PERMON libraries for large scale quadratic programming

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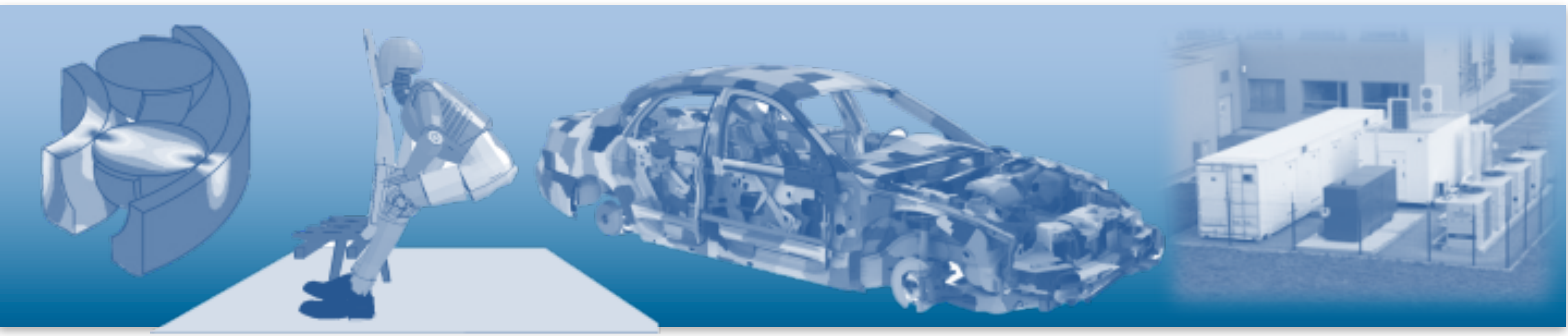

PETSc User Meeting 2016, Vienna, June 28-30, 2016

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permon.it4i.cz

IT4Innovations

- HPC infrastructure
- 8 research programmes

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national111010
supercomputing
center1££0#110

2013

2014

2015

Anselm - 94 TFLOPs system operational since June 2013

Salomon – 2 PFLOPs system from June/July 2015

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Salomon in numbers

- 1008 compute nodes
- 24,192 Intel Haswell cores
  - 2 x 12 per node
- 129,024 GB RAM
  - 128GB per node, 5.3GB per core
- 864 2nd generation MICs (KNC)
  - Intel Xeon Phi 7120P
  - 52,704 cores
- Rpeak 2.01 Pflop/s
- Rmax 1.46 Pflop/s (LINPACK)

largest European installation of MICs
⇒ interested in PETSc on MIC

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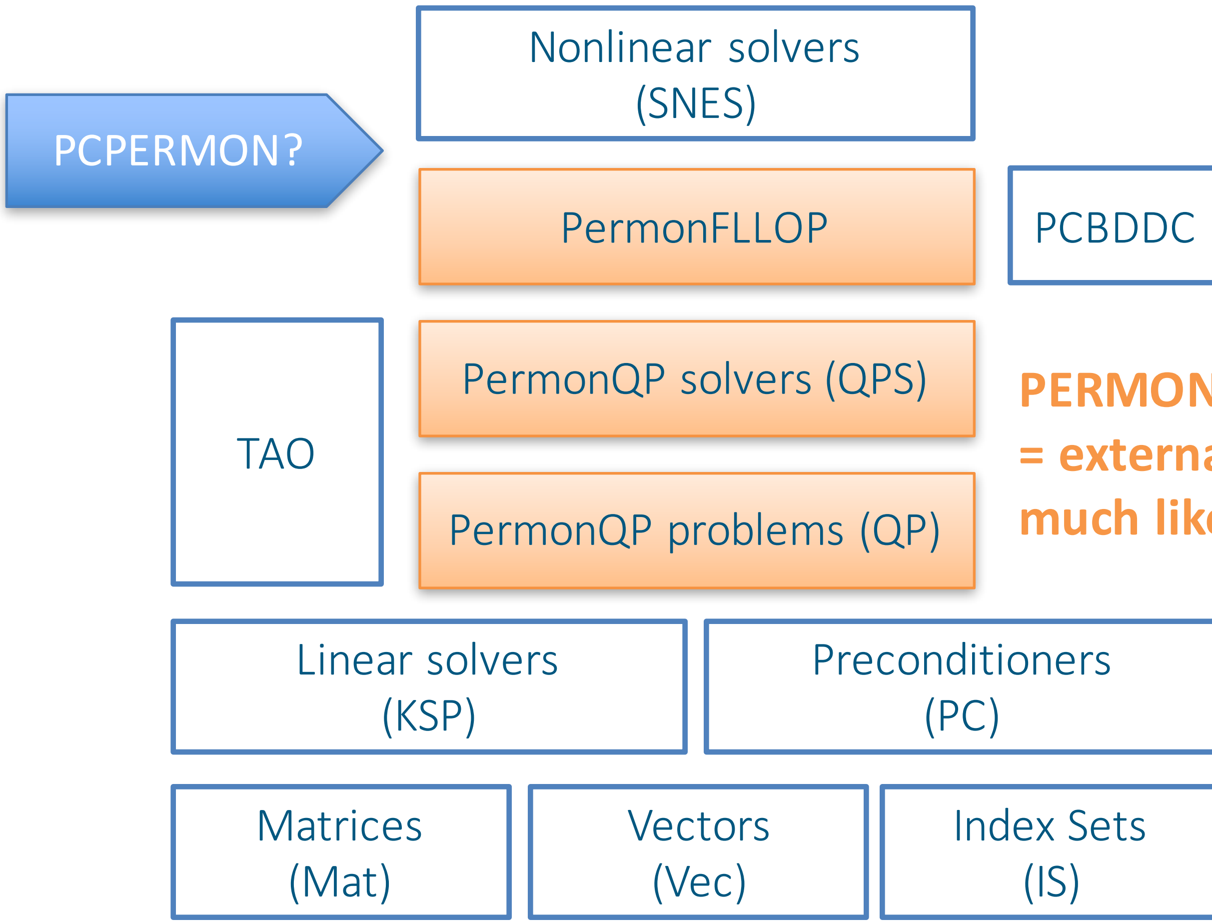
PERMON in a nutshell

Parallel, **E**fficient, **R**obust, **M**odular, **O**bject-oriented, **N**umerical

http://permon.it4i.cz/

- **PermonQP**
  - generic QP solution framework
  - QP problems, transforms, solvers
- **PermonFLLOP**
  - FETI DDM implementation
  - extends PermonQP
- **both**
  - based on/extending **PETSc** open-source framework for sci. comp.
  - together solve large contact mechanics problems
- started in 2011, ~30 000 lines of effective C code

PETSc + PERMON



PERMON
= external PETSc extension
much like SLEPc

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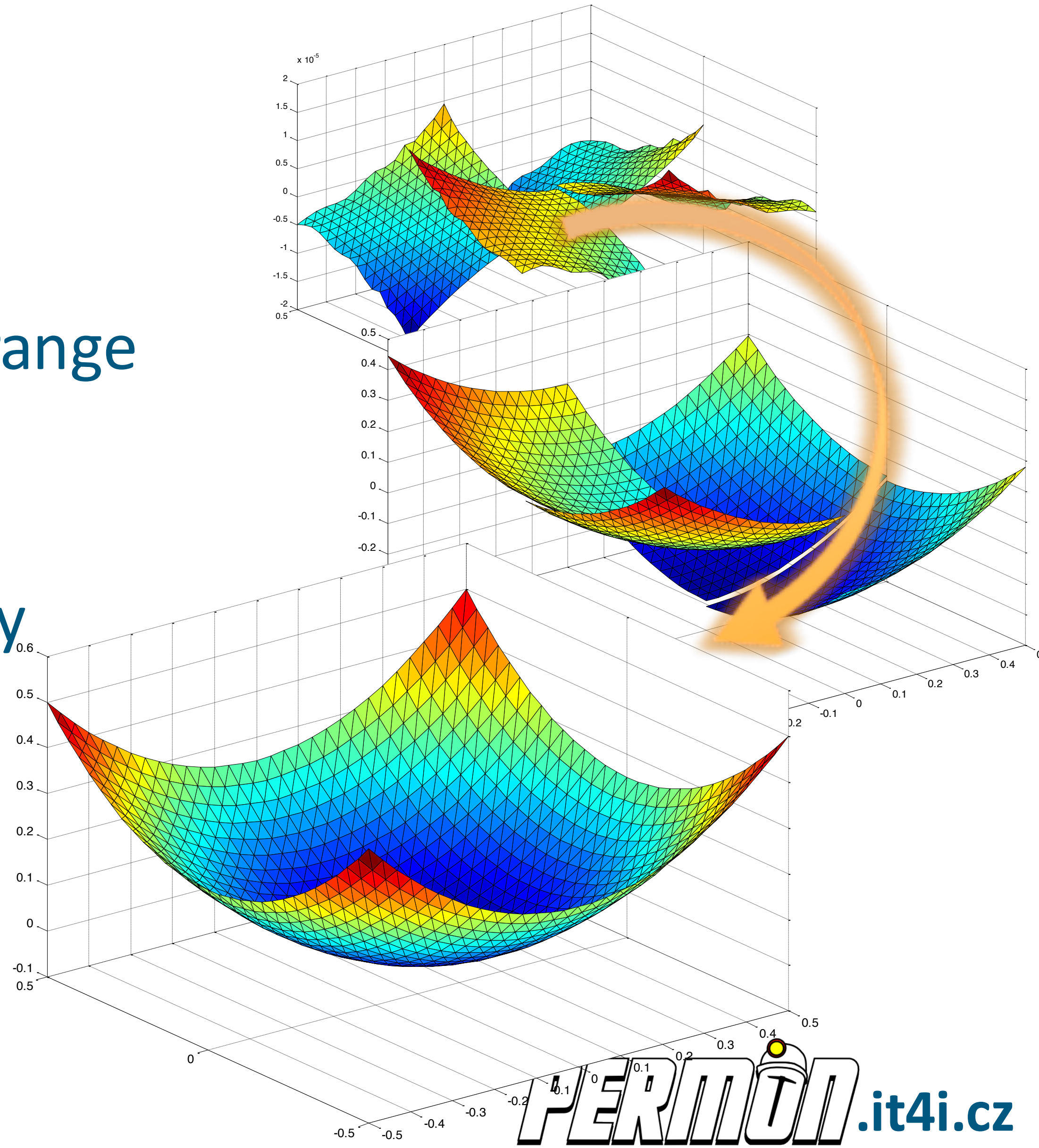
Build

