathbf{B}^T\lambda - \lambda^T\left(\mathbf{BK}^{-1}\mathbf{f} - \hat{\mathbf{c}}\right)$

for $\lambda^I \geq \mathbf{o}$

Optimal estimates for coercive FETI-DP - model problem (nodal/normalized mortar multipliers)

Theorem: The following bounds for $\mathbf{F} = \mathbf{B}\mathbf{K}^{-1}\mathbf{B}^T$ hold:



$$C_1 \le \lambda_{\min}(\mathbf{F}) \le \lambda_{\max}(\mathbf{F}) \le C_2 \left(\frac{H}{h}\right)^2$$

Z.D., D.Horák, D.Stefanica IMA J. Numer. Anal. 2005

Dual formulation (2): semicoercive FETI-DP coercive/semicoercive FETI1 and Total FETI

Convexity of $L(\,.\,,\lambda)$ and gradient argument:

$$\mathbf{Kx} - \mathbf{f} + \mathbf{B}^T\lambda = \mathbf{o}$$

$\mathbf{R}$ full rank matrix, $\operatorname{Im}\mathbf{R} = \operatorname{Ker}\mathbf{K}$

Solvable for $\mathbf{f} - \mathbf{B}^T\lambda \in \operatorname{Im}\mathbf{K} \Leftrightarrow \mathbf{R}^T\left(\mathbf{f} - \mathbf{B}^T\lambda\right) = \mathbf{o}$

$\mathbf{K}^+$ generalized inverse $\mathbf{K}\mathbf{K}^+\mathbf{K} = \mathbf{K}$, $\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^T & \mathbf{C} \end{bmatrix}^+ = \begin{bmatrix} \mathbf{A}^{-1} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix}$

$$(\mathrm{D}_{SC})\ \textit{Find}\ \min\ \lambda^T\mathbf{B}\mathbf{K}^+\mathbf{B}^T\lambda - \lambda^T\left(\mathbf{B}\mathbf{K}^+\mathbf{f} - \hat{\mathbf{c}}\right)$$

$$\textit{for}\quad \lambda^I \geq \mathbf{o},\ \ \mathbf{R}^T\left(\mathbf{f} - \mathbf{B}^T\lambda\right) = \mathbf{o}$$

FETI notation and homogenization

Notation :

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

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

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

$$\textit{subject to} \quad \lambda_{I} \geq 0 \quad \textit{and} \quad \mathbf{G}\lambda = \mathbf{e}$$

Homogenization :

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

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

$$\lambda \geq \mathbf{o} \quad \Leftrightarrow \quad \mu \geq -\hat{\lambda}$$

$$(\text{FETI}) \quad \tfrac{1}{2}\lambda^{T}\mathbf{F}\lambda - \lambda^{T}\mathbf{d} \rightarrow \min$$

$$\textit{subject to} \quad \lambda_{I} \geq -\hat{\lambda}_{I} \quad \textit{and} \quad \mathbf{G}\lambda = \mathbf{o}$$

Natural coarse grid projectors (semicoercive FETI-DP, FETI1, total FETI) and penalty approximation

Natural coarse grid projectors :

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

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

$$(\text{FETI-NCG}): \ \tfrac{1}{2}\lambda^T\mathbf{PFP}\lambda - \lambda^T\mathbf{Pd} \rightarrow \min$$

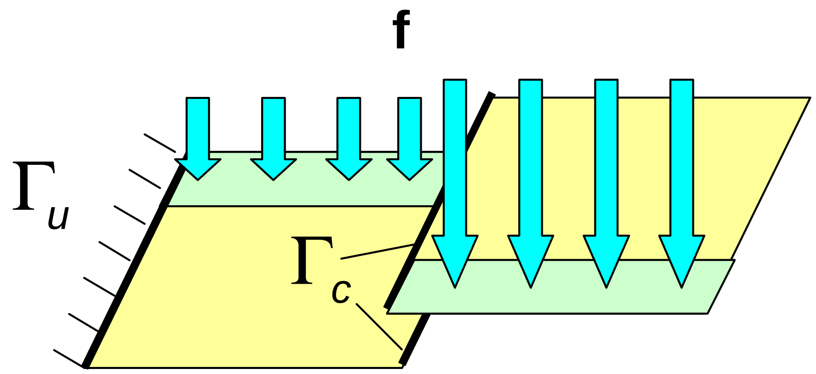
$$\textit{subject to} \ \ \lambda_I \geq -\hat{\lambda}_I \ \ \textit{and} \ \ \mathbf{G}\lambda = \mathbf{o}$$

$$(\text{FETI-NCG}_\rho): \ \tfrac{1}{2}\lambda^T(\mathbf{PFP} + \rho\mathbf{Q})\lambda - \lambda^T\mathbf{Pd} \rightarrow \min$$

$$\textit{subject to} \ \ \lambda_I \geq -\hat{\lambda}_I$$

Optimal estimates for semicoercive FETI-DP – model problem

Theorem : The following bounds for $\mathbf{F}$ hold :



$$C_1 \le \lambda_{\min}(\mathbf{F} \,|\, \mathrm{Im}\,\mathbf{F}) \le \lambda_{\max}(\mathbf{F}) \le C_2 \left(\frac{H}{h}\right)^2$$

Proof in Z.D., D.Horak, D.Stefanica 2005

Optimal estimates for FETI1, TFETI and BETI (D2, D3)

Theorem: The following bounds for $\mathbf{F}$ hold:

$$C_1 \leq \lambda_{\min}(\mathbf{F} \mid \operatorname{Im}\mathbf{F})$$

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

$$\kappa(\mathbf{F} \mid \operatorname{Im}\mathbf{F}) \leq C_3 \frac{H}{h}$$

Proof in C.Farhat, J.Mandel and F.-X.Roux CMAME 1994

BETI J.Bouchala, Z.D., M.Sadowska in preparation

Optimality of dual penalty for FETI1, semicoercive FETI-DP and Total FETI

Theorem: **For** $H/h \le C_1$

$$\left\|\mathbf{G}\lambda_\rho^{H,h}\right\| \le C_2 \frac{1+\varepsilon}{\sqrt{\rho}}\left\|\mathbf{Pd}\right\|$$

Moreover,

$$\left\|\mathbf{G}\lambda_\rho^{H,h}\right\| \le C_2(H,h)\frac{1+\varepsilon}{\rho}\left\|\mathbf{Pd}\right\|$$

Proof in Z.D. and D. Horak Num.Lin.Alg.Appl. 2004 (coercive) and Contemporary Math. 2004 (semicoercive)

$\left\|\mathbf{G}\lambda\right\| / \left\|\mathbf{Pd}\right\|$ for varying ρ and H/h

ρ	1152/591	139392/7551	2130048/29823
1	1.32e-1	1.20e-1	1.12e-1
1000	1.40e-3	1.28e-3	1.19e-3
100 000	1.40e-5	1.28e-5	1.19e-5

Primal formulation of problems with given (Tresca) friction

(P) *Find* $\min J(\mathbf{v})$ *for* $\mathbf{v} \in K$

$$J(v) = \tfrac{1}{2} a(\mathbf{v},\mathbf{v}) - l(\mathbf{v}) + j(\mathbf{v})$$

$$a: \mathrm{V} \times \mathrm{V} \to \mathbb{R}, \qquad l, j: \mathrm{V} \to \mathbb{R} \qquad \mathrm{V} = \mathrm{V}^1 \times \mathrm{V}^2 \times \ldots \times \mathrm{V}^s$$

$$j(\mathbf{v}) = \int_{\Gamma_c} g \left| \mathbf{v}_t \right| d\Gamma$$

$$\mathrm{V}^i = \left\{ \mathbf{v} \in H^1\left(\Omega^i\right) : \mathbf{v} = \mathbf{o} \ \ on \ \ \Gamma^i \cap \Gamma_u \right\}$$

$$K^E = \left\{ \mathbf{v} \in \mathrm{V} : \mathbf{v}^i = \mathbf{v}^k \ \ on \ \ \Gamma^i \cap \Gamma^k \right\}$$ **gluing**

$$K^I = \left\{ \mathbf{v} \in \mathrm{V} : (\mathbf{n}^k, \mathbf{v}^i - \mathbf{v}^k) \le \mathbf{g} \ \ on \ \ \Gamma^i \cap \Gamma^k \cap \Gamma_c \right\}$$ **non-penetration**

$K = K^E \cap K^I$ closed convex

Discretized primal problem

$$J_h(\mathbf{u}) = \mathbf{u}^T\mathbf{K}\mathbf{u} - \mathbf{f}^T\mathbf{u} + j_h(\mathbf{u})$$

$$j_h(\mathbf{u}) = g\mathbf{e}^T|\mathbf{u}|, \mathbf{u} = [|u_1|,\ldots,|u_1|], \quad \mathbf{e} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$ non-differentiable

"gluing" $\Rightarrow \mathbf{B}^E\mathbf{u} = \mathbf{o}$

non-penetration $\Rightarrow \mathbf{B}^I\mathbf{u} \leq \mathbf{g}$

$$K_h \equiv \left\{ \mathbf{u} : \mathbf{B}^E\mathbf{u} = \mathbf{o} \quad \textit{and} \quad \mathbf{B}^I\mathbf{u} \leq \mathbf{g} \right\}$$

$$(\mathrm{P}_h) \quad \textit{Find} \quad \min \; J_h(\mathbf{v}) \quad \textit{for} \quad \mathbf{v} \in K_h$$

