Abstract

Existing approaches to exploring design space in thermo-fluid domains are human-labor intensive and not easily automatable. As a result they can typically generate only minor variations of pre-existing designs. In this paper, we discuss results from an AI-assisted design-space exploration tool built at our organization for such domains.

Introduction

Constraint-satisfaction problems (CSP) arise in diverse application areas, including software and hardware verification, scheduling, planning, design-space exploration, etc (Rossi, Van Beek, and Walsh 2006). Mathematical formulations of such problems typically involve constraints defined using a combination of Boolean, Integer, and Real-valued variables. The problem size and complexity of constraints in such formulations typically render naive approaches (e.g., random assignments, simple heuristic search techniques) ineffective (Rossi, Van Beek, and Walsh 2006). Design-space exploration (DSE) problems are a class of CSPs where solutions represent feasible designs (Saxena and Karsai 2010). The term exploration refers to the activity of exploring design alternatives prior to implementation. The power to operate on the space of potential design candidates renders DSE useful for many engineering tasks, including rapid prototyping, optimization, and system integration. A majority of existing DSE approaches in various domains focus on incremental variations of existing designs. As a result, they typically lead to only marginally better performing new designs (Kanajan et al. 2006).

In the context of discovery of candidate designs for thermo-fluid domains, existing approaches are largely based on costly and time-consuming trial-and-error, with only a very small fraction of the entire possible design space having been explored. The space of feasible designs for such problems is enormously large and it is quite often also challenging to estimate the total size of design space given a variety of constraints imposed on feasible designs (manufacturability, physics, etc.). Hence brute force approaches do not scale. As an example, for a design domain with \(10^6\) Boolean design variables, without the use of sophisticated search techniques, one would need to compute and then verify about \(2^{10^6}\) design candidates. Hence, when considering the vastness of the design space together with complex constraints, it is clear that scalable and automated DSE strategies are critical for exploration.

Figure 1: Current best practice in heat-transfer surface design: iterative parametric opt. w/ limited design freedom and days/iteration. Figure adapted from (Kirsch and Thole 2017).

DSE on Thermo–Fluid Domains

State-of-the-art (SoA) heat-transfer (HT) components used in energy systems are typically designed to contain incremental improvements over past designs. This approach, where previous designs dictate the form of these components, is conservative; the designs have been validated, as have their models to predict performance. However, achieving a step change in performance is unlikely with this conservative approach. Efforts to push the limits on these complex designs are ongoing, but are limited in two key ways. First, optimization schemes can be costly, especially when the optimization considers multiple objectives across multiple physics. In topology optimization, for example, solutions may get stuck in a local minimum. Rerunning the optimization with different constraints or different optimization parameters may help push the solution out of a potential local minimum, but these approaches cannot guarantee a global optimum. Second, engineers generally limit the geometric
Figure 2: Overview of our AI-driven DSE framework. The framework leverages capabilities from artificial intelligence to efficiently and comprehensively search the design space. The explored designs are then used to learn design choices that lead to better performance by leveraging SoA ML approaches. The learned ML models are used to synthesize feasible designs that satisfy a given set of performance requirements.

AI-driven DSE framework

As part of ongoing research, the team has developed a novel requirements-driven AI design framework, shown in Figure 2, for thermo-fluid domains. The main steps in this approach are outlined at the top in Figure 2. In the first two steps, the designs are generated using various approaches, including conventional designs, topology optimized designs, and those generated using the team’s AI design framework. Using this wide collection of candidates to train ML algorithms leads to fundamentally new conceptual designs suitable for a variety of applications that perform closer to the theoretical highest performance. The framework leverages capabilities from artificial intelligence to efficiently and comprehensively search the design space. The explored de-
Figure 3: Heat Transfer surface design space exploration using AI-driven framework. More than 20000 feasible designs were automatically synthesized and evaluated for performance. The framework discovered a variety of designs, e.g., thin pin array like designs, and designs with fat channels for fluid flow.

Designs are then used to learn design choices that lead to better performance by leveraging SoA machine learning (ML) approaches. The ML-based model is then used to synthesize near-optimal feasible designs that satisfy a given set of performance requirements.

An example ongoing case study of using the approach for the design of a heat transfer surface is shown in Figure 3. This case study specifically explores heat sink and cold plate designs, where heat transfer performance is quantified through thermal resistance: high heat transfer corresponds to a low thermal resistance. In the performance plot, therefore, the best designs are in the lower left corner, where frictional loss and thermal resistance are both low. More than 20000 feasible designs were automatically synthesized and evaluated for performance. Note that this number of feasible designs is orders of magnitude larger than what a human expert designer could hand craft and evaluate in any reasonable amount of time. The framework discovered a variety of designs, e.g., thin pin array like designs, and designs with fat channels for fluid flow. The diverse set of candidate designs are being currently used to learn good design choices using machine learning approaches.

Figure 3 highlights an important criteria for heat sink design, namely that surface area is key. In the AI-driven designs, two classes of designs emerged that mimic those used by human designers: channel-like structures and discrete fins. The AI-driven channel-like structures show low frictional losses, but high thermal resistance; large channels lead to slow flow and, consequently, poor convection. On the other hand, the AI-driven discrete fin examples show comparable, if not better, performance than a human-designed staggered pin fin array. These discrete fin layouts can be used to learn effective design strategies.

An estimation of a pareto frontier for highest performing designs is included as the dotted line in Figure 3. A gap can be seen between the pareto front and the candidate designs in the lower left corner of the performance plot. Given the massive design space that the team is exploring, the expectation is that the ongoing work to generate effective designs will fill that gap. The heuristics developed for the team’s framework continue to produce designs with lower thermal resistance and lower frictional losses. Further, as the team refines the ML-based model, the learning based on these initial candidates can be used to generate innovative designs that will fill any performance gaps that currently exist.

Conclusions

In this paper, we have presented an AI-driven design space exploration framework for thermo-fluid domains. The framework continues to be under active development and improving accuracy and computational speedup within the framework remain part of ongoing and future efforts.

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