- easy
- just build PETSc
- set PETSC_DIR and PETSC_ARCH
- set PERMON_DIR
- make

PermonFLLOP

- implements FETI non-overlapping DDM
- dual formulation
- unknown optimal Lagrange multipliers found by iterative process
- they enforce continuity across subdomains
- mix iterative and direct solvers



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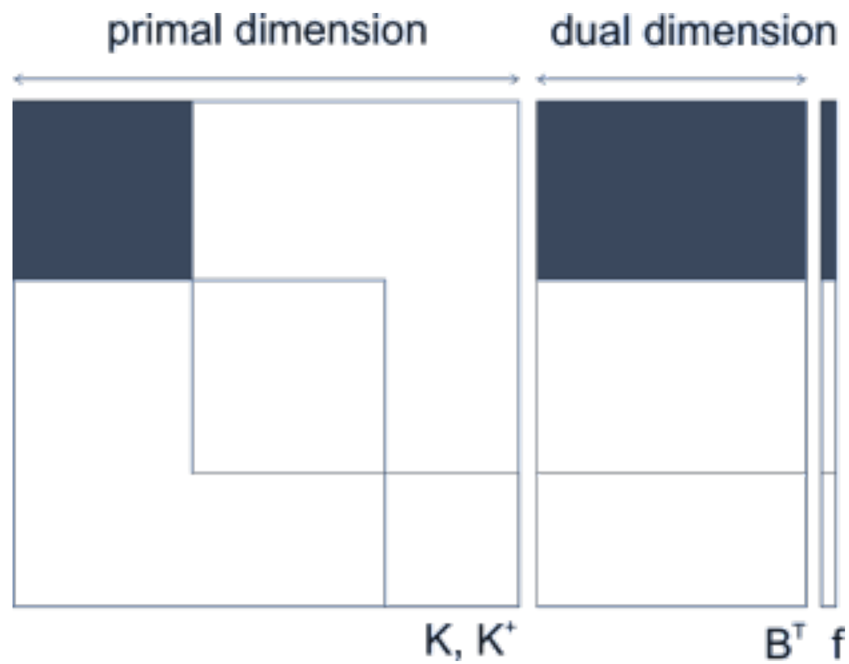
FETI: primal formulation

$$\begin{bmatrix} \mathbf{K} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{O} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{o} \end{bmatrix}$$

- $\mathbf{K}$ SPD block-diagonal stiffness matrix (blocks ~ subdomains)
- $\mathbf{R}$ columns span kernel of $\mathbf{K}$
- $\mathbf{f}$ load vector
- $\mathbf{B}$ signed boolean gluing matrix (can enforce also Dirichlet BC - TFETI)



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FETI: QP formulations

- $\begin{bmatrix} \mathbf{K} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{O} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{o} \end{bmatrix}$ (primal)
- $\begin{bmatrix} \mathbf{BK}^+\mathbf{B}^T & -\mathbf{BR} \\ -\mathbf{R}^T\mathbf{B}^T & \mathbf{O} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\alpha} \end{bmatrix} = \begin{bmatrix} \mathbf{BK}^+\mathbf{f} \\ -\mathbf{R}^T\mathbf{f} \end{bmatrix}$ (dual)

- $\min_{\mathbf{u}} {}^1\!/_2\, \mathbf{u}^T\mathbf{Ku} - \mathbf{u}^T\mathbf{f}$ s.t. $\mathbf{Bu} = \mathbf{o}$ (primal)

  $\mathbf{F} = \mathbf{BK}^+\mathbf{B}^T,\ \mathbf{d} = \mathbf{BK}^+\mathbf{f},\ \mathbf{G} = -\mathbf{R}^T\mathbf{B}^T,\ \mathbf{e} = -\mathbf{R}^T\mathbf{f}$

  $\mathbf{u} = \mathbf{K}^\dagger(\mathbf{f} - \mathbf{B}^T\boldsymbol{\lambda}) + \mathbf{R}\boldsymbol{\alpha}$

  $\boldsymbol{\alpha} = -(\mathbf{GG}^T)^{-1}\mathbf{G}(\mathbf{F}\boldsymbol{\lambda} - \mathbf{d})$

- $\min_{\boldsymbol{\lambda}} {}^1\!/_2\, \boldsymbol{\lambda}^T\mathbf{F}\boldsymbol{\lambda} - \boldsymbol{\lambda}^T\mathbf{d}$ $s.t.$ $\mathbf{G}\boldsymbol{\lambda} = \mathbf{e}$ (dual)

FETI: improving the dual formulation

1) $\min_{\boldsymbol{\lambda}} {}^{1}/_{2}\, \boldsymbol{\lambda}^T \mathbf{F} \boldsymbol{\lambda} - \boldsymbol{\lambda}^T \mathbf{d}$ s.t. $\mathbf{G}\boldsymbol{\lambda} = \mathbf{e}$

$\boldsymbol{\lambda} = \overline{\boldsymbol{\lambda}} + \boldsymbol{\lambda}_{\mathrm{P}}$

$\boldsymbol{\lambda}_{\mathrm{P}} = \mathbf{G}^T (\mathbf{G}\mathbf{G}^T)^{-1} \mathbf{e} \in \mathrm{Im}\mathbf{G}^T$

$\bar{\mathbf{d}} = \mathbf{d} - \mathbf{F}\boldsymbol{\lambda}_{\mathrm{P}}$

$\overline{\boldsymbol{\lambda}} \in \mathrm{Ker}\mathbf{G}$ unknown

2) $\min_{\overline{\boldsymbol{\lambda}}} {}^{1}/_{2}\, \overline{\boldsymbol{\lambda}}^T \mathbf{F} \overline{\boldsymbol{\lambda}} - \overline{\boldsymbol{\lambda}}^T \bar{\mathbf{d}}$ s.t. $\mathbf{G}\overline{\boldsymbol{\lambda}} = \mathbf{o}$

$\mathbf{P} = \mathbf{I} - \mathbf{G}^T (\mathbf{G}\mathbf{G}^T)^{-1} \mathbf{G}$, [$(\mathbf{G}\mathbf{G}^T)^{-1}$ is coarse problem]

3) $\min_{\overline{\boldsymbol{\lambda}}} {}^{1}/_{2}\, \overline{\boldsymbol{\lambda}}^T \mathbf{PFP} \overline{\boldsymbol{\lambda}} - \overline{\boldsymbol{\lambda}}^T \mathbf{P}\bar{\mathbf{d}} \iff \mathbf{PFP}\overline{\boldsymbol{\lambda}} = \mathbf{P}$ [solve with CG]

FETI: inequality constraints

- **primal formulation**

  $\min_{\mathbf{u}} \, {}^1\!/_2 \, \mathbf{u}^T \mathbf{K} \mathbf{u} \; - \mathbf{u}^T \mathbf{f}$ s.t. $\mathbf{B}_{\mathrm{E}} \mathbf{u} = \mathbf{o}$ and $\mathbf{B}_{\mathrm{I}} \mathbf{u} \leq \mathbf{c}_{\mathrm{I}}$

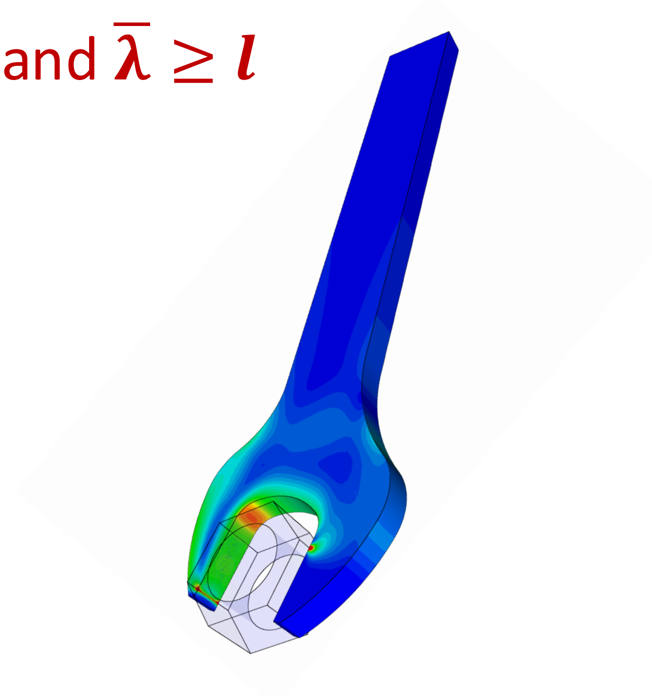
  (nonpenetration - mortar conditions)

- **dual formulation**

  $\min_{\overline{\boldsymbol{\lambda}}} \, {}^1\!/_2 \, \overline{\boldsymbol{\lambda}}^T \mathbf{P} \mathbf{F} \mathbf{P} \overline{\boldsymbol{\lambda}} - \overline{\boldsymbol{\lambda}}^T \mathbf{P} \overline{\mathbf{d}}$ s.t. $\mathbf{G} \overline{\boldsymbol{\lambda}} = \mathbf{o}$ and $\overline{\boldsymbol{\lambda}} \geq \boldsymbol{l}$

  (is no more a linear system !)