A simple observation (2D)

$$g\left|u\right| = \max\{\lambda u : \lambda \in [-g, g]\}$$

$$\Downarrow$$

$$J(v) = \tfrac{1}{2}a\left(\mathbf{v},\mathbf{v}\right) - l\left(\mathbf{v}\right) + \max_{-g \le \lambda \le g} \boldsymbol{\lambda}^T \mathbf{v}$$

Mixed (saddle point) formulation

$$L_h(\mathbf{u},\lambda) = \tfrac{1}{2}\mathbf{u}^T\mathbf{K}\mathbf{u} - \mathbf{u}^T\mathbf{f} + \lambda_{IN}^T(\mathbf{B}^{IN}\mathbf{u} - \mathbf{g}_N) + \lambda_{IT}^T\mathbf{B}^{IT}\mathbf{u} + \lambda_E^T\mathbf{B}^E\mathbf{u}$$

$$\mathbf{B} = \begin{bmatrix}\mathbf{B}^{IN}\\ \mathbf{B}^{IT}\\ \mathbf{B}^{E}\end{bmatrix}, \quad \lambda = \begin{bmatrix}\lambda_{IN}\\ \lambda_{IT}\\ \lambda_{E}\end{bmatrix}, \quad \begin{matrix}\lambda_{IN} \ge \mathbf{o},\\ -\mathbf{g}_T \le \lambda_{IT} \le \mathbf{g}_T,\end{matrix} \quad \lambda_I = \begin{bmatrix}\lambda_{IN}\\ \lambda_{IT}\end{bmatrix}$$

$$(\mathrm{SP}_h)\quad \textit{Find}\quad \min_{\mathbf{u}}\ \max_{\lambda_I \in \Omega} L_h(\mathbf{u},\lambda) = \max_{\lambda_I \in \Omega}\ \min_{\mathbf{u}} L_h(\mathbf{u},\lambda)$$

Drawback : 2 sets of variables

Dual formulation (3): coercive/semicoercive FETI1 and Total FETI with given friction 2D

Convexity of $L(\ .\ ,\lambda)$ and gradient argument:

$$\mathbf{Kx} - \mathbf{f} + \mathbf{B}^T\lambda = \mathbf{o}$$

$\mathbf{R}$ full rank matrix, $\operatorname{Im}\mathbf{R} = \operatorname{Ker}\mathbf{K}$

Solvable for $\mathbf{f} - \mathbf{B}^T\lambda \in \operatorname{Im}\mathbf{K} \Leftrightarrow \mathbf{R}^T\left(\mathbf{f} - \mathbf{B}^T\lambda\right) = \mathbf{o}$

$\mathbf{K}^+$ generalized inverse $\mathbf{K}\mathbf{K}^+\mathbf{K} = \mathbf{K}$, $\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^T & \mathbf{C} \end{bmatrix}^+ = \begin{bmatrix} \mathbf{A}^{-1} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix}$

$(\mathrm{D_{TF}})$ *Find* $\min\ \lambda^T\mathbf{B}\mathbf{K}^+\mathbf{B}^T\lambda - \lambda^T\left(\mathbf{B}\mathbf{K}^+\mathbf{f} - \hat{\mathbf{c}}\right)$

for $\lambda_{IN} \geq 0,\ -\mathbf{g}_T \leq \lambda_{IT} \leq \mathbf{g}_T,\ \mathbf{R}^T\left(\mathbf{f} - \mathbf{B}^T\lambda\right) = \mathbf{o}$

FETI notation and homogenization

Notation :

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

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

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

subject to $\lambda_{IN} \geq 0, -\mathbf{g}_{T} \leq \lambda_{IT} \leq \mathbf{g}_{T}$ *and* $\mathbf{G}\lambda = \mathbf{e}$

Homogenization :

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

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

$$\lambda \geq \mathbf{o} \quad \Leftrightarrow \quad \mu \geq -\hat{\lambda}$$

$$(\mathrm{FETI}) \quad \tfrac{1}{2}\lambda^{T}\mathbf{F}\lambda - \lambda^{T}\mathbf{d} \rightarrow \min$$

subject to $\lambda_{IN} \geq \mathbf{g}_{N}$ $-\mathbf{g}_{T} \leq \lambda_{IT} \leq \mathbf{g}_{T}$ *and* $\mathbf{G}\lambda = \mathbf{o}$

Natural coarse grid projectors (semicoercive FETI-DP, FETI1, total FETI) and penalty approximation

Natural coarse grid projectors:

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

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

$$(\text{FETI-NCG-TF}): \ \tfrac{1}{2}\lambda^T\mathbf{PFP}\lambda - \lambda^T\mathbf{Pd} \to \min$$

$$\textit{subject to} \ \ \lambda_{IN} \ge \mathbf{g}_N, -\mathbf{g}_T \le \lambda_{IT} \le \mathbf{g}_T \ \ \textit{and} \ \ \mathbf{G}\lambda = \mathbf{o}$$

$$(\text{FETI-NCG}_\rho\text{-TF}): \ \tfrac{1}{2}\lambda^T(\mathbf{PFP} + \rho\mathbf{Q})\lambda - \lambda^T\mathbf{Pd} \to \min$$

$$\textit{subject to} \ \ \lambda_{IN} \ge \mathbf{g}_N, -\mathbf{g}_T \le \lambda_{IT} \le \mathbf{g}_T$$

Bound constrained problems

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

$$f_i(\mathbf{x}) = \tfrac{1}{2}\mathbf{x}^T \mathbf{A}_i \mathbf{x} - \mathbf{b}_i^T \mathbf{x}, \quad \Omega_i = \{\mathbf{x} : \mathbf{x} \geq \mathbf{c}_i\},$$

$$\mathbf{A}_i = \mathbf{A}_i^T, \quad \mathbf{x}^T \mathbf{A}_i \mathbf{x} > 0 \text{ for } \mathbf{x} \neq \mathbf{o}$$

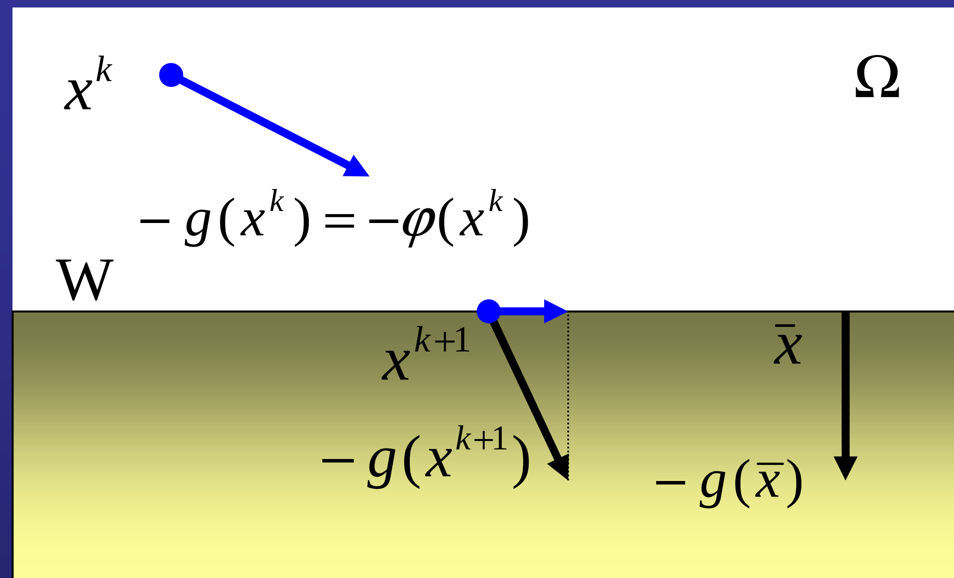
$$C_1 \|\mathbf{x}\|^2 \leq \mathbf{x}^T \mathbf{A}_i \mathbf{x} \leq C_2 \|\mathbf{x}\|^2 \quad \text{and} \quad \|\mathbf{c}_i^+\| \leq C_3$$

(QPB_i) Find: $\min_{\Omega_i} f_i(\mathbf{x})$

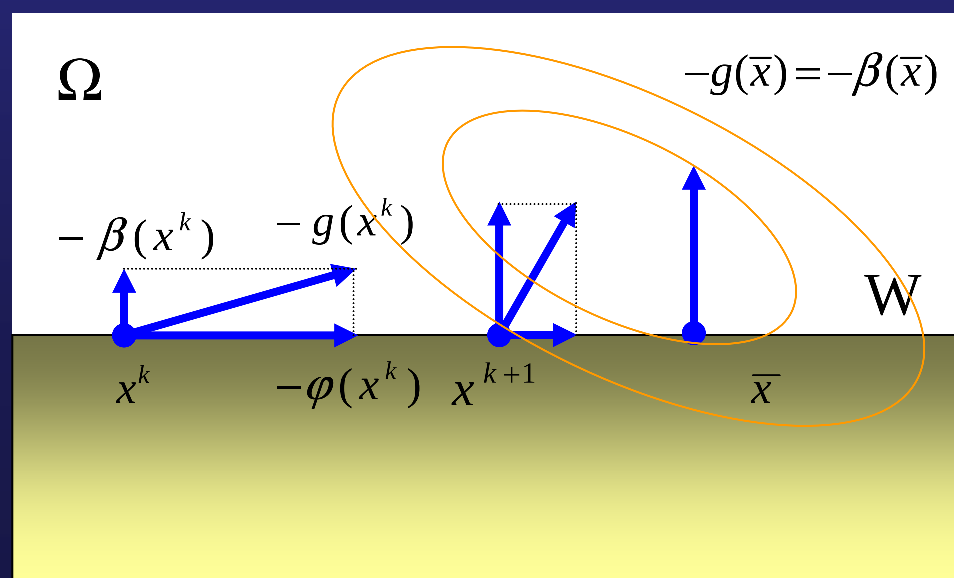
Goal: find approximate solution at *O(1)* iterations !!!

