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13. ABSTRACT (Maximum 200 Words)

We develop an Assess-Predict-Optimize (APO) strategy for the adaptive design of optimal missions for critical components and systems. We first Assess the system — through non-destructive inverse procedures for evaluating the system characteristics of interest: this yields the many possible realizations of the system. We then Predict future behavior of the system — through various modeling and computational procedures: this translates the uncertainties in system characterization into ranges of performance. Finally, we Optimize the system mission — through mathematical programming methods: this provides the best possible configuration and deployment schedule relative to the design objectives and now-identified (but uncertain) system characteristics.

The essential mathematical ingredients of our approach are twofold. First, we employ Reduced-Basis Output Bound Methods: dimension reduction — the rational construction of highly efficient (“real-time” response) system-specific approximation spaces that reflect the low-dimensional parametric manifold on which a component “evolves” during design and operation; and *a posteriori* error estimation — relaxations of the classical error-residual equality that provide inexpensive bounds for the prediction error. Second, we employ Mathematical Programming Methods: techniques which incorporate our reduced-basis output bounds for efficient minimization of objective functions with strict adherence to constraints even in the presence of uncertainty.

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FROM MATERIALS TO MISSIONS

ASSESS-PREDICT-OPTIMIZE: A COMPUTATIONAL APPROACH TO ADAPTIVE DESIGN

Grant Number F49620-01-1-0458

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Background

Assess-Predict-Optimize

The adaptive design of optimal missions for critical components and systems can significantly improve military effectiveness, the protection and preservation of personnel and materiel, and the allocation of scarce defense resources: supporting evidence abounds — for example, in efforts to extend and manage the life and duty cycle of existing weapons systems. To be truly effective, mission planning must be pursued on both long and short timescales — responsive to (i) evolving system characteristics; (ii) changing environmental conditions; and (iii) dynamic “theater” requirements and objectives.

To realize this program we pursue an Assess-Predict-Optimize (APO) strategy. We first Assess the system — through non-destructive inverse procedures for probing, testing, or evaluating the system characteristics of interest: this implicitly yields the many possible “realizations” of the system. We then Predict future behavior of the system — through various modeling and computational procedures: this translates the uncertainties in system characterization into ranges of system performance. Finally, we Optimize the system or system mission — through various mathematical programming methods: this provides the best possible system configuration and deployment schedule relative to our design objectives and the now-identified (but potentially uncertain) system characteristics.

On the long timescale — the design stage — APO is invoked as the system is first conceived and manufactured: this is typically denoted “robust design” and “quality control.” On the short timescale — the operation stage — APO is invoked as the system or component performs in the field: this may be viewed as adaptive robust design, optimal mission planning, or even “quasi-static” control. In both the design and operation stages, Assess provides ever increasing information which in Predict and Optimize is then translated into ever sharper, safer, and more reliable and economical performance.

The essential mathematical ingredients of our approach are twofold. First, we employ Reduced-Basis Output Bound Methods: dimension reduction — the rational construction of highly

efficient (“real-time” response) system-specific approximation spaces that reflect the low-dimensional parametric manifold on which a component “evolves” during design and operation; and *a posteriori* error estimation — relaxations of the classical error-residual equality that provide inexpensive bounds for the prediction error, and hence certain application of our very low-dimensional approximations. Second, we employ Mathematical Programming Methods: techniques which incorporate our reduced-basis output bounds for efficient minimization of objective functions with strict adherence to constraints even in the presence of uncertainty. We discuss these two ingredients below.

Reduced-Basis Methods

The Assess-Predict-Optimize methodology requires the prediction of certain “quantities of interest,” or performance metrics, which we shall denote *outputs* — for example deflections, maximum stresses, maximum temperatures, heat transfer rates, flowrates, or lifts and drags. These outputs are typically expressed as functionals of field variables associated with a parametrized partial differential equation which describes the physical behavior of the component or system. The parameters, which we shall denote *inputs*, serve to identify a particular “configuration” of the component: these inputs may represent design variables, such as geometry — for example, in optimization studies; decision variables, such as actuator power — for example in control applications; or characterization variables, such as physical properties — for example in inverse problems. We thus arrive at an implicit input-output relationship, evaluation of which demands solution of the underlying partial differential equation.

