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Differentiable Physics in Multidisciplinary Design Optimization: Implicit Gradients, Adjoint Tricks, and Robustness under Distribution Shift

Elif Yılmaz[1], Katharina Weiss[2*], Markus Keller[3]

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Abstract

This study aimed to synthesize and critically evaluate the role of differentiable physics frameworks in advancing multidisciplinary design optimization (MDO), focusing on implicit gradient computation, adjoint-based sensitivity analysis, and robustness of optimization performance under distributional shifts. A qualitative review design was adopted to examine sixteen peer-reviewed articles published between 2015 and 2025 that addressed differentiable physics, adjoint methods, and robust optimization in MDO contexts. Data collection relied exclusively on systematic literature review procedures across Scopus, Web of Science, IEEE Xplore, and ScienceDirect databases. Studies were selected through purposive sampling until theoretical saturation was achieved. Data were analyzed thematically using Nvivo 14 software through open, axial, and selective coding stages. Emergent concepts were organized into four major themes: differentiable physics foundations, adjoint-based optimization, robustness under distribution shift, and future integration challenges. The synthesis revealed that implicit differentiation and adjoint-based gradient computation form the computational backbone of differentiable physics in MDO, enabling scalable and memory-efficient sensitivity analysis across coupled physical domains. However, computational efficiency, gradient stability, and numerical conditioning remain significant challenges that limit generalization across problem types. The findings also indicate that while differentiable frameworks have achieved theoretical maturity, their robustness under distributional shift—such as environmental or boundary condition changes—remains underexplored. Integration with uncertainty quantification, Bayesian robustness, and domain adaptation is emerging as a promising solution. Additionally, the analysis underscored the lack of standardized benchmarks and reproducibility protocols, which constrains cross-study validation. Differentiable physics represents a paradigm shift in engineering optimization by bridging first-principles simulation and gradient-based learning. Yet, realizing its full potential requires methodological advancements in implicit solvers, cross-domain adjoint coupling, and robustness-aware design. Future work should emphasize scalable algorithms, reproducible benchmarking, and integration with real-world uncertainty modeling to foster reliable and interpretable differentiable MDO systems.

Keywords: Differentiable physics; multidisciplinary design optimization; implicit differentiation; adjoint methods; distribution shift; robust optimization; uncertainty quantification; automatic differentiation.

1. Department of Mechatronics Engineering, Middle East Technical University, Ankara, Turkey
2. Department of Transportation Engineering, Vienna University of Technology, Vienna, Austria
3. Department of Systems Engineering, ETH Zurich, Zurich, Switzerland

*Correspondence: e-mail: katharina.weiss@tuwien.ac.at

1. Introduction

In contemporary engineering and scientific computing, the integration of physics-based simulation with gradient-driven optimization has become a transformative paradigm for enabling design that is both physically consistent and data-aware. Among these trends, differentiable physics—that is, simulation engines or models which provide differentiable mappings from input (design, parameters, boundary conditions) to outputs (fields, responses, performance metrics)—has garnered intense interest. Such systems allow gradients to propagate through physical models, thereby facilitating end-to-end optimization, system identification, sensitivity analysis, and co-design in high-dimensional settings. Over the past decade, the fusion of differentiable physics with multidisciplinary design optimization (MDO) has promised to unify traditionally disjoint design disciplines (e.g., aerodynamics, structural mechanics, thermal analysis) under a common gradient-based optimization pipeline. However, this promising intersection is accompanied by formidable methodological and robustness challenges. In particular, the use of implicit differentiation, adjoint-based gradient techniques, and the need for robustness under distribution shifts represent three intertwined frontiers that remain under-explored in the literature. This article aims to synthesize and push forward the intellectual boundary of these interrelated themes, by surveying, analyzing, and critiquing existing approaches, and by pointing toward future pathways for more reliable and generalizable differentiable MDO systems.

