Massachusetts Institute of Technology
Department of Aeronautics and Astronautics

Ph.D. Proposal Document

Advancing the Usability, Interpretability, and Practicality of Conceptual Aircraft Design Optimization with Code Transformations

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Abstract

TODO abstract

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Chapter 1

Introduction

TODO background

1.1 Project Definition and Thesis Overview

1.2 Proposal Document Organization

The latest doctoral handbook for the MIT Department of Aeronautics and Astronautics requires the following elements in a PhD proposal, which, for reader convenience, are mapped to specific portions of this document:

Table 1.1: Requirement-to-section mapping for the PhD proposal document.

Requirement	Section
A clear, specific statement of the technical problem and the objectives of the proposed research	Section 1.1, 3.1
A thorough, adequately referenced, summary of previous work done on the problem	Section 2
A plan for the initial approach to the problem	Section 3.2
An outline of the major foreseeable steps to a solution of the problem	Section 3.2, 4.4
An estimate of the time that might be required	Section 4.4
A list of the facilities needed	Section 4.5

Chapter 2

A Review of Aircraft Design Optimization

2.1 Early Promises, Predictions, and Pitfalls

> *"When an aircraft designer hears that a new program will use multidisciplinary optimization, the reaction is often less than enthusiastic. Over the past 30 years, aircraft optimization at the conceptual and preliminary design levels has often yielded results that were either not believable, or might have been obtained more simply using methods familiar to the engineers. Even 5-20 years ago, actual industry application of numerical optimization for aircraft preliminary design was not widespread."*
>
> -Ilan Kroo, 1997 [1]

These are the opening lines of a landmark 1997 paper that reviewed the state of the art and future directions in the then-nascent field of aircraft multidisciplinary design optimization (MDO) [1]. The paper, by aircraft designer and MDO pioneer Ilan Kroo, not only reviewed the status of the field's academic research, but also took the key step of assessing whether these research advances had translated to practical industry impact. As a later review by an MDO technical organizing committee would emphasize, "the ultimate benchmark of a research field's impact is indicated by the realization of its theories into successful products throughout industry." [2]

Kroo's assessment of the field is generally optimistic, though he also hedged this with some important reservations. On one hand, he notes the auspicious progress of aircraft MDO research during the preceding decades by all traditional metrics: problem size, analysis fidelity, runtime speed, and so on. He credits these successes largely to both algorithmic advances and the exponential growth of computational power over time (Moore's law[1]). Extrapolating these trends forward, he concludes that the field is poised to make a significant impact on the aircraft design process across both academia and industry. The promise of MDO is made clear in a remark that many aircraft designers would agree with today: "In a very real sense, preliminary design is MDO." [1]

On the other hand, Kroo notes that actual industry applications of aircraft MDO remained conspicuously limited as of the paper's 1997 publication, and "many difficulties remain in the routine application of MDO." [1] Other works from the early days of aircraft MDO corroborate this dearth of industry adoption. For example, in a 1982 AIAA lecture titled *On Making Things the Best – Aeronautical Uses of Optimization*, optimization advocate Holt Ashley notes the "keen disappointment felt by many [optimization] specialists because their theories have received so little practical application." [3] Ashley goes further by conducting an exhaustive industry-wide survey to identify "successful practical applications" of aircraft design optimization. The survey received "overwhelming" industry interest and encouragement; however, "the yield of examples which met the criterion of having been incorporated into a vehicle that actually operates in the Earth's atmosphere was painfully, perhaps shockingly small."

Perhaps the reason why Ashley's disappointment was so poignant is that, even at the time, aircraft designers in industry widely recognized the immense potential of MDO tools to fundamentally transform engineering design workflows. As two Lockheed engineers stated in 1998 [4], "The technical community knows the power of MDO and not having a cradle-to-grave example has been a continual source of frustration, as voiced by AIAA MDO technical committee members [for] years." Similarly, a 2002 Boeing paper identifies MDO as one of four key technologies poised to define the next generation of aircraft design[2] [5].

Motivated by this gap between promise and practice, Kroo and other luminaries offer several reasons for the lack of industry adoption of MDO technologies:

1. **Inadvertently-violated model assumptions:** When optimization is applied to an analysis toolchain, it acts adversarially, disproportionately seeking out the "weakest link" in the analysis chain and exploiting it. Simplified models that are acceptable in a manual sizing study are often unacceptable in an optimization study, because implied assumptions that an engineer would naturally cross-check during manual design are prone to optimizer exploitation. This can lead to unrealistic results from

[1] "Moore's law" is an empirical observation that chip transistor density (a surrogate for computational power) has tended to double roughly every two years, a trend that has held true for the past half-century.

[2] With the others being computational simulation, small uncrewed aircraft, and newly-emphasized design considerations such as environmental footprint and operations optimization.

MDO tools that degrade user trust in optimization processes. Kroo contends that the solution to this problem is to implement higher-fidelity models that account for more edge cases, an approach we explore later in Section 2.3.1.

2. **Missing models and constraints:** Critical aircraft design choices are often determined by tradeoffs spanning multiple disciplines. If an MDO tool does not incorporate relevant disciplines (e.g., it performs aerodynamic, propulsive, and structural analyses, but the true design driver is noise), then the resulting design will be fundamentally flawed with no indication to the user whatsoever. This can lead to costly design mistakes. Indeed, Kroo suggests that a flawed MDO tool is not only useless, but worse, due to the false confidence it can instill.

3. **Challenges of managing complexity:** As computational power grows, MDO tools can incorporate increasingly numerous and higher-fidelity models. To first order, when the number of models N grows, the potential number of cross-discipline couplings to manage tends to scale as $\mathcal{O}(N^2)$. Therefore, in the limit of growing computational power, the practical bottleneck is less about implementing individual analyses, but more about managing this communication overhead and architecting the optimization code itself.

