Multidisciplinary Design Optimization Techniques: Implications and Opportunities for Fluid Dynamics Research

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MULTIDISCIPLINARY DESIGN OPTIMIZATION TECHNIQUES: IMPLICATIONS AND OPPORTUNITIES FOR FLUID DYNAMICS RESEARCH

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Abstract
A challenge for the fluid dynamics community is to adapt to and exploit the trend towards greater multidisciplinary focus in research and technology. The past decade has witnessed substantial growth in the research field of Multidisciplinary Design Optimization (MDO). MDO is a methodology for the design of complex engineering systems and subsystems that coherently exploits the synergism of mutually interacting phenomena. As evidenced by the papers, which appear in the biannual AIAA/USAF/NASA/ISSMO Symposia on Multidisciplinary Analysis and Optimization, the MDO technical community focuses on vehicle and system design issues. This paper provides an overview of the MDO technology field from a fluid dynamics perspective, giving emphasis to suggestions of specific applications of recent MDO technologies that can enhance fluid dynamics research itself across the spectrum, from basic flow physics to full configuration aerodynamics.

Introduction
The phrase "multidisciplinary design optimization" does not admit a universally accepted interpretation. For some, it encompasses all of the aerospace design process used in industry and perforce has been in use since the advent of aviation. For others, it refers to a particular set of computational technologies of fairly recent provenance that enable enhanced design processes in which (1) there is more knowledge about the design available earlier in the design cycle; and (2) there is more freedom to alter the design later in the design cycle. Consistent with the latter perspective, we adopt here the definition: Multidisciplinary Design Optimization (MDO) is a methodology for design and analysis of complex engineering systems and subsystems which coherently exploits the synergism of mutually interacting phenomena. The stress is on a systematic methodology, rather than heuristic or ad hoc approaches, and on exploiting interdisciplinary interactions to achieve a better overall system than can be achieved by ignoring the interactions. MDO methods treat interdisciplinary interactions as opportunities rather than as nuisances or liabilities.

Probably the earliest MDO developments recognizable from our current perspective occurred in the 1970s. By the early 1980s there was a sufficiently large community of researchers to warrant the start of a continuing biannual symposium on Multidisciplinary Analysis and Optimization, and by 1989 the AIAA had established its Technical Committee on MDO. In 1992 it assumed cosponsorship of this biannual Symposium. The most recent Symposium consisted of several hundred technical papers. A healthy fraction of these papers involved aerodynamics. But it was not always thus. The roots of MDO lie within the structures discipline, and until about 1990 the aerodynamics discipline was usually a passive player in MDO—serving merely as a source of loads for structural optimization processes. (Of course, optimization had been applied to airfoil design many years ago.)

The crucial development that furnished aerodynamics with its bona-fide MDO credentials was aerodynamics sensitivity analysis. (A sensitivity derivative is the derivative of an output quantity with respect to an
input quantity; a simple example for a computational fluid dynamics (CFD) code is the derivative of the lift with respect to the thickness of a particular airfoil section.) At a 1986 conference Sobieski challenged the aerodynamics community to develop a general sensitivity analysis capability, and the first papers on exact aerodynamic sensitivity analysis appeared a few years afterwards. Of course, there had been earlier related developments. Sensitivity analysis of a limited sort was implicit in the aerodynamic optimization methods utilizing adjoint equations that originated in the late 1970s. Brute-force finite differences had certainly been employed for a number of years, but the development of efficient methods for solving the exact sensitivity equations was essential for accuracy and robustness. Aerodynamic optimization with exact aerodynamic sensitivities has now become almost routine. We are even beginning to see demonstrations of combined aerodynamic-structural optimization of aircraft using nonlinear CFD (Euler or Navier-Stokes) and full finite-element models of the structure, as well as the first steps towards earlier integration of the controls discipline into design by using aerodynamic sensitivity analysis for estimating stability and control derivatives.

Most MDO applications to date have been at the level of vehicle design. A significant portion of this forum is more interested in the performance of vehicle components and in basic flow physics issues. Our aim in this paper is to describe the MDO technology field and to propose some opportunities for exploiting these technologies in fluid dynamics research and applications at the vehicle, the component, and the flow physics levels. For the most part, we will confine our references to that portion of the literature that has a strong fluid dynamics connection. We will also usually refer to recent articles, in archival form whenever feasible, from which lines of research can be traced back; our choice of references does not imply priority. Those interested in a recent broad survey of MDO, complete with an extensive reference list, should consult Sobieski & Haftka. A recent special issue of Journal of Aircraft was devoted to MDO; it contains 28 papers covering both methodology and applications, including a half-dozen papers focusing on aerodynamics. Several individual papers from this volume will be cited below as general references for certain areas of MDO. An informative set of papers on applications of MDO in industry was presented at the 7th AIAA/USAF/NASA/ISSMO Symposium on Multidisciplinary Analysis and Optimization.

In this paper we shall first give an overview of two specific MDO applications. These two examples will serve as a background for the subsequent discussion of the contents of the “MDO discipline.” Then we shall comment on some opportunities and implications for fluid dynamics research.

**MDO Examples**

Let us start then with two examples of NASA-industry MDO technology demonstrations. We will use these both as settings for discussion of the MDO discipline and to point out some practical issues.

**Aerospike Nozzle**

In 1995 the MDO Branch at NASA Langley and Rocketdyne, Inc. started a joint development of MDO methods, focused on the design of the nozzle of an aerospike engine, an engine concept used for the X-33. Fig. 1 illustrates the two-dimensional physical model of the nozzle employed in this study, and Fig. 2 illustrates the design variables for the nozzle structure and for the nozzle ramp geometry. The flow on the nozzle ramp was computed by a marching Euler method, and the structural response (stress, deformation, buckling) by a commercial finite-element code; the base flow region was represented by a simple model, and a lookup table was used to estimate the gross lift-off weight (GLOW) of the launch vehicle from the engine specific impulse (Isp) and thrust-to-weight ratio (T/W). The nozzle structure was parameterized by 14 structural design variables and the nozzle ramp by 5 geometry variables. The initial geometry design variables were selected from previous Rocketdyne design studies on aerospike nozzles that used conventional design methods and were expected to be close to an optimized aerodynamic shape.