Differentiable physics frameworks have proliferated across domains, from fluid dynamics and contact mechanics to solid mechanics and thermal systems. Recent surveys (e.g. Newbury, et al., 2024) provide a panoramic view of the design trade-offs inherent in differentiable simulators—namely, balancing gradient fidelity, computational overhead, solver robustness, and modular flexibility. Newbury et al. (2024) articulate how choices in discretization, solver coupling, and autodiff integration shape the practical performance of differentiable simulation frameworks, and how these choices interact with downstream optimization performance. In many cases, researchers employ explicit differentiation or unrolled solvers to bypass some of the complexity associated with implicit systems; yet explicit formulations often limit stability and scalability when applied to stiff or constrained physical systems. Implicit differentiation offers a theoretically cleaner alternative, allowing gradients to be computed through equilibrium or fixed-point conditions by solving linearized systems rather than relying on unrolling entire trajectories. However, effective use of implicit differentiation in large-scale multiphysics simulation requires careful handling of Jacobian and Hessian structure, memory constraints, and solver-conditioning issues (e.g., implicit differentiation with second-order derivatives in finite-element based physics) (see, e.g., research on second-order implicit differentiation) (Implicit differentiation with second-order derivatives…, 2025). Moreover, in domains such as hydrology and environmental modeling, recently proposed "discretize-then-optimize" adjoint schemes enable differentiable implicit models in contexts that previously resisted gradient integration (Song et al., 2024). The adoption of such schemes exemplifies the delicate balance between fidelity in physical discretization and tractability of gradient propagation.

Within the MDO context, adjoint-based optimization stands out as a central tool for efficiently computing sensitivities across large numbers of design variables. Historically, adjoint methods have been staples in aerodynamic shape optimization, structural topology optimization, and computational fluid dynamics, because they make gradient computation cost largely independent of the number of design variables (Giles & Pierce, 2000; Martins & Hwang, 2013). The coupling of adjoint solvers across disciplines—such as aero-structural, thermo-fluid, or fluid–electrical–structural systems—requires chaining sensitivity backpropagation across domain-specific modules, while preserving accuracy and scalability. However, the direct composition of adjoints in an MDO architecture introduces challenges: memory bottlenecks, management of intermediate state variables, numerical noise accumulation, and the necessity of checkpointing or reversible integration schemes. Researchers have thus proposed variant strategies such as checkpointed adjoint propagation, modular adjoint "pipelines," and sparse Jacobian estimation techniques to mitigate these burdens. Meanwhile, validation and consistency checking via finite-difference approximations or adjoint verification remain essential to confirm correctness. The literature presents concrete applications in aerostructural optimization, topology design, and systems integration (e.g. Martins et al., 2021), yet the full, generalized treatment of adjoint-enabled MDO remains at an early, exploratory stage.

One aspect that increasingly draws attention is how differentiable physics–based optimization performs under distribution shift—namely, when the design, operating, or environmental conditions at deployment diverge from those assumed during the design optimization. Distributional shifts may stem from unmodeled changes in boundary conditions, materials, external loads, or environmental factors. In broader machine learning and statistical learning, robustness to such shifts has been a central concern: a model that generalizes well on training distributions may fail catastrophically under even modest changes in input distribution (Wiles et al., 2021). In differentiable physics, this manifests as sensitivity to perturbations in inputs or simulation environments, which can undermine gradient reliability, degrade objective predictions, and misguide design decisions. To counteract this, researchers have begun to explore robust optimization techniques, such as worst-case (min–max) formulations, Bayesian approaches, or distributionally robust optimization (DRO) that optimize over uncertainty sets (Sutter et al., 2021). Moreover, embedding uncertainty quantification within differentiable pipelines—sometimes via differentiable Monte Carlo estimation (Zhang et al., 2023) or variance-aware adjoint formulations—helps expose the sensitivity of optimized designs to input perturbations. Complementary strategies such as regularization, adversarial reweighting, and domain adaptation—borrowed from the machine learning robustness literature—have also been adapted (or remain ripe for adaptation) to physics-aware optimization. For instance, reweighting loss functions to emphasize worst-case performance or injecting adversarial perturbations in simulation inputs can promote designs that generalize better across possible operating regimes. Notably, the ability to compute gradients through such robustness-enhancing perturbations is a particularly powerful advantage of differentiable physics frameworks, enabling robust design criteria to be directly optimized. Yet, the theoretical foundations, practical instantiation, and benchmarking of distribution-shift–resilient differentiable MDO remain underdeveloped and ripe for systematic synthesis.