Kroo primarily attributes these early barriers to practical industry adoption to the limited computational power of the era, noting: "This convergence between computational capability and computational requirements for interesting design problems is one of the reasons that MDO is considered to be such a promising technology, despite the limited acceptance of pioneering MDO efforts." A contemporaneous review by Sobieski and Haftka agreed, identifying "very high computational demands" as a "major [obstacle] to realizing the full potential of MDO". [6]

However, some works recognized that not all challenges would recede with increasing computational power. A 2002 review paper by a Boeing Technical Fellow in *Journal of Aircraft* [5] cautions: "New [MDO] strategies need to be developed...which take advantage of the assumptions and techniques that airplane designers use, rather than letting a computer churn away and come up with theoretically possible, but practically impossible, configurations." Likewise, Kroo, Sobeiski, and Haftka all cite "managing complexity" as a growing challenge of MDO [1, 6], which hints at a human-computer interface problem, rather than simply a need for more CPU cycles. Drela's aptly-titled 1998 work *Pros & Cons of Airfoil Optimization* also demonstrates a similar issue [7]. Here, Drela shows that even seemingly-simple aerospace design optimization problems will only yield practical results if the problem formulation, assumptions, and results are all precisely understood by an expert designer. These works presciently foreshadow modern concerns around MDO interpretability and other user frictions, urging the development of human-centered MDO approaches that synthesize mathematical optimization with designer intuition.

In summary, while computational limits were a clear early barrier, foundational challenges around managing complexity and aligning optimization with real-world design constraints were already emerging. These issues would become increasingly central as MDO research rapidly expanded in scope.

2.2 A Retrospective on Aircraft Design Optimization in Industry

Current Status

With the benefit of an additional quarter-century of hindsight since the date of these early MDO assessments, we can begin to assess how these forecasts have played out. In many ways, these predictions by Kroo and others were remarkably accurate. The scale and speed of optimization problems solved today has indeed grown exponentially in the years since. This is not only due to increasing computational power, but also from algorithmic and architectural improvements in MDO and optimization more broadly[3]. Numerous high-quality aircraft MDO case studies and post-hoc design studies have been published in the years since, including the D8 transport aircraft [8, 9], the STARC-ABL aircraft [10], and the Aerion AS2 [11]. Some of these studies leverage relatively-high-fidelity models (e.g., RANS CFD) that would have been computationally-intractable for optimization studies in prior eras.

However, many of the barriers to practical industry use Kroo identified have not disappeared; to the contrary, as computational power increases, the challenges of interpretability and managing complexity ring even truer today. As a result, this gap between academic research and practical industry adoption has not closed, and in some ways is wider than ever before. A 2010 review paper [2] concludes that "the actual use of genuine MDO methods within industry at large...is still rather limited." In 2013, Hoburg and Abbeel lamented that "despite remarkable progress in MDO, the complexity and diversity of modern aerospace design tools and teams makes fully coordinated system-level optimization a monumental undertaking." [12] As recently as 2017, a team of Airbus engineers and MDO researchers concurred: "While the field of MDO techniques has tremendously grown since [the 1980s] in the scientific community, its application in industry is still often limited[...] A major challenge remains to apply MDO techniques to industrial design processes." [13]

Despite the prevalence of on-paper design studies using MDO, it remains somewhat rare to see *built-and-flown* airplanes developed with documented, significant use of MDO methodologies. Indeed, the industry norm for aircraft conceptual design remains largely unchanged: expert-driven manual design guided primarily by point analyses and parametric surveys. Here, the human designer informally fulfills an optimizer-like role, but the

[3] discussed later in Section 2.3

requirements are never explicitly translated into a formal mathematical optimization problem[4]. High-quality aircraft design case studies that implement this expert-driven manual approach successfully are those of the Joby Aviation S2 eVTOL [14] and Perdix micro-UAV [15] aircraft. Anecdotally, the *industry* conceptual designer's computational weapon of choice is still more often an Excel spreadsheet than a formalized MDO framework.

To assess the magnitude of this gulf between academic and industry use of MDO, we surveyed industry literature and design reviews to identify aircraft development programs showing three minimal criteria:

1. A design optimization problem for a complete aircraft coupling at least three disciplines (e.g., aerodynamics, structures, and propulsion) that is solved computationally.
2. Evidence that the optimization result (or at least, some insight gained from it) was used to inform the design of aircraft.
3. Evidence that the aircraft was subsequently built and flown.

It is worth pausing to discuss why this restrictive *built-and-flown* aircraft requirement is used, since it accounts for the majority of the aircraft design studies that were excluded from this survey. Successful optimization on built-and-flown aircraft forces a level of completeness, trust, and durability that may not be present in a paper study. Ashley notes that a practical MDO result "must also survive the gauntlet of ground testing, reliability, demonstration, flight verification, and the like without further special attention". [3] Myriad other practical considerations could be added to this list – certifiability, manufacturability, lifecycle costs, maintainability, robust off-design performance, and the realities of engineering culture (e.g., can the MDO tool give not only a result, but sufficient evidence that it should be believed?), to name only a few. To justify the substantial capital of building and flying a new aircraft, optimization results must withstand a much higher standard of scrutiny and reviewability than they might otherwise.

Consistent with previous surveys and reviews [1–3, 6, 13], we find that relatively few programs meet these criteria; here, we make note of some that do. The Lockheed Martin F-22 Raptor program was one of the first programs to leverage an MDO-like process for a complete, flown aircraft design, as reported by Radovcich and Layton [4]. However, the workflow documented in this 1998 work differs significantly from modern MDO processes in that it was remarkably manual – a fusion of traditional and MDO-based design processes. While some disciplines (aerodynamics, structures, and control law design) are coupled computationally, many other disciplines (low-observability, manufacturability,

[4]i.e., with a precisely specified objective, defined variables, and enumerated constraints

etc.) are coupled in by querying teams of subject-matter experts at iterates within the optimization loop itself, essentially serving as a black-box function call. When contrasted with more-typical MDO processes where all interdisciplinary communication is computational, this manual approach has some pros and cons. One one hand, intermediate optimization iterates are continuously human-reviewed, which could cause a poorly-posed problem to be identified as such more quickly. On the other hand, it also sharply increases the optimization runtime, which may take months instead of hours. Even allowing for this broader definition of MDO, however, the authors note the rarity of their experience in industry: "Documented experiences of MDO applications during the engineering, manufacturing, and design phases of fighter aircraft programs are not numerous. Documentation is even rarer for aircraft that have flown."

The Lockheed Martin X-59 Quiet Supersonic Transport (QueSST) is another program that leveraged an MDO-based design process throughout aircraft development, unifying aerodynamics, acoustics, and structural analyses for outer mold line design and composite ply scheduling [16–18]. (Although the X-59 has not yet met the "flown" criterion at the time of writing, industry reports credibly suggest this is imminent with no remaining obvious barriers.) The X-59 program builds upon several decades of successful MDO research for sonic-boom-minimization problems, a topic where computational shape optimization has proven particularly useful due to the non-intuitive and sensitive nature of the design problem [19].

