A reduced Sequential Quadratic Programming method for large systems exploiting existing simulators

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The optimisation of real industrial systems is a formidable task, mainly because of the complexity of the models that are employed for the simulation of those systems. Those models typically consist of, or include, sets of Partial Differential Equations (PDEs) which are discretized over a computational mesh resulting in a large scale lumped system. For the solution of such systems of equations direct or iterative methods can be employed, the latter being more efficient as the size of the system increases. The simulators' technology has advanced significantly in recent times. It is safe to claim that for most processes, there are simulators available which are both computationally efficient and approximate the physics of the problem very well. The simulators delineated may either be open source (e.g. home-made) or input/output (e.g. commercial) and can be exploited for optimisation, using either deterministic, or stochastic/meta-heuristic methods. Stochastic methods are more suitable for moderate-sized problems [1], as they typically include a large number of function evaluations, i.e. system simulations. On the other hand, deterministic methods require a lot more information (usually Jacobians and sensitivities) which are usually not made available to the user in the case of commercial simulators. This renders the task at hand problematic or unrealistic. Even if those difficulties are surmounted, the obstacle of most deterministic optimisation methods having increased requirements in computing power and memory size remains.

We have recently developed a model reduction-based framework for steady-state [2] and dynamic [3] deterministic optimisation using input/output dynamic simulators. In this work we extend this methodology by presenting a novel optimisation algorithm that employs black-box steady-state simulators based on solvers using iterative linear algebra methods. It follows the nested analysis and design (NAND) approach, thus it allows the use exploitation of state-of-the-art simulators for finding feasible points. The proposed technique is a reduced Hessian one [4] and includes only low-dimensional Jacobian and reduced Hessian matrices. Those are adaptively computed using a basis which corresponds to the dominant modes of the system, calculated through subspace iterations. The reduced Jacobian matrices are computed through a few numerical perturbations to the direction of the dominant modes of the system, whereas the reduced Hessian matrices are computed according to a 2-step projection scheme, firstly onto the dominant subspace of the system and secondly onto the subspace of the independent variables. In this context, inequality constraints can be handled either by introducing slack variables, or by aggregating the inequality constraints in a conservative fashion and incorporating them in the objective function

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following the KS approach [5]. In both cases it actually is projections of the inequality constraints onto the dominant subspace that are used. However the KS approach leaves the most expensive part of the algorithm, updating of the basis of the aforementioned eigenspace, unmodified. Hence it is more efficient than the slack variable-based one, although not as precise.

The performance of the proposed algorithm, as well as its efficiency in handling large-scale input/output simulators is demonstrated through illustrative realistic applications using the state-of-the-art massively parallel finite element code MPSALSA developed at SANDIA National Laboratories [6] and the commercial package FLUENT [7]. We discuss the convergence of the proposed framework and its efficiency in handling equality and inequality constraints by presenting comparative case studies.

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