In light of these three clusters—implicit differentiation, adjoint-based coupling, and robustness under distribution shift—this review seeks to weave a coherent narrative that elucidates the state of the art, identifies gaps, and charts directions for future research. Specifically, we pose the following guiding questions: (1) What algorithmic strategies currently enable implicit gradient propagation in physics-based simulations, and how do they interface with MDO structures? (2) How are adjoint pipelines architected to handle coupling across physics modules, and what compromises do practitioners make between computational cost and accuracy? (3) How do existing works treat distributional perturbations in the context of differentiable physics, and to what degree do they ensure generalizability and resilience? Through a qualitative synthesis of 16 seminal articles across simulation, optimization, and robustness literatures, we extract thematic insights, compare methodological choices, and highlight emergent tensions. Our analysis reveals cross-cutting themes: trade-offs between solver tractability and gradient fidelity; memory–compute scaling limitations; sensitivity of gradient paths to modeling perturbations; and limited empirical evaluations under real-world shift conditions.

The contributions of this review are threefold. First, we offer a conceptual taxonomy that connects implicit differentiation techniques, adjoint coupling paradigms, and robustness-oriented strategies within the unifying frame of differentiable MDO. Second, we critically examine the strengths, limitations, and design trade-offs in representative implementations, emphasizing their practical implications and scalability barriers. Third, we advance a set of future research hypotheses and design criteria aimed at more robust, scalable, and interpretable differentiable optimization systems capable of real-world deployment under uncertainty. In so doing, we hope to guide researchers toward unified frameworks that leverage the best of physics-based simulation, gradient optimization, and robustness-aware design, overcoming the fragmentation that otherwise characterizes current approaches.

In sum, the confluence of differentiable physics and MDO offers remarkable promise for next-generation engineering design. Yet, realizing that promise demands deeper methodological rigor—particularly in the implicit gradient mechanics, adjoint coupling architectures, and distribution-shift resilience. This review represents a deliberate effort to agglomerate, interrogate, and project the maturation of this field. From this vantage, we anticipate that the next wave of breakthroughs will not merely refine individual subsystems, but bridge across them, yielding cohesive, interpretable, and trustworthy differentiable MDO frameworks for complex, uncertain engineering domains.

2. Methods and Materials

This study adopted a qualitative review design aimed at synthesizing the existing body of knowledge on the integration of differentiable physics in multidisciplinary design optimization (MDO), focusing specifically on implicit gradients, adjoint-based differentiation, and robustness challenges under distributional shifts. Unlike empirical research, this review did not involve human participants; instead, the "participants" were peer-reviewed scientific articles that directly addressed differentiable simulation frameworks, MDO coupling techniques, and robustness analysis in computational design optimization. The qualitative review design was chosen to facilitate a deep interpretive understanding of theoretical, methodological, and computational advancements in differentiable physics-based optimization, enabling cross-comparison of frameworks and analytical paradigms used across engineering disciplines.

Data were collected exclusively through systematic literature review procedures, employing major academic databases including Scopus, Web of Science, IEEE Xplore, and ScienceDirect. The search strategy incorporated keywords such as *"differentiable physics," "adjoint method," "implicit differentiation," "gradient-based optimization," "MDO," "distribution shift,"* and *"robust optimization."* Inclusion criteria required that articles be:

1. Published between 2015 and 2025,
2. Written in English,
3. Peer-reviewed journal or conference publications, and
4. Explicitly discuss differentiable simulation or optimization under uncertainty or multi-physics coupling contexts.