The Airbus *Vahana*, a single-seat eVTOL demonstrator flown in 2018, is perhaps one of the most recent public examples of an MDO-based process used to develop a flown aircraft [20–22]. The initial sizing study considered aerodynamics, structures, propulsion, and cost analysis to drive conceptual trade studies between various vehicle configurations. This study included practical constraints and margins, such as reserve mission energy, battery cycle life, and engine-out safety (by enforcing either autorotation capability, motor redundancy, or a mass allocation for a ballistic parachute, depending on configuration).

Several other programs have built and flown uncrewed research aircraft with MDO use, such as the Facebook *Aquila* solar-powered UAV [23], the MIT *Jungle Hawk Owl* long-endurance UAV [24], and the X-48B blended-wing-body demonstrator [25–27]. Other programs document MDO usage for narrower subsystem- or component-level design, as in the detailed design of the Boeing 787 Dreamliner [2].

Outside of these cases, documented *industrial* use of MDO for complete-aircraft conceptual design remains rare, relative to the vast number of industry programs conducted in the past few decades. This observation is especially surprising in light of the widely-recognized potential utility of MDO in industry.

One compelling partial explanation for this lack of use is a lag effect stemming from long timelines of new aircraft development programs – it takes time for new tools (such as MDO methods) to proliferate throughout industry, due to sunk-costs on design pipelines for existing programs. Indeed, although the present literature review finds that documented industry use of MDO is scarce, the situation appears somewhat less dire than older surveys indicate [1–3, 6, 13]; this suggests that industry use may be gradually increasing. However, considering that aircraft MDO research and industry interest in optimization has existed for over forty years [3, 28], this lag effect alone does not constitute a complete explanation for the lack of adoption.

Ashley considers another possible explanation for the lack of visible MDO use in industry: that of "military classification or company proprietary considerations." [3] However, after exhaustive correspondence with dozens of aircraft design industry contacts, Ashley concludes that this limitation was only occasional and "not to an extent that would affect the principal conclusions." Therefore, it seems that the limited observations of formal mathematical optimization processes in industrial aircraft design are genuine, representing a missed opportunity for the field to make an practical impact.

2.3 Pivotal Advances in Design Optimization Research

On a more optimistic note, MDO's substantial academia-industry gap is equally attributable to academia's remarkable advances in design optimization research over recent decades. This progress is readily apparent from analyzing trends in academic literature. As shown in Figure 2.1, the fraction of aircraft design publications directly referencing MDO has grown from near-zero in 1985 to 10% today.

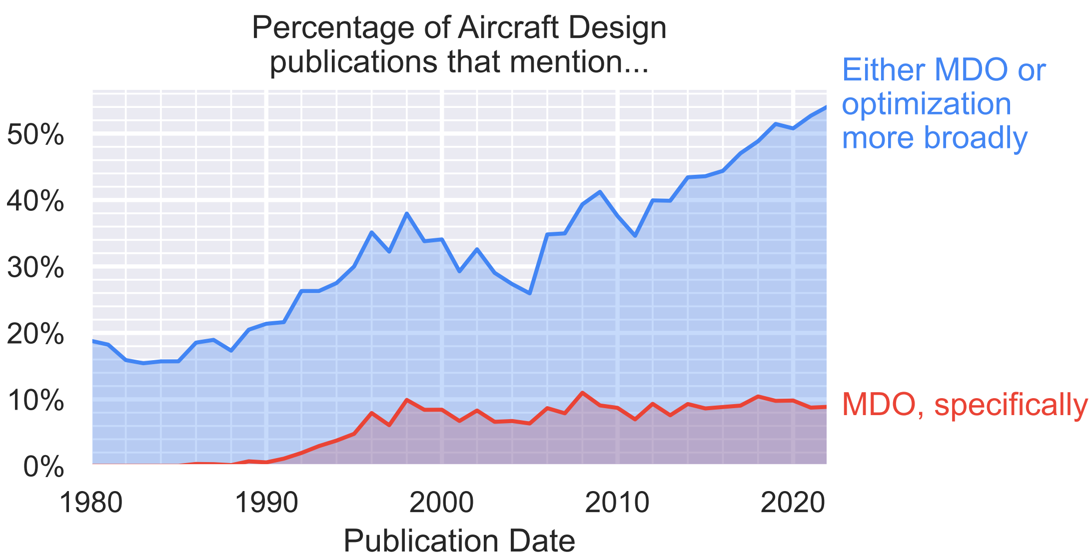

Figure 2.1: Prevalance of optimization-related keywords in academic literature with the keyword "aircraft design". Data from Google Scholar; includes industry-standard texts such as AIAA journals and conference proceedings. MDO-specific keywords (red line) include any of: "multidisciplinary design optimization", "MDO", and "MDAO". The blue line adds the keyword "optimization" to this list.

Moreover, this statistic alone understates the true magnitude of MDO's impact. Arguably the most pivotal contribution of MDO research to aircraft design has been to catalyze a shift towards an *optimization mindset*: the recognition that optimization is not only a useful tool, but also a principled mathematical framework that can represent complete design problems. Figure 2.1 shows that this mindset is a relatively recent development – the fraction of aircraft design publications mentioning optimization in any form has tripled since the advent of MDO, reaching a majority share today.

These optimization-based design processes have shown several benefits when used to augment traditional design methods such as point analyses, parametric surveys, and carpet plots [29]. Most obviously, formal optimization methods can lead to improved design results and allow the consideration of many more design variables. Optimization can also help human designers discover clever cross-discipline synergies that might otherwise be overlooked [7], and its rigor can reduce the likelihood of biased decisions [29]. In cases where designer intuition is exhausted, such as with unconventional configurations, optimization provides a means to identifying useful directions for further exploration [7]. Torenbeek argues that an optimization-based design process can respond more quickly to unexpected changes in program requirements, whereas manual processes often require substantial redesign effort [29]. Finally, the optimization mindset itself has benefits, even beyond the results of an optimization study. for example, discussions about problem formulation (how to translate given requirements into a quantified optimization problem) can help a team of engineers align on design goals and expose subtle discrepancies in perceived requirements[5].

Another important area where MDO research has made significant progress is in defining the relationship between the human designer and the optimizer. The prevailing view in the early days of aircraft design optimization was that optimization would eventually advance to the point that computational tools could yield complete, production-ready designs with minimal human oversight – as evidenced by encouraging titles such as "Automating the Design Process" [28, 30, 31]. Over time, this has largely given way to a more balanced view: although the optimization solve itself may be well-served by computational means, this forms only one small part of the larger design process. Inputting the engineer's design intent into the optimizer accurately ("problem specification") and extracting intuition from the results ("interpretation") are challenges in their own right, and best addressed by iterative human-computer teams. As described by Drela in a 1998 optimization study [7], "[Engineering optimization] is still an iterative cut-and-try undertaking. But compared to [traditional] techniques, the cutting-and-trying is not on the geometry, but rather on the precise formulation of the optimization problem."