- use SMALXE + MPGP (discussed later)
  to solve this dual formulation



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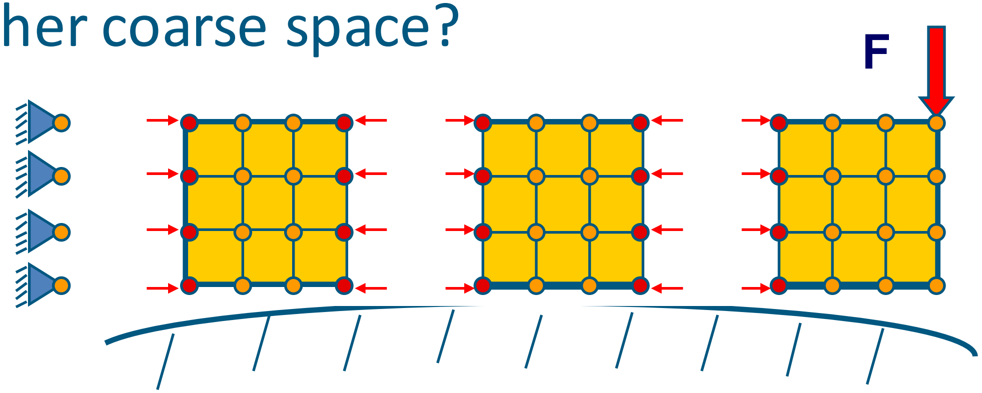
Total FETI (TFETI)

- **Dirichlet** boundary conditions handled **same way as gluing**
- all subdomain **floating**
  - all stiffness matrices singular
  - no need to detect it
  - same nullspaces in typical cases
  - uniform handling
- additional rows of **B** matrix
- effect of richer coarse space?



PermonFLLOP calls PermonQP

```
MPI_Comm comm;
Mat K, BE, BI;
Věc f, cE, cI, x;
QP qp;

QPCreate(comm, &qp);
QPSetOperator(qp, K);
QPSetRhs(qp, f);
QPSetEq(qp, BE, cE);
QPSetIneq(qp, BI, cI);

QPFetiPrepare(qp);

QPSCreate(comm, &qps);
QPSSetQP(qps, qp);
QPSSetFromOptions(qps);
QPSSolve(qps);
QPGetSolutionVector(qp,&x);
```

```
PetscErrorCode QPFetiPrepare(QP qp)
{
  …
  QPTDualize(qp);
  QPTHomogenizeEq(qp);
  QPTEnforceEqByProjector(qp);
  …
}
```

Sequence of QP transforms

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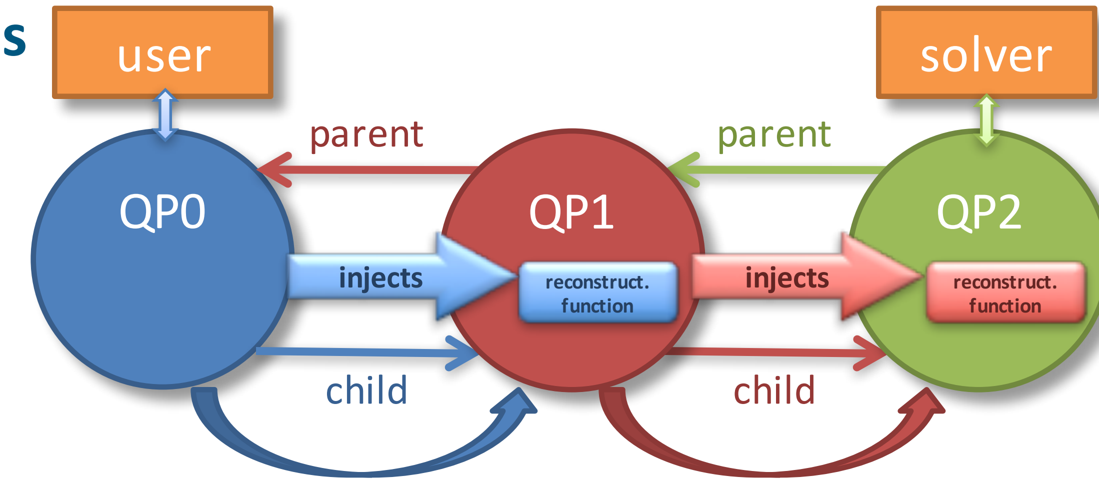
PermonQP

- QP solution **framework**
- **separation of concerns**
  - QP **problems** (QP)
  - QP **transforms** (QPT) and corresponding **backward reconstructions**
  - QP **solvers** (QPS)



- *"gradually get rid of difficulties in the original formulation"*
- modularity/composability
- automatic/manual **choice of solver**
- **applications:** contact problems, data fitting, support vector machines, ...

PermonQP and PETSc TAO

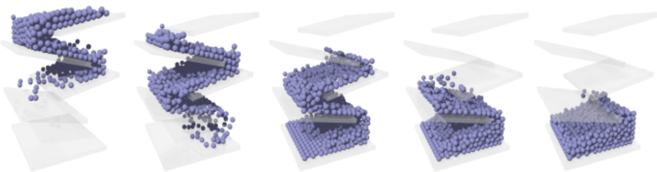
TAO

- general objective function
- only unconstrained and box constrained

PermonQP

- specific objective function (convex quadratic), Mat, Vec
- more like KSP, less like SNES
- can be coupled with FETI DDM (PermonFLLOP)
- more general constraints
  - linear equality
  - linear inequality
  - separable convex constraints – next slide
    - applicable to any subset of indices (IS)
    - simple bound / box constraints
    - quadratic constraints (spherical, elliptical)
    - conical constraints, …

Generalizing box constraints - QPC



- separable convex constraints
- applicable to any subset of indices (IS)
- simple bound / box constraints
- quadratic constraints (spherical, elliptical)
- conical constraints, …

$$\min \, {}^{1}\!/_{2}\, \mathbf{x}^T \mathbf{A} \mathbf{x} - \mathbf{x}^T \mathbf{b}$$
s.t. …

QPC
index set

QPCBOUND
lower bound
$\mathbf{x} \geq \boldsymbol{l}$

QPCBOX
lower bound
upper bound
$\mathbf{l} \leq \mathbf{x} \leq \mathbf{u}$

QPCELLIPTIC
major axis
minor axis
$\left(\frac{x_1}{a}\right)^2 + \left(\frac{x_2}{b}\right)^2 \leq 1$

QPCQUADRATIC
radii
$x_1^2 + x_2^2 \leq r^2$

QPCCONICAL
angles
$x_1^2 + x_2^2 \leq \mu x_3^2$

PermonQP – print KKT satisfaction

```
====================
QPChainViewKKT output
QP Object: 4 MPI proce
  type: QP
  #0 in chain, derived
|| x|| = 4.75e+00    max( x) = 2.00e-06 =   x    )    min( x) = -3.23e-01 =
|| b|| = 4.75e-02    max( b) = -4.17e-04 =           min( b) = -2.50e-03 =
||cE|| = 0.00e-00    max(cE) = 0.00e-00 = cE(0)    min(cE) = 0.00e-00 = cE(
||cI|| = 1.63e+00    max(cI) = 4.34e-01 = cI(0)    min(cI) = 3.01e-01 = cI(
r = ||A*x - b + BE'*lambda_E + BI'*lambda_I|| = 6.78e-06    r0/||b|| = 1.43
r = ||BE*x-cE||             = 1.58e-05    r/||b|| = 3.32e-04
r = ||max(BI*x-cI,0)||      = 0.00e+00    r/||b|| = 0.00e+00
r = ||min(lambda_I,0)||     = 0.00e+00    r/||b|| = 0.00e+00
r = lambda_I'*(BI*x-cI)     = -1.39e-07    r/||b|| = -2.92e-06
------------------
QP Object: 4 MPI processes
  type: QP
  #1 in chain, derived by QPTScal
|| x|| = 4.75e+00    max( x) = 2.0
|| b|| = 4.75e-02    max( b) = -4.
||cE|| = 0.00e-00    max(cE) = 0.0
||cI|| = 1.63e+00    max(cI) = 4.3
r = ||A*x - b + BE'*lambda_E + BI'
r = ||BE*x-cE||             = 1.58e-0
r = ||max(BI*x-cI,0)||      = 0.00e+0
r = ||min(lambda_I,0)||     = 0.00e+0
r = lambda_I'*(BI*x-cI)     = -1.39e-
------------------
QP Object:(dual_) 4 MPI processes
  type: QP
  #2 in chain, derived by QPTDuali
|| x|| = 4.47e-01    max( x) = 1.3
|| b|| = 2.62e+00    max( b) = 3.9
||cE|| = 5.00e-01    max(cE) = -2.
||lb|| = inf    max(lb) = 0.00e+00
r = ||A*x - b + BE'*lambda_E - lam
r = ||BE*x-cE||             = 6.78e-0
r = ||min(x-lb,0)||         = 0.00e+0
r = ||min(lambda_lb,0)||    = 1.67e-05    r/||b|| = 6.37e-06
r = |lambda_lb'*(lb-x)|     = 2.47e-06    r/||b|| = 9.42e-07
------------------
```

-qp_chain_view_kkt

$$\min \tfrac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x} - \mathbf{x}^T\mathbf{b} \text{ s.t. } \mathbf{B}_E\mathbf{x} = \mathbf{c}_E \text{ and } \mathbf{x} \geq \boldsymbol{l}$$

$$\mathbf{A}\mathbf{x} - \mathbf{b} + \mathbf{B}_E^T\boldsymbol{\lambda}_E - \boldsymbol{\lambda}_l = \mathbf{o}$$

$$\mathbf{B}_E\mathbf{x} = \boldsymbol{c}_E$$

$$\mathbf{x} \geq \boldsymbol{l}$$

$$\boldsymbol{\lambda}_l \geq \mathbf{o}$$

$$\boldsymbol{\lambda}_l(\boldsymbol{l} - \mathbf{x}) = \mathbf{o}$$


```
QP Object:(dual_) 4 MPI processes
  type: QP
  #2 in chain, derived by QPTDualize
|| x|| = 4.47e-01    max( x) = 1.30e-01 =   x(112)    min( x) = -1.47e-01 =   x(106)
|| b|| = 2.62e+00    max( b) = 3.90e-01 =   b(21)    min( b) = -5.61e-01 =   b(133)
||cE|| = 5.00e-01    max(cE) = -2.50e-01 = cE(3)    min(cE) = -2.50e-01 = cE(0)
||lb|| = inf    max(lb) = 0.00e+00 = lb(30)    min(lb) = -4.49e+307 = lb(0)
r = ||A*x - b + BE'*lambda_E - lambda_lb|| = 5.31e-05    r0/||b|| = 2.03e-05
r = ||BE*x-cE||             = 6.78e-06    r/||b|| = 2.59e-06
r = ||min(x-lb,0)||         = 0.00e+00    r/||b|| = 0.00e+00
r = ||min(lambda_lb,0)||    = 1.67e-05    r/||b|| = 6.37e-06
r = |lambda_lb'*(lb-x)|     = 2.47e-06    r/||b|| = 9.42e-07
```

PermonQP – how to solve any QP?

