# PERMON

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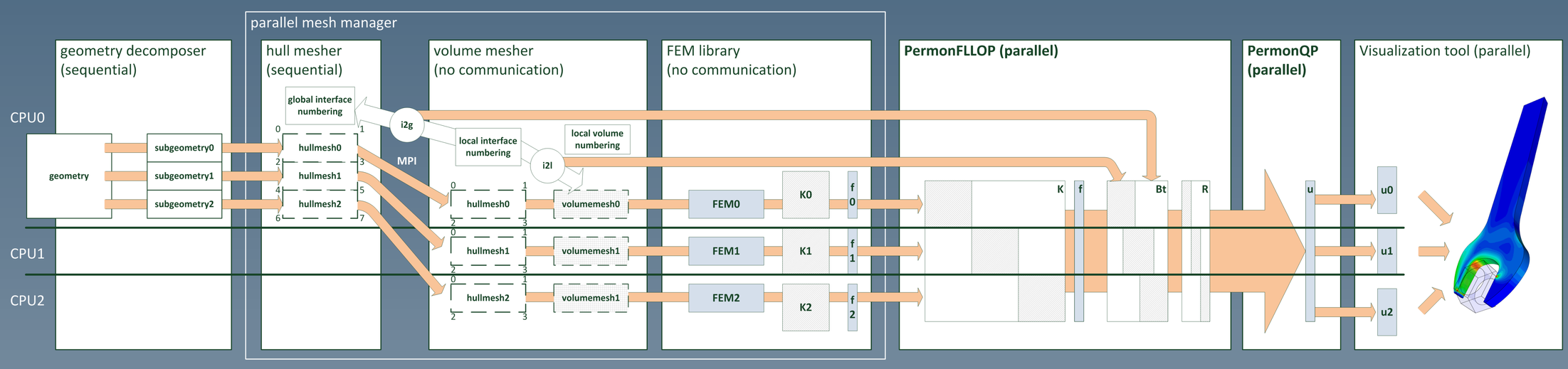
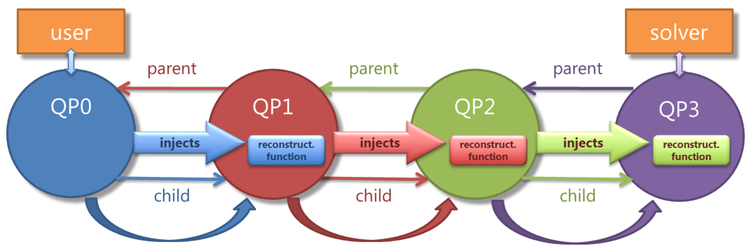
**Parallel, Efficient, Robust, Modular, Object-oriented, Numerical simulations**

- discretization methods
- domain decomposition methods
- linear system solvers
- quadratic programming solvers
- application-specific modules
- PETSc extension




## PermonQP

- framework and concrete solvers quadratic programming (QP)
- QP problems, transforms, solvers
- easy-to-use / HPC-oriented
- workflow
  1. QP problem specification
  2. QP transforms
  3. automatic/manual choice of an appropriate solver
  4. the solver is called




```
QP
QP parent, child; /* QP chain objects */
Vec x; /* solution */

Mat A; /* Hessian matrix */
Vec b; /* right-hand side */

Mat BE; Vec cE; /* linear equality constraints */
Vec lambdaE; /* equality Lagrange multipliers */

QPC constraint; /* inequality constraints */
```

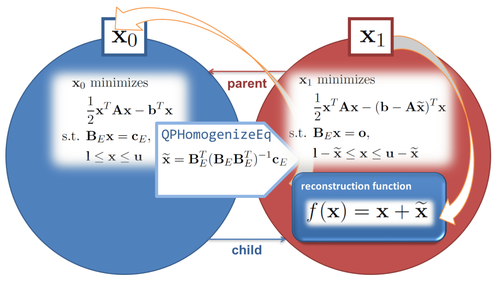
```
QPS
QP topQP, solQP; /* QP chain objects */
PetscReal rtol, atol, divtol; /* alg. tolerances */

PetscReal rnorm; PetscInt it; /* current state */
QPSMonitor monitor;
```

```
QPT
QPTDualize()
QPTEnforceEqByProjector()
QPTEnforceEqByPenalty()
QPTOrthonormalizeEq()
QPTHomogenizeEq()
QPTFetiPrepare()
```

$$\min_{\substack{l_b \le x \le u_b \\ B_{eq}x = c_{eq} \\ B_{ineq}x \le c_{ineq}}} \frac{1}{2}x^T Ax - x^T b$$

### Homogenization of equality constraints

- an example of QP transformation for problem




## PermonFLLOP

- extends PermonQP with domain decomposition methods of the FETI type
- problems without / with contacts
- scalability up to tens of thousands of CPU cores, billions of unknowns
- assembly of FETI-specific objects