When considering this full design process (i.e., from initial requirements to product delivery), the scope of challenges becomes even broader. Indeed, industry adoption of MDO is often limited by non-computational user frictions [32–34]. In the present work, we deliberately term these user frictions "costs", borrowing optimization nomenclature to emphasize that minimizing these frictions is an implied part of the objective function of any optimization-driven design process.

Figure 2.2 summarizes a variety of design literature to present a holistic view of this complete process as applied to aircraft design [29, 32, 34–38]. Frictions that a designer

[5]For example, is the objective to minimize fuel burn, or to maximize range? Is operating cost a quantity that should be strictly capped (a constraint), or instead only penalized (an objective)?

may experience from a computational optimization framework at each step are shown in red.

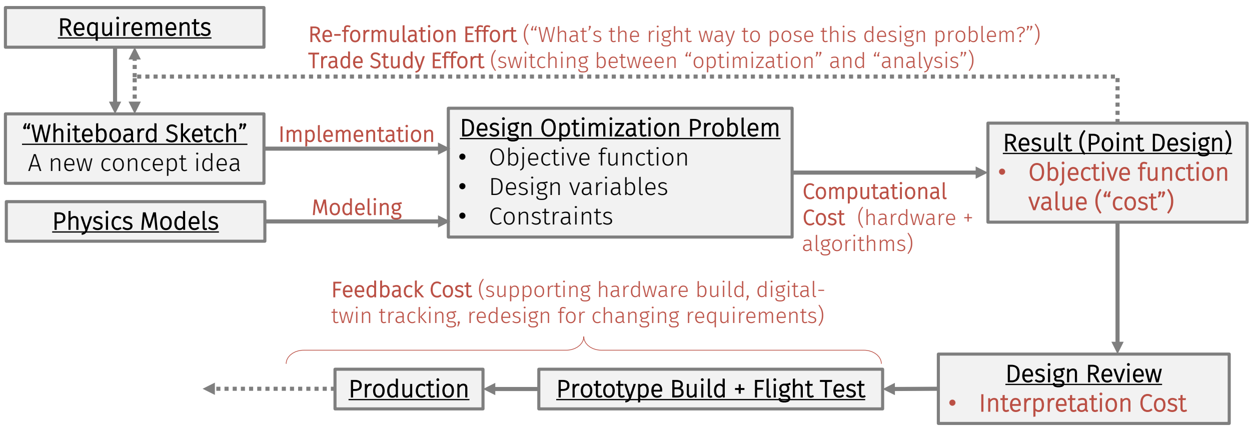

Figure 2.2: A high-level overview of the optimization-driven design process, as applied to aircraft design. "Costs" (user frictions to be minimized) associated with each step are shown in red.

In the aircraft design process model of Figure 2.2, the initial point of departure is a set of high-level requirements [29, 36]. The first design step is to develop a set of candidate concepts ("sketches"), a qualitative process that largely leverages designer creativity and experience [35, 37]. Concepts and the associated requirements are then translated into a design optimization problem consisting of an objective function, design variables, and constraints.

The remainder of this section will discuss some of the most important advances in design optimization research that have helped to reduce the costs incurred at various steps of this holistic process.

2.3.1 Two Directions: "Wide" vs. "Deep" MDO

Before proceeding further, it is important to clarify the scope of aircraft design optimization problems that are of interest in this thesis, as the definition of "MDO" is somewhat overloaded. More precisely, the modern field of MDO can be decomposed into two related but distinct subfields which have developed different strategies and mindsets to address different design needs. Figure 2.3 illustrates this distinction.

The first subfield, and the subject of the present work, is that of **conceptual**, or **"wide" MDO**. This is essentially a formalization of the conceptual sizing problem and typically involves casting a wide net to capture as many first-order dependencies as possible. The intended use case is often clean-sheet design of a complete aircraft, and the end goals are

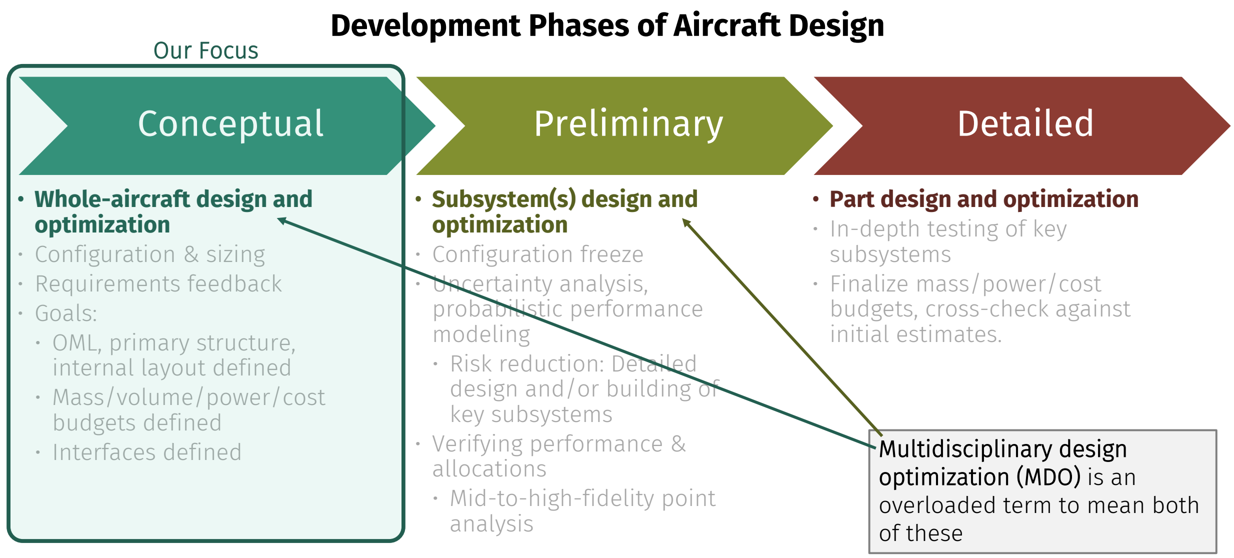

Figure 2.3: Multiple definitions of the term "multidisciplinary design optimization".

often initial identification of strong design drivers and assessment of concept feasibility. Sensitivity analysis is also a key desired output of a wide MDO process.