KKT conditions and active set method

KKT and minimization on the face with the solution:



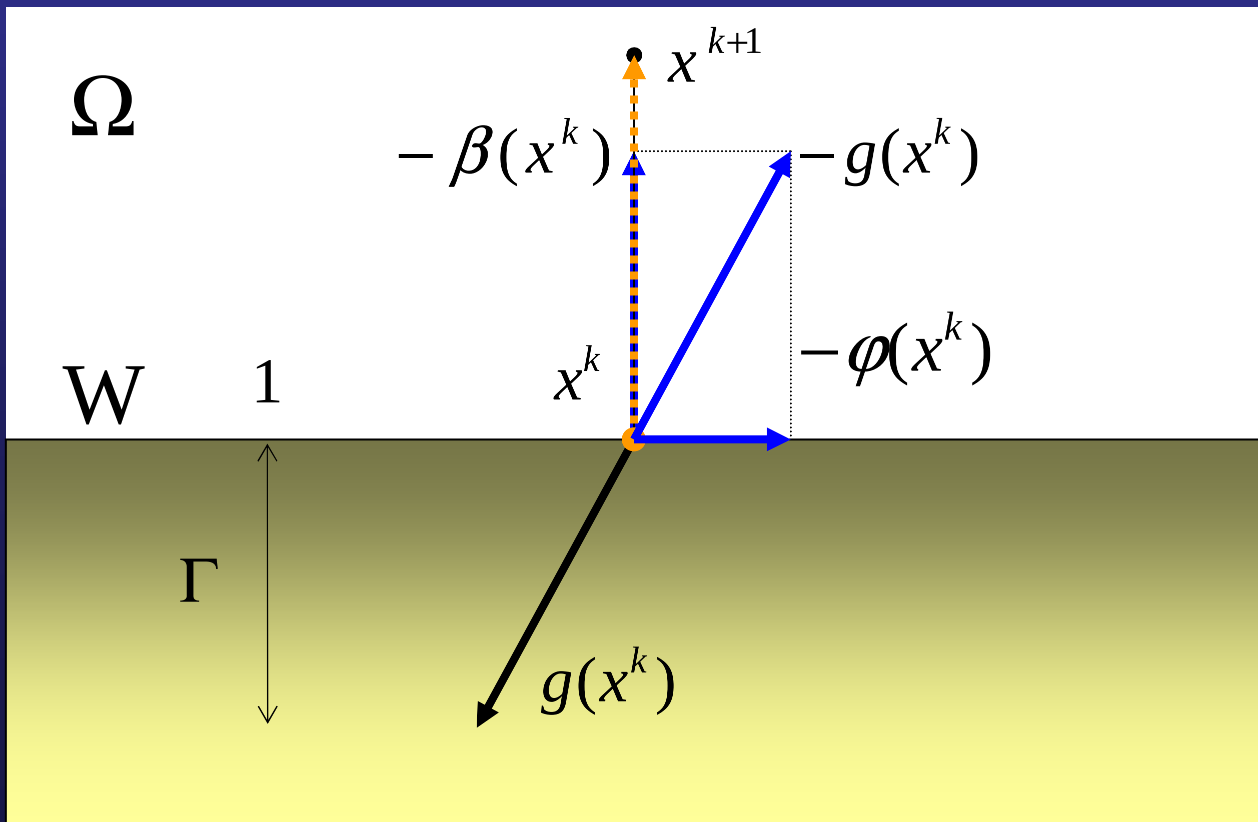
Typical minimization:



Proportioning

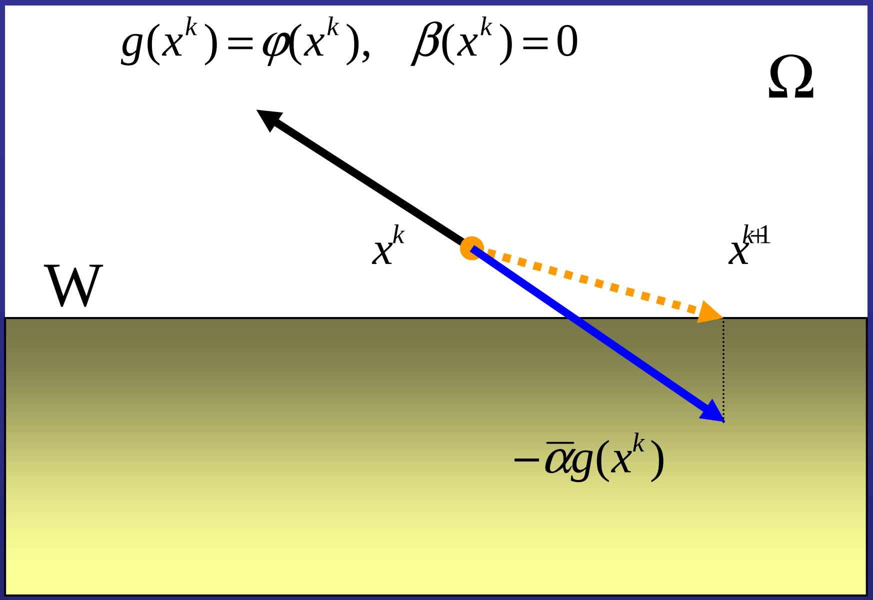
x **proportional:** $$\Gamma^2 \tilde{\varphi}^T(x)\varphi(x) \le \|\beta(x)\|^2$$

Reduction of the active set for non-proportional iterations

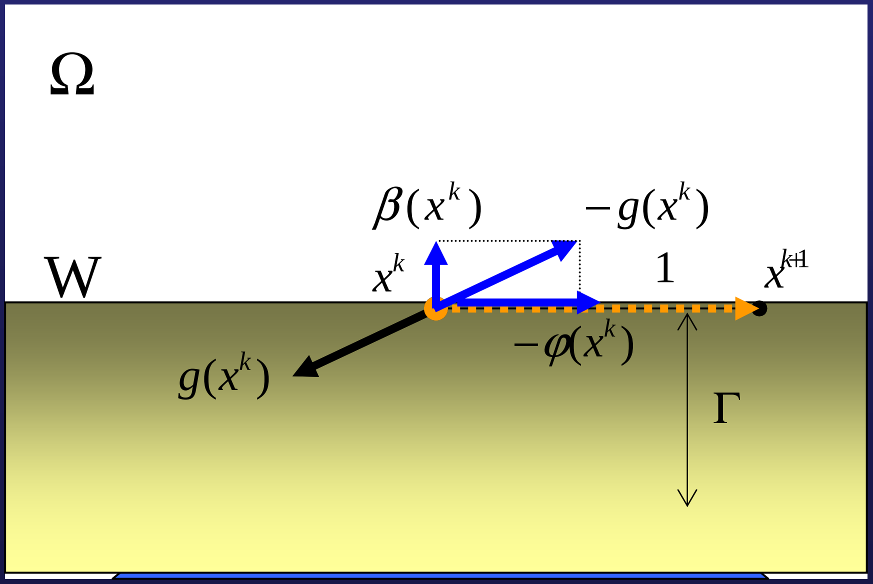


Proportional iterations

Projection step: expansion of the active set



Feasible conjugate gradient step:



Optimality of MPRGP

Theorem:

Let $\Gamma > 0, \hat{\Gamma} = \max\{\Gamma, \Gamma^{-1}\}$, $\bar{\mathbf{x}}_i$ solution of (QPB$_i$),

$\{\mathbf{x}_i^k\}$ generated with $\bar{\alpha} \in (0, C_2^{-1}]$ and $\mathbf{x}_i^0 = \max\{\mathbf{c}_i, \mathbf{o}\}$.

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

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

is found at

$$O(1) \quad \text{matrix-vector multiplications}$$

Z.D., J. Schoeberl, Comput. Opt. Appl. (2005), Z.D. (2004)

Optimality of FETI-DP for coercive model problem (frictionless/Tresca friction)

Theorem:

The solutions of the discretized coercive model problem with

$$H/h \leq C$$

to a given precision by SMALBE/MPRGP may be obtained at

$O(1)$ **matrix/vector multiplications**

frictionles Z.D., D. Horak, D.Stefanica IMA J. Num. Mat. 2005
Tresca friction (2D) in preparation

Bound and equality constrained problems

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

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

$$\Omega_i = \{\mathbf{x} : \mathbf{x} \ge \mathbf{c}_i \text{ and } \mathbf{D}_i \mathbf{x} = \mathbf{o}\}, \quad \|\mathbf{D}_i\| \le C_0$$

$$\mathbf{A}_i = \mathbf{A}_i^T, \ \mathbf{x}^T \mathbf{A}_i \mathbf{x} > 0 \text{ for } \mathbf{x} \ne \mathbf{o}$$

$$C_1 \|\mathbf{x}\|^2 \le \mathbf{x}^T \mathbf{A}_i \mathbf{x} \le C_2 \|\mathbf{x}\|^2 \quad \text{and} \quad \|\mathbf{c}_i^+\| \le C_3$$

(QPBE_i) Find: $\min_{\Omega_i} f_i(\mathbf{x})$

Goal: find approximate solution at *O(1)* iterations !!!