![Fig. 1 Aerospike nozzle physical model.](image)

In this idealized problem the "single discipline design" is produced by first fixing the structural shape and optimizing the nozzle contour for maximum thrust, and then fixing the nozzle contour and...
optimizing the structural sizing variables for minimum weight. The full "multidisciplinary design" permits both the aerodynamic and structural design variables to be optimized simultaneously. The comparison between results from the two approaches, illustrated in Fig. 3, is a clear example of multidisciplinary synergy achieved by the MDO method. It achieves a better overall system (lower GLOW) by sacrificing some thrust for lower engine weight. Even greater gains are possible from the MDO method when the nozzle length is permitted to vary. We emphasize that this was a technology development study and did not impact the actual X-33 engine, as that design was fixed by the time this study was complete.

**High-Speed Civil Transport**

From the inception of the High Performance Computing and Communications Program in late 1991, NASA Langley's application focus under NASA's Computational Aerosciences element has been on demonstrating MDO for a high-speed civil transport (HSCT). A series of increasingly complex applications has been developed. The complexity is associated both with increasing fidelity of the analysis codes, e.g., from vortex-lattice (WINGDES) to marching Euler (ISAAc) to global Euler (CFL3D) codes, and with increasing complexity of the design problem. Table 1 lists the salient characteristics of the two applications that have been completed—HSCT 2 and HSCT 3—along with the one currently under development—HSCT 4.

![Fig. 4 Some geometric design variables for HSCT 4.](image)

Fig. 4 illustrates some of the planform (geometry) and wing section design variables of the HSCT 4 application. As Table 1 indicates, there are also several hundred structural sizing design variables. The problem definition of this application drew upon prior HSCT applications at NASA Langley dating back to the HiSAIR (High-Speed Airframe Integration Research) Pathfinder problem. It was heavily influenced by discussions over a period of several years with industry engineers working on HSCT designs under the auspices of the NASA High Speed Research Program, as well as by long-standing interactions with MDO researchers at Georgia Institute of Technology, Stanford University and Virginia Polytechnic Institute and State University.

The HSCT 4 problem is far more complex than the aerospike nozzle problem. Even with the benefit of

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American Institute of Aeronautics and Astronautics
more than 6 years of experience with several related, but smaller scale, HSCT MDO applications, the NASA Langley team of roughly ten members (civil servants and contractors) took over 2 years to define, assemble, and debug just the HSCT 4 analysis process.

Table 1. NASA Langley HPCCP Applications 1991–1999

<table>
<thead>
<tr>
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<td>Total time/cycle</td>
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Table 2. MDO Conceptual Elements

<table>
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<tr>
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<th>Analysis Capabilities and Approximations</th>
<th>Design Formulations and Solutions</th>
<th>Management and Cultural Implementation</th>
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<tr>
<td>• MDO Framework and Architecture</td>
<td>• Analysis and Sensitivity Capability</td>
<td>• Design Problem Objectives</td>
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<td>• Databases, Data Flow, and Standards</td>
<td>• Parametric Geometric Modeling</td>
<td>• Design Problem Decomposition and Organization</td>
<td>• MDO Operation in IPD Teams</td>
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<td>• Effective Inclusion of High-Fidelity Analyses/Tests</td>
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</table>
MDO Conceptual Elements

Our list of the components of MDO methodology is influenced by what methods are needed to achieve multidisciplinary synergy in practice. Multidisciplinary analysis, even when accompanied by optimization, does not suffice by itself. In other words, MDO does not consist merely of linking together disciplinary analysis tools and wrapping an optimizer around them. This may well be the manner in which most multidisciplinary optimization problems have been approached, including the two examples in the previous section, but as this overview will demonstrate, there are many alternative approaches.

A delineation of the contents of the "MDO discipline" has progressed through three generations, evolving from an academic perspective to an industry perspective. The first proposal was an individual one made by Sobieski. A modified version was used at NASA Langley for several years. Recent activities by the AIAA MDO Technical Committee have led Giesing & Barthelemy to propose a third generation MDO taxonomy summarized here in Table 2. The latter paper has the distinction of including a discussion of the state-of-the-art of each element in industrial applications. Note also the fourth major category, Management and Cultural Implementation. This new category (absent from the first two generations) acknowledges explicitly the nontechnical challenges that must be addressed in order for MDO to be adopted in industry.

Our discussion of the MDO conceptual elements is complementary to that of Giesing & Barthelemy. Whereas they focused on the industry perspective, we shall focus on the research and methods development perspective.

For future reference, we state here in abstract terms the general optimization problem:

$$\min f(x,u(x))$$

s.t. $$h(x,u(x)) = 0$$

$$g(x,u(x)) \leq 0$$

in terms of design variables $$x$$, the state variables $$u$$ (from the corresponding multidisciplinary analysis problem), the objective function $$f$$, the equality constraints $$h$$, and the inequality constraints $$g$$.

Information Management and Processing

The general category of information management and processing refers to the enabling information technology infrastructure for MDO; many of the new developments have originated in computer science technology advancements. The issues discussed here may not be as critical for adaptation of MDO techniques to enhance investigations of basic flow physics, but they grow more significant as fluid dynamics strives to become more closely linked with other disciplines.

A theme that permeates this section is the desirability of automating as much of the MDO process as is feasible. Nevertheless, let us stress that MDO does not purport to furnish a push-button design capability. Rather, MDO seeks to provide the human designer with improved tools for achieving better designs. The MDO tools should be used to assist the designer by automating routine tasks, by furnishing useful information on interdisciplinary trades, and by conducting design space searches.

