Optimization Under Uncertainty for Magnetic Confinement Fusion

D. Kouri, D. Ridzal, and B. van Bloemen Waanders* (Sandia National Laboratories)†
S. Uryasev (University of Florida)

April 27, 2015

Motivation. Considerable effort is devoted to improving numerical predictive capabilities for magnetic confinement fusion with the ultimate goal of designing and controlling reactors to realize the full potential and economic viability of fusion energy. A succesful reactor design and operating process will be challenged by many complexities, including micro-turbulence, instabilities (Alfvén and MHD modes), tearing phenomena, dynamical interactions between different spatial scales, and operating disruptions (sawtooth and edge localized modes causing erosion) [10]. Aside from the challenges associated with continuously improving our phenomenological models, additional challenges arise when solving optimal reactor design and control problems. First, the overall computational requirements for forward simulations are significant, the success of which is pinned on future computational architectures. Optimal design and control problems will further increase this cost. Second, the number of design and control variables is potentially enormous and therefore analysis must consider efficient, possibly embedded, optimization approaches. Embedding optimization-specific linear objects in forward simulation code requires a paradigm shift in the code development process. Third, we must accomodate uncertainties resulting from model approximation and unknown model inputs to achieve resilient optimal solutions. The incorporation of uncertainty further increases the already large computational requirements. Additional challenges include the demand for high resolution, implicit coupling of disparate physical models at multiple scales, large numbers of design variables spanning various system components, and the need to characterize high-dimensional random fields that arise from the numerous sources of uncertainty. The purpose of this paper is to describe various concepts from PDE-constrained and stochastic optimization that could provide a possible foundation for efficient design under uncertainty.

General Strategy. To address these challenges, we require an approach that is rooted in the coupling of partial differential equation (PDE) constrained optimization [2, 1], often used in engineering design, and stochastic programming, the mathematical backbone of risk management in many financial applications [7, 6, 11, 8, 9]. We have recently developed algorithms for solving optimization problems governed by PDEs with uncertain coefficients whose performance, for certain classes of problems, is nearly independent of the number of uncertain variables [4, 5, 3]. To extend such approaches to solve realistic large-scale optimization problems for magnetic confinement fusion, we must explore the following three key areas: optimization algorithms that leverage inexact computations, the risk quadrangle and buffered probabilities. Optimization algorithms that permit inexact objective function and gradient evaluations provide a foundational technology to manage varying model fidelities, including mesh refinement and adaptive sampling. The risk quandrangle provides the statistical synergy between risk-averse optimization and statistical estimation. Finally,

*communicating author (no oral presentation is requested), SAND2015-3310 C

†Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000

buffered probabilities provide a numerically tractable and conservative surrogate for addressing rare events. Next, we discuss each concept in more detail.

Inexactness in Risk-Averse Optimization. The incorporation of uncertain inputs in PDE-constrained optimization significantly increases the computational size of the optimization problem. In addition, uncertainty in the objective function must be appropriately handled to produce meaningful solutions that are resilient to uncertainty. One approach is through risk measures. Risk refers to the hazard associated with an uncertain performance metric such as the objective function. There are several challenges associated with risk measures, including the differentiability and smoothness of particular measures, and the consistent and efficient approximation of risk-averse quantities. These approximations often depend on controllable tolerances that must be managed and refined throughout the outer optimization loop. Exploiting inexactness computations will be critical in achieving efficient solutions. The next section discusses concepts to help bridge risk-averse optimization and statistical estimation.

Risk Quadrangle. The new mathematical formalism known as the *risk quadrangle* [7] unifies risk-averse optimization and statistical estimation. The risk quadrangle facilitates injection of expert knowledge to handle uncertainties, by defining measures of risk, deviation, error and regret. Similar to risk, regret numerically quantifies ones displeasure associated with the uncertain performance. On the other hand, deviation quantifies how non-constant a random variable is and error measures how close a random variable is to zero. In the design of magnetic fusion reactors, it is critical that we employ physically relevant risk measures. Given a measure of regret that quantifies the designers displeasure for large objective function values, the risk quadrangle relationships provide an error measure, often biased to overestimation, that can be used to judicially calibrate models. From a calibrated model, the variability can be determined using the associated deviation measure and the risk can by computed using the associated risk measure risk measure. An overall research challenge will be to formulate physically meaningful regret measures for different aspects of a reactor design. In addition to designing an economically viable reactor, a key design challenge will be to avoid catastrophic scenarios. In the next section we introduce the concept of buffered probabilities for handling rare events.