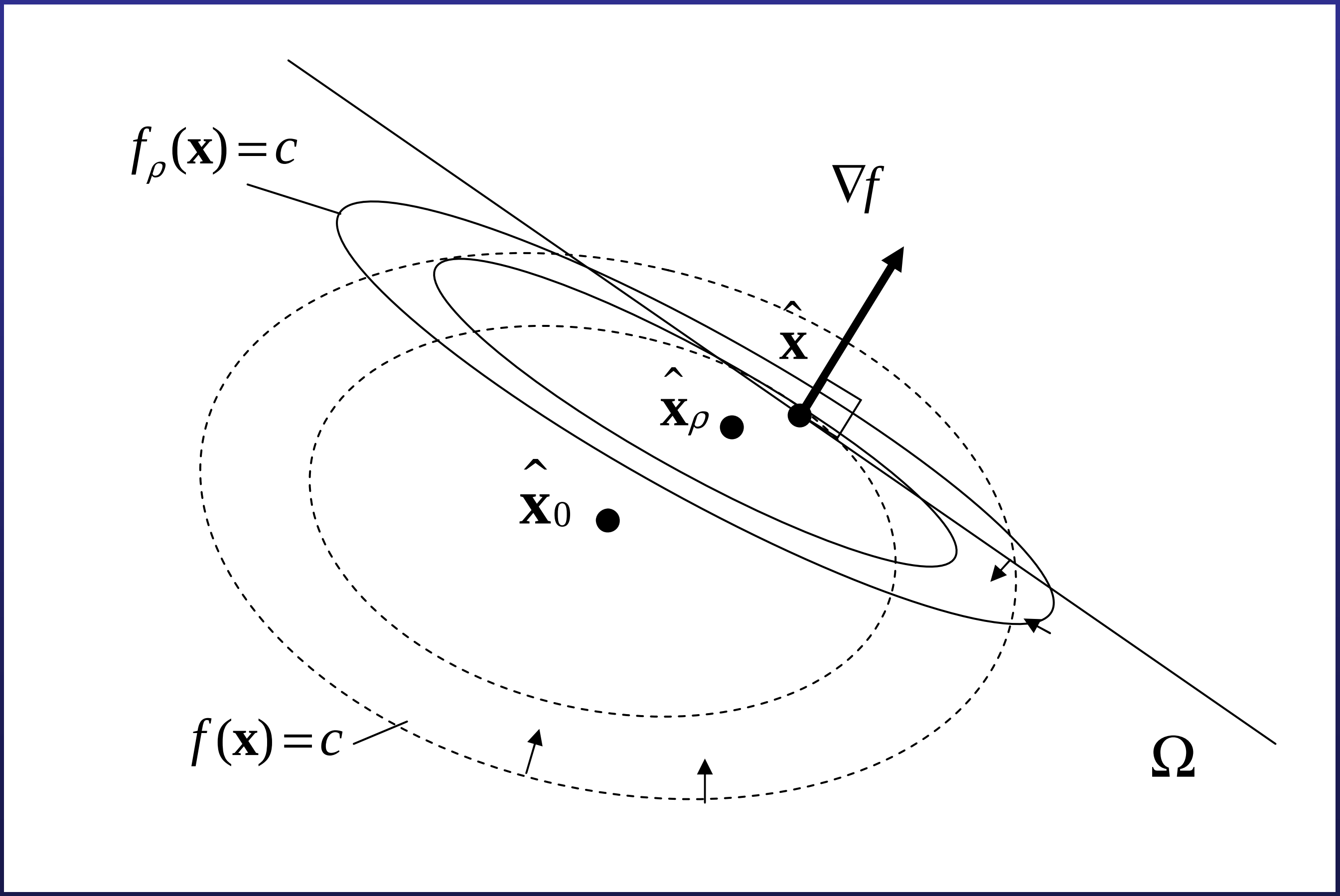
Augmented Lagrangian and projected gradient

$$L(\mathbf{x},\mu,\rho) = f(\mathbf{x}) + \mu^T \mathbf{Dx} + \frac{1}{2}\rho \left\|\mathbf{Dx}\right\|^2$$

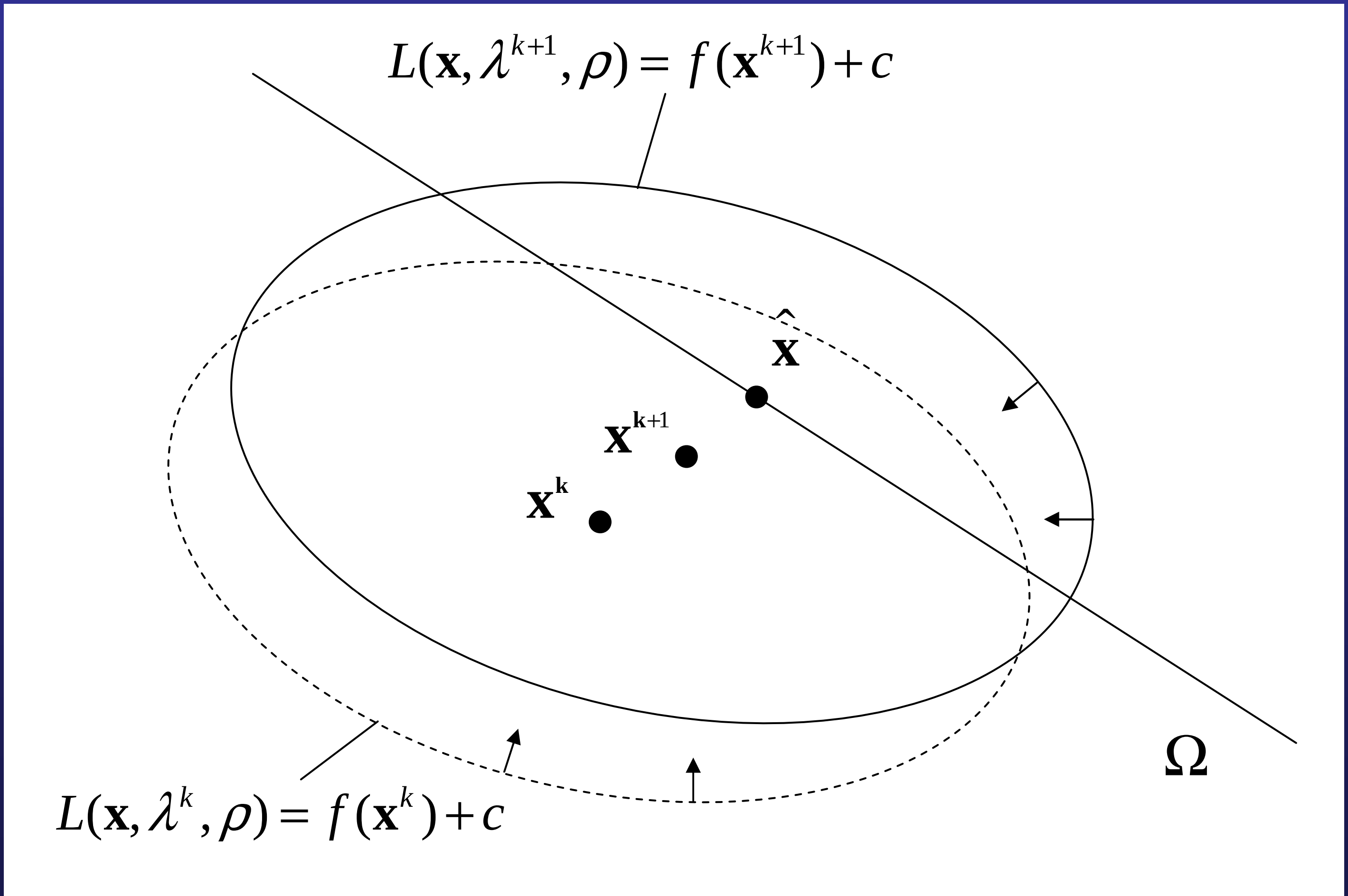
$$g(\mathbf{x},\mu,\rho) = \nabla_x L(\mathbf{x},\mu,\rho)$$

$$g^P = g^P(\mathbf{x},\mu,\rho) = \varphi(\mathbf{x},\mu,\rho) + \beta(\mathbf{x},\mu,\rho)$$

Effect of penalization



Modification of linear term (Lagrange multipliers)



Computational engine II: SMALBE (Semimonotonic augmented Lagrangians)

{Initialization}

Step 0 $1 < \beta, \rho_0 > 0, \eta > 0, M > 0, \mu^0$

{Approximate solution of bound constrained problem}

Step 1 Find $x^k \geq c$ such that $\left\| g^P\left(x^k, \mu^k, \rho_k\right)\right\| \leq \min\left\{M \left\|Dx^k\right\|, \eta\right\}$

{Test}

Step 2 If $\left\| g^P\left(x^k, \mu^k, \rho_k\right)\right\|$ and $\left\|Dx^k\right\|$ are small then x^k is solution

{Update Lagrange multipliers}

Step 3 $\mu^{k+1} = \mu^k + \rho_k\left(Dx^k\right)$

{Update penalty parameter}

Step 4 If $L\left(x^{k+1}, \mu^{k+1}, \rho_{k+1}\right) \leq L\left(x^k, \mu^k, \rho_k\right) + \frac{\rho_{k+1}}{2}\left\|Dx^{k+1}\right\|^2$

then $\rho_{k+1} = \beta \rho_k$

else $\rho_{k+1} = \rho_k$

{Repeat loop}

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

Basic relations for SMALBE

Theorem:

Let $\{\mathbf{x}^k\}, \{\mu^k\}$ and $\{\rho^k\}$ be generated with $\bar{\alpha} \in (0, \|\mathbf{A}\|^{-1}]$ and $\Gamma > 0$.