After an iterative screening process based on title, abstract, and full-text relevance, a total of 16 articles were selected for in-depth qualitative analysis. The selection process followed the theoretical saturation principle, meaning that literature inclusion continued until no new conceptual themes or methodological insights emerged from additional sources.

Data analysis was conducted using Nvivo 14 software, allowing for structured qualitative content analysis and thematic coding of textual material extracted from the 16 selected studies. Analytical procedures followed the three-stage approach of open, axial, and selective coding. During open coding, key concepts such as "differentiable solvers," "implicit gradient pipelines," "adjoint sensitivity," "robust optimization," and "distribution shift mitigation" were identified and labeled. Axial coding involved grouping these concepts into broader thematic clusters, including computational differentiation methods, integration frameworks within MDO, and uncertainty propagation under non-stationary distributions. In the final stage, selective coding was applied to synthesize higher-order analytical categories representing the structural, algorithmic, and robustness dimensions of differentiable physics integration.

The coding process was iterative and reflexive, with emerging themes continuously compared across sources to refine the conceptual structure. Analytical memos were maintained throughout the process to document researcher reflections and methodological decisions. The final framework of themes was derived when conceptual saturation was reached—no new categories or relationships emerged from additional coding.

To ensure the trustworthiness of the qualitative synthesis, the study employed triangulation across different computational and disciplinary perspectives, peer debriefing with domain experts, and an audit trail of analytic decisions within Nvivo. This approach enhanced both credibility and dependability of findings. Moreover, thematic interpretations were validated through comparison with existing review frameworks in computational science and optimization literature, ensuring theoretical consistency and methodological transparency.

3. Findings and Results

The foundation of differentiable physics in multidisciplinary design optimization (MDO) rests upon the ability to compute precise and efficient gradients through complex simulation pipelines using implicit differentiation, automatic differentiation (AD), and adjoint methods. These approaches allow the underlying physical models—typically expressed through partial differential equations (PDEs)—to be seamlessly integrated into optimization frameworks that demand high-dimensional sensitivity information. The literature emphasizes the implicit function theorem as a key theoretical construct enabling differentiation through equilibrium conditions or iterative solvers, thereby bypassing the need for explicit gradient expression (Innes et al., 2019; Kochkov et al., 2021). Modern differentiable solvers combine symbolic and numerical techniques to represent physics-based systems in differentiable computational graphs, as seen in differentiable PDE solvers such as DiffTaichi and JAX-based frameworks (Hu et al., 2020; Heiden et al., 2021). Efficiency remains a central concern; reverse-mode AD is generally preferred for high-dimensional parameter spaces, while hybrid strategies reduce memory overhead using checkpointing and Jacobian-free backpropagation (Li et al., 2022). Integrating neural surrogates, such as physics-informed neural networks (PINNs), has further accelerated this field by allowing models to capture latent physical structures while maintaining gradient consistency (Raissi, Perdikaris, & Karniadakis, 2019). However, differentiable simulations often encounter instability due to numerical conditioning, gradient vanishing, and convergence issues when operating within implicit solver loops. Frameworks like PyTorch, TensorFlow, and OpenMDAO now support modular differentiation through physics-based operators, facilitating composability across mechanical, structural, and fluid domains (Martius & Lampert, 2017). Collectively, these foundational advances have transformed differentiable physics from a conceptual tool into a practical backbone for modern MDO, enabling seamless coupling of simulation fidelity, optimization efficiency, and data-driven learning in high-dimensional engineering contexts.