These goals requires an enormous breadth of models to be considered, as practical aircraft designs are shaped by an enormous number of constraints that do not appear in first-principles performance analysis (e.g., the Breguet range equation). For example, a drag reduction of the vertical stabilizer is of little interest if engine-out performance constraints preclude certification; likewise, a more efficient engine is of little interest if acoustic constraints preclude customer acceptance. This need for analysis breadth can lead to design problems with many hundreds of models spanning anywhere from five to twenty relevant disciplines. To illustrate this breadth, consider the following non-exhaustive list of example disciplines that might be included:

- Aerodynamics
- Structures and weights estimation
- Propulsion
- Power systems and thermal management
- Flight dynamics (trim, stability, and control)
- Internal geometry and packaging
- Mission design (concept of operations) and trajectory optimization
- Takeoff and landing field length analysis
- Certifiability, safety, and engine-out performance

- Life-cycle emissions
- Cost modeling and manufacturability
- Acoustic signature
- Ride quality
- Survivability and stealth

Each of these disciplines might include dozens of submodels [39]. To keep problems tractable despite their large scope, these models are typically low-fidelity; often, they are either derived from first principles physics with appropriate simplifications or regressions to statistical data. Despite the reduced accuracy of these models, they fulfill two critical functions. First, they apply *optimization pressure* to steer the optimizer towards realistic designs, often in subtle, interdisciplinary ways. For example, increasing fuselage length requires increased landing gear length and mass to maintain a proper takeoff rotation angle, reducing the attractiveness of such design changes. Secondly, these low-fidelity models provide information on which constraints might be active near the optimum, allowing computational resources to be devoted to fidelity improvement only where it is needed. Often, these wide MDO problems are posed as large single-level optimization problems, which allows the large number of cross-disciplinary constraints to be computationally represented in a shared namespace [12].

The second subfield of MDO is that of **preliminary**, or **"deep" MDO**. Here, the goal is often to provide detailed design refinement of a very close initial guess. Because the low-hanging fruit has often been picked by this stage, the design problem is often more local in nature, and the number of models is typically smaller than in wide MDO. Likewise, continued improvement from a good initial guess requires high-fidelity models, since the objective function tends to be relatively flat near the optimum and hence highly sensitive to model inaccuracy. For example, RANS-based CFD[6] models are often used for aerodynamics, at significant cost: optimization runtimes of 1,000 to 100,000 CPU-hours are not uncommon [40]. To maintain tractability, relatively few disciplines are considered – often only aerodynamics and structures. The intended use case is often detailed design of a single component or subsystem, such as a wing. Due to computational challenges that tend to be more prevalent in high-fidelity models (e.g., PDE-constrained optimization, adjoint-based gradients, numerical stiffness of models, and convergence of models that use iterative solvers), the subfield of "deep" MDO has placed a large focus on MDO architectures that allow multi-level decomposition of the original optimization problem [41].

While both subfields share broad similarities, they are fundamentally attacking different problems: wide MDO is aimed at clean-sheet design, while deep MDO tends to aim

[6] Reynolds-averaged Navier-Stokes; Computational fluid dynamics

at refinement of an existing design. Historically, this schism began to emerge roughly in the 1990s and 2000s, as various research groups began "spending" their increasing computational budgets in either model depth or model breadth.

2.3.2 Advances in Optimization Algorithms

Gradient-Based Methods with Analytical Gradients

Disciplined Optimization Methods

2.3.3 Advances in Design Optimization Practice

A recent notable shift in aircraft design optimization perspectives has been a renewed focus on geometry representation and parameterization. For example, Haimes and Drela [42] contended in 2012 that "constructive solid geometry (CSG) is the natural foundation for [aircraft design optimization]". This publication extended prior work by Lazzara, Haimes, and Willcox [43] that introduced the concept of "multifidelity geometry". Together, these works advocated for accurate 3D outer mold line representations from the earliest stages of conceptual design, with degenerate representations of this central geometry used to drive individual discipline analyses. Furthermore, they recognized the fundamental limitations of general-purpose (e.g., Parasolid-based) CAD tools in aircraft design optimization: because aerospace geometries tend to use complex, lofted surfaces, the resulting CAD models can be brittle with respect to parameter changes. This observation, along with later developments such as differentiable discretization techniques [44], led to renewed research on how aircraft geometry should be parameterized for optimization. For example, in recent years aircraft-specific geometry tools like OpenVSP [45] and Engineering Sketch Pad [44] have been developed for design optimization workflows, a trend that arguably stems from this line of research.

A notable area where computational methods for aircraft design have long made inroads to industry is in inverse design tools. (An example of successful industry adoption in aerodynamics the inverse approach used by the XFoil airfoil design code [46] and others [26] to recover a shape from a specified pressure distribution.) Like optimization methods, these inverse methods can aid designers because they offer fundamentally different capabilities than traditional design methods (e.g., carpet plots). While traditional methods focus on the "forward problem" (design $\rightarrow$ performance), inverse methods and optimization methods both focus on the "inverse problem" (performance $\rightarrow$ design). Drela [7] shows that this inverse approach can lead to more robust designs than optimization, if the user is not familiar with the risks of an improperly-specified optimization problem.

2.3.4 Advances in Numerical Methods

Automatic Differentiation

Here, we review literature on *automatic differentiation*, an advanced technique borne out of the machine learning community that fundamentally accelerates gradient-based optimization algorithms. A complete survey is available by Baydin et al. [47]

As previously discussed, gradient-based optimization methods

In the adjacent field of machine learning, application of these techniques[7] have ignited a revolution of progress [47]. Rackauckas in 2021 [48] states: "[Automatic differentiation] has become the pervasive backbone behind all of the machine learning libraries."

Automatic Sparsity Detection and Jacobian Coloring

Other Numerical Advances

2.4 Motivation for Improving Industry Access to Design Optimization

[7] in particular, automatic differentiation and backend-agnostic computing enabling GPU acceleration

Chapter 3

Thesis Approach, Methodology, and Contributions

3.1 The Technical Gap: Practical Limitations of MDO Frameworks in Industry

The stark dichotomy of MDO – its immense potential to improve the aircraft design process contrasted with its barriers to practical adoption – is the fundamental motivation for this thesis. The goal of this work is to identify and address the root causes of this gap between academic research and practical industry use. In particular, we will focus on the challenges of *interpretability* and *reviewability* of large-scale engineering design optimization problems. These challenges are not unique to MDO, but rather are a fundamental challenge of large-scale computational tools in general. The field of aircraft design optimization is no exception to this, and it is one that has been recognized for decades. However, the problem remains unsolved.