Buffered Probability. In the context of reactor design, it is pivotal that we not only quantify the probability that a rare event will occur, but also quantify the "weight" of this distribution tail. For example, we must be able to quantify the high-consequence rare events that result in system failures. A possible approach to handling rare events is through *buffered probabilities* [6, 11]. Buffered probabilities provide a general approach to quantify not only the tail probability but also the magnitude of tail events. Thus, buffered probabilities provide a conservative proxy for quantifying rare events. In addition, one can reformulate buffered probabilities as a convex optimization problem. This permits the numerically stable and tractable evaluation of buffered probabilities. Moreover, the evaluation of buffered probabilities motivates research on statistical estimation approaches that preserve distribution tails as well as on efficient nonsmooth optimization algorithms.

Summary. Magnetic confinement fusion motivates a range of large-scale optimization under uncertainty problems. Based on the complexity and computational resource requirements, efficient large-scale optimization methods combined with concepts from stochastic optimization must be considered as part of future numerical development efforts. The use of the risk quadrangle and buffered probabilities offer capabilities to address different optimization formulations and handle catastrophic rare events. Although the computational resource demands seem intractable for the foreseeable future, simulation technologies have reached sufficient levels of maturity that suggests the timing is right to consider efficient optimization and uncertainty quantification interfaces.

References

[1] L. Biegler, O. Ghattas, M. Heinkenschloss, D. Keyes, and B. van Bloemen Waanders, editors. *Real-Time PDE-Constrained Optimization*. SIAM, 2007.

[2] L. Biegler, O. Ghattas, M. Heinkenschloss, and B. van Bloemen Waanders, editors. *Large-Scale E-Constrained Optimization*. Springer-Verlag, 2003.

[3] D. P. Kouri. A multilevel stochastic collocation algorithm for optimization of PDEs with uncertain coefficients. *SIAM/ASA Journal on Uncertainty Quantification*, 2(1):55–81, 2014.

[4] D. P. Kouri, M. Heinkenschloss, D. Ridzal, and B. G. van Bloemen Waanders. A trust-region algorithm with adaptive stochastic collocation for PDE optimization under uncertainty. *SIAM Journal on Scientific Computing*, 35(4):A1847–A1879, 2013.

[5] D. P. Kouri, M. Heinkenschloss, D. Ridzal, and B. G. van Bloemen Waanders. Inexact objective function evaluations in a trust-region algorithm for PDE-constrained optimization under uncertainty. *SIAM Journal on Scientific Computing*, 36(6):A3011–A3029, 2014.

[6] R. T. Rockafellar and J. O. Royset. On buffered failure probability in design and optimization of structures. *Reliability Engineering & System Safety*, 95(5):499 – 510, 2010.

[7] R. T. Rockafellar and S. Uryasev. The fundamental risk quadrangle in risk management, optimization and statistical estimation. *Surveys in Operations Research and Management Science*, 18(12):33 – 53, 2013.

[8] A. Ruszczyński and A. Shapiro. Optimization of risk measures. In G. Calafiore and F. Dabbene, editors, *Probabilistic and Randomized Methods for Design under Uncertainty*, pages 117–158. Springer-Verlag, London, 2005.

[9] A. Shapiro, D. Dentcheva, and A. Ruszczynski. *Lectures on Stochastic Programming: Modeling and Theory (second edition)*. SIAM, Philadelphia, 2014.

[10] W. Tang, D. Keyes, N. Sauthoff, N. Gorelenkov, J. Cary, A. Kritz, S. Zinkle, J. Brooks, R. Betti, W. Mori, A. Bhttacharjee, W. Daughton, and A. Shoishani. Scientific grand challenges" fusion energy sciences and the role of computing at the extreme scale. Technical report, Department of Energy, Office of Fusion Energy Sciences and the Office of Advanced Scientific Computing Research, 2009.

[11] S. Uryasev. Buffered Probability of Exceedance and Buffered Service Level: Definitions and Properties. University of Florida, Research Report, ISE Dept., 2014-3, 2014.