(i) If $\rho_k \geq M^2 / \lambda_{\min}(\mathbf{A})$ then

$$L(\mathbf{x}^{k+1}, \mu^{k+1}, \rho_{k+1}) \geq L(\mathbf{x}^k, \mu^k, \rho_k) + \frac{\rho_{k+1}}{2}\|\mathbf{D}\mathbf{x}^{k+1}\|^2$$

(ii) There is $C = C(C_1, C_2, \bar{\alpha}, \Gamma, M)$ such that

$$\sum_{k=1}^{\infty} \frac{\rho_k}{2}\|\mathbf{D}\,\mathbf{x}^k\|^2 \leq C$$

Z.D. SINUM (2005), Z.D. (2004)

Optimality of SMALBE

Corollary :

Let $\{\mathbf{x}_i^k\}, \{\mu\}$ and $\{\rho^k\}$ be generated with $\bar{\alpha} \in (0, \|\mathbf{A}_i\|^{-1}], \Gamma > 0.$

(i)

$$\rho_k \le \beta M^2 / \lambda_{\min}(\mathbf{A})$$

(ii) SMALBE generates $\mathbf{x}^k$ that satisfies

$$\|g^P(\mathbf{x}^k)\| \le \varepsilon \|\mathrm{b}_\mathrm{i}\| \quad \text{and} \quad \|\mathbf{D}_i \mathbf{x}^k\| \le \varepsilon \|\mathrm{b}_\mathrm{i}\|$$

at $O(1)$ outer iterations

(ii) SMALBE with MPRGP in inner loop generates x^k that satisfies

$$\|g^P(\mathbf{x}^k)\| \le \varepsilon \|\mathrm{b}_\mathrm{i}\| \quad \text{and} \quad \|\mathbf{D}_i \mathbf{x}^k\| \le \varepsilon \|\mathrm{b}\|$$

at $O(1)$ matrix-vector multiplications

Z.D. SINUM (2005), Z.D.(2004)

Computational engine II: SMALBE
Semimonotonic augmented Lagrangians

Theorem: $H/h \leq C \Rightarrow$ SMALBE *finds* $\bar{\lambda}, \mu$ *such that*

$$\mathbf{g}^P(\bar{\lambda}, \mu, 0) \leq \varepsilon \|\mathbf{b}_{H,h}\| \quad \text{and} \quad \|\mathbf{G}\bar{\lambda}_{H,h}\| \leq \varepsilon \|\mathbf{b}_{H,h}\|$$

in $O(1)$ iterations

Z.D., SINUM (2005)

Optimality of FETI/BETI for semicoercive/coercive problems (Tresca 2D, frictionless 2D/3D)

Theorem:

The solutions of the discretized model problem
with

$$H/h \leq C$$

to a given relative precision by SMALBE/MPRGP
may be obtained at

$O(1)$ **matrix/vector multiplications**

Z.D,D.Horak, submitted

J. Bouchala, Z.D., M.Sadowská, in preparation

Convergence of Lagrange multipliers

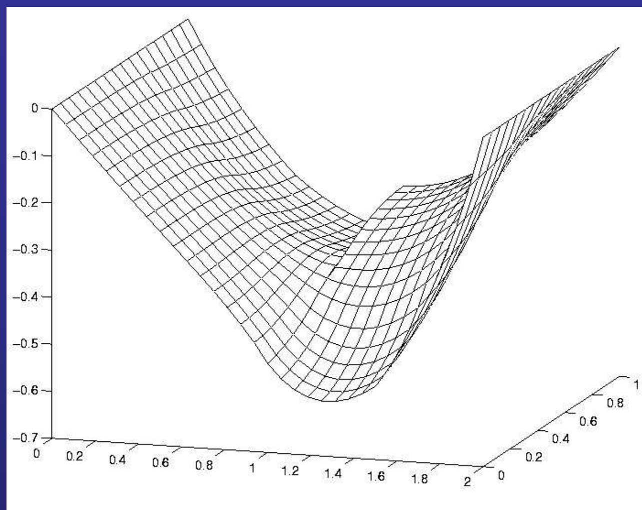
- Lagrange multipliers $\lambda^k \to \lambda_{LS}$ when

  $\lambda^0 \in \mathrm{Im}\,\mathbf{B}$ and λ_{LS} is range regular (i.e $\mathrm{Im}\,\mathbf{B}_{F(\lambda_{LS}),*} = \mathrm{Im}\,\mathbf{B}$)

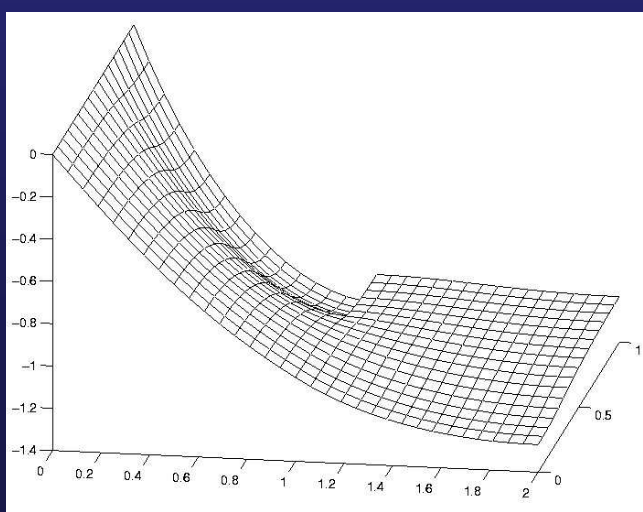
- Lagrange multipliers are unique when

  B is full row rank

FETI-DP: Numerical experiments for nodal Lagrange multipliers

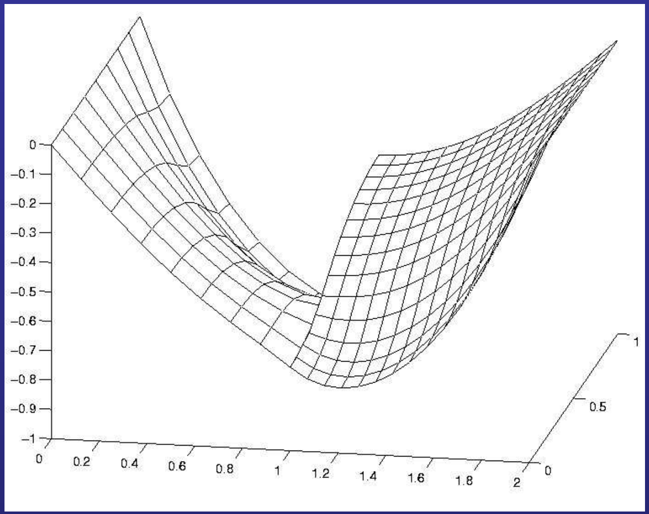


H	1/2	1/4	1/8
H/h=4	200/33/10 **17**	800/161/42 **21**	3200/705/154 **27**
H/h=8	648/73/10 **22**	2592/369/42 **36**	10365/1633/154 **38**
H/h=16	2312/153/10 **27**	9248/785/42 **48**	36992/3489/154 **51**

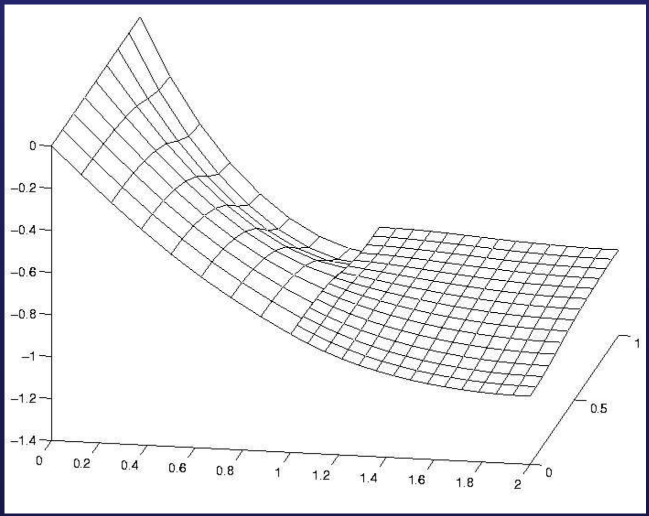


H	1/2	1/4	1/8
H/h=4	200/33/10 **24**	800/161/42 **24**	3200/705/154 **31**
H/h=8	648/73/10 **27**	2592/369/42 **39**	10365/1633/154 **46**
H/h=16	2312/153/10 **41**	9248/785/42 **57**	36992/3489/154 **63**