- **Dualization**
  - crucial QP transform
  - new QP with **smaller dim**, **better conditioned** and **simpler constraints**

$$\min \tfrac{1}{2}\mathbf{u}^T\mathbf{K}\mathbf{u} - \mathbf{u}^T\mathbf{f} \text{ s.t. } \mathbf{B}_E\mathbf{u} = \mathbf{o} \text{ and } \mathbf{B}_I\mathbf{u} \le \mathbf{c}_I$$

$$\min \tfrac{1}{2}\boldsymbol{\lambda}^T\mathbf{A}\boldsymbol{\lambda} - \boldsymbol{\lambda}^T\mathbf{b} \text{ s.t. } \mathbf{C}\boldsymbol{\lambda} = \mathbf{d} \text{ and } \boldsymbol{\lambda} \ge \boldsymbol{l}$$

- **SMALXE**
  - **"pass-through"** solver taking care of **equality constraints**
    - moved to the Hessian matrix by means of penalty term
  - **aux. problem** with the rest of constraints solved by **inner solver**

$$\min \tfrac{1}{2}\boldsymbol{\lambda}^T\mathbf{A}\boldsymbol{\lambda} - \boldsymbol{\lambda}^T\mathbf{b} \text{ s.t. } \cancel{\mathbf{C}\boldsymbol{\lambda} = \mathbf{d}} \text{ and } \boldsymbol{\lambda} \ge \boldsymbol{l}$$

- **concrete solvers** for convex QP
  - **unconstrained** – PETSc KSP wrapper (QPSKSP)
  - **bound/box constraints**
  - MPGP, APGD, PBBf, SPG-QP, ...
  - PETSc TAO wrapper

$$\min \tfrac{1}{2}\boldsymbol{\lambda}^T\mathbf{A}\boldsymbol{\lambda} - \boldsymbol{\lambda}^T\mathbf{b} \text{ s.t. } \boldsymbol{\lambda} \ge \boldsymbol{l}$$

SMALXE for $\min_{\mathbf{Bx}=\mathbf{o}} \frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x} - \mathbf{x}^T\mathbf{b}$ (SMALE)

- **Mainstream:** solve KKT system $\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{O} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \boldsymbol{\mu} \end{bmatrix} = \begin{bmatrix} \mathbf{b} \\ \mathbf{o} \end{bmatrix}$
  - using **direct/iterative linear system solver**
  - $\boldsymbol{\mu}$ is equality constraint Lagrange multiplier
  - inequality constrained → slacks, nonlin. eq. → **Interior Point Method**
- **SMALXE:** solve directly QP $\min \frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x} - \mathbf{x}^T\mathbf{b}$ s.t. $\mathbf{Bx} = \mathbf{o}$
  - using **Augmented Lagrangians** and inner **iterative** solver
  - easier to extend for **inequality constraints**
  - equality and inequality constraints handled completely **separately**, **one after another**, in a specialized manner
  - **matrix structure agnostic** - both A and B may be even implicit

Lagrangian

$$L(\mathbf{x}, \boldsymbol{\mu}) = \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} - \mathbf{x}^{\mathrm{T}}\mathbf{b} + \boldsymbol{\mu}^{\mathrm{T}}\mathbf{B}\mathbf{x}$$ (Lagrangian)

$$\mathbf{g}(\mathbf{x}, \boldsymbol{\mu}) = \mathbf{A}\mathbf{x} - \mathbf{b} + \mathbf{B}^{\mathrm{T}}\boldsymbol{\mu}$$ (Lagrangian gradient)

Augmented Lagrangian

$\tilde{L}(\mathbf{x},\boldsymbol{\mu},\rho) = \frac{1}{2}\mathbf{x}^T\mathbf{A}\mathbf{x} - \mathbf{x}^T\mathbf{b} + \boldsymbol{\mu}^T\mathbf{B}\mathbf{x} + \frac{1}{2}\rho\|\mathbf{B}\mathbf{x}\|^2$ (augmented Lagrangian)

$\tilde{\mathbf{g}}(\mathbf{x},\boldsymbol{\mu},\rho) = \mathbf{A}\mathbf{x} - \mathbf{b} + \mathbf{B}^T\boldsymbol{\mu} + \rho\mathbf{B}^T\mathbf{B}\mathbf{x}$ (augmented Lagrangian gradient)

Note1: $\tilde{L}$ is Lagrangian of penalized problem

$$\min_{\mathbf{B}\mathbf{x}=\mathbf{o}} \frac{1}{2}\mathbf{x}^T(\mathbf{A} + \rho\mathbf{B}^T\mathbf{B})\mathbf{x} - \mathbf{x}^T\mathbf{b} \qquad \text{(QPP)}$$

$$\tilde{L}(\mathbf{x},\boldsymbol{\mu},\rho) = \frac{1}{2}\mathbf{x}^T(\mathbf{A} + \rho\mathbf{B}^T\mathbf{B})\mathbf{x} - \mathbf{x}^T(\mathbf{b} + \mathbf{B}\boldsymbol{\mu})$$

Note2: Solution $\hat{\mathbf{x}}$ of unconstrained penalized problem

$$\min \frac{1}{2}\mathbf{x}^T(\mathbf{A} + \rho\mathbf{B}^T\mathbf{B})\mathbf{x} - \mathbf{x}^T\mathbf{b} \qquad \text{(QPPU)}$$

approximates that of original QP: $\|\tilde{\mathbf{g}}\| \le \varepsilon\|\mathbf{b}\| \Longrightarrow \|\mathbf{B}\mathbf{x}\| \le \frac{1+\varepsilon}{\sqrt{\lambda_{\min}(\mathbf{A})\rho}}$

Exact aug. Lag. method for $\min_{\mathbf{Bx}=\mathbf{o}} \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{Ax} - \mathbf{x}^{\mathrm{T}}\mathbf{b}$

(Method of multipliers)

initialize: $\mathbf{x}_0$ $[\mathbf{o}]$, $\rho_0 > 0$ $[2\|\mathbf{A}\|]$

$\boldsymbol{\mu}_0 = \mathbf{o}, \; k = 0$

while $\|\tilde{\mathbf{g}}(\mathbf{x}_k, \boldsymbol{\mu}_k, \rho_k)\| > \varepsilon\|\mathbf{b}\| \; \vee \; \|\mathbf{Bx}_k\| > \varepsilon\|\mathbf{b}\|$

$\quad \boldsymbol{\mu}_{k+1} = \boldsymbol{\mu}_k + \rho_k \mathbf{Bx}_k$

$\quad \mathbf{x}_{k+1} = \arg\min_{\mathbf{x}} \tilde{L}(\mathbf{x}, \boldsymbol{\mu}_{k+1}, \rho_k)$ starting with $\mathbf{x}_k$

$\quad k = k + 1$

end

$$\mathbf{x}_{k+1} = \arg\min_{\mathbf{x}} \frac{1}{2}\mathbf{x}^{\mathrm{T}}(\mathbf{A} + \rho_k \mathbf{B}^{\mathrm{T}}\mathbf{B})\mathbf{x} - \mathbf{x}^{\mathrm{T}}(\mathbf{b} + \mathbf{B}\boldsymbol{\mu}_{k+1})$$

- inner QP with penalized Hessian and updated RHS
- unconstrained QP ~ solving linear system
- solve with CG

Dostál, Z.:
Optimal Quadratic Programming Algorithms,
Springer Optimization and Its Applications,
2009, ISBN 978-0387848051

SMALXE for $\min_{\mathbf{Bx}=\mathbf{o}} \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x} - \mathbf{x}^{\mathrm{T}}\mathbf{b}$ (SMALE)

initialize: $\mathbf{x}_0$ $[\mathbf{o}]$, $\beta > 0$ $[10]$, $M_0 > 0$ $[100\|\mathbf{A}\|]$, $\rho_0 > 0$ $[2\|\mathbf{A}\|]$, $\eta > 0$ $[0.1\|\mathbf{b}\|]$

$\boldsymbol{\mu}_0 = \mathbf{o}$, $k = 0$

while $\|\tilde{\mathbf{g}}(\mathbf{x}_k, \boldsymbol{\mu}_k, \rho_k)\| > \varepsilon\|\mathbf{b}\| \;\vee\; \|\mathbf{B}\mathbf{x}_k\| > \varepsilon\|\mathbf{b}\|$

$\boldsymbol{\mu}_{k+1} = \boldsymbol{\mu}_k + \rho_k \mathbf{B}\mathbf{x}_k$

find $\mathbf{x}_{k+1}$ such that $\|\tilde{\mathbf{g}}(\mathbf{x}_{k+1}, \boldsymbol{\mu}_{k+1}, \rho_k)\| \leq \min(M_k\|\mathbf{B}\mathbf{x}_{k+1}\|, \eta)$

if $\tilde{L}(\mathbf{x}_{k+1}, \boldsymbol{\mu}_{k+1}, \rho_k) > \tilde{L}(\mathbf{x}_k, \boldsymbol{\mu}_k, \rho_{k-1}) + \frac{1}{2}\rho_k\|\mathbf{B}\mathbf{x}_{k+1}\|^2$

