PERMON toolbox combining discretization, domain decomposition, and quadratic programming

[Extended Abstract]

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ABSTRACT

Quadratic programming (QP) problems result e.g. from certain methods in image processing or particle dynamics, or finite element discretization of contact problems of mechanics.

Domain decomposition methods solve an original large problem by splitting it into smaller subdomain problems that are almost independent, allowing naturally massively parallel computations on supercomputers.

We are mostly interested in combining non-overlapping DDMs, namely FETI (Finite Element Tearing and Interconnecting), with optimal QP algorithms. FETI combines both iterative and direct solvers and allows highly accurate computations scaling up to tens of thousands of processors.

Due to limitations of commercial packages, problems often have to be adapted to be solvable and it takes a long time before recent numerical methods needed for HPC are implemented into such packages. These issues lead us to establish the PERMON (Parallel, Efficient, Robust, Modular, Object-oriented, Numerical) toolbox.

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Categories and Subject Descriptors

G.1.3 [**Numerical Analysis**]: Numerical Linear Algebra—*linear systems (direct and iterative methods)*; G.1.6 [**Numerical Analysis**]: Optimization—*quadratic programming methods*; G.1.8 [**Numerical Analysis**]: Partial Differential Equations—*domain decomposition methods*; G.4 [**Mathematical Software**]: Miscellaneous

Keywords

PERMON, PermonQP, PermonFLLOP, quadratic programming, domain decomposition methods, FETI

1. INTRODUCTION

The **PERMON** toolbox makes use of theoretical results in discretization techniques, quadratic programming (QP) algorithms, and domain decomposition methods (DDM). It incorporates our own codes, and makes use of renowned open source libraries. We focus on engineering applications (linear elasticity, contact problems with friction, elasto-plasticity, shape optimization and others) as well as altruistic ones (medical imaging, image processing, ice-sheet melting modelling, climate changes modelling, multi-body simulations, and others). The combination of DDM and QP algorithms is what makes **PERMON** unique.

PERMON consists of autonomous modules forming several layers:

- problem-specific modules - **PermonPlasticity**, **PermonMultiBody**, **PermonImage**, etc.
- discretization modules - **PermonCube** and interfaces with external libraries
- solver modules - **PermonQP** abd **PermonFLLOP**

- utility modules

The core solver layer of **PERMON** depends on PETSc [2, 1] and uses its coding style. It is formed by the **PermonFLLOP** and **PermonQP** modules. The QP problem reads

$$\min_{x \in \Omega} \frac{1}{2} x^T A x - b^T x$$

where $A \in \mathbb{R}^{n,n}$ is symmetric positive (semi)definite matrix, $b \in \mathbb{R}^n$, and $\Omega \subset \mathbb{R}^n$ is feasible set described by the combination of linear equality constraints and separable convex inequalities.

2. PERMONQP

PermonQP is a package providing a framework as well as concrete solvers for solution of QP problems. It separates QP problems, transforms and solvers. Its API is carefully designed to be easy-to-use, and at the same time efficient and suitable for HPC. The poster provides the solution process from the user's point of view.

The package allows solving unconstrained QP problems (i.e. linear systems with a positive semidefinite matrix) and equality constrained ones. In both cases it makes use of the **PETSc KSP** package which includes both direct and iterative solvers, including interfaces to many external solvers.

Special algorithms for solution of box constrained QP problems (**PermonIneq**) are also included. The QPC class enables solution of problems with more general separable convex inequality constraints. It supports feasible sets described by bound, box, quadratic, elliptic, and/or conical constraints. These are motivated e.g. by contact problems with friction. Currently, the package contains implementations of the following QP algorithms [4, 14, 7, 3]

- MPRGP (Modified Proportioning with Reduced Gradient Projections),
- SPG-QP (Spectral Projected Gradient method for QP problems),
- PBBf (Projected Barzilai-Borwein method with fallback),
- APGD (Accelerated Projected Gradient Descent method).

The QP transformation Dualize transforms original problem to new one with better properties and simpler (bound) inequality constraints. Solvers include special "pass-through" solver SMALXE (generalization of SMALBE [5, 4]) which takes care of equality constraints, which "filtered-out" and moved to the Hessian matrix. An auxiliary problem is then solved by an arbitrary inner solver compatible with the rest of constraints.

All these ingredients together form a powerful tool for solution of any kind of QP in a slightly generalized sense (QPQC), and an alternative to interior point methods.

3. PERMONFLLOP

PermonFLLOP is an extension of **PermonQP**, implementing the algebraic part of DDM of the FETI type [9, 8, 6, 11, 10, 12, 15].

In the poster, we present our recent numerical results in solution of large-scale linear elasticity problems. We demonstrate efficiency of our algorithms and their implementations on academic benchmarks generated using the PermonCube package and on benchmarks with realistic geometries. We are interested in problems with either permanent or potential contact between bodies. The latter are much harder to solve.

At the moment, **PermonFLLOP** and **PermonQP** are being prepared for publishing under an open source license. Let us mention that open source DDM and QP codes are relatively rare and we hope the codes will be of interest for community of PETSc and related libraries such as FEniCS.

4. PERMONPLASTICITY, PERMONIMAGE, PERMONMULTIBODY

Our poster presents results from three selected problem-specific modules which form "adapters" from problem-specific inputs to QP formulation.

- **PermonPlasticity** solves plasticity (contact) problems. A pseudo-time stepping schema is exploited and systems of non-linear equations are solved by Newton method. This approach generates a sequence of QP problems.
- **PermonMultiBody** is a package for numerical simulations of rigid-body motion. The Newton laws are discretized by Euler method. To determine contact forces in every time-step, a QP problem with bound constraints has to be solved. Moreover, if we consider problems with friction, we obtain QP with separable conical constraints.
- **PermonImage** includes specific methods for image registration [13], reconstruction, and segmentation.

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