The primary remaining explanation, which has become increasingly accepted in the past decade [2, 13, 29, 33], is that MDO faces a set of related organizational, culture, and practical challenges that must be addressed before widespread industry adoption can occur.

Summarizing this body of work yields a list of MDO's current major challenges:

1. MDO can be time-consuming to set up. As stated by Torenbeek in 2013 [29] on contemporaneous MDO tools, "the MDO methodology can be used at any design stage although its complexity does not justify application in the early conceptual phase."

2. MDO can be time-consuming to run [33].

3. MDO faces interpretability challenges, particularly as problem size grows. If MDO is not interpretable and

4. If practitioners are not experienced, it is easy to inadvertently produce designs with poor off-design performance, overly aggressive margins, and violated assumptions [7, 29, 49]. This often leads to non-credible designs or program failures.

5. Most MDO frameworks are syntactically complex, requiring users to be joint experts not only in aircraft design, but also in applied math and computer science [2, 32, 33]. This "expertise barrier", as termed by Grant [50], is a severe impediment to widespread adoption among "users whose focus is the application".

TODO

Interestingly, many of the challenges identified by early MDO works [1, 3] are the same ones that the field is grappling with today.

[32]

TODO

Contemporaneous publications from leading voices in the field of aircraft design around the time of Kroo's work paint a similar story - expressing optimism about the field's growing potential while highlighting (or in some cases, urging) hesitation by industry practitioners.

3.2 Proposed Contributions

The Ph.D. thesis will make the following novel conceptual contributions to address the technical gap described in Section 3.1:

1. **Code Transformation Paradigm:** Introduce a new computational paradigm for MDO frameworks that offers most of the benefits of state-of-the-art paradigms with significantly fewer user frictions.

2. **Differentiable Physics Models:** Provide the first implementations of several key aerospace physics models that are amenable to code transformations.

3. **Sparsity Tracing via NaN-Propagation:** Introduce the new idea of "NaN-propagation" as a method to trace sparsity through black-box numerical analyses, accelerating gradient-based optimization.

4. **Strategies for Black-Box Functions:** Demonstrate that physics-informed machine learning surrogates provide a viable method of incorporating aerospace-related black box functions into a code-transformation-based design framework.

5. **Framework Requirements for Interpretability:** Identify the set of features that a design optimization framework must provide to enable the *interpretability* and *reviewability* of large-scale engineering design optimization problems. Implement these features in a *code transformation* design optimization framework.

6. **System Identification**

7. Build a computational framework for engineering design optimization based on the paradigm of *code transformations*, which enables the use of modern techniques in computer science and applied math (detailed more in Section TODO). This framework will act as a "proving ground" on top of which subsequent research objectives will be implemented and evaluated.

8. Demonstrate that this *code transformation* paradigm enables the formulation of large-scale engineering design optimization problems at the conceptual stage, to an extent that is not otherwise possible with existing public aircraft design frameworks. To satisfy this objective, the framework will demonstrate (on at least one applied aircraft design case study) performance equaling-or-exceeding the state-of-the-art across the following metrics:

- Runtime speed (i.e., scalability of computational resources, and runtimes compatible with human-in-the-loop interactive design).
- Problem implementation and re-implementation speed (i.e., scalability of engineering time resources).
- Mathematical flexibility: the ability to achieve the above metrics without imposing restrictions on user models that can force undue deviations from physical reality (e.g., log-convexity).

9. Demonstrate the double-edged sword of the large-scale conceptual design optimization capabilities enabled by this framework:

   (a) **Benefit:** Demonstrate that enabling large-scale engineering design at the conceptual stage offers measurable performance gains in the resulting aircraft designs compared to those produced with existing methods. Specifically, the thesis will present at least one applied aircraft design case study, which is then solved with two separate approaches:

      i. A first-order sizing study where an aircraft is designed by coupling only "core" aircraft design disciplines (aerodynamics, structures, and propulsion) and traditional sizing relations (e.g., W/S and T/W diagrams)

      ii. A higher-order sizing study where more "non-core" disciplines (e.g., stability and control, trajectory and mission optimization, cost analysis, field lengths, noise, manufacturability) are added to the aircraft design problem. Geometric flexibility, as measured by the number of design variables describing the aircraft geometry, will also be increased.

      The resulting designs from these two studies will then be compared (post-optimality) to assess their performance on both stated objectives (to assess how much large-scale modeling expands the feasible design space) and secondary metrics (to assess how well core disciplines act as a surrogate for non-core disciplines).

   (b) **Risk:** Demonstrate the major pitfall of the new large-scale conceptual design optimization: the lack of result *interpretability*. Show that the system complexity enabled by large-scale optimization leads to results are more difficult to communicate, interpret, review, and trust.

10.

11. Identify framework features and characteristics that aid in the *interpretability* and *reviewability* of large-scale engineering design optimization problems. This should be

based on a combination of literature review, aircraft design case studies, and (as resources allow) discussions with framework users and aircraft designers. Fundamentally, this is more a communication question than a technical one: setting up a large-scale optimization problem is doable with state-of-the-art aircraft design optimization tools, but TODO ("how do we communicate whether we can trust the results of a design optimization study?").

12. Implement some of these practical This should include, at minimum:

    - A constraint activity log, which

3.2.1 Code Transformation Paradigm

The thesis will introduce the idea of *code transformations* as a new computational paradigm on top of which an MDO framework can be built. Here, code transformations are defined as a generalized set of computational techniques that intercept the original optimization problem posed by the user (at runtime), apply some improvement based on analysis of the code itself, and then solve a modified optimization problem instead. This encompasses a variety of recent advanced techniques in scientific computing, such as:

- Automatic differentiation [51]
- Automatic sparsity detection [52]
- Problem transformations:
    - Auto-scaling [53]
    - Log-transformation of variables, constraints, and objectives (similar to geometric programming) [54, 55]
    - Redundant constraint elimination
- Backend-agnostic programming (CPU/GPU, different math library backends, just-in-time compilation, automatic vectorization and parallelization) [56]

The benefit of introducing this abstraction is to recognize that all of these advanced techniques essentially share one major requirement to use: the optimization framework must be able to inspect the actual code driving the design problem. This code inspection is done either via direct source code analysis or by creating a computational graph of the optimization model at runtime. The latter approach, which is called *tracing* in machine learning literature [47, 56, 57], is widely preferred to the former in modern, syntactically-rich languages[1]. Therefore, for the purposes of this work, *traceability* is effectively synonymous with code transformability.