$\rho_{k+1} = \beta\rho_k$ or $M_{k+1} = M_k/\beta$

SMALE or SMALE-M

end

$k = k + 1$

end

again solving $\min_{\mathbf{x}} \frac{1}{2}\mathbf{x}^{\mathrm{T}}(\mathbf{A} + \rho_k\mathbf{B}^{\mathrm{T}}\mathbf{B})\mathbf{x} - \mathbf{x}^{\mathrm{T}}(\mathbf{b} + \mathbf{B}\boldsymbol{\mu}_{k+1})$

BUT with early termination

- inner QP with penalized Hessian and updated RHS
- unconstrained QP ~ solving linear system
- solve with e.g. CG

SMALXE for $\min_{\substack{\mathbf{Bx}=\mathbf{o} \\ \mathbf{x} \geq \boldsymbol{l}}} \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{Ax} - \mathbf{x}^{\mathrm{T}}\mathbf{b}$ (SMALBE)

initialize: $\mathbf{x}_0$ $[\mathbf{o}]$, $\beta > 0$ $[10]$, $M_0 > 0$ $[100\|\mathbf{A}\|]$, $\rho_0 > 0$ $[2\|\mathbf{A}\|]$, $\eta > 0$ $[0.1\|\mathbf{b}\|]$

$\boldsymbol{\mu}_0 = \mathbf{o}$, $k = 0$

$\mathbf{g}^P$ ... projected gradient – see next slide

while $\|\tilde{\mathbf{g}}^P(\mathbf{x}_k, \boldsymbol{\mu}_k, \rho_k)\| > \varepsilon\|\mathbf{b}\| \vee \|\mathbf{Bx}_k\| > \varepsilon\|\mathbf{b}\|$

$\boldsymbol{\mu}_{k+1} = \boldsymbol{\mu}_k + \rho_k \mathbf{Bx}_k$

find $\mathbf{x}_{k+1} \geq \boldsymbol{l}$ such that $\|\tilde{\mathbf{g}}^P(\mathbf{x}_{k+1}, \boldsymbol{\mu}_{k+1}, \rho_k)\| \leq \min(M_k\|\mathbf{Bx}_{k+1}\|, \eta)$

if $\tilde{L}(\mathbf{x}_{k+1}, \boldsymbol{\mu}_{k+1}, \rho_k) > \tilde{L}(\mathbf{x}_k, \boldsymbol{\mu}_k, \rho_{k-1}) + \frac{1}{2}\rho_k\|\mathbf{Bx}_{k+1}\|^2$

$\rho_{k+1} = \beta\rho_k$ or $M_{k+1} = M_k/\beta$

SMALBE or SMALBE-M

end

now solving $\min_{\mathbf{x} \geq \boldsymbol{l}} \frac{1}{2}\mathbf{x}^{\mathrm{T}}(\mathbf{A} + \rho_k\mathbf{B}^{\mathrm{T}}\mathbf{B})\mathbf{x} - \mathbf{x}^{\mathrm{T}}(\mathbf{b} + \mathbf{B}\boldsymbol{\mu}_{k+1})$

but using the same $\tilde{L}$ corresponding to $\min_{\mathbf{Bx}=\mathbf{o}} \frac{1}{2}\mathbf{x}^{\mathrm{T}}\mathbf{Ax} - \mathbf{x}^{\mathrm{T}}\mathbf{b}$

$k = k + 1$

end

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Dostál, Z.: Optimal Quadratic Programming Algorithms, Springer Optimization and Its Applications, 2009, ISBN 978-0387848051

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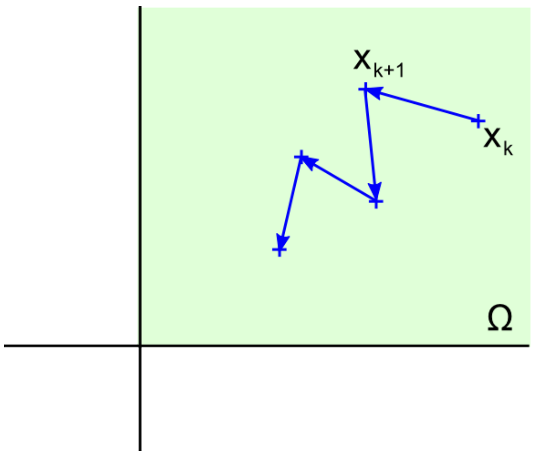
Projected gradient

- $\tilde{\mathbf{g}}^P = [g_i^P]$, $\tilde{\mathbf{g}} = [g_i]$, $\mathbf{x} = [x_i]$, $\boldsymbol{l} = [l_i]$
- M … set of indices of inequality constrained entries of $\mathbf{x}$

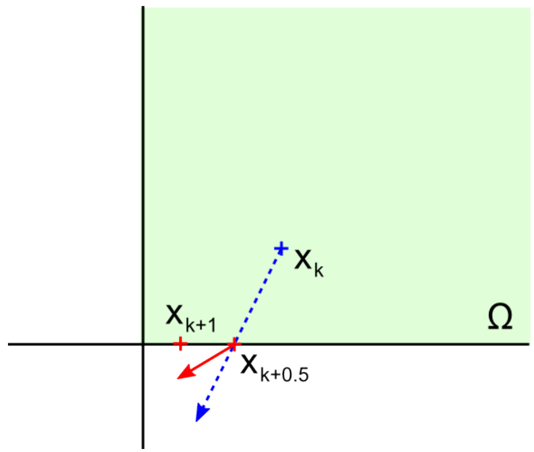
$$g_i^P = \begin{cases} g_i & \text{for} \quad x_i > l_i \ \vee \ i \notin M \\ \min(g_i, 0) & \text{for} \quad x_i = l_i \ \wedge \ i \in M \end{cases}$$

Dostál, Z.:
Optimal Quadratic Programming Algorithms,
Springer Optimization and Its Applications,
2009, ISBN 978-0387848051

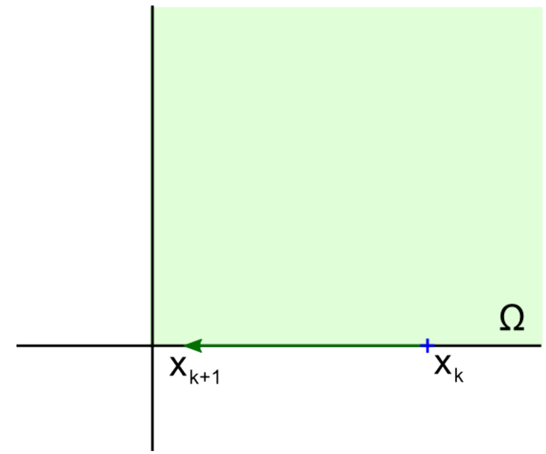
MPGP (Modified Proportioning with Gradient Projection)



CG-step



CG-halfstep
+ expansion step
- expand active set



optimal step on active set
(proportioning step)
- reduce active set

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Dostál Z., Pospíšil L.: Minimization of the quadratic function with semidefinite Hessian subject to the bound constraints, Computers and Mathematics with Applications, (2015).

MPGP (Modified Proportioning with Gradient Projection)

Choose $x_0 \in \Omega$, $\overline{\alpha} \in (0, 2/\lambda_{\max})$,
for $k = 0, 1, 2, \ldots$ **do** (while $\|g^P(x_k)\|$ is not small)
if $\|\varphi(x_k)\| >> \|\beta(x_k)\|$ (proportioning condition)
CG-step or *CG-halfstep*
- do CG-step for the solution of the problem on free set
- if this means leaving Ω,
do only feasible step, expansion step and restart CG

else
Proportioning step
- do optimal step to solve problem on active set, restart CG

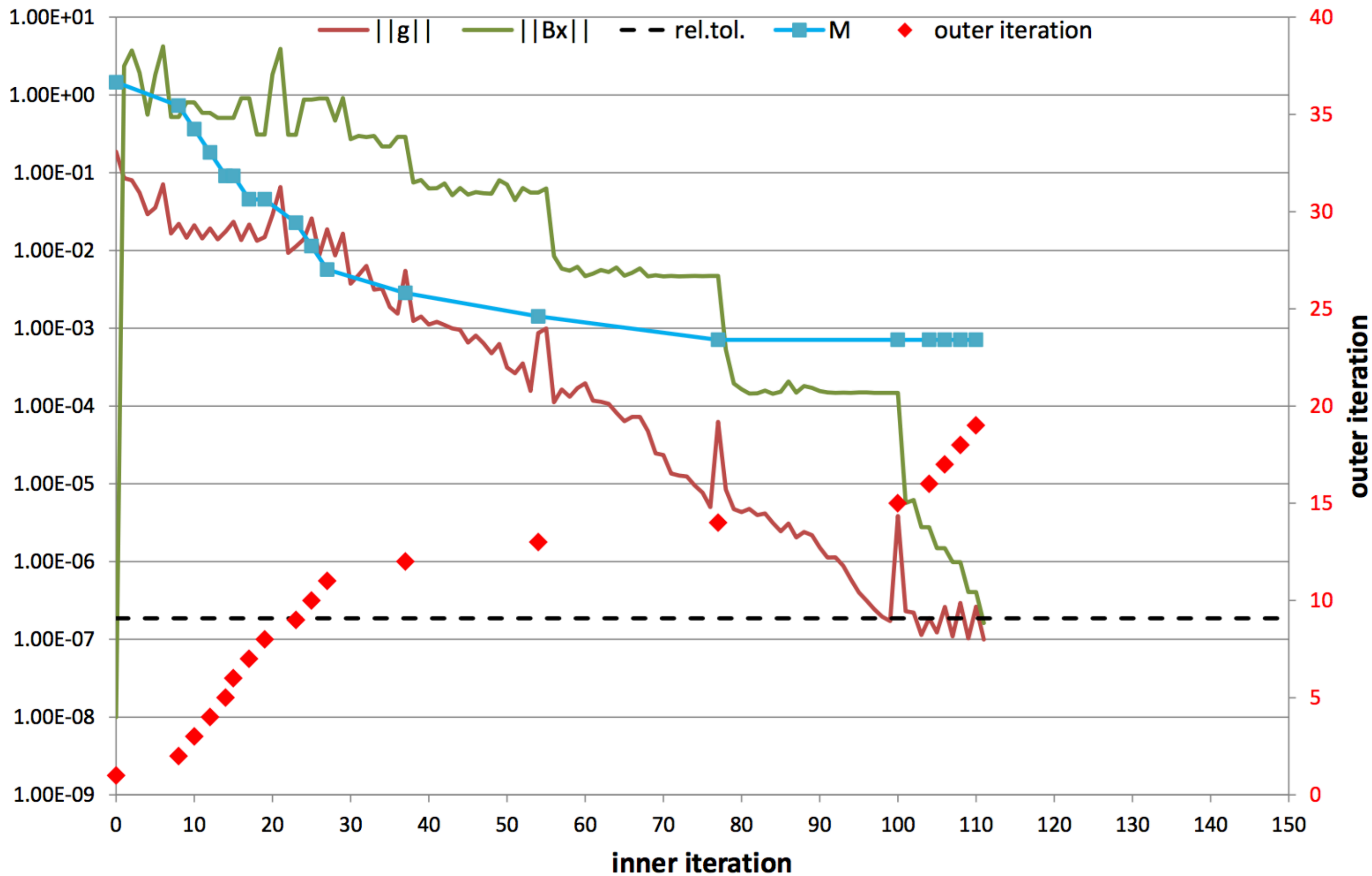
endif
$k = k + 1$
endfor
$\bar{x} \approx x_k$