MDO Framework and Architecture

The phrase MDO framework and architecture refers to the abstract design (architecture) and the specific software tools for implementing and controlling (framework) a multidisciplinary design process. For those MDO practitioners who have attempted significant applications, such as the aerospike nozzle and even more so the sequence of HSCT applications, the need for appropriate architectures and useful frameworks is abundantly clear. Well over 90% of the human effort on the implementation of these applications went into preparing the analysis codes for use in a multidisciplinary application and into linking these codes together in the proper control sequence.

A variety of framework research activities have been conducted, and several commercial frameworks are now on the market. Although none of these commercial frameworks yet presents a complete solution, their progress in the past few years has been impressive. Our advice to any group contemplating a nontrivial MDO application is to acquire the best available frameworks rather than hard-wiring the application or attempting an in-house framework development activity. We would especially caution fluid dynamics researchers to avoid succumbing to the temptation to build their own frameworks; leave this task to the information technology specialists. Above all, exploit tools that automate the repetitious activities involved in preparing the analysis codes for integration.

The HSCT 4 application is obviously a significant software development activity. The ad hoc "configuration management" approaches typically
used in the research community are not feasible for this scale of problem. On the other hand, the rigorous software engineering methods applied to the development of flight critical software are surely overkill. The HSCT 4 team is currently experimenting with the use of formal configuration management procedures and utilities in the hopes of effectively managing the software development while permitting the experimentation necessary for a research project. As might be expected, this use of formal configuration management initially met with considerable resistance from the team members. As time has passed, however, and more and more team members have been affected by problems arising from multiple, uncontrolled versions of other members' software, greater acceptance has developed.

Databases, Data Flow, and Standards

Development of the problem definition for an MDO research application is quite challenging. In the application of MDO methods in an industry setting one often seeks to make an incremental improvement in an existing design process. Here the existing disciplinary and interdisciplinary processes are likely to have well-understood and well-documented data flow, interfaces, and standards. In the research case, there is unlikely to be an existing process that can serve as a starting point. Researchers, especially those with no prior experience on diverse, multidisciplinary teams, typically have little appetite for the extended discussions, compromises, and documentation necessary to achieve the detailed problem definition essential for implementation. The aerospike nozzle application was still small enough that it could reasonably be developed without a formal requirements document, but the HSCT 4 application sorely needed such a document. The HSCT 4 team eventually assembled a detailed requirements document. It took nearly 100 pages just to define the analysis process, the tools used, and the data flow. The requirements document necessarily went through several drafts as the process understanding evolved. It took more than a year to extract this definition from the researchers on the team. The overall process would have been more efficient had time for this been set aside at the very start of HSCT 4, but it is next to impossible to persuade researchers of the value of this process until they have seen firsthand the consequences of delaying the requirements definition.

Managing the sheer volume of data for the HSCT 4 application is quite a challenge. More than 10 GBytes of data is exchanged in a single execution of the analysis process. The volume of data exchange for a full system sensitivity analysis is estimated to exceed one TByte. A formal database system is used judiciously in the HSCT 4 implementation.

Computing Requirements

The aerospike nozzle application was run on several UltraSPARC™ workstations and typically took a day to reach an optimal solution. Even for this relatively small-scale application, automation of the individual processes was essential to achieve this 1-day turnaround. For the HSCT 4 application, it takes roughly a day to generate a single analysis on a workstation even with full automation of the entire process. This can possibly be reduced to several hours by use of parallel processing, but load balancing is very challenging for this heterogeneous application. Bear in mind that the workhorse aerodynamic code for most of the HSCT 4 computations is a (linear) panel code (USSAERO); in order to keep the computational time within reasonable bounds, the nonlinear code CFL3D (in Euler mode) is used only for occasional nonlinear corrections. Recall from Table 1 that there are approximately 70 distinct subprocesses in the HSCT 4 application and that numerous iterative loops between subprocesses are needed to enforce full multidisciplinary consistency. Such iterations are characteristic of multidisciplinary problems.

And yet, the complexity of the HSCT 4 problem pales in complexity beside the industry design process. In practice, thousands of load conditions (rather than a mere seven), higher fidelity analyses (such as Reynolds-averaged Navier-Stokes computations), and many more effects, such as flutter, controls, layout, propulsion, manufacturing, and operations, must be examined even at the preliminary design stage. Hence, for the foreseeable future, MDO applications will have to consider carefully the computing requirements.

Design Space Visualization

The sophisticated graphical tools presently available for flow field visualization are not particularly useful for MDO applications: detailed flow-field features are of far less interest than representations of the effects of the design variables upon the overall system objective(s) and constraints. Suffice it to be said here that what tools do exist for this purpose are woefully inadequate. The fluid dynamics community could certainly make a useful contribution by demonstrating how to provide intuitive views of the optimization process to the fluids and systems specialists.
Analysis Capabilities and Approximations

The analysis capabilities that are needed for MDO applications go beyond what is usually included in traditional discipline analysis tools, where the one-of-a-kind analysis paradigm often prevails. This section will discuss some techniques that the "MDO discipline" has promoted because of their generic utility.

Analysis and Sensitivity Capability

From the MDO perspective it is important that each significant disciplinary analysis code be robust, automated (or at least readily automated), computationally efficient, well documented, and equipped with accurate, efficient sensitivity analysis. The first three requirements in the preceding list are necessary to permit timely incorporation into a multidisciplinary analysis system. A major trap of current tool development is the dependence on graphical user interfaces (GUIs) for the input, execution, and output of CFD and especially grid generation codes. GUIs are appropriate for initial problem setup and for off-line visualization and interpretation, but their use in other portions of the analysis process embedded within optimization loops is a dead end. The documentation must target the general user whose main interest is the vehicle and not the esoterica of fluid dynamics. The requirement for sensitivity analysis is driven by the use of gradient-based optimization at the system level.