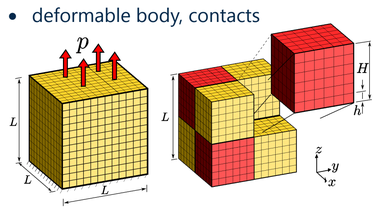
```
Mat Ks, BIs; Vec fs, cI, coords;
IS l2g, dbcis; MPI_Comm comm;
FLLOP fllop;

/*  generate the data */

/*  create FLLOP living in communicator */
FllopCreate(comm, &fllop);

/*  set the subdomain stiffness matrix and load vector */
FllopSetStiffnessMatrix(fllop, Ks);
FllopSetLoadVector(fllop, fs);

/*  set the local-to-global mapping for gluing */
FllopSetLocalToGlobalMapping(fllop, l2g);

/*  specify the Dirichlet conditions in the local numbering and tell FLLOP to enforce them by means of the B matrix */
FllopAddDirichlet(fllop, dbcis, FETI_LOCAL, FETI_DBC_B);

/*  set vertex coordinates for rigid body modes */
FllopSetCoordinates(fllop, coords);

/*  set the non-penetration inequality constraints */
FllopSetIneq(fllop, BIs, cI);

FllopSolve(fllop);
```

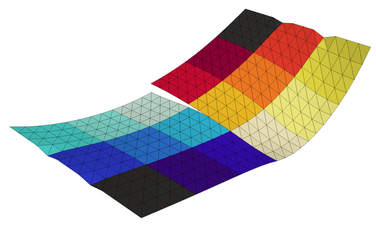
```
/* FllopSolve() function */

/*  subdomain data */
Mat Ks, BIs, Bgs, Bds, Rs;  Vec fs;
/* global data */
Mat K, BI, Bg, Bd, R;  Vec f, cI, cd;
/*  QP problem, QP solvers */
QP qp; QPS qps;

/*  create a QP data structure */
QPCreate(comm,&qp);

/*  Globalise the data. */
MatCreateBlockDiag(Ks,&K);
MatCreateBlockDiag(Rs,&R);
MatMerge(Bgs,&Bg); MatMerge(Bds,&Bd);
MatMerge(BIs,&BI); VecMerge(fs,&f);

/*  Insert the data into the QP. */
QPSetOperator(qp, K);
QPSetOperatorNullspace(qp, R);
QPSetRHS(qp, f);
QPAddEq(qp, Bg, NULL);
QPAddEq(qp, Bd, cd);
QPSetIneq(qp, BI, cI);

/*  Basic sequence of QP transforms
    giving (T)FETI method.
    QP chain is created in backend. */
QPTDualize(qp);
QPTHomogenizeEq(qp);
QPTEnforceEqByProjector(qp);

/*  Create a PermonQP solver. */
QPSCreate(comm, &qps);

/* Set the QP to be solved. */
QPSSetQP(qps,qp);

/*  Solve, i.e. hand over to PermonQP.
    The last QP in the chain is solved. */
QPSSolve(qps);
```

## PermonCube

## PermonMembrane

- benchmark generation - mesh with billion of unknowns in parallel over the cubical or membrane domain
- FEM assembly
- deformable body, contacts

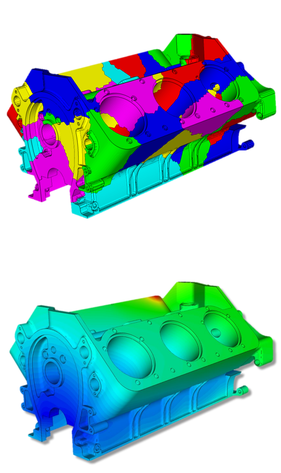


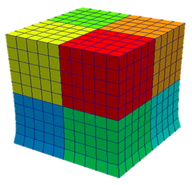



## Numerical experiments

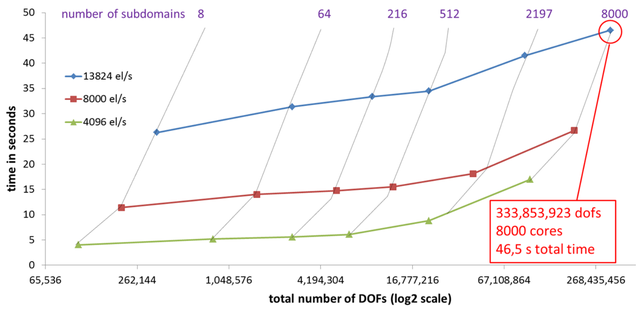
- realistic linear elasticity problem
- displacement computed
- boundary conditions prescribed in one cylinder
- quadratic tetrahedral elements with midnodes
- METIS mesh decomposition
- benchmark prepared by Tomáš Brzobohatý (IT4Innovations)

| | | | |
|---|---|---|---|
| **# DOF** | 98,214,558 | | |
| **# constraints (dual dim.)** | 13,395,882 | | |
| **# subdomains = # cpus** | 5,012 | | |
| **# CG iter.** | 181 | | |
| **computer** | HECToR | CURIE | Hermit |
| **total setup time** | 28 s | 64 s | 30 s |
| **total solution time** | 233 s | 283 s | 283 s |