Dostál Z., Pospíšil L.: Minimization of the quadratic function with semidefinite Hessian subject to the bound constraints, Computers and Mathematics with Applications, (2015).

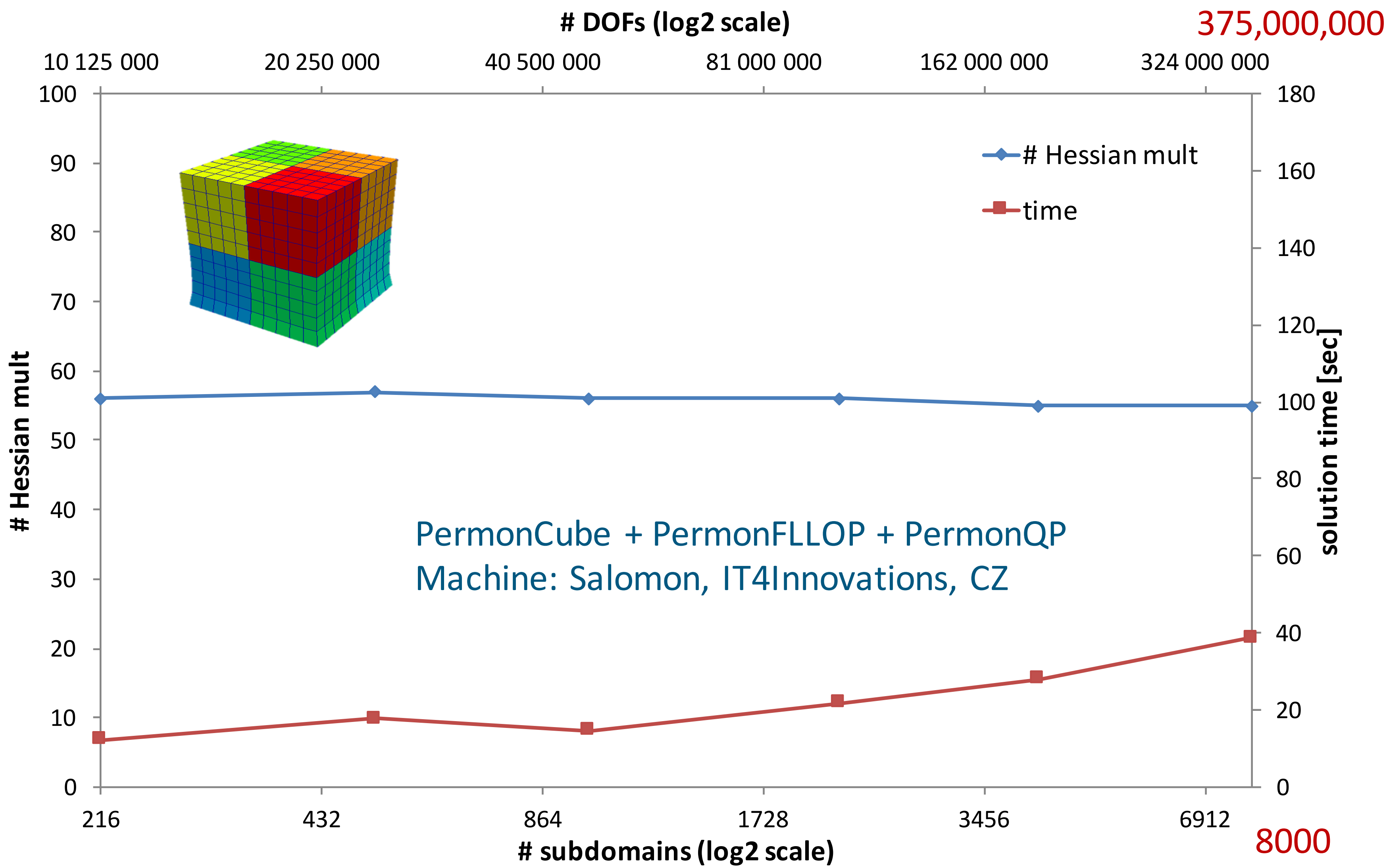
SMALXE+MPGP iteration progress

Inner stopping criterion: $\|\tilde{\mathbf{g}}^P\| \leq \min(M\|\mathbf{Bx}_k\|, \eta) \ \wedge \|\tilde{\mathbf{g}}^P\| < \varepsilon$

Start to increase penalty ρ by factor of 2 each outer iteration once $\|\tilde{\mathbf{g}}^P\| < \varepsilon$ is reached



Experiments – linear elasticity



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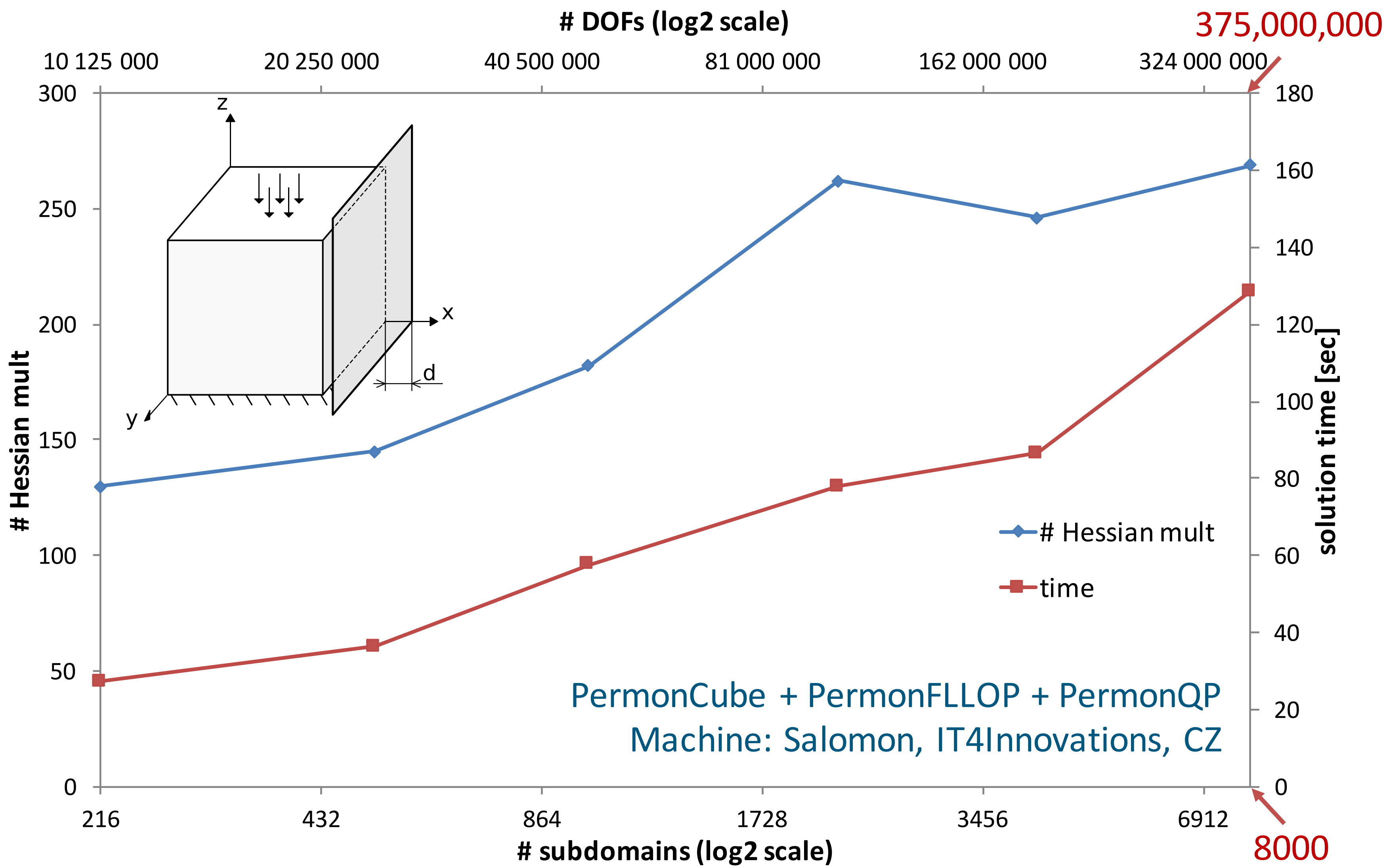
Experiments – contact elasticity