If code transformation techniques can be applied to engineering design optimization, they offer order-of-magnitude speedups over the black-box optimization methods that form the vast majority of industry use today [34, 59]. These achievable speeds are comparable to those of state-of-the-art optimization methods in academia, such as disciplined optimization methods[2] [33, 50, 55, 60] and gradient-based methods using user-provided analytic gradients[3] [61–63].

However, code transformations offer a key advantage over these state-of-the-art methods in that they can be applied *automatically* – most of the benefits of these advanced techniques can be gained without requiring any additional effort (or mathematical expertise) from the user. This ease-of-use is critical for practicality – Grant notes that existing paradigms are hamstrung by a "expertise barrier" of existing methods, as described by Grant [50]. Table 3.1 compares code transformations to existing MDO paradigms across three key practical metrics. In short, code transformations offer the best of both worlds: the computational speed of latest academic methods with the ease-of-use of methods already accepted by industry today.

[1] Maclaurin provides a comprehensive discussion of the tradeoffs between these techniques, and why tracing is often preferable in practice [58]

[2] such as geometric programming and disciplined convex programming

[3] sometimes referred to as "adjoint methods" in reference to a common method for manually deriving these gradients for more-complex analyses

Table 3.1: A subjective comparison of tradeoffs between existing MDO framework paradigms and the proposed *code transformation* paradigm. The industrial state-of-the-art is largely *black-box optimization*. The academic state-of-the-art has two major branches: *gradient-based methods with analytical gradients*, and *disciplined optimization methods*. More detailed discussion of these assessments, including definitions and reasoning, is given in Appendix A.

MDO Framework Paradigm	**Example Frameworks and Tools**	**Ease of Implementation** (idea-to-code)	**Runtime Speed and Scalability** (code-to-result)	**Modeling Flexibility**
Black-box Optimization	SUAVE [64], OpenMDAO* [61], TASOPT [9], PASS [65], FAST [66], FLOPS [67], FBHALE [23], **almost all industry codes**	**Great**	**Limited**	**Best**
Gradient-based with Analytic Gradients	MACH-Aero [68], OpenMDAO* [61], OpenConcept [69]	**Limited**	**Best**	**Great**
Disciplined Optimization	GPkit [33], other convex methods [50, 60, 70], most algebraic modeling languages	**Good**	**Good**	**Limited**
Code Transformations	AeroSandbox† [71], JAX‡ [56], ModelingToolkit.jl‡ [72]	**Good**	**Great**	**Good**

* Can use either paradigm, depending on user's implementation

† Part of the present work, as detailed in Section 4.1

‡ These are computational tools to facilitate code transformations, rather than frameworks themselves

This leads to a compelling value proposition: if we can develop new methods for industry engineers to easily write traceable design code, then we gain access to an host of advanced scientific computing techniques that can significantly shrink the academia-industry MDO gap described in Section 3.1.

Thus, this contribution is twofold. First, the thesis will conceptually introduce code transformations as a new paradigm for engineering MDO frameworks. Secondly, the thesis will demonstrate strategies that allow traceability of engineering design code with minimal user effort, enabling the use of code transformations in practice.

3.2.2 Differentiable Physics Models

The thesis will also contribute the first computational implementations of several key physics models for aircraft design that are compatible with a code transformations paradigm (i.e., traceable).

The broad motivation stems from the observation that "ease-of-implementation" has historically proven to be one of the most important factors for determining whether an MDO paradigm can achieve use in industry. More specifically, the goals of this contribution are to:

1. Stress-test the feasibility of code transformations in practice – How much added user effort and expertise is required to bring typical engineering analyses into a code-transformations-based MDO tool? To what extent can existing code be used as-is? Finally, the thesis aims to identify any specific computational elements that cause "pain points" when attempting to make an analysis traceable.

2. Jump-start future applied research by providing a set of modular, plug-and-play analyses that can be used to quickly build a variety of aircraft design optimization problems. Since the long-term goal of this research direction is to establish whether the proposed MDO paradigm improves practicality, it follows that many practical aircraft design problems must be posed. By creating the building blocks for such problems, we aim to accelerate future research.

To achieve these goals, the thesis will contribute the first traceable implementations of the common aircraft design analyses given in Table 3.2. This set of analyses was deliberately chosen to be diverse, spanning a wide range of common computational attributes. The types of attributes that each analysis is intended to stress-test are given in the right-most column of Table 3.2. By contributing this breadth of analyses within a traceable paradigm, we aim to cover a wide and representative gamut of engineering code patterns.

Table 3.2: A list of aircraft design analyses that the thesis will implement within a code transformations framework. The middle column lists the non-traceable tools for each analysis that are commonly used in industry today. The right-most column lists the computational attributes that each analysis is intended to stress-test.

Analysis To Contribute	**Non-Traceable Analogue**	**Tests tracing through...**
Vortex-Lattice Method Aerodynamics Analysis	AVL [73]	An aerospace geometry engine and discretization; large, vectorized matrix methods, like linear solves.
Nonlinear Lifting Line Aerodynamics Analysis	Phillips & Snyder [74], Reid [75]	Nonlinear systems of equations (i.e., implicit), which often lead to value-dependent computational graphs (via convergence loops).
Workbook-style Aerodynamics Buildup	USAF Digital DATCOM [76]	Table lookups, large amounts of conditional logic (yielding a wide, branching graph), and scalar-heavy math
Rigid-Body Equations of Motion	ASWING (dynamics) [77]	Ordinary differential equations, which are often implemented in a loop-heavy way (yielding a deep graph)
Linearized Aircraft Stability Modal Decomposition	AVL [73]	More advanced matrix methods, such as an eigenvalue decomposition

These traceable implementations offer value within the context of the thesis itself (in stress-testing the practicality of code transformations), but they also have value as a standalone contribution to the aircraft design community – even outside of design optimization. For example, a traceable workbook-style aerodynamics buildup would seamlessly enable GPU-accelerated evaluations and automatic vectorization, offering significant speedups; an example application might be real-time performance estimation for model predictive controllers.

3.2.3 Sparsity Tracing via NaN-Propagation

The third contribution of the thesis will be a novel idea about how to trace sparsity through black-box numerical analyses.