FETI-DP: Numerical experiments for mortars (orthogonalized constraints)

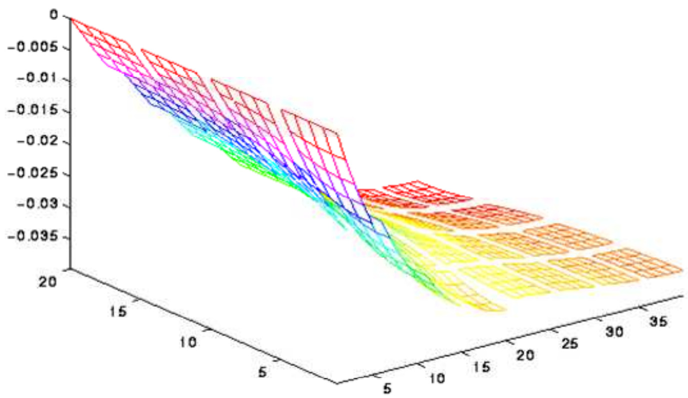


N_1 N_2	1x2 1x3	2x4 2x5	4x8 4x11
$H_1/h_1=4$	242/23/6	840/122/25	3616/620/97
$H_2/h_2=7$	**15**	**34**	**49**
$H_1/h_1=8$	750/47/6	2608/256/25	11216/1298/97
$H_2/h_2=13$	**29**	**49**	**59**
$H_1/h_1=16$	2606/95/6	9072/524/25	38992/2654/97
$H_2/h_2=25$	**33**	**57**	**78**

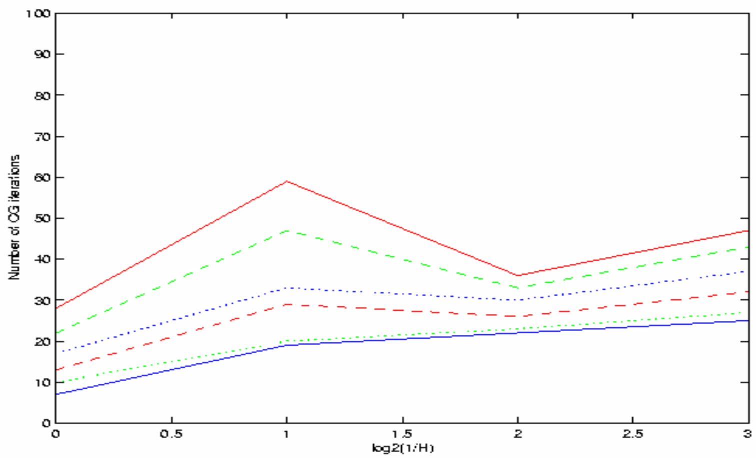


N_1 N_2	1x2 1x3	2x4 2x5	4x8 4x11
$H_1/h_1=4$	242/23/6	840/122/25	3616/620/97
$H_2/h_2=7$	**20**	**37**	**52**
$H_1/h_1=8$	750/47/6	2608/256/25	11216/1298/97
$H_2/h_2=13$	**36**	**56**	**70**
$H_1/h_1=16$	2606/95/6	9072/524/25	38992/2654/97
$H_2/h_2=25$	**39**	**65**	**84**

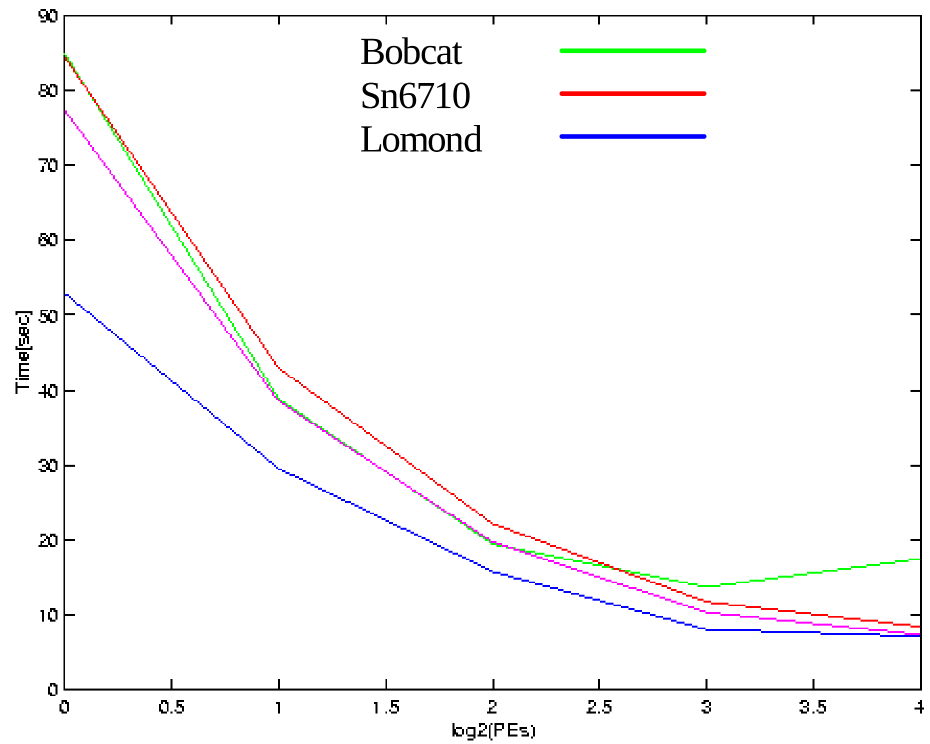
Solution and numerical scalability of FETI for *n* ranging from 50 to 2 130 048 (C/PETSc)



H	1/2	1/4	1/8
H/h=8	648/87 **20**	2592/447 **23**	10365/1983 **27**
H/h=32	8712/327 **33**	34848/1695 **30**	139392/7551 **37**
H/h=128	133128/1287 **59**	532512/6687 **36**	2130048/29823 **47**



Numerical scalability



$h = 1/256, \quad H = 1/4,$

primal dimension 135 200, dual dimension 3359

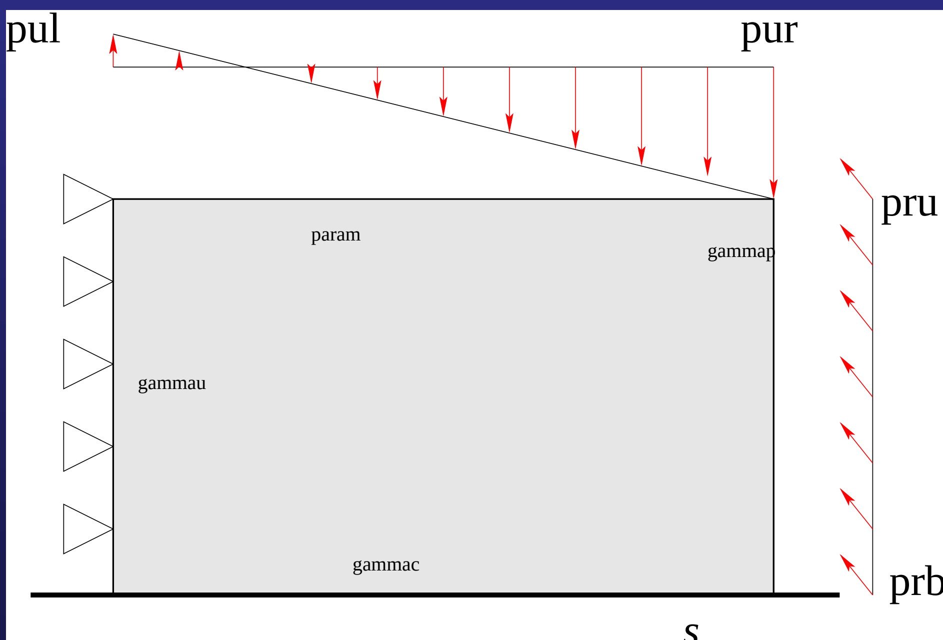
2 outer iterations, 33 cg iterations

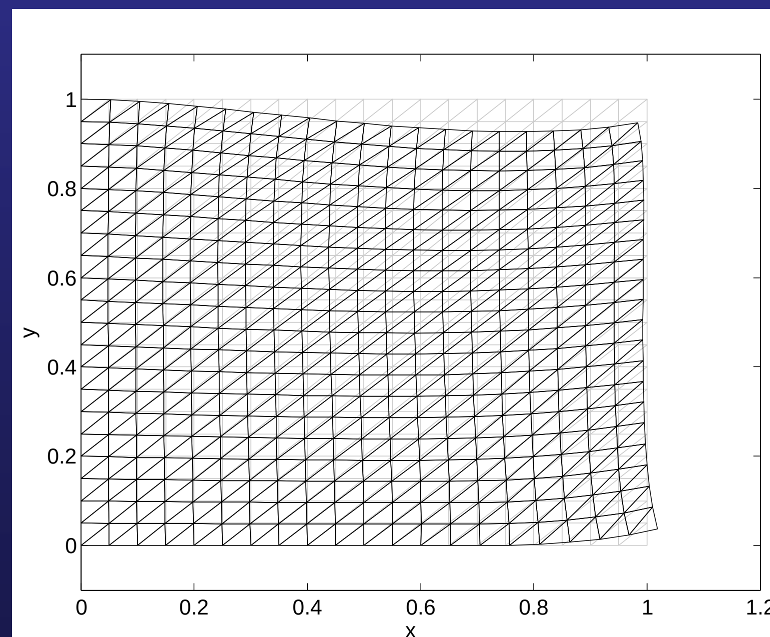
Best results for FETI with SMALBE

primal dimension	**2 130 048**	**8 454 272**
dual dimension	29 823	59 519
number of subdomains	128	128
number od SGI-Origin processors	32	64
number of outer iterations	2	2
number of cg iterations	**47**	**65**
time [sec]	**167**	**1281**