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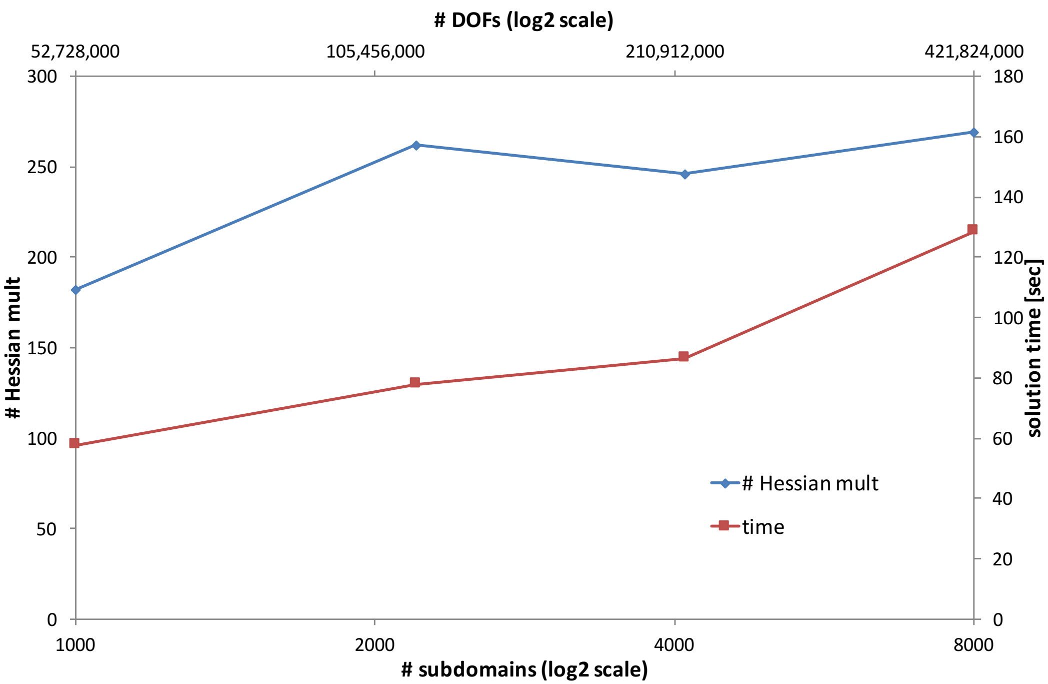
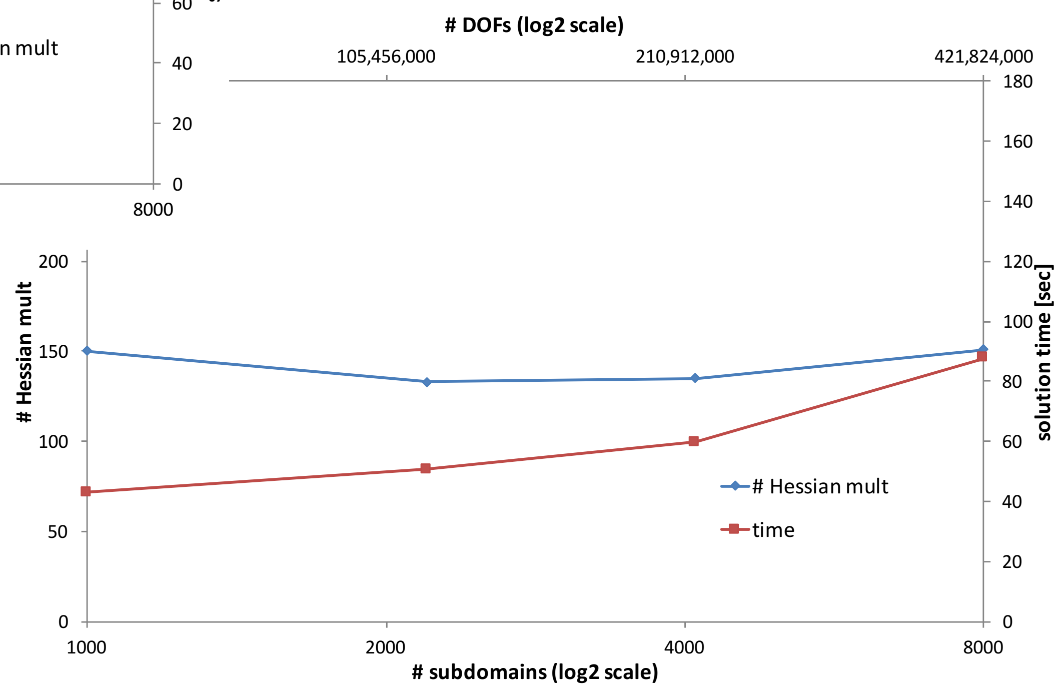
Very recent improvement



adaptive length
of expansion step
(computed yesterday)



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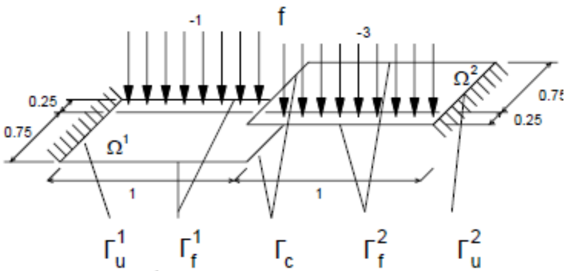
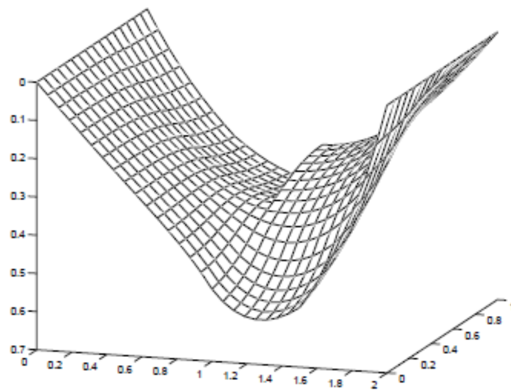
Coercive and semicoercive variational inequalities

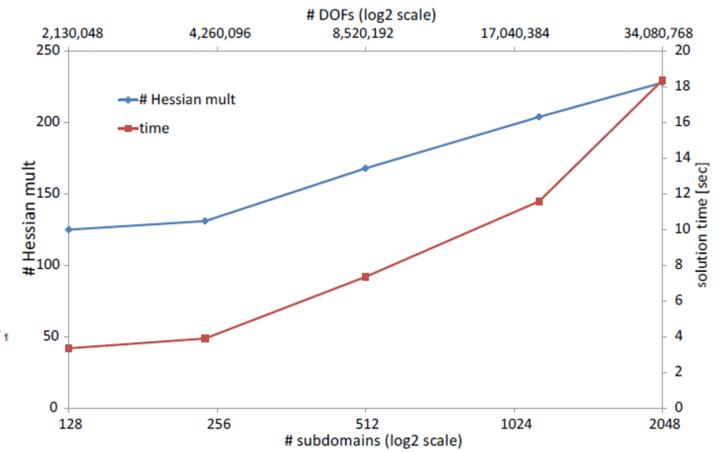
(older PERMON version)

Coercive membrane problem

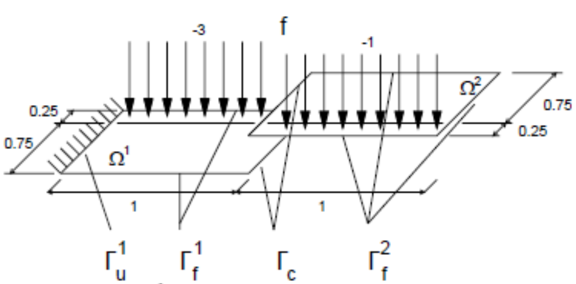


$$f(x,y) = \begin{cases} -1 & \text{for } (x,y)\ (0,1)\times[0.75,1) \\ 0 & \text{for } (x,y)\ (0,1)\times[0,0.75) \\ & \text{and } (x,y)\ (1,2)\times[0.25,1) \\ -3 & \text{for } (x,y)\ (1,2)\times[0,0.25) \end{cases}$$

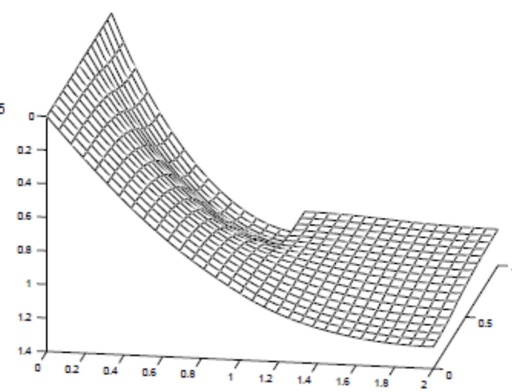


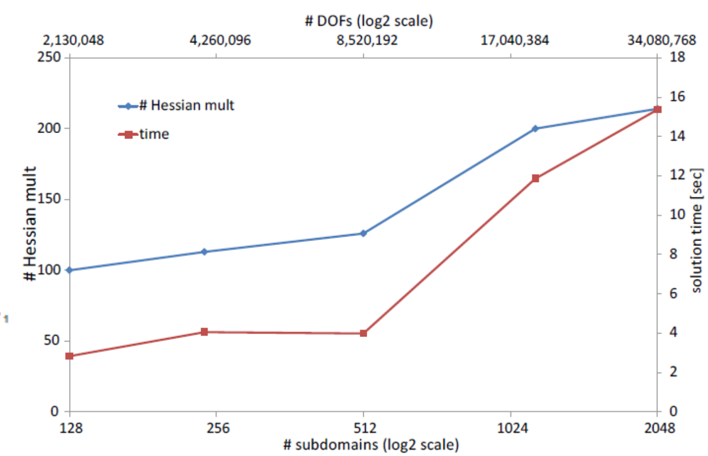


Semicoercive membrane problem



$$f(x,y) = \begin{cases} -3 & \text{for } (x,y)\ (0,1)\times[0.75,1) \\ 0 & \text{for } (x,y)\ (0,1)\times[0,0.75) \\ & \text{and } (x,y)\ (1,2)\times[0.25,1) \\ -1 & \text{for } (x,y)\ (1,2)\times[0,0.25) \end{cases}$$