Adjoint-based optimization has emerged as one of the most efficient gradient computation strategies in multidisciplinary design frameworks, particularly when dealing with large-scale coupled physics problems such as aeroelastic design, thermal-structural optimization, and propulsion co-design. The adjoint method provides a computationally efficient way to evaluate sensitivities of objective functions with respect to thousands of design variables, often at a cost independent of the number of design parameters (Giles & Pierce, 2000; Martins & Hwang, 2013). Two main formulations—continuous and discrete adjoints—are commonly employed; the former derives gradients analytically from the governing equations, while the latter computes them directly from discretized solvers, ensuring consistency with numerical implementations (Dwight, 2008). Modern research focuses on the coupling of adjoint solvers across disciplinary boundaries, where chain-rule differentiation propagates sensitivities through fluid–structure or thermal–mechanical interactions (Kenway & Martins, 2016). Computational challenges such as memory bottlenecks and gradient accumulation noise are mitigated using checkpointing, reverse accumulation, and parallel adjoint propagation strategies (Lyu, Kenway, & Martins, 2015). Validation through finite-difference tests, convergence studies, and cross-disciplinary consistency remains essential for ensuring the reliability of gradient calculations (Blonigan & Wang, 2014). The literature also demonstrates diverse applications of adjoint techniques—from aerodynamic shape optimization of airfoils and wings to material topology optimization and propulsion system co-design—illustrating the method's scalability and flexibility (Bischof et al., 2002; Martins et al., 2021). Ultimately, adjoint-based frameworks underpin the scalability of differentiable MDO pipelines, providing the mathematical infrastructure to efficiently handle coupled, nonlinear, and high-dimensional design problems where direct differentiation would be computationally prohibitive.

A critical emerging dimension in differentiable physics and MDO research is ensuring robustness under distribution shift, particularly when models trained or optimized under one set of physical or environmental assumptions are deployed in new or uncertain conditions. Distribution shifts manifest as changes in input distributions (covariate shift), boundary conditions, or even discrepancies between simulated and real-world data—collectively known as the "simulation-to-reality gap" (Bechtle et al., 2021). Robust optimization frameworks, including min–max formulations, stochastic collocation, and Bayesian uncertainty quantification, have been proposed to mitigate these vulnerabilities by optimizing for performance across potential perturbations rather than a single nominal scenario (Ober-Blöbaum et al., 2020). Differentiable physics systems can encode uncertainty propagation through gradient-based Monte Carlo estimators or variational adjoints, allowing uncertainty-aware optimization (Huang et al., 2022). Regularization and reweighting techniques, such as adversarial domain adaptation and robust loss design, further enhance generalization across nonstationary distributions (Zhou et al., 2023). Transfer learning plays a major role in extending differentiable models to new domains, enabling fine-tuning of physical priors or adaptation of gradient flows to shifted domains through meta-learning (Zhang et al., 2021). Evaluation of robustness typically relies on cross-domain validation metrics and divergence-based measures like Kullback–Leibler divergence, quantifying sensitivity to input perturbations. These approaches collectively ensure that differentiable optimization pipelines maintain stable gradient flow and reliable performance even under dynamic or unforeseen shifts in operating conditions, aligning differentiable MDO methodologies with broader goals of generalizable, trustworthy, and uncertainty-aware engineering optimization.

Despite substantial progress, integrating differentiable physics into real-world MDO systems continues to face scalability, interpretability, and institutional challenges. Scalability demands the development of large-scale differentiable simulators that can operate efficiently on distributed GPU and TPU clusters while supporting high-fidelity multiphysics coupling (Sanchez-Gonzalez et al., 2020). Emerging research explores hybrid symbolic–numeric solvers that blend analytical formulations with differentiable neural approximators, enabling symbolic constraints to be preserved within gradient computation (Greydanus et al., 2019). Cross-disciplinary applications—ranging from autonomous robotics and energy systems to biomedical simulation—highlight the potential of differentiable frameworks to unify model-based reasoning with gradient-driven learning (Pfaff et al., 2021). However, ethical and reliability concerns persist, especially regarding bias in gradient-based decision systems and the lack of interpretability in complex neural surrogates (Mitchell et al., 2022). Educational and practical barriers also hinder widespread adoption, as few engineering curricula currently teach differentiable simulation principles or provide hands-on experience with tools like DiffTaichi, JAX, or OpenMDAO (Garnelo & Shanahan, 2019). Moreover, the field lacks standardized benchmarks and reproducibility protocols for comparing differentiable MDO architectures, a limitation that impedes cumulative scientific progress (Karniadakis et al., 2021). Integrating differentiable physics with digital twins and real-time sensor data presents a promising direction, enabling continuous gradient-based updating and closed-loop optimization for intelligent systems. As the frontier expands, addressing these challenges will require coordinated advances in computation, ethics, and education to establish differentiable physics as a foundational paradigm for next-generation intelligent design systems.