Fortunately, pre-processing tools for equipping analysis codes with accurate and efficient sensitivity analysis capability are nearing maturity. One such tool is ADIFOR (Automatic Differentiation of Fortran), developed by Argonne National Laboratory and Rice University. (A similar tool, ADIC, handles C code.) ADIFOR works as a preprocessor— it accepts as input a Fortran code along with specifications of the input and output variables, and it produces as output an augmented Fortran code that contains the original analysis capability plus the capability for computing the derivatives of all the specified output quantities with respect to all the specified input quantities. Applications of ADIFOR to nonlinear CFD codes began in 1991 and have involved a close interaction with the ADIFOR tool developers. When ADIFOR 3.0 is officially released in 1999, it will also contain the capability to produce the adjoint code.

Recent experience indicates that a complete multigrid, multiblock, turbulent CFD code can be equipped with sensitivity analysis capability in less than a week by using ADIFOR (assuming that the code is written in the Fortran 77 ANSI standard). The typical time for equipping a laminar Navier-Stokes code with quasi-analytic sensitivity analysis appears to be about a year. Of course, the hand-coded algorithm will be more efficient in terms of both CPU time and computer memory, by factors of perhaps 3 to 10.

Another attractive alternative is the use of the complex variable technique. Each of these three approaches—hand-coded sensitivities, automatic differentiation, and the complex variable technique—has its place, but there is certainly no excuse today for not providing sensitivity analysis capability along with the CFD tools. Some exploratory work has been performed on obtaining accurate second derivatives from CFD codes, and the forthcoming ADIFOR 3.0 tool will include Hessian-generation capability.

A number of CFD groups have developed adjacent capabilities for their codes. There has been some question recently about precisely how to define adjoints appropriately, especially in the presence of flow or grid discontinuities or singularities. Having witnessed first hand the enormous impact numerical analysis had upon spectral methods in the 1980s, the first author became a firm believer in the advantages of the weak formulation of numerical methods. We therefore have little hesitation in recommending the work of Lewis for resolving these debates for those who prefer to derive the adjoint first and then discretize the equations.

One can choose first to derive the sensitivity equations from the basic continuous equations of the problem and then discretize them or else first to discretize the basic continuous equations and then derive the sensitivity equations from this discrete problem. (Automatic differentiation tools such as ADIFOR compute the sensitivities from the discrete equations.) While the jury is still out on just when the sensitivities (or adjoints) need to be derived from the discrete equations, we side with those who place greater importance on having gradients consistent with the function evaluation. This avoids the possibility that inconsistent gradients would point the optimizer in the wrong direction in some delicate situations. In our view, consistency in the (unreachable) limit of sufficiently fine discretization may mollify some mathematicians but is perilous for the practitioner.

An important but rather underdeveloped area, especially for fluid dynamics, is smart reanalysis. This term refers to efficient reanalysis techniques that minimize the computations required in simulating a
system with perturbed input parameters. There is no reason to believe that the best that can be done in CFD is to redo the entire computation with the initial condition taken from the previous solution, or even a linear extrapolation of the previous solution based on the sensitivity derivatives.

**Parametric Geometric Modeling**

Parametric geometric modeling is a prerequisite for full use in optimization of common geometry and discretization models. The models need to be consistent across the disciplines even for multidisciplinary analysis. The different types of models that are needed just in the HSCT 4 application are shown in Fig. 5, taken from the work of Samareh. Note that the various analysis processes use different features and different levels of detail. The additional requirement that the underlying common model be parametric is essential for effective use of optimization in design processes. Ideally, the common model should be tied directly to a commercial computer-aided design (CAD) system, with the input to the MDO processes coming directly out of the CAD representation and the improved model output from the MDO process imported directly back into the CAD representation. The present barriers to this goal are discussed at length by Samareh.

For fluid dynamics applications, the focus is on the surface geometry (outer mold line) model of the vehicle and on the field grid for the CFD computations. Keep in mind the importance of obtaining accurate sensitivity derivatives of the performance measure $f$ (a functional of the CFD solution $u$) with respect to the model parameters $x$. The following notional equation indicates the components that contribute to the overall sensitivity:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial u} \frac{\partial u}{\partial v} \frac{\partial v}{\partial s} \frac{\partial s}{\partial x},$$

(2)

where $v$ represents the volume grid and $s$ the surface grid. Although there has been enormous progress on equipping CFD codes with accurate sensitivities with respect to the flow variables ($\partial f/\partial u$, $\partial u/\partial v$), there has been more limited progress on inserting this feature into volume grid generation codes for $\partial v/\partial s$, and no analytical capability exists for extracting from a CAD system the sensitivity of the surface with respect to the model parameters ($\partial s/\partial x$). There is no conceptual difficulty in doing this extraction; CAD vendors have not yet felt a compelling need for providing this capability. The approach used in HSCT 4 includes analytical sensitivities of the parameterized NURBS representation.

The message for those contemplating optimization with CFD tools is to choose surface modeling, grid generation, and flow solver tools that provide parametric and sensitivity analysis capabilities.

**Approximation & Correction Processes**

While most disciplinary specialists envision that their sophisticated tools would be incorporated directly into MDO processes, the sober reality is that the lengthy run times of many of these disciplinary codes, especially CFD codes, preclude their direct use. (Recall the time it takes for a single multidisciplinary analysis in HSCT 4.) In practice, heavy use is made of approximation and corrections processes. The approach is to rely on a lower fidelity model for most of the computations, but to invoke the high-fidelity model occasionally for corrections.