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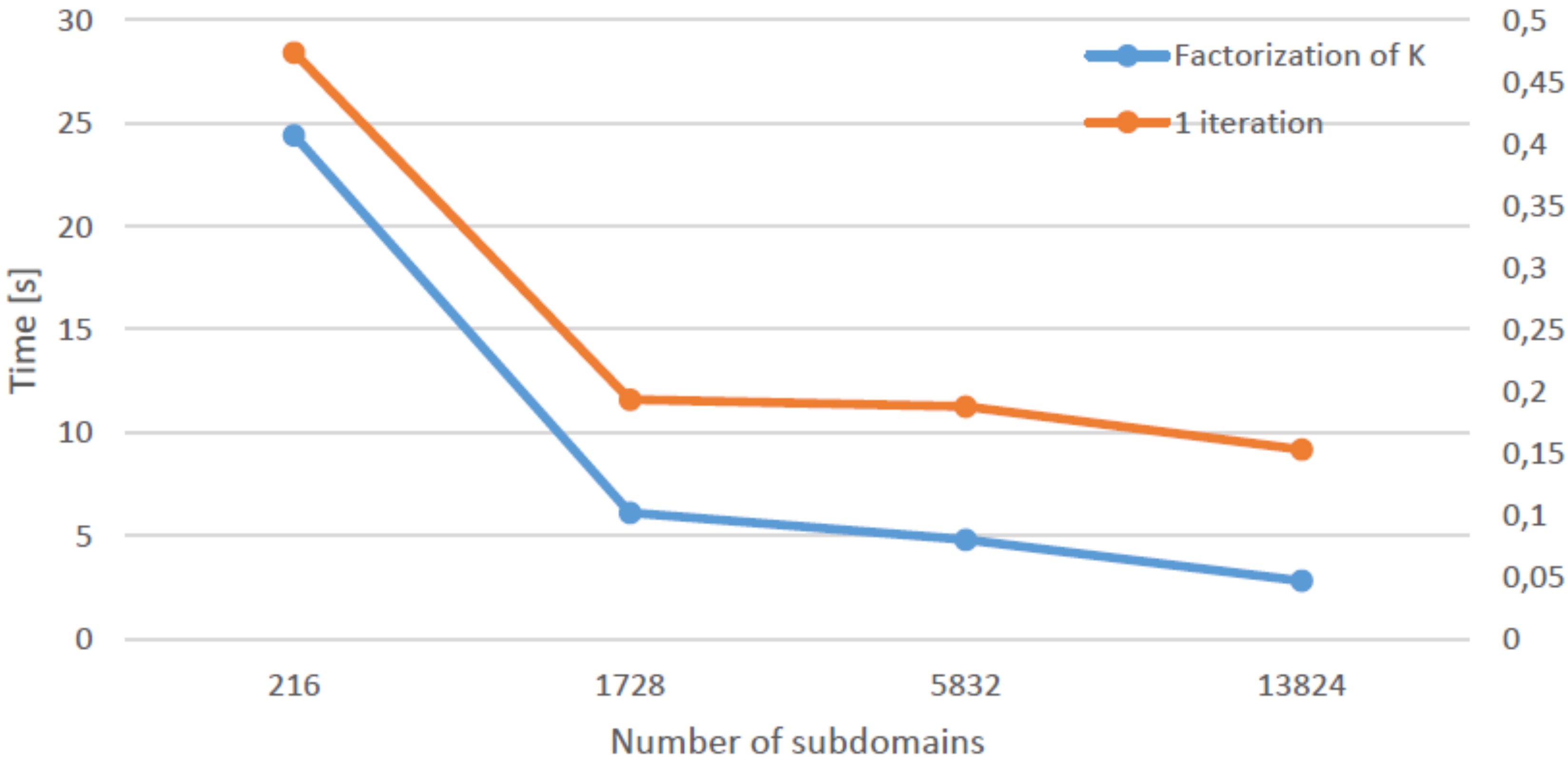
Experiments show

- **FETI DDM numerical scalability**
  - condition number is O(n) for constant local problems size n
- **parallel scalability** of PermonFLLOP's FETI implementation
- **SMALXE numerical scalability**
  - number of iterations given by Hessian spectrum
- **PermonQP** infrastructure does **not slow** it **down**

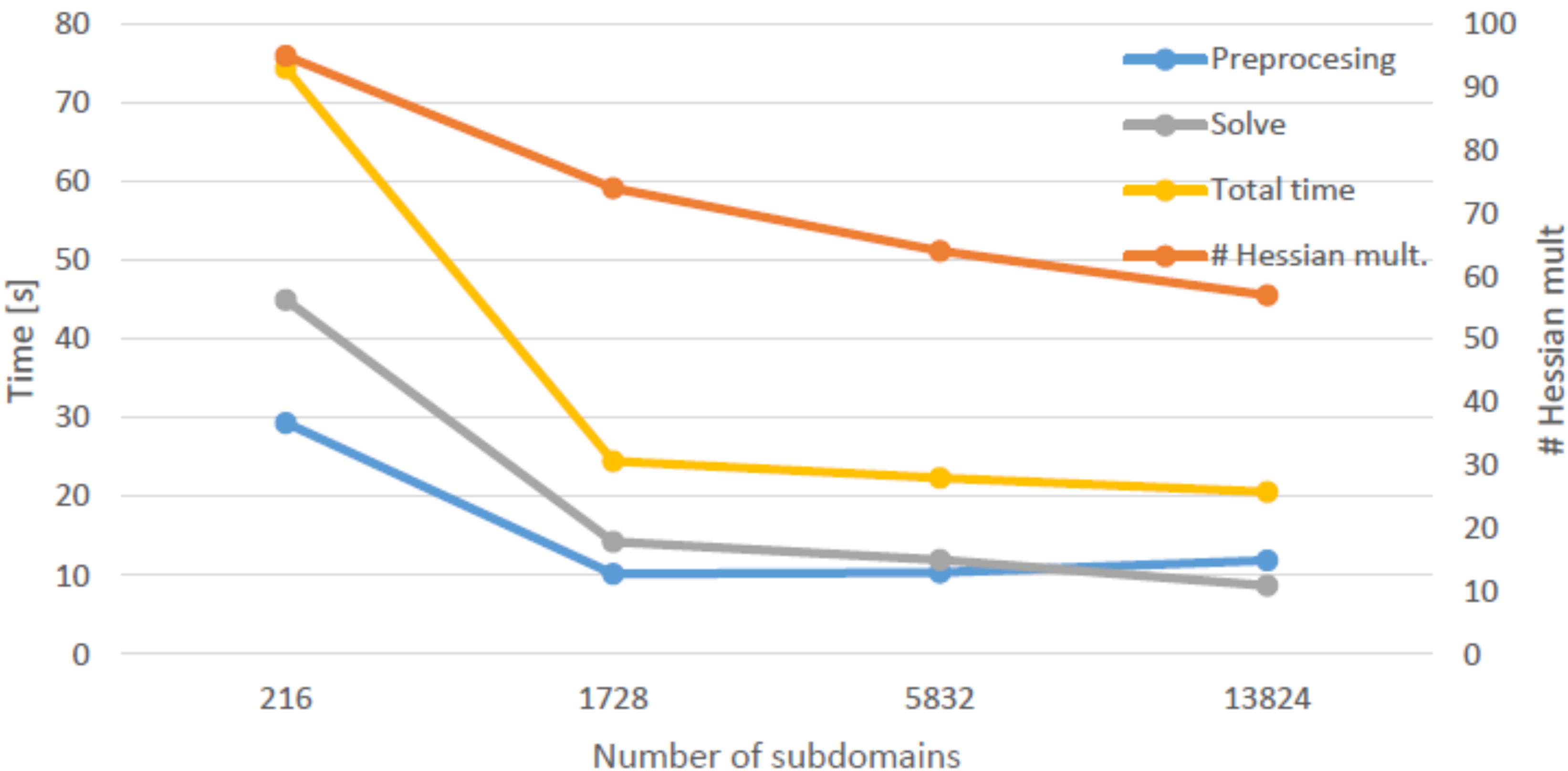
New feature: >1 subdomains per rank

- 216 MPI processes/cores
- cost of factorization and one iteration
- MUMPS



New feature: >1 subdomains per rank

- 216 MPI processes/cores
- time of setup phase and solve phase and total time
- effect of improving condition number



Bleeding edge

- optimized assembly and storage of mortar **B** matrices
  - support for non-conforming submeshes – hanging nodes at interfaces
- stiffness matrix kernel **R** black-box stochastic generation
- other applications of QP – *do you use some*?
  - support vector machines, data fitting, SQP, Proximal Bundle Method,…
- condensation of local problems
  - improve arithmetical density, accelerators
- real-world problems using existing FEM software
  - libMesh, FEniCS, Sifel, Elmer, ViennaMesh/Grid tools
- other QP algorithms – IP, semismooth Newton
- gitpublish under FreeBSD (2-clause BSD) license this year
  - merge separable convex constraints (QPC)
  - finish splitting into PermonQP and PermonFLLOP
  - basic documentation

Acknowledgements

READEX
Runtime Exploitation of Application Dynamism for Energy-efficient eXascale computing

The EXA2CT European Project (EXascale Algorithms and Advanced Computational Techniques)

EXA2CT

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Účinné metody odhadu životnosti pro obecné víceosé namáhání
(Efficient methods for life prediction for general multiaxial fatigue)
GA15-18274S

PRACE

MŠMT
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Additional acknowledgement

"Coffee-driven research"

1^{st} parallel machine @ IT4I *

* It is able to prepare 2 espressos in parallel.

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PERMON team @ IT4I
is your PETSc partner in Czechia ☺

Thank you for your attention!

Do you have any questions?

See you also at our poster.

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