An Inertia Revealing Preconditioning Method For Large-Scale Nonconvex PDE-Constrained Optimization

Olaf Schenk
Department of Computer Science, University of Basel
Klingelbergstr. 50, 4056 Basel, Switzerland
olaf.schenk@unibas.ch

We propose an inertia revealing preconditioning approach for the solution of nonconvex PDE-constrained optimization problems. If interior methods with second-derivative information are used for these optimization problems, a linearized Karush-Kuhn-Tucker system of the optimality conditions has to be solved. The main issue addressed is how to ensure that the Hessian is positive definite in the null-space of the constraints while neither adversely affecting the convergence of Newton's method or incurring a significant computational overhead. In the nonconvex case, it is of interest to find out the inertia of the current iteration system so that the matrix may be modified a posteriori to obtain convergence to a minimum. However, in order to not destroy the rapid convergence rate of the interior method, the modification has only be performed in the cases where the inertia is not correct and factorization methods are very often used in order to compute the inertia information [3, 6]. However, in this work we propose a new inertia revealing preconditioned Krylov iteration to solve the linearized Karush-Kuhn-Tucker system of optimality conditions.

The generally most efficient methods for solving large scale nonlinear programming problems are of Newton type, including sequential quadratic programming methods for equality and inequality constrained problems as well as primal and primal-dual interior point methods for inequality constrained problems. Common to these methods is that they exploit second order information, which usually leads to superlinear local convergence towards some local minimum. The downside is, that in general the methods do indeed converge only locally. Thus, globalization techniques have to be designed unless a sufficiently good starting iterate is provided. Stepsize damping can enlarge the domain of convergence considerably. It is, however, limited to convex problems, since otherwise the Newton direction — if it exists in the first place — may point upwards, and convergence to arbitrary critical points, including maxima, can occur.

For general nonconvex nonlinear programming problems it is therefore of utmost importance to modify the method in such a way that no ascent steps are taken and finally to check that the delivered solution is indeed a local minimum. For both tasks it is necessary to compute the inertia of the Karush-Kuhn-Tucker system of the optimality conditions, which is relatively easy using direct factorization methods. For very large scale problems, in particular discretized 3D partial differential equations, direct factorizations are prohibitively expensive both in terms of computing time and storage requirements. How to reliably obtain the inertia from iterative methods, however, is essentially an open problem.

We propose an algebraic multilevel preconditioning technique using maximum weighted matchings [1, 5] for revealing the inertia to be used in a primal interior point method [7]. Our preconditioning approaches for the symmetric indefinite Karush-Kuhn-Tucker systems are based on maximum weighted matchings and algebraic multi-level inverse-based incomplete LBL^T factorizations [4, 2]. We present numerical results on several large-scale three-dimensional examples of PDE-constrained optimizations in the full space of states, control and adjoints variables with equality and non-equality constraints and test them with artificial as well as clinical data from biomedical cancer hyperthermia treatment planning. The largest nonconvex optimization problem from three-dimensional PDE-constrained optimization with the inertia revealing preconditioning approach has more than one million control state variables and one million state variables with both lower and upper bound.

The beneficial impact of the method is finally demonstrated on a biomedical application. Hyperthermia treatment planning (HTP) is an important therapeutical option in biomedical cancer medicine. Hyperthermia is a promising, relatively new method to treat various types of cancer by heating the tumor, thereby inducing preferential apoptosis of cancerous cells. In patient therapy planning, the therapeutically optimal antenna parameters for the applicator are determined for each patient. The specific absorption rate values are obtained by solving the Maxwell equations, and the temperature distribution

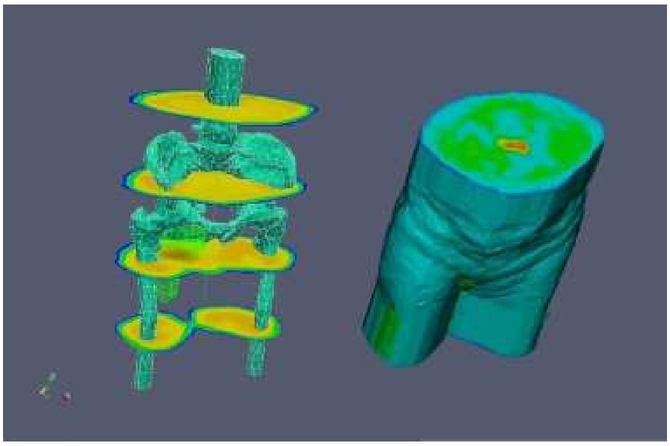

Figure 1: Inertia revealing optimal control in nonconvex PDE-constrained optimization of biomedical hyperthermia cancer treatment planning.

is predicted by variants of the bio-heat transfer equation. Although this can be a demanding task, a planning tool greatly improves the medical treatment quality with a "virtual experiment", i.e. to model, simulate and optimize the therapy in great detail and with high precision.

Optimal hyperthermia can be formulated as a nonlinear optimization problem, in which the Maxwell equations appear as additional constraints — a mathematical task known as *PDE-constrained optimization*. It refers to the optimization of systems governed by partial differential equations (PDEs). The *simulation problem* involves solving the PDE for the temperature distribution, given the patient geometry. The *constrained optimization problem* seeks to determine the temperature distribution given performance goals in the form of an objective function and possibly (in-)equality constraints. Since the temperature distribution is modeled by a PDE, it appears as equality constraints in the optimization problem. Solving the PDE constrained optimization problem presents significant challenges and is a frontier problem in combinatorial scientific computing.

This is joint work with Andreas Wächter (IBM Research, Yorktown, US) and Martin Weiser (Konrad-Zuse Institute, ZIB, Berlin, Germany)

References

[1] I. S. Duff and S. Pralet, *Strategies for scaling and pivoting for sparse symmetric indefinite problems*, SIAM J. Matrix Analysis and Applications, 27 (2005), pp. 312–340.

[2] M. Hagemann and O. Schenk, *Weighted matchings for the preconditioning of symmetric indefinite linear systems*, SIAM Journal of Scientific Computing, 28 (2006), pp. 403–420.

[3] *Harwell Subroutine Library, AEA Technology, Harwell, Oxfordshire, England catalogue of subroutines*, 2004.

[4] O. Schenk, M. Bollhöfer, and R. Römer, *On large-scale diagonalization techniques for the Anderson model of localization*, SIAM Journal of Scientific Computing, 28 (2006), pp. 963–983.

[5] O. Schenk and K. Gärtner, *On fast factorization pivoting methods for symmetric indefinite systems*, Electronic Transaction of Numerical Analysis, 23 (2006), pp. 158–179.

[6] O. Schenk, A. Wächter, and M. Hagemann, *Matching-based preprocessing algorithms to the solution of saddle-point problems in large-scale nonconvex interior-point optimization*, Journal of Computational Optimization and Applications. To appear, http://www.maths.ed.ac.uk/ gondzio/coapLAIPM/Welcome.html.

[7] A. Wächter and L. T. Biegler, *On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming*, Tech. Rep. RC 23149, IBM T.J. Watson Research Center, Yorktown Heights, USA, March 2004. To appear in Mathematical Programming.