The use of variable-fidelity approximations is now quite common. Fig. 6 illustrates the basic idea. Think of the high-fidelity model as a Navier-Stokes CFD code, with $f$ and $\nabla f$ representing the objective function and its gradient with respect to the design variables, as evaluated using the high-fidelity model. Let $a$ and $\nabla a$ denote the approximate objective function and gradient, as evaluated using the lower fidelity model. Many choices are available for the lower fidelity model. It could be a simpler physical

**Fig. 5 HSCT geometry models.**

In the meantime, stopgap measures must be employed. In the aerospike nozzle application, MATLAB™ scripts were used in a novel way to parameterize a conventional NASTRAN™ model of the structure. In the HSCT 4 application, the CAD representation was exported to a NURBS (nonuniform rational B-spline) representation and shape deformation methods were applied to yield the parameterization illustrated above in Fig. 4.
model, such as an Euler code, a panel code, or a vortex-lattice code; alternatively, it could be a formal approximation (what has been called a metamodel in some quarters23), such as a response surface, a neural network, or a kriging approximation. In the past few years there has been considerable work toward putting variable-fidelity approximations on a sound mathematical footing.52,53 There are now variable-fidelity optimization algorithms that have been proven to converge to the solution of the high-fidelity problem. However, the available mathematical results do not address the practical issue of whether the high-fidelity model will be invoked sufficiently infrequently in the variable-fidelity approximation to yield an overall reduction in computational time (compared with always invoking the high-fidelity model). The empirical experience with these rigorous methods is still too limited for any conclusions to be drawn at this point.

![Variable-fidelity approximation diagram](image)

**Fig. 6 Variable-fidelity approximation.**

A related area of research is devoted to developing rigorous error estimates for the approximations. Patera and his colleagues54–56 have pioneered this work for CFD applications. Fig. 7 illustrates the current focus of this group. Note that the design question is not the traditional: Given input heat flux $q = 1$, what is $\bar{T}$, but rather what is $\bar{T}$ and what are the upper and lower bounds due to discretization errors? This work provides rigorous, quantitative bounds on the chosen figure of merit. These bounds are obtained from global calculations on a coarse grid and *local* calculations on a more highly refined grid; consequently, the computational cost of obtaining the bounds in addition to the coarse-grid solution is essentially the cost of the coarse-grid solution. In this example, $\bar{T}_{\text{initial}}$ represents the mean value of the temperature as computed on the initial, coarse mesh, and $\bar{T}_{\text{adapted}}$ represents the improved value of the temperature as computed on the adaptively refined mesh. The methodology relies upon the solution of an adjoint equation for each output function of interest. It also provides a rigorous context for adapting the grid in precisely those regions that produce the greatest errors in the figure or merit.

**Fig. 7 Error estimates for a Boussinesq problem.**56

**Breadth vs. Depth Requirements and Effective Inclusion of High-Fidelity Analyses/Tests**

The most difficult decision for any MDO application is how to strike the right balance between the breadth of the effects that are considered and the depth of the tools used to analyze the effects. The narrower the breadth and the shallower the analysis tools, the more likely the application is to produce an unrealistic design. The broader the breadth and the deeper the analysis tools, the more likely the application is to produce an unrealistic design. In this case the phrase “design improvement” better characterizes the goal than does “optimization.” Here formal optimization techniques are utilized more to guide movement in the direction of an improvement to the design than to locate the mathematical optimum.

**Design Formulations and Solutions**

The use of the word “optimization” in conjunction with design often conjures up the impression that the designer is seeking a mathematically optimal solution to his problem. In reality, the designer’s goal is often to improve an existing design. In this case the phrase “design improvement” better characterizes the goal than does “optimization.” Here formal optimization techniques are utilized more to guide movement in the direction of an improvement to the design than to locate the mathematical optimum.

**Design Problem Objectives**

In practice, there is considerable art to specifying the details of the problem statement, Eq. (1). Optimization is notorious for finding the weaknesses in the analysis codes and the problem formulation. In the context of aerodynamics, casual optimization frequently drives the solution towards regimes in which the CFD code is unreliable (e.g., highly separated flow) or for which the surface geometry
model or the volume grid breaks down. A related difficulty for CFD-based optimization is that great care must be exercised in parameterizing the surface. Virtually everyone who has attempted aerodynamic wing design has been disconcerted by spanwise corrugations in the "optimal" wing. Arian and Ta'asan have provided a mathematical explanation of this phenomenon. They demonstrated that it is an inherent difficulty. Only well-chosen parameterizations or constraints can mitigate this tendency.

In most cases the precise problem formulation evolves in the course of the investigation. This makes methods that are able to reuse information from previous optimization formulations quite useful.

Design Problem Decomposition & Organization

An MDO method for a given problem consists of an MDO formulation and an optimization algorithm. The former deals with problem decomposition, and mathematical issues such as equivalence to the original problem and to alternative formulations are germane. The latter deals with the solution procedures applied to the MDO formulation, and the properties of optimization algorithms as applied to the formulation are of interest.

Fig. 8 Multidisciplinary feasible (MDF) formulation.

We shall use a coupled aerodynamics-structures problem to illustrate a few of the many formulations (decompositions) that have been proposed. The most obvious formulation is to stay with the original problem statement by constructing a full multidisciplinary analysis of the problem and wrapping an optimizer around it (Fig. 8). This multidisciplinary feasible (MDF) approach has the feature that at each cycle of the optimization, the current trial point is a consistent solution to the multidisciplinary analysis (MDA) problem. If there is a significant coupling between the disciplines, the solution of the MDA problem requires iterations (usually of fixed-point type) through all the disciplinary codes. The use of the word "feasible" in the name of the MDF formulation may be misleading. It is feasible only in the sense that the multidisciplinary analysis is consistent with respect to all the disciplines; the consistent multidisciplinary analysis may still represent a point infeasible with respect to the optimization problem (some constraints are violated).

Fig. 9 Individual discipline feasible (IDF) formulation.

The MDF formulation is hardly the only approach, however. Fig. 9 illustrates the individual discipline feasible (IDF) formulation. At each optimization cycle IDF requires feasible solutions for each discipline analysis but not for the full multidisciplinary analysis. The disciplinary coupling variables become part of the design variable set in IDF and compatibility constraints are added at the system level; consistent multidisciplinary analysis is guaranteed only at the convergence of the optimization.

Fig. 10 Collaborative optimization (CO) formulation.