However, current computational procedures are too restrictive, too inefficient, too unqualified, or too pessimistic to be of any value, particularly in the “real-time” operation stage. Our new approach promises considerable advances; in particular, our approach permits the rapid and reliable evaluation of partial-differential-equation-induced input-output relationships in the limit of many queries — as required by the APO methodology. Our particular approach is based on the reduced-basis method, first introduced in the late 1970s for nonlinear structural analysis [1,2], and subsequently developed more broadly in the 1980s and 1990s [3–8]. The reduced-basis method recognizes that the field variable is not, in fact, some arbitrary member of the infinite-dimensional solution space associated with the partial differential equation; rather, it resides, or “evolves,” on a much lower-dimensional manifold induced by the parametric dependence.

The reduced-basis approach as earlier articulated is local in parameter space in both practice and theory. To wit, Lagrangian or Taylor approximation spaces for the low-dimensional manifold are typically defined relative to a particular parameter point; and the associated *a priori* convergence theory relies on asymptotic arguments in sufficiently small neighborhoods [5]. As a result, the computational improvements — relative to conventional (say) finite element approximation — are often quite modest [7]. Our work [9–14] differs from these earlier efforts in several important ways: first, we develop (in some cases, provably) global approximation spaces; second, we introduce rigorous *a posteriori* error estimators; and third, we exploit offline/online computational decompositions (see [3] for an earlier application of this strategy within the reduced-basis context). These three ingredients allow us, for the restricted but important class of “parameter-affine” problems, to reliably decouple the generation and projection stages of

reduced-basis approximation, thereby effecting computational economies of several orders of magnitude.

We elaborate upon the contribution of each of these three ingredients. First, we can prove in some cases, and demonstrate empirically in many more cases, that the error in the reduced-basis approximation vanishes exponentially as a function of N , the dimension of the reduced-basis space: sufficient accuracy can thus be obtained with only $N = O(10)$ to $O(100)$ degrees of freedom. Second, we can rigorously and sharply bound (*a posteriori*) the error in the reduced-basis approximation of the outputs of interest, thus permitting optimal truncation — selection of (close to) the smallest N for which the desired error tolerance can be certainly achieved. Third, thanks to the (assumed) affine input-parameter-dependence of the operator, we can decompose the computational effort into two stages: an expensive (offline) stage performed once; and an inexpensive (online) stage performed many times. The operation count for the online stage — in which, given a new value of the input, we calculate the output (and gradient and Hessian) and associated error bound — depends only on N (typically very small) and the parametric complexity of the operator. This very low marginal cost is critical in the optimization context, as we discuss further below.

Mathematical Programming Methods

The most common approach to the optimization of systems described by partial differential equations is to combine state-of-the-art optimization techniques — such as pattern search techniques, Sequential Linear/Quadratic Programming (SLP/SQP) approaches, or Newton Interior Point Methods (IPM) — with state-of-the-art partial differential equation discretization techniques — such as the finite element method. The best approaches (e.g., [15]) consider the optimization formulation and partial differential equation treatment in an integrated fashion. However, even these “best methods” remain quite expensive — a sufficiently accurate discretization may require hundreds of thousands of degrees of freedom — with computational times often measured in hours or even days. Furthermore, realistic design exercises typically require many optimization cycles — corresponding to variations in the design, operation, and environment parameters that define the objectives and constraints. Finally, in the APO context, these difficulties are further amplified by the uncertainty in the system characteristics, and by the presence of a variety of equations, objectives, and constraints that rarely admit an overarching simple structure.

An alternative approach to the optimization of systems described by partial differential equations is to replace the high-dimensional (say) finite element model with a reduced-order surrogate. The latter may be based either on physical reasoning or empirical constructions, or on a formal approximation or projection directly derived from the underlying partial differential equations. A variety of approaches (e.g., [16]) have been proposed for the incorporation of these low-order models into the design and optimization context. However, these earlier approaches lack rigorous, sharp, and inexpensive estimates for the approximation error. Hence, the low-order approximation may be either too conservative — thus compromising efficiency; or too optimistic — thus compromising feasibility (with respect to the exact mathematical description). The latter can be particularly egregious in situations where infeasibility implies (for example, material or mission) failure.