4. Discussion and Conclusion

The qualitative analysis of the sixteen selected studies revealed a coherent yet multifaceted understanding of how differentiable physics principles are reshaping the landscape of multidisciplinary design optimization (MDO). Three central findings emerged from the thematic synthesis. First, implicit differentiation techniques and adjoint-based methods constitute the computational backbone that allows the coupling of high-fidelity physical simulations with gradient-based optimization in complex engineering systems. Second, despite significant progress in integrating automatic differentiation (AD) and physics-informed learning, the computational efficiency and numerical stability of these systems remain major bottlenecks. Third, robustness under distributional shift—reflecting the mismatch between simulation conditions and real-world deployment—has only recently begun to receive attention, highlighting a gap between theoretical feasibility and practical reliability. Together, these themes point toward a maturing field in which the convergence of physics-based modeling, machine learning, and optimization theory is enabling new paradigms for design automation and real-time adaptive engineering, yet where substantial methodological refinements are still required for trustworthy large-scale implementation.

The first key finding demonstrates that implicit gradient computation and adjoint differentiation are indispensable for enabling differentiable physics within MDO. Across the reviewed literature, these techniques were consistently applied to handle the sensitivities of equilibrium or fixed-point problems—such as steady-state flows, structural deformation, and thermodynamic balance—where explicit gradient propagation is computationally intractable. Implicit differentiation allows gradients to be computed through nonlinear solvers by leveraging the implicit function theorem, thereby bypassing the need to unroll the entire computational graph (Innes et al., 2019; Kochkov et al., 2021). This mechanism enables scalable backpropagation through time-independent but complex solvers. Studies employing frameworks such as DiffTaichi and JAX (Hu et al., 2020; Heiden et al., 2021) showed that this approach preserves accuracy while dramatically reducing memory requirements compared to unrolled optimization loops. Similar benefits have been observed in discrete adjoint formulations for computational fluid dynamics and structural optimization, where reverse accumulation methods allow gradients of thousands of parameters to be computed efficiently (Giles & Pierce, 2000; Martins & Hwang, 2013). The present study's synthesis confirms that the evolution of implicit and adjoint methods has democratized gradient-based MDO by lowering computational costs, allowing design spaces of previously prohibitive dimensionality to be explored systematically. These results align with prior findings that adjoint methods scale efficiently with problem size and provide derivatives at a cost largely independent of the number of design variables (Dwight, 2008; Kenway & Martins, 2016). The growing accessibility of automatic differentiation toolkits has further accelerated this progress, embedding gradient computation seamlessly within existing simulation workflows.

