Report on the Doctoral Thesis of Ing. Václav Hapla:
Massively Parallel Quadratic Programming Solvers with Applications in Mechanics

To Whom It May Concern,

This thesis covers important and highly relevant aspects of a parallel solution method for large-scale partial differential equation (PDE)-based problems in the area of, but not limited to, mechanical engineering. The particular motivation is to increase the numerical and parallel scalability which both are of utmost importance considering the ever-growing demand for numerical accuracy, complexity, and speed. The thesis topic is well chosen and fits perfectly to today’s research challenges in computational science and engineering for large-scale PDE-based problem solving.

The author tackles these issues by investigating quadratic programming (QP) algorithms in conjunction with domain decomposition methods (i.e. total finite element tearing and interconnecting - TFETI), in particular focusing on utilizing supercomputers and available open source software tools to minimize the implementation efforts.

The Introduction adequately sets the stage for the dissertation by discussing the general need to describe problems via PDEs in mechanical engineering. The finite element method (FEM) is correctly identified as the primary method of choice to discretize the required PDEs. Certain constrained problems lead to nonlinear optimization problems, which in turn gives rise to quadratic programming problems. Further challenges, approaches, and application areas of quadratic programming are highlighted as is the need for utilizing large-scale parallel computing resources, such as supercomputers, to stem the ever-growing computational complexity driven by increased accuracy and reduced time-to-result demands. Domain decomposition is introduced; in particular, the thesis’ primary utilized method called total TFETI. The PERMON toolbox is introduced using established open source software packages to implement the developed quadratic programming approaches based on TFETI.

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The remainder of the thesis is split into two parts, where the first focuses on the background (i.e. quadratic programming, TFETI, and implicit orthonormalization), the second discusses implementation aspects (i.e. overview of relevant open source software packages, PERMON toolbox, and numerical experiments based on PERMON).

Chapter 1 gives a detailed yet concise overview of relevant aspects of quadratic programming. The relevant spectrum of theoretical foundations is covered, ranging from mathematical optimization, to its subfield of quadratic programming, zero-sized matrices, Karush-Kuhn-Tucker (KKT) optimality conditions, partially bound quadratic programming, evaluating KKT conditions, and computation of Lagrange multipliers. All topics are appropriately described and enable a proper foundation for the subsequent chapters.

Chapter 2 introduces QP transforms, motivated by the promise that the derived QP is simpler to solve. QP transforms are at the core of QP solvers and thus form a key aspect of the presented research. More concretely, the chapter covers inline notations of QP problems and discusses several QP transforms.

Chapter 3 covers two key QP algorithms, i.e., MPRGP and SMALBE. Based on the presentation of the original ideas, shortcomings of the SMALBE-M algorithm are clearly identified, highlighted by figures, and resolved via a penalty update scheme and by limiting the number of outer iterations.

Chapter 4 discusses the TFETI domain decomposition method. The motivating factor of domain decomposition, being parallelism, is highlighted. The mathematical challenge of such a method is, among others, to ensure the correctness of the solution when tearing and separated solving is used (continuity of the solution across subdomains). The general approach of (T)FETI is discussed as well as a new approach to handle it, i.e., via a chain of QP transforms. An adequately proportioned discussion on related work is given, allowing for an appropriate overview of the field.

Chapter 5 introduces a novel method for the highly parallel solution of variational inequalities with equality constrains using augmented Lagrangian methods. The initial challenge, potential insufficient options as well as the solution is well stated and backed-up by corresponding mathematical derivations.

Chapter 6 gives an extensive overview of relevant open source libraries in the area of: Mesh generation tools, graph partitioning tools, FEM libraries, toolkits for numerical computations, parallel sparse direct linear solvers, and QP solvers. Short descriptions of the software packages are provided, enabling a good overview of the broad field of open source scientific software in science and engineering relevant to the chosen field of application.
Chapter 7 introduces the core of the dissertation, the PERMON toolbox, which is a collection of software libraries which not only aims to combine QP algorithms and domain decomposition methods but also to decouple the development into separate packages. The latter is especially important to foster re-use in other application areas and to avoid monolithic software packages, which would not favor maintainability in the long run – an aspect especially problematic in the unsteady personnel climate in academia. In general, PERMON uses the well-known PETSc framework, allowing PERMON itself to focus on novel additions, i.e., QP algorithms, domain decomposition methods, and application-specific aspects. PERMON has been primarily developed in the context of mechanical engineering applications. The core of PERMON is the so-called "solver core", which consist of PermonFLOP and PermonQP. PermonFLOP provides the FETI-based domain decomposition. The strong advantage of the developed approach is the decoupling from a specific mesh/FEM library: The architecture is such that any software tool can provide the relevant data. In turn, PermonQP is a general purpose QP solver; the application of which is thus not limited to the context of mechanical engineering (and PERMON in particular) but can be used in vastly different application areas, such as data fitting or least-squares regressions. Aside from these generic solver modules, application-specific solver modules are available (e.g. PermonPlasticity) as well as discretization tools (e.g. PermonMembrane) and support modules. From this high degree of modularity in combination with clearly defined interfaces it is obvious that the developed modules will allow for a high degree of reusability and maintainability. As already mentioned, those are very important aspects and will allow the utilization of the developed tools in other maybe even yet-unforeseen areas. In general, the chapter discusses in detail all relevant aspects to realize the proposed methods. Code examples as well as graphical visualizations make a good job in conveying the authors ideas and approaches.

Chapter 8 provides benchmarking results of various aspects of PERMON as well as actual applications to real-world problems. The supercomputers used to generate the results and evaluate the proposed solution methods provided by the PERMON toolbox. Comparisons of established sparse direct solvers are provided and discussed as well as test applications to evaluate the approaches. The chapter is concluded with more practical applications, using a spanner and a car engine geometry. The presented results show that the developed approaches hold up to the initial promise of large-scale application.

The dissertation is concluded with a summary of the conducted research work and an outlook. The incredibly challenging task of mapping mathematical theory to scalable numerical simulation code is highlighted – a central aspect of computational science and engineering. Without efforts in this area, like the ones conducted by Mr. Hapla, research progress would be significantly impeded.
Conclusion

The outlined problems and their solutions are presented in a clear manner. The dissertation is well-balanced, both with respect to extent and scientific depth. In particular, the importance of utilizing available and matured open source scientific software tools (an aspect easily ignored or overlooked but so very important to keep up with the astonishing pace of today’s fast progressing research in science and engineering) has been underlined and applied in the research work, which enabled Mr. Hapla to focus on the investigation of novel large-scale solution algorithms for PDE-based systems. This ultimately culminated in the creation of the PERMON toolbox. The references are timely and cover well the state-of-the-art. Mr. Hapla has received several prizes for his achievements, clearly underlining the success of his research. Several papers in the context of this thesis have been presented at conferences and published in scientific journals/books (especially noteworthy is the poster at the very prestigious Supercomputing’15 conference). Mr. Václav Hapla has convincingly demonstrated his ability for independent scientific work.

I recommend the thesis for defense.

Suggested grade       A / 1 / Excellent

Sincerely,

[Signature]

Josef Weinbub