Numerous multilevel formulations have been developed, including concurrent subspace optimization (CSSO), collaborative optimization (CO), MAESTRO, and bilevel integrated systems synthesis (BLISS). Multilevel methods are distinguished by using optimization both at the upper or system level and at the lower or subsystems levels. Fig. 10 illustrates the CO formulation (a two-level formulation). Note that at the subsystem
(disciplinary) level, the optimization problem is not a traditional discipline optimization problem, but rather an optimization to reduce the incompatibility between the variables shared by the disciplines. This formulation permits considerable disciplinary autonomy. Fig. 11 illustrates the MAESTRO formulation. Along with most of the other multilevel formulations, it uses more traditional discipline optimization problems at the subsystem levels and permits some degree of disciplinary autonomy as well.

![Fig. 11 MAESTRO formulation.](image)

Some of these formulations, such as CO and IDF, dispense completely with the requirement to perform a full MDA. Others, such as CSSO and BLISS only require occasional uses of full MDA. At least two classifications for MDO formulations have been proposed, but not every extant MDO formulation fits cleanly into either classification system.

One should not lose sight of the point that the formulations discussed above (aside from MDF) remain merely candidate approaches until proven to be equivalent to the MDF formulation and to be practical in the sense that they can be coupled with an effective optimization algorithm. Thorough discussions of the mathematical properties of the CO formulation and the MAESTRO formulation are available. MAESTRO has been proven rigorously to be equivalent to MDF, whereas there are some subtle difficulties with CO.

The choice of formulation should be strongly influenced by the nature of the coupling between the disciplines. This interdisciplinary coupling may be characterized in two dimensions. The coupling is narrow if few variables are interchanged and broad if many variables are interchanged. The coupling is weak if a consistent multidisciplinary analysis can be achieved in a small number of iterations and strong if many iterations are needed. For problems with weak, narrow coupling, just about any formulation appears to work. For problems with strong, broad coupling, only the MDF and the MAESTRO formulations apply. The effectiveness of the various MDO formulations is very much an open question for the other two combinations.

Another aspect of problem decomposition, which becomes increasingly important as the number of subprocesses involved in the design process increases, is the identification of the best sequence for executing the individual subprocesses. One needs to recognize that in complex design processes there is both feed-forward and feedback of information. There are usually subprocesses that depend upon the information from downstream subprocesses. This dependence can only be handled iteratively. Tools for assisting in the overall structuring of the design process are available.

**Optimization Procedures and Issues**

A wide variety of optimization algorithms and software is available for solving the particular MDO formulations. There is certainly quite a selection of gradient-based optimization algorithms. The main issue with these is ensuring that accurate and efficient derivative information (sensitivity analysis) is available from all the codes. Sobieski has provided an algorithm—the generalized sensitivity equations—for combining the constituent disciplinary sensitivities into the full multidisciplinary sensitivities for the MDF formulation. Especially when there are iterative subprocesses involved in the MDA, just validating that the system sensitivities are correct is quite time consuming.

Most optimization software assumes complete control over the calls to the analysis and sensitivity analysis (gradients) processes as illustrated in the left half of Fig. 12. For most multidisciplinary problems the analysis and sensitivity analysis calls are quite time consuming, and this "direct insertion" approach is prohibitively expensive. This problem is not inherent in the optimization algorithms, but is due to the inadequate user control provided by many of the software packages. Many MDO practitioners prefer to exert more control over the optimization and have adopted the sequential approximate programming (SAP) approach illustrated in the right half of Fig. 12. This approach couples the optimization software with an approximation; the figure illustrates an approximation based on zero- and first-order information, but the method has been used with a variety of approximations. Not only does the SAP approach usually reduce the number of invocations of...
the expensive analysis and sensitivity analysis computations, but it also provides readily for periodic human intervention whenever the approximation is updated. The SAP approach is so common in current MDO applications that one is hard pressed to find a complex application that used the direct insertion approach. The aerospike nozzle application used the direct insertion approach to optimization, whereas the plan for HSCT 4 is to use the SAP approach. The computational demands of the former were sufficiently modest to permit use of direct insertion.

**Fig. 12 Direct insertion and sequential approximate programming (SAP) approaches.**

In many MDO applications involving aerodynamics modeled at the nonlinear CFD level, the run-time of the aerodynamics code dominates the overall run-time of the MDA. Because nonlinear CFD codes are invariably solved via iterative methods, the MDF formulation yields an iterative CFD process nested inside the iterative optimization process. This has led several groups to propose turning the aerodynamics optimization process “inside out” and nesting the optimization iterations inside the CFD iterations. Fig. 13, loosely taken from Newman et al., illustrates the multidisciplinary extension of this simultaneous analysis and design (SAND) procedure as it would appear for an aerodynamics-structures problem. This approach has met with demonstrable success for some structures problems, but has yet to reach its full potential for aerodynamics, let alone for coupled aerodynamics-structures problems. Robust strategies for ensuring convergence have yet to be demonstrated for flows with discontinuities. One barrier to acceptance of this approach is that if the optimization process is stopped short of convergence, as might occur if one simply runs out of time, one may not have a feasible solution to the individual disciplinary problems, let alone one to the complete multidisciplinary problem. This consideration appears to have limited the use of this approach within the structures discipline.

**Fig. 13 Simultaneous analysis and design (SAND) algorithm.**

One cannot yet provide reliable guidelines on matching the method to the problem. (Remember that an MDO method consists of both a formulation and an algorithm.) Some comparisons are available in the original papers cited above for these methods. There have been the beginnings of third-party comparisons between methods. However, these comparisons are invariably on quite simple problems due to the tremendous effort required to implement even one MDO method on a complex problem. NASA Langley has established the MDO Test Suite, a collection of MDO problems, has to serve as test cases.

There is an increasing selection of available optimization methods that do not exploit gradient information. These include novel pattern search methods, evolutionary algorithms (including genetic algorithms and simulated annealing methods), and discrete search methods. Such methods appear to have significant difficulties with problems with a large number of variables and constraints. Since formulations such as CO, IDF, BLISS and CSSO all add a large number of constraints to the original MDF formulation, non-gradient-based methods may have difficulty with the alternative formulations.