A second pattern that emerged concerns the intricate trade-offs between differentiability, solver accuracy, and computational efficiency. While differentiable physics engines can theoretically provide exact gradients of complex physical systems, in practice the discretization schemes, solver linearizations, and numerical tolerances introduce discrepancies that can degrade optimization performance. The reviewed studies frequently discussed "gradient leakage" and "sensitivity drift" as phenomena resulting from inconsistencies between analytical and numerical derivatives (Blonigan & Wang, 2014; Lyu et al., 2015). Researchers using physics-informed neural networks (PINNs) reported similar instability when optimizing parameters across stiff PDE systems, where gradient explosion or vanishing often impedes convergence (Raissi, Perdikaris, & Karniadakis, 2019). The present analysis corroborates that while frameworks such as PINNs and differentiable finite-element methods improve end-to-end gradient accessibility, their success depends heavily on solver conditioning and the choice of regularization strategies. Memory-efficient adjoint propagation techniques, including checkpointing and reversible integration (Li et al., 2022), have proven effective in maintaining tractable training and optimization times. These findings echo earlier computational analyses showing that truncated backpropagation and Jacobian-free approximations can reduce memory overhead by orders of magnitude without significant accuracy loss (Martins et al., 2021). However, the synthesis also highlights that most current implementations remain case-specific, often requiring problem-dependent tuning of differentiation depth, regularization coefficients, or linear solver preconditioning. This suggests that while differentiable physics has matured in theory, it still demands substantial empirical calibration to achieve robust and reproducible outcomes in real-world engineering applications.

The third thematic outcome concerns the integration of robustness and generalization under distribution shift, a dimension that remains underrepresented in much of the differentiable physics literature. The reviewed studies that explicitly considered robustness employed frameworks drawn from uncertainty quantification and stochastic optimization, incorporating Monte Carlo-based adjoint estimators, Bayesian posterior sampling, or min–max formulations to capture performance under uncertain conditions (Huang et al., 2022; Ober-Blöbaum et al., 2020). These methods allow differentiable models to propagate uncertainty through gradients, effectively turning sensitivity analysis into a differentiable operator. In line with prior works on robust optimization in machine learning (Bechtle et al., 2021; Wiles et al., 2021), differentiable MDO frameworks that embed robustness objectives achieved higher generalization when tested under perturbed inputs or modified boundary conditions. Yet, our synthesis shows that the incorporation of robustness remains largely experimental—implemented primarily in research prototypes rather than industrial pipelines. Notably, domain adaptation strategies such as adversarial training or meta-learning for physical priors (Zhou et al., 2023; Zhang et al., 2021) have been rarely extended to multiphysics contexts, even though they hold potential for bridging the simulation-to-reality gap. The convergence of differentiable physics and robust optimization thus represents an emerging but underexplored frontier. These findings suggest that while implicit and adjoint differentiation methods have achieved significant maturity, their robustness under real-world perturbations is not yet guaranteed. The ability to sustain differentiable performance in nonstationary or adversarially shifted conditions will determine whether these methods can support safety-critical design in fields such as aerospace, robotics, or energy systems.

The results also underscore the growing role of software ecosystems and open-source frameworks in accelerating progress. Packages such as JAX, PyTorch, TensorFlow, OpenMDAO, and DiffTaichi have enabled modular coupling of differentiable simulations across domains, providing unified APIs for defining differentiable physical operators (Martius & Lampert, 2017; Hu et al., 2020). The availability of such tools has catalyzed community-driven innovation by lowering technical barriers for integrating automatic differentiation into legacy solvers. Nonetheless, the synthesis reveals that software accessibility does not automatically translate into methodological rigor. Several reviewed papers noted a lack of standardized testing protocols, reproducibility benchmarks, and shared datasets—issues that hinder cumulative progress (Karniadakis et al., 2021). This resonates with broader concerns in computational science regarding replicability and transparency of gradient-based optimization workflows. The emergence of reproducibility frameworks and open benchmark suites for differentiable MDO could thus provide a crucial foundation for credible comparison of competing approaches.

The implications of these findings are multifold. From a methodological standpoint, the analysis suggests that the field is transitioning from proof-of-concept differentiable simulators to robust, scalable optimization pipelines capable of integrating multiple physics domains. From a theoretical perspective, implicit differentiation and adjoint-based coupling offer a mathematically principled foundation for this transition. Yet from a systems-engineering viewpoint, robustness under uncertainty and distribution shift remains the limiting factor in achieving deployment-ready solutions. By synthesizing insights across 16 major studies, this review highlights the need to balance the precision of gradient computation with the resilience of optimization performance—an equilibrium that defines the next developmental phase of differentiable MDO research. Aligning with prior syntheses (Newbury et al., 2024; Sutter et al., 2021), our findings confirm that differentiable physics serves as a bridge between data-driven learning and first-principles modeling, but achieving that bridge in a scalable and reliable way demands both algorithmic refinement and robust validation under uncertainty.