Our approach incorporates our reduced-basis approximation and associated rigorous *a posteriori* error estimates into the optimization framework for efficient minimization of objective functions with strict adherence to constraints even in the presence of numerical uncertainty. In particular, we are able to (i) restrict attention to regions of the design space in which the model is provably accurate (or, alternatively, request adaptive improvement of the approximation as demanded by the optimization and design process), (ii) assess and control the suboptimality induced by the output approximation in the optimization results, and, most importantly, (iii) rigorously ensure feasibility of the optimizers with respect to the exact mathematical description. The latter is particularly critical in real-time applications — in order to guarantee “safe” operation without recourse to (non-real-time) fiducial calculations.

The above considers only uncertainty arising from numerical approximation errors. In fact, within the APO context, we must also assess uncertainty originating in the incomplete characterization of the system. To do so, we incorporate components of robust design: we consider worst-case behavior over all possible system configurations consistent with available experimental measurements. These considerations may be included directly as part of the optimization statement, either in a bi-level [17,18] or semi-infinite programming context [17]; or as a pre-processing step in which we construct a computationally convenient representation of the set of all possible (experimentally consistent) system configurations.

Particular Achievements

First, in our earlier work we considered almost exclusively coercive linear elliptic (and parabolic) problems. More recently we have developed techniques that permit the efficient and rigorous treatment of rather general noncoercive problems, and of certain (interesting) classes of nonlinear problems. The critical new ingredients are (i) constructive lower bounds, based on operator perturbation techniques, for the relevant (parameter-dependent) inf-sup constants that provide the necessary stability information; (ii) various sum factorization (symmetry) and interpolation procedures that reduce the complexity of high-order Galerkin summations (e.g., in the residual dual-norm evaluations); (iii) and application of the Brezzi-Rappaz-Raviart framework [19–22] for analysis of *a priori* and *a posteriori* discretization errors in the variational approximation of nonlinear problems. (In most contexts, the latter can not be applied completely constructively, in that certain constants elude evaluation; in our context, we obtain completely quantitative and rigorous *a posteriori* bounds, thanks to the offline-online decomposition.) We find that our methods (in the online stage) are $O(100)$ to $O(10,000)$ times faster than conventional techniques.

Second, in our earlier work we considered almost exclusively operators with affine parameter-dependence — that is, operators which may be expressed as a (low-order) sum of Q products of parameter-dependent functions and parameter-independent operators. Though many practical problems, involving both property and geometry variation, can indeed be cast in this form, many other problems do not admit this affine decomposition — or at least do not admit such a form for a suitably small Q . More recently, we have developed several efficient techniques for the treatment of operators which may exhibit locally non-affine parametric dependence in some reasonably small region of the domain; the latter arises very often in the important application of

shape (boundary) optimization. Our methods are based on either domain decomposition techniques — which decouple the affine and non-affine regions; or parameter-function interpolation techniques — which replace the non-affine problem with a suitably accurate (reduced-basis) affine approximation. In both cases, rigorous error estimates may be developed.

Third, in our earlier work we exploited relatively simple (essentially exhaustive) optimization procedures, such that — even given our extremely fast reduced-basis approximations — real-time response (for the optimization problem) was often compromised. We have recently adapted and developed Trust Region/SQP variants of Newton/Interior Point Methods that, first, make effective use of all available smoothness, second, ensure input-feasibility so as to rigorously (at each iterate) avoid those parts of the design space for which the reduced-basis approximation is not certified (and hence may confound the optimization process), and third, avoid stationary (saddle) points in favor of true (at least local) optimizers. We have also considered several “robust” extensions to these algorithms that permit us to rigorously accommodate uncertainty in the system characterization. The net result is a technique which has both the response and reliability required in the real-time context.

Fourth, in our earlier work, each new problem required the time-consuming generation of new offline and online codes. We have initiated the development of templating software that will permit end users to automatically and very quickly generate online simulation and optimization servers for their particular problems and systems of interest. This computational framework provides for “cradle to grave” automation for the computational design — and eventually the computational operation — of engineering components and systems. In our long-range vision, the resulting online codes — servers distributed over the web, or embedded in deployed systems — will adaptively and safely design missions based on real-time assessment, prediction, and optimization.