Finally, we should mention that most MDO problems have multiple objective functions, rather than a single objective function for a dominant discipline plus constraints for the remaining disciplines. An obvious, but simplistic, approach is to construct a single weighted objective function out of all the objective functions. More promising approaches are available. Perhaps these will
ultimately prove useful for applications to aerodynamic multipoint optimization.

Management and Cultural Implementation

In many respects the technical challenges within the MDO field pale against the organizational and cultural barriers the research community faces. Giesing and Barthelemy\textsuperscript{26} discuss this from an industry perspective. Here we’ll just comment on some team issues that arise in a government research laboratory. In a research environment, discipline specialists participating in MDO applications naturally want to use the latest tools from their discipline, but these tools usually are not yet robust enough for inclusion in an automated process and take large amounts of computer time. Researchers, however, receive very negative feedback from their discipline peers if they resort to use of established tools that are more suited for a complex MDO application.

Another common obstacle is that developing a multidisciplinary problem statement, which includes detailed process definition along with specific tool selection, takes considerable time. (It took well over a year to arrive at the final technical definition of the HSCT 4 application.) This process is excruciating for most researchers. Researchers from a discipline accustomed to a dominant role in the organization find it especially difficult to make the compromises that are essential for an effective team. In all likelihood, more prospective MDO research projects have come to naught for human reasons than for technical ones. We have begun to make systematic studies of these issues.\textsuperscript{83–85}

Fluid Dynamics for a Multidisciplinary Age

Here we shall reinforce some of our earlier comments and point out some potential new opportunities for fluid dynamics research.

Sensitivity Analysis

Our principal message is a recapitulation of Sobieski’s 1986 call for aerodynamic sensitivity analysis,\textsuperscript{4} but with a twist: whereas Sobieski recommended that sensitivity analysis should be a standard feature of the CFD codes to be used in vehicle design, our recommendation is that sensitivity analysis should also be a standard feature of the codes used to study flow physics.

Sensitivity derivatives are useful for a variety of purposes beyond their obvious use in gradient-based optimization. Consider an issue that has recently received significant attention—uncertainty analysis. There are many contributions to the uncertainty in results from CFD codes.\textsuperscript{66} Certainly spatial and temporal discretization, iterative convergence tolerances, artificial viscosity, transition and turbulence modeling, and plain coding errors all must be examined. Some aspects of these and other sources of errors can be quantified through sensitivity analysis. Figure 14 illustrates how sensitivity derivatives can be used to estimate the effect of uncertainties in flow variables, such as Mach number $M$ and angle of attack $\alpha$, upon the uncertainties in outputs such as the lift coefficient. We have performed some preliminary calculations for the uncertainties in CFD outputs for a high-lift case\textsuperscript{87} with $M = 0.2$ and $\alpha = 19^\circ$, which is near maximum lift. The computations were performed by the CFL3D code augmented with sensitivity derivatives by the ADIFOR tool. These calculations suggest that for these conditions $\frac{\partial C_L}{\partial M} = O(1)$ and $\frac{\partial C_L}{\partial \alpha} = O(10^{-3})$.

\begin{align*}
\Delta C_L &= \left(\frac{\partial C_L}{\partial M}\right) \Delta M \\
\Delta C_L &= \left(\frac{\partial C_L}{\partial \alpha}\right) \Delta \alpha
\end{align*}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{uncertainty_analysis.png}
\caption{Uncertainty analysis via sensitivities.}
\end{figure}

The use of sensitivities in this context goes far beyond quantification of the effect of flow field uncertainties. They can be used to determine the effects upon the code outputs arising from variations in any input variable or continuous parameter of a CFD code. Obvious examples are the uncertainties from transition onset location, transition region extent, turbulence model coefficient, surface manufacturing variability, and elastic surface deflections. One can, of course, compute these sensitivities with the finite-difference approach, i.e., by performing one additional CFD run for each desired sensitivity with a small perturbation in the appropriate input or parameter variable. But a CFD code equipped with sensitivity analysis can compute all the desired sensitivities in the same run as the original analysis, usually far more efficiently and
always more accurately. The accuracy suffers when finite differences are used to estimate the sensitivities because one is forced to subtract nearly equal numbers; with the other approaches the sensitivity derivatives are obtained from the most significant digits of the computation. As noted above, one can hand-code the sensitivities, use the complex variable method, or employ automatic differentiation.

The use of automatic differentiation for obtaining sensitivities from CFD codes with respect to Mach number, angle of attack, turbulence model coefficient, some algorithmic parameters such as artificial viscosity coefficients, and geometry perturbations has already been demonstrated 6 years ago. The accuracy problems with the finite-difference approach to sensitivities can be severe for transition and turbulence modeling coefficients, as models for these phenomena tend to be nonanalytic. Nevertheless, the automatic differentiation approach was conclusively shown to yield the correct sensitivities. This may be the only viable approach if one wishes to tune the model coefficients by what amounts to a gradient-based optimization method.

Some preliminary calculations we have performed for a multielement airfoil near maximum lift, such as illustrated in Figure 14, suggest that first derivatives alone may not suffice for accurate estimation of the effect upon forces and moments of inherent uncertainty in tunnel settings. Contributions from second derivatives may also be needed. Park et al. reached a similar conclusion in their use of sensitivity derivatives to estimate control effectiveness. Second derivatives may be obtained fairly easily by combining the complex variable technique with use of ADIFOR or by exploiting the forthcoming Hessian capability of ADIFOR, although the computational expense will be high. This second derivative capability should provide fluid dynamicists with a variety of new opportunities.

The example above was for a (nearly) steady flow. Sensitivities can be useful for time-dependent fluid dynamical problems as well. A meteorological application of automatic differentiation has been made to the computation of propagation of small disturbances in time-dependent nonlinear simulation codes.