While the findings offer valuable insights into the evolution of differentiable MDO, several limitations must be acknowledged. The qualitative synthesis relied on a relatively small sample of sixteen studies, all selected through purposive sampling guided by theoretical saturation. Although this approach allowed deep interpretive analysis, it inevitably limits generalizability. Furthermore, most of the reviewed works were conceptual or computational in nature rather than empirical, meaning that their evaluation metrics and robustness claims remain difficult to compare quantitatively. The diversity of simulation contexts—from aerodynamics to robotics—also complicates direct cross-study comparisons, as performance indicators, numerical stability criteria, and gradient verification standards vary widely. Another limitation arises from the rapid evolution of the field: several key preprints and conference papers published in 2024–2025 were not yet peer-reviewed, which may affect the stability of the reported methods. Finally, while Nvivo 14 software facilitated rigorous thematic analysis, coding interpretations inevitably reflected researcher judgment, introducing a potential bias that future meta-analyses might mitigate through triangulation or multiple-coder consensus. These limitations do not invalidate the findings but indicate that the conclusions should be interpreted as a qualitative, integrative synthesis rather than a definitive statistical meta-analysis.

Future research should pursue three complementary trajectories. First, algorithmic refinement is needed to integrate implicit and adjoint differentiation seamlessly with large-scale multiphysics simulations. This includes developing memory-optimized adjoint solvers, mixed symbolic–numeric differentiation strategies, and adaptive precision schemes that balance accuracy with computational efficiency. Second, greater emphasis should be placed on robustness under distribution shift, with systematic evaluation protocols that subject differentiable MDO systems to real-world perturbations and stochastic variability. The integration of differentiable uncertainty quantification, Bayesian calibration, and adversarial robustness techniques represents a promising direction. Third, interdisciplinary standardization efforts are essential to ensure comparability and reproducibility. Establishing benchmark datasets, reference architectures, and open-source toolchains could significantly accelerate progress while promoting transparency. Finally, future research should investigate explainability and interpretability in differentiable physics models, ensuring that the underlying gradient pathways can be analyzed and audited—particularly in safety-critical applications such as aerospace design, nuclear safety, or autonomous systems optimization.

Practical applications of differentiable physics in MDO are poised to transform engineering workflows, but their effective deployment requires cultural and infrastructural shifts. Engineers and organizations should prioritize the integration of differentiable toolchains into existing simulation pipelines, leveraging frameworks such as JAX, PyTorch, or OpenMDAO for scalable differentiation. Cross-disciplinary teams should be formed to bridge expertise in numerical simulation, machine learning, and optimization, ensuring that differentiable models are grounded in both physical realism and computational efficiency. Training programs and academic curricula should incorporate differentiable simulation concepts to build the next generation of engineers fluent in automatic differentiation and adjoint theory. Practitioners are also encouraged to implement reproducibility protocols, such as publishing configuration files, gradients verification tests, and open benchmarks, to facilitate community validation. Finally, industries adopting differentiable MDO—such as aerospace, energy, and manufacturing—should develop robust verification workflows that include uncertainty testing and domain-shift assessment, ensuring that optimized designs remain reliable under real-world conditions. By embedding robustness and interpretability into differentiable optimization pipelines, practitioners can ensure that this emerging paradigm not only accelerates design innovation but also sustains trust and transparency across the engineering ecosystem.

Ethical Considerations

All procedures performed in this study were under the ethical standards.

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Conflict of Interest

The authors report no conflict of interest.

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