Benchmark for 2D Tresca friction

$$E = 21.19$$
$$\nu = 0.277$$
$$tol = 1e-5$$

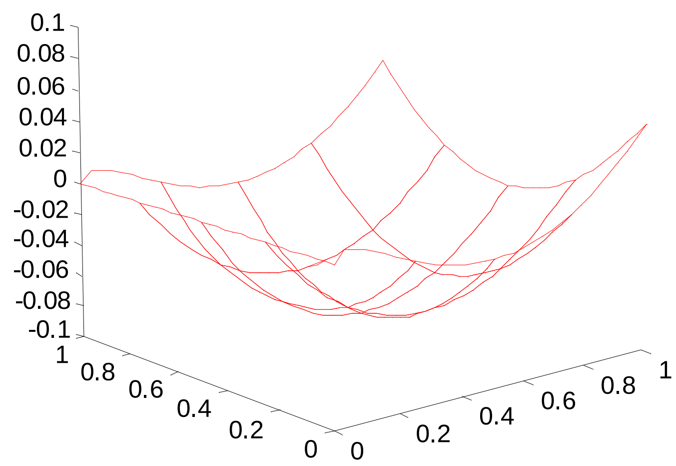




FETI-DP 2D contact problem frictionless and with given (Tresca) friction

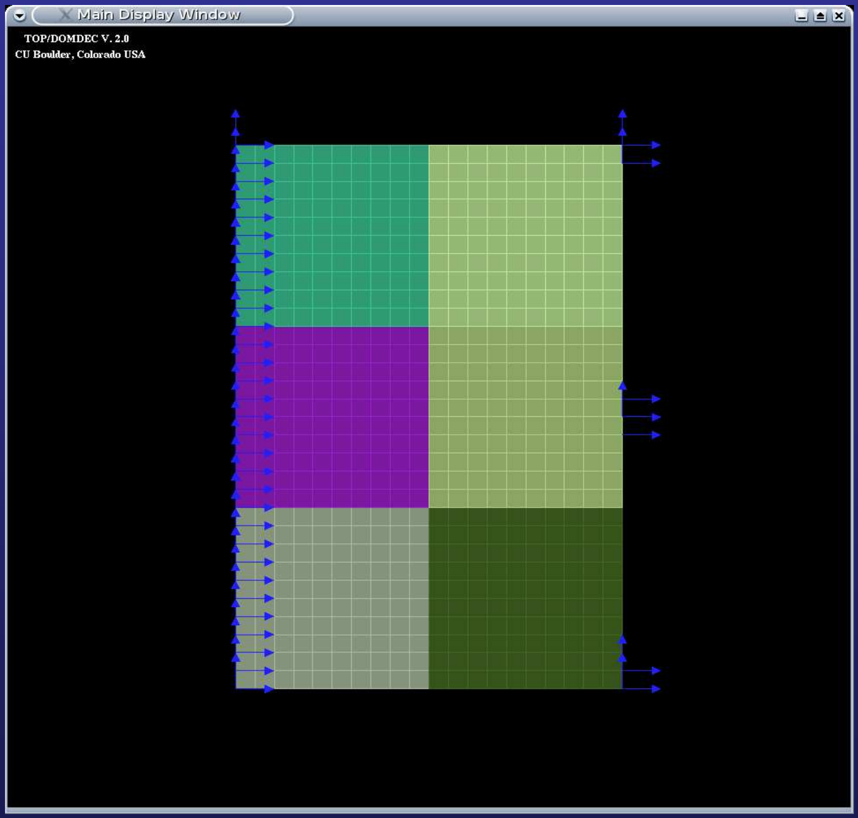
subdomains	Primal dimension	Dual dimension	Iterations frictionless	Iterations Tresca
16	3872	512	50	63
64	15488	2176	62	87
144	34846	4992	77	130
256	61952	8960	81	129
400	96800	14080	101	175
900	217800	31920	107	187

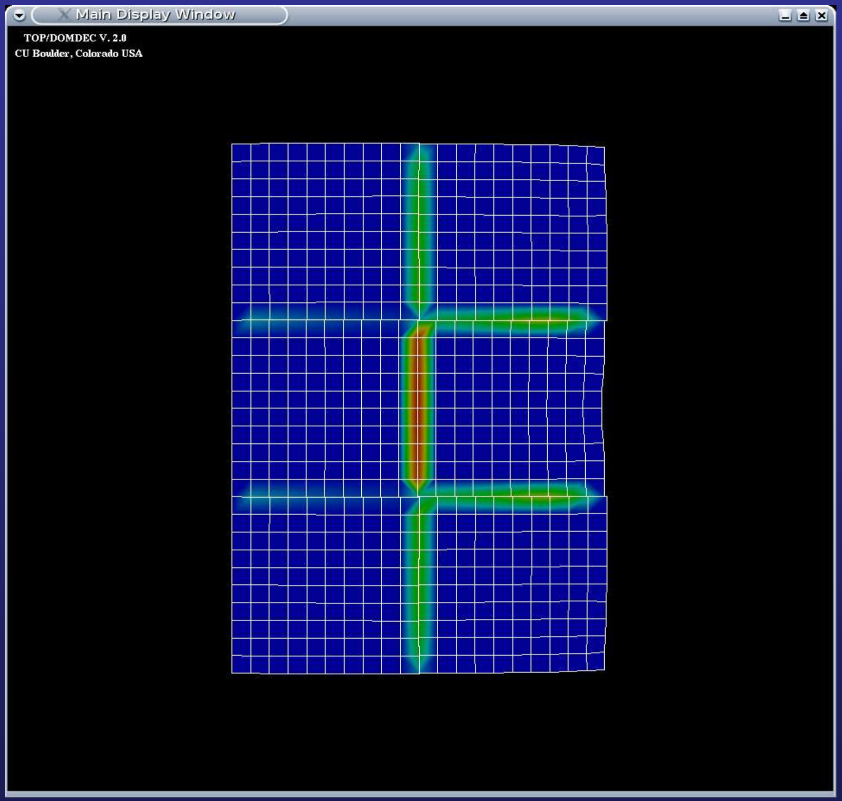
BETI for 2nd kind variational inequality



$H/h \setminus H$	1/2	1/4	1/6	1/8
24	384/100/0.04 14	1536/592/0.86 21	3456/1476/9.40 25	6144/2752/25.40 25
16	256/68/0.02 10	1024/400/0.36 14	2304/996/2.54 20	4096/1856/6.50 17
8	128/36/0.02 8	512/208/0.12 11	1152/516/0.59 15	2048/960/1.52 12
4	64/20/0.04 7	256/112/0.06 9	576/276/0.17 10	1024/512/0.39 10