Recent trends suggest that the CFD tools of choice for the next decade will have sensitivity analysis as well as rigorous discretization error estimates (recall the work leading to Fig. 7). Together these will provide the user with a firm handle on many aspects of the uncertainties in the code results.

Sensitivity analysis is clearly applicable to the task of computing stability and control derivatives from CFD codes. Most past attempts at this have simply used the CFD code to mimic how these quantities are approximated, by what amounts to finite differencing or curve fitting, in wind tunnel experiments and flight tests. Why not use sensitivity analysis to solve the exact equations that govern the stability and control coefficients?

Aerodynamic Design Methods

There has been significant progress this decade in gradient-based aerodynamic design methods, with the most efficient methods utilizing hand-coded sensitivities and adjoints (although no one has yet been masochistic enough to produce a hand-coded adjoint that includes the turbulence model). The next challenge in this line is to adapt these methods to multidisciplinary problems, e.g., to aerodynamics-structures problems. This extension is not straightforward. If one is using a loose coupling between aerodynamics and structures codes, there will be many surface interface variables, and the requirement for sensitivities for each of these variables diminishes the advantage of the adjoint methods.

This difficulty can be avoided if one develops a tightly coupled aerodynamics-structures code, but the tools of choice for the structures community are commercial codes, and one does not have access to the source code.

The gradient-based optimization methods that have been the focus of much of this paper are certainly not always the method of choice for aerodynamic design problems. Inverse design methods are often far more efficient. For example, the DISC and CDISC methods can typically match a desired pressure distribution at an additional cost that is less than 10% of the underlying cost of a single analysis, and rules have been developed that allow reasonable guesses for desired pressure distributions and for incorporation of a variety of constraints. Generally speaking, however, this approach is confined to situations in which the design variables and the objective function are taken from the same surface; they don't apply, for example, to the design of the shape of an engine nacelle to optimize the performance of a wing. When effective estimates of desired pressure distributions cannot be made and for cases in which there may be many local minima, the DACE (Design and Analysis of Computer Experiments) approach used in the 3DOPT tool and/or methods such as genetic algorithms can be used to explore the design space. The DACE and genetic algorithm approaches do
suffer, however, from the curse of dimensionality, rapidly becoming impractical as the number of design variables increases. (Parallel processing can reduce the impact of the curse of dimensionality.) Gradient-based optimization appears the best choice when a desired pressure distribution is not available, when multiple surfaces are involved, when there are a large number of design variables, or when one is content with a local minimum.

Inverse aerodynamic design methods do not appear to have yet been used effectively in multidisciplinary optimization problems. Surely they can be exploited somehow in multilevel MDO methods. But even in the context of their use in aerodynamic optimization there is an opportunity, using techniques developed for structural optimization, to apply sensitivity analysis to these inverse design methods to address such issues as sensitivity of the optimal design with respect to parameters.

Aerodynamic design methods generally view the problem deterministically. A different perspective is taken by optimization methods that seek to account explicitly for uncertainties. This “optimization under uncertainties” approach arose in the civil engineering community and is starting to make inroads in parts of aeronautics. Two distinct aspects of this approach are reliability-based design and robust design. In the former case one designs to a prescribed probability of failure, whereas in the latter case one seeks relatively flat local optima, i.e., designs that remain effective (robust) in a broad neighborhood of the putative optimal point. In both cases one needs to characterize the distribution of uncertainties. For reliability-based design one is most interested in the tail of the distribution, whereas for robust design one is most interested in its low-order moments. One can foresee fluid dynamics applications in both areas—reliability-based approaches to the aerodynamics of systems which operate in an uncertain environment and robust design approaches to the fluid dynamics of devices which cannot be modeled at all accurately.

Aerodynamic Approximations

Accurate, but affordable, approximations to aerodynamic analyses are desperately needed for fluid dynamics to make an impact in broad MDO processes. A wide variety of approximations have been used for MDO problems in general and for aerodynamics optimization. This variety includes response surfaces, neural networks, DACE models, kriging methods, and low-fidelity methods. Approximations are especially needed for time-dependent problems. The aeroservoelastic community has developed a variety of methods that they call reduced-order models. Some aspects of these models are useful for purely fluid dynamics problems as well. An approach that may be intriguing to parts of the turbulence physics community is the use of proper orthogonal decompositions in design.

Experimental Validation

Experimental validation of aerodynamic optimization is very challenging. There is as yet no satisfactory approach to experimental validation of the predictions of optimization studies, at least with respect to shape design variables. The issue here is not just validating the performance predictions of a specific “optimized” design, but rather experimentally exploring the design space in a neighborhood of the supposed optimum to determine whether it is indeed an optimal design. The obvious difficulty is that testing the region around the optimal design requires an inexpensive, rapid capability to make specific small changes in the shape of the test article and to retest it. Similar difficulties beset experimental validation of sensitivity analyses.

A Cultural Reminder

If a multidisciplinary approach to a problem is to have any hope of producing a beneficial, synergistic result, then there must be genuine interdependency among the contributing disciplines. This interdependency of disciplines invariably requires that the individual members of the multidisciplinary team be interdependent upon each other, i.e., that they be a true team and not just a working group in which the team leader merely collates isolated, independent contributions. This requirement is probably the largest barrier that any fluid dynamicist must overcome before entertaining serious thoughts of conducting multidisciplinary research; most researchers are very uncomfortable depending on someone else. This discomfort barrier is one reason there are so many examples of very simple structures codes linked to state-of-the-art CFD codes and so many examples of sophisticated finite-element codes obtaining the loads from vortex-lattice codes. There are few opportunities for synergy in such approaches.

The fluid dynamicist who wishes to participate in multidisciplinary activities should ensure that his analysis tools are design oriented: that they contain sensitivity analysis, use approximations to the maximum extent possible, allow for rapid reanalysis,
are robust, are built on parametric model descriptions, and are automated. The fluid dynamics researcher should also be prepared to invest considerable time in understanding the other disciplines and to participate fully in the arduous process of defining the multidisciplinary problem.

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