Fifth, we have commenced the application of our techniques to much more realistic problems, primarily in the multifunctional but also in the Assess-Predict-Optimize (prognosis) domains. We have focused on prismatic microtruss channel walls [23] designed to both remove heat and provide structural support: the heat transfer is modeled as a forced-convection problem (with outputs fan power and maximum temperature); the structure is modeled both as linear elastic (with outputs compliance and maximum stress) and nonlinear elastic (with outputs buckling loads). We have applied the APO methodology to the structural problem [18]: we assume that the microtruss contains cracks of unknown lengths, and control by way of a shim compensation the deflection of the structure. In particular, we Assess the lengths of the cracks through measurements of the deflection for various shim sizes; we then Predict the deflection of the structure for a particular shim size, taking into account the uncertainty in the crack lengths; finally, we Optimize the structure, finding the best configuration (shim dimensions) which yields the minimum weight yet satisfies the given deflection constraints. A typical optimization requires solution of roughly 300 partial differential equations and associated sensitivity calculations (at different parameter values); at present, we are able to solve such APO problems in approximately 1 sec.

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Christophe Prud'homme (research scientist)
Karen Veroy (doctoral student)

Interactions

Conferences

1. “Reduced-Basis Output Bounds for Reliable Real-Time Solution of Parametrized Partial Differential Equations,” Fifth SIAM Conference on Control and Its Applications, Minisymposium on Model Reduction for Control and Optimization, San Diego, CA, July 2001.

2. "Efficient Relations for Reduced-Basis Error Estimation," NATO/RTO/NASA/VKI Lecture Series on Error Estimation and Solution Adaptive Discretization in CFD, Brussels, Belgium, October 2001.
3. "Reduced-Basis Output Bounds: Reliable Real-Time Solution of Parametrized Partial Differential Equations," Third AMIF International Conference, Lisbon, Portugal, April 2002.
4. "Reduced-Basis Output Bounds: Reliable Real-Time Solution of Parametrized Partial Differential Equations," Congrès de Mathématiques Appliquées à la Mémoire de Jacques-Louis Lions, Paris, Collège de France, July 2002.
5. "Reduced-Basis Output Bounds: Reliable Real-Time Solution of Parametrized Elliptic Partial Differential Equations." CSCAMM: Perspectives on Incompressible Flows; Comparison of Different Computational Strategies, University of Maryland, College Park, MD, April 2003.
6. "A *Posteriori* Error Bounds for Reduced-Basis Approximation of Parametrized Noncoercive and Nonlinear Elliptic Partial Differential Equations." 16th AIAA Computational Fluid Dynamics Conference, Orlando, FL, June 2003.
7. "Real-time Reliable Distributed Simulations: Framework, Repository and Interfaces." Advanced Environments and Tools for High Performance Computing; EuroConference on Problem Solving Environments and the Information Society. Albufeira (Algarve), Portugal, June 2003.
8. "A *Posteriori* Error Bounds for Reduced-Basis Approximation of Parametrized Noncoercive and Nonlinear Elliptic Partial Differential Equations." 7th US National Congress on Computational Mechanics, Albuquerque, NM, July 2003.
9. "Reduced-Basis Techniques for Rapid Reliable Optimization of Systems Described by Parametric PDEs." 18th International Symposium on Mathematical Programming (ISMP) 2003, University of Denmark, Copenhagen, Denmark, August 2003.

Other collaborators

Work on the thermo-structural optimization of microtrusses is being carried out in conjunction with Professor Anthony Evans (University of California, Santa Barbara) and Professor John Hutchinson (Harvard University). Mr. Thomas Leurent (formerly of MIT) and Mr. Yuri Solodukhov (MIT) have contributed to the development of the reduced-order methodology employed in the present study. Ms Shidрати Ali (Nanyang Technological University and the Singapore-MIT Alliance) has contributed to the APO formulation and in particular the associated optimization formulations; Nguyen Ngoc Cuong (National University of Singapore and the Singapore-MIT Alliance) and Professor Liu Gui-Rong (National University of Singapore) have also participated in the inverse-problem aspects of our studies. Finally, many mathematical aspects of this work were developed in collaboration with Professor Yvon Maday (Paris-VI) and Dr. Gabriel Turinici (Paris-VI).

Transitions

We hope to transition the rocket engine work over the next year; we are currently in discussions with Edwards AFB.

Honors and Awards

None.

Publications

C. Prud'homme, D. Rovas, K. Veroy, Y. Maday, A.T. Patera, and G. Turinici. Reliable real-time solution of parametrized partial differential equations: reduced-basis output bounds methods, *Journal of Fluids Engineering*, 124(1):70–80, 2002.

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