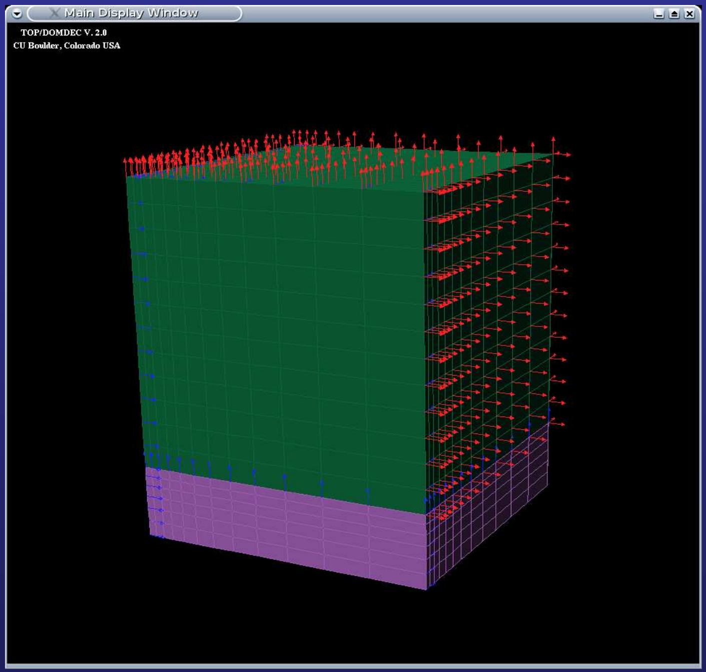
2D coercive test

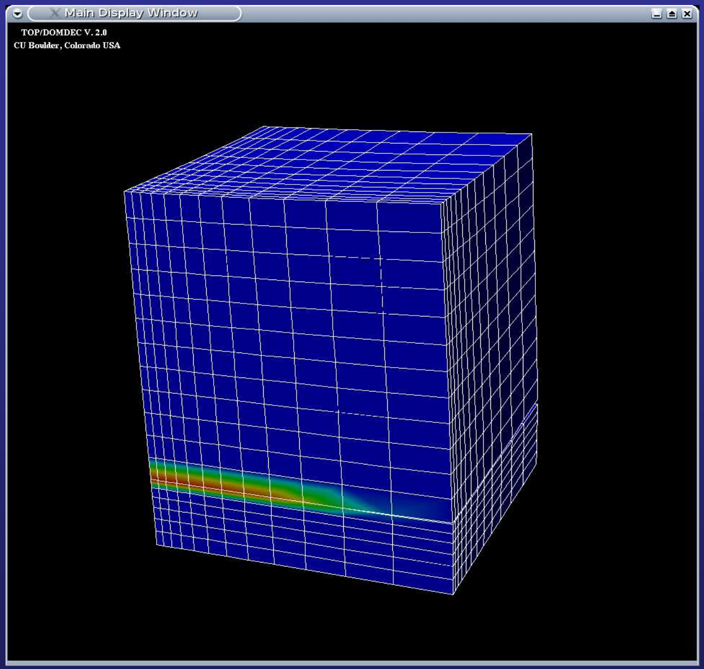




MPRGP	12

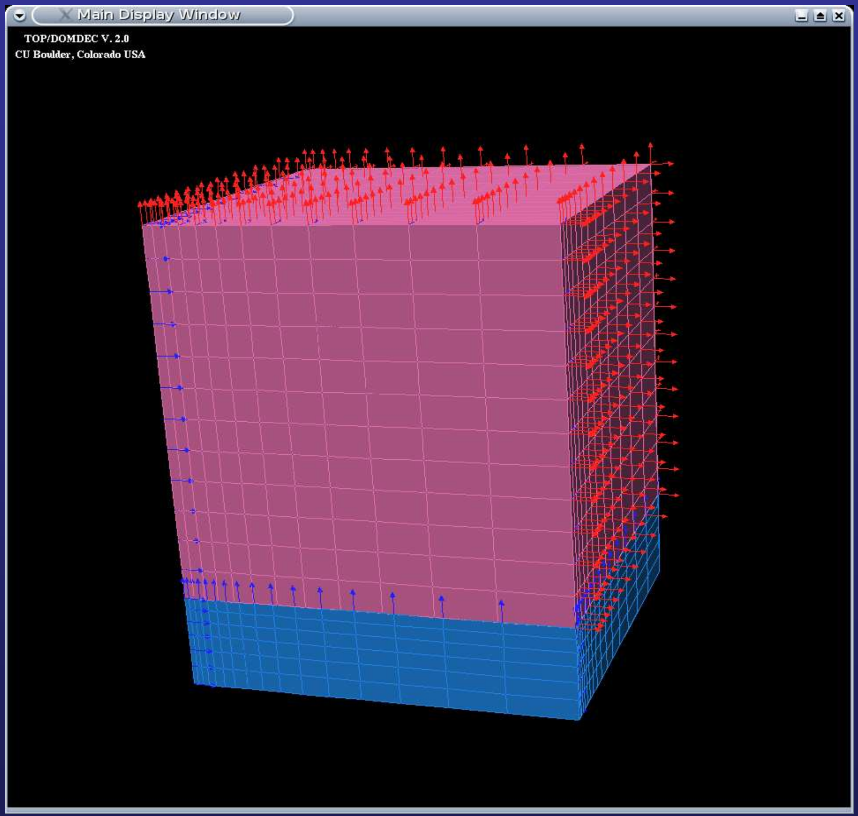
3D 2 blocks problem matching grids

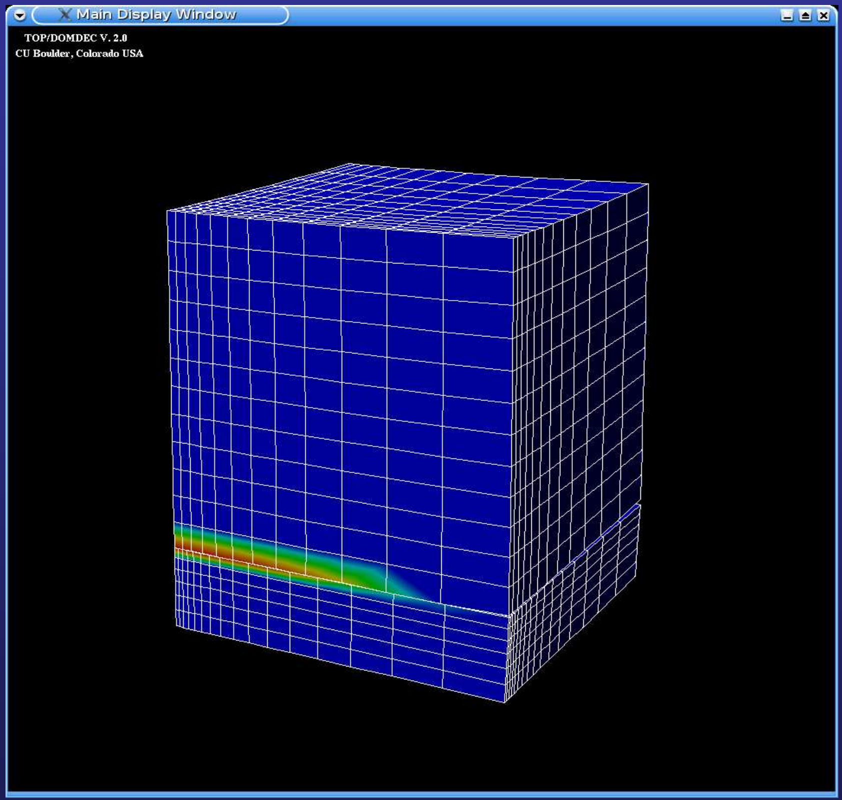




	inner	outer
SMALBE	13	29

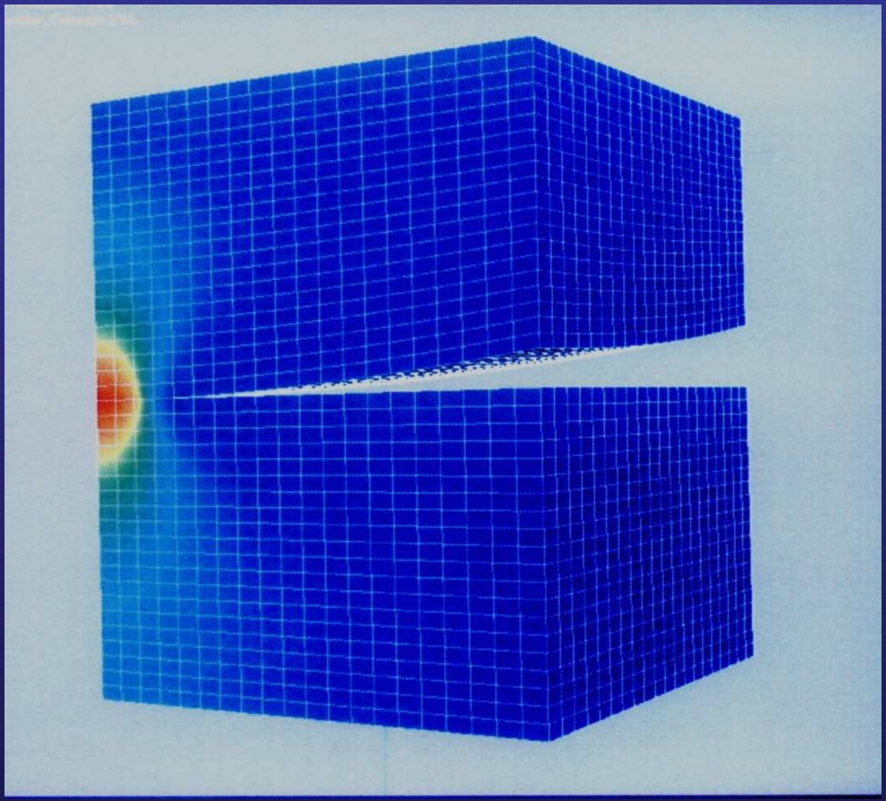
3D 2 blocks problem:non-matching grids





	inner	outer
SMALBE	10	29

FETI-DP 3D elasticty Hertz model problem



55666	DOFs
47	iterations
61	matrix-vector OPs
38.5 s	time

Optimal preconditioner and adaptive strategy for $\bar{\alpha}$ (proposed by M. Lesoinne)

Related research in variational inequalities

- FETI-NCG by C. Farhat, Duraiseix (based on FETI)
- FETI-C C. Farhat, M. Lesoinne , P. Avery, … (based on FETI-DP)
- Optimal dual penalty Z. D., D. Horák
- Large deformation J. Dobias, V. Vondrák, …
- Applications to contact shape optimization V. Vondrák, Z. D.
- Applications in composites Z.D., O. Vlach
- Quasistatic problems J. Haslinger, O. Vlach, Z.D.,
- Applications in biomechanics V. Vondrák, J.Rasmussen, …
- Problems with Coulomb friction R. Kučera, J. Haslinger, Z.D., …
- Some others (R. Kornhuber, R. Krause, B. Wohlmuth, …) gave evidence of optimality of various algorithms, J. Schoeberl even the first proof.

Conlusions

1. New algorithms for bound and equality constrained QP problems were introduced
2. Qualitatively new results were shown
3. The results were applied to develop scalable algorithms for elliptic boundary variational inequalities including contact problems
4. Theoretical results are in agreement with numerical experiments
5. Engineering application in progress (joint with C. Farhat)
6. Recently extended to 3D Tresca