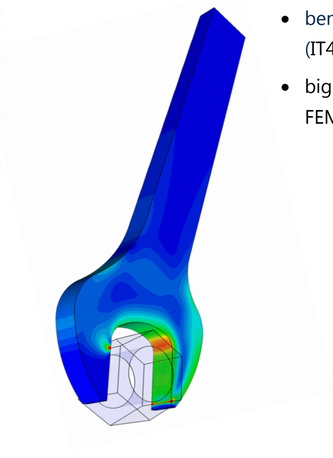




- linear elasticity problem
- problem generated using PermonCube
- computed on HECToR (EPCC)

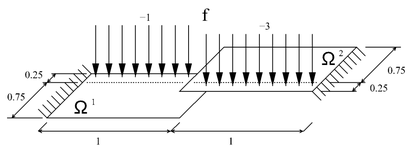


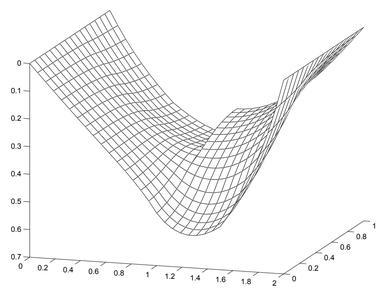

- realistic elasticity problem with contact
- displacements computed
- gluing and non-penetration constraints
- METIS mesh decomposition
- benchmark prepared by Tomáš Brzobohatý (IT4Innovations)
- bigger problems currently limited by the FEM implementation, work in progress

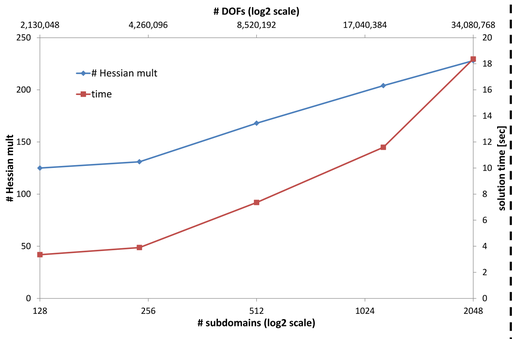


| | |
|---|---|
| **# DOF** | 193,227 |
| **# constraints (dual dim.)** | 24380 |
| **# subdomains = # cpus** | 39 |
| **# outer SMALSE iter.** | 12 |
| **# inner MPRGP iter.** | 588 |
| **computer** | Salomon |
| **total setup time** | 0.5 s |
| **total solution time** | 24.4 s |

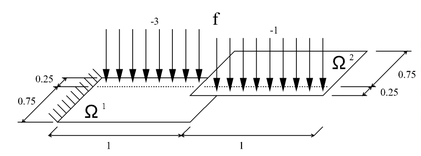
### Coercive membrane problem

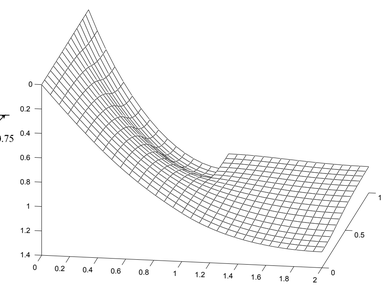


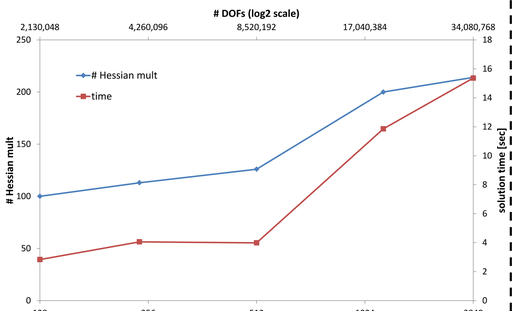





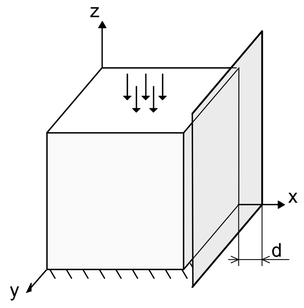

### Semicoercive membrane problem

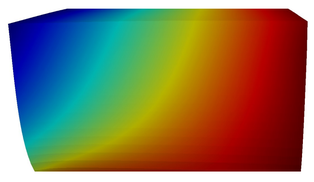


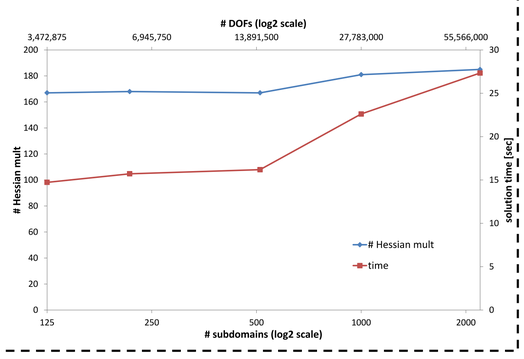



### Elastic cube in potential contact with obstacle



computed on Archer (EPCC)

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

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