3.2.4 Physics-Informed Machine Learning Surrogates for Black-Box Functions

3.2.5 Aircraft System Identification from Minimal Sensor Data

Chapter 4

Status and Proposed Schedule

4.1 Results to Date

4.1.1 Code Transformation Paradigm

In machine learning, traceability has largely been achieved through the rise of domain-specific languages (DSLs): a sub-language implemented within a programming language. These DSLs, such as Theano, TensorFlow, PyTorch, JAX, and others, have quickly become ubiquitous, empirically demonstrating that DSLs are a viable path to industry adoption. However, there are several downsides if machine-learning-oriented DSLs are applied to engineering design as-is. DSLs tend to differ substantially in syntax from their underlying language, which adds a barrier for new users, and more importantly, requires existing engineering analysis code to be rewritten. DSLs for machine learning also make architectural choices that tend to be ill-suited for typical engineering problems. For example, most deep learning applications consist predominantly of highly-vectorized mathematical operations on large tensors, with a high amount of compute per operator. Engineering analysis, by contrast, tends to be much more scalar-heavy, with many more intermediate steps and a lower amount of compute per operator.

These DSLs restrict users to a narrow set of mathematical operators

Before that, algebraic modeling languages (AMLs) in the field of mathematical optimization

Which is typically achieved through type-flexible programming (through either dynamic typing or multiple dispatch)

4.2 Fields of Study and Coursework

At the first meeting with the thesis committee (Apr. 5, 2023), the following major and minor programs of study were proposed:

- Major: **Computation for Design and Optimization**
  - 16.920: Numerical Methods for Partial Differential Equations
  - 6.255: Optimization Methods
  - 16.888: Multidisciplinary Design Optimization
  - 18.337: Parallel Computing and Scientific Machine Learning
  - 16.842: Fundamentals of Systems Engineering
- Minor: **Flight Physics**
  - 16.110: Flight Vehicle Aerodynamics
  - 16.13: Aerodynamics of Viscous Fluids
  - 16.885: Aircraft Systems Engineering
- Doctoral math requirement:
  - 16.920: Numerical Methods for Partial Differential Equations
  - 6.255: Optimization Methods

The program of study was approved by the committee at the Apr. 2023 meeting, with no further coursework recommendations made. All listed classes have been completed for credit with A/A+ grades, satisfying grade requirements. The Doctoral Research and Communication Seminar course (16.995) has been completed, satisfying the department prerequisite for the thesis proposal defense.

4.3 Degree Milestones

Major degree milestones, both past and future, are listed in Table 4.1.

Table 4.1: Tentative planned timeline for PhD degree milestones.

Complete?	Date	Milestone
✓	Fall 2019	Began studies at MIT
✓	Summer 2021	S.M. thesis submitted
✓	Summer 2021	S.M. degree awarded
✓	Fall 2022	Formation of doctoral committee
✓	Spring 2023	Committee Meeting #1
	Fall 2023	Ph.D. Thesis Proposal Defense
	Spring 2024	Committee Meeting #2
	Fall 2024	Committee Meeting #3
	Winter 2024	Ph.D. Thesis Defense

4.4 Research Schedule

Spring 2024

1. Motivate the optimization framework developed in the thesis.

   (a) Identify or develop an aircraft design benchmark problem suitable for comparing existing frameworks and their associated paradigms. The design problem should be realistic (incorporating all core aircraft disciplines), but it should not be overly complex. Potential suitable problems could include:

   - SimPleAC, a small aircraft design problem initially proposed by Warren Hoburg [12] and further refined by Berk Ozturk [78].
   - The solar seaplane design problem developed and implemented as part of TA work for MIT 16.821 in Spring 2023 [79].
   - An aircraft design problem adapted from the AIAA Graduate Aircraft Design Competition, where the 2023-24 problem is a self-launching electric sailplane.
   - Long-haul liquid-hydrogen-powered transport aircraft design, which was studied and developed for MIT 16.886 in Fall 2022 and MIT 16.885 in Fall 2023 [80, 81].

   (b) Implement the benchmark problem in several frameworks that are representative of state-of-the-art and/or industry-standard paradigms: AeroSandbox, OpenMDAO, GPkit, and a "optimizer wrapped around black-box analysis" method[1].

   (c) Compare the implementations on the basis of the three framework-level metrics identified in Section 3.2: runtime speed, problem implementation speed, and mathematical flexibility. Document this thoroughly. Use this exercise as a jumping-off point to write a thesis chapter on how specific framework design choices affect each of these three metrics.

   (d) Show that the thesis framework makes large-scale optimization practical to implement at the conceptual design stage.

2. Quantitatively illustrate the performance benefit associated with large-scale optimization in conceptual-level aircraft design:

[1]Typical of industry methods, such as those seen in the development of the Facebook HALE aircraft development effort[23]

(a) Identify or develop an aircraft design benchmark problem suitable for comparing various levels of model fidelity at the conceptual design level. The design problem should be sufficiently complex such that it can be solved with or without the inclusion of secondary disciplines. Potential suitable problems could include:

- MIT Firefly, a rocket-propelled micro-UAV design problem coupling packaging constraints, transonic aerodynamics, trajectory design, and propulsion design.
- Dawn One, a high-altitude-long-endurance solar-powered aircraft.

Fall 2024

1. Present the idea that implicit model assumptions and constraint-satisfaction information as "metadata" that should be

4.5 Facilities Required

No special facilities are required for this work beyond those already available at MIT AeroAstro.

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Appendix A

Comparison of MDO Framework Paradigms

This appendix aims to provide more detailed discussion of the comparisons made in Table 3.1.

In this Table, three qualitative metrics are defined over which MDO framework paradigms are enabled. These metrics represent framework needs derived from the barriers to industry adoption that are identified in Section 3.1. The metrics are:

1. **Ease of implementation:** How much effort is required to implement a typical aircraft design problem (from "concept idea" to "working code") in this paradigm? How much optimization or programming expertise is required, beyond the basics needed to write engineering analysis code?

2. **Computational speed and scalability:** How fast is the resulting design optimization problem to run, and how does this scale with problem size and number of disciplines? Are there other fundamental limits to scaling up analysis fidelity?

3. **Mathematical Flexibility:** What kinds of restrictions are present on the mathematical form of the optimization problem? This has important follow-on effects for backwards-compatability, as highly-restrictive frameworks preclude the use of existing engineering code and instead require from-scratch rewrites.

Black-box optimization refers to the common industry approach of wrapping