# Predictive Methods: overview

Predictive methods, which aim to anticipate future events never before seen are the cornerstone of science and engineering. These methods typically involve reducing the number of degrees of freedom in the system to be modeled, as most problems in life are intractable in their full extent. This reduction results in a closure problem, which requires assumptions about the physics of the missing degrees of freedom. Therefore, the predictive power of a method stems from the quality of its underlying physical assumptions, along with the tools used for its implementation. Predictive approaches should not be confused with other practices in the field, such as surrogate modeling, where an already known model is made computationally more efficient for real-time prediction (e.g., control systems and digital twins) or design (e.g., parametric sweeps and optimization). Nor should predictive modeling be mistaken for curve fitting—the art of replicating already known data—which offers no true predictive capability. This distinction is particularly important in the current AI/data-driven era, where curve fitting has increasingly become a tempting practice. The true beauty of predictive modeling lies in its ability to address new, unseen situations based solely on knowledge from the past. While this approach is undeniably challenging, it is simply a reflection of the fact that "life can only be understood backwards; but it must be lived forwards" (Kierkegaard).

During the 2024 CTR Summer Program, seven projects dedicated to turbulence modeling for engineering applications contributed to the development of groundbreaking ideas in the field. The group focused on the common theme of predictive modeling, with 22 participants from 11 institutions, supported by eight hosts, working together for a month. The teams addressed problems of both fundamental and technological significance, with topics ranging from novel large-eddy simulation (LES) modeling strategies for complex flows to the effects of floating-point precision on quantities of interest.

The project by Domino aimed to evaluate the capability of wall-modeled LES (WMLES) in predicting heat flux migration and combustion efficiency for fire-engulfed objects in crosswind scenarios. The study demonstrated the potential of WMLES to accurately predict windward-to-leeward migration of hydrocarbon fire heat flux, driven by interactions between vortical structures and boundary layer separation. Senga *et al.* focused on simulating methane-oxygen combustion in rotating detonation engines using a flamelet-based progress variable approach. The team achieved stable detonation wave modeling and showed that detonation speed is sensitive to initial fuel-oxidizer mixing. Ma *et al.* devised a generalizable model for WMLES in high-speed flow scenarios. Using turbulent channel flows with varied roughness and Mach numbers, they identified key nondimensional inputs and outputs to maximize predictive capabilities. Validation revealed an average error of 10%, demonstrating the broad applicability of the model and its potential use for hypersonic vehicles.

The project by Huang *et al.* addressed the gap between *a priori* and *a posteriori* results in training subgrid-scale (SGS) models. By increasing the explicit filter size, the team reduced numerical error and improved the correlation between modeled and actual flow behaviors. Karp *et al.* studied the impact of lower floating-point precision on computational fluid dynamics (CFD) simulations of turbulent flows. Their findings revealed that sensitivity to reduced precision is lower than previously expected, with accurate simulations achievable even at reduced precision. Przytarski *et al.* characterized turbulence and unsteady interactions in multistage compressors. By using high-fidelity simulations and large-scale data decomposition, the team developed a phenomenological description of energy cascades and worked toward reduced-order models to replace empirical correlations in industrial design tools. Bellosta *et al.* investigated the geometric scales needed to predict aerodynamic loads on iced airfoils. Their results indicated that small ice roughness scales are crucial for accurate load predictions in streamlined rime icing, while larger features dominate aerodynamic behavior in glaze icing.

After the summer program, it is fair to ask: What can we do now that we couldn't do before? Or what can we do better? The projects described above have reinforced the credibility of WMLES for multiphysics applications and analyses, including compressor multiscale analysis, airfoil icing in multiphase flows, combustors, fire-engulfed objects, and entry vehicles. These demonstrate that we have overcomed the trainability barrier in SGS models for WMLES beyond canonical flows while deepening our understanding of the impact of limited precision in CFD. The advancements in modeling, numerics, and best practices achieved during the program are poised to make transformative contributions to the community. From sustainable aviation solutions and certification by simulation to reliable predictions for space exploration and extreme engineering environments, these developments lay the groundwork for driving innovation across a wide array of problems.

Finally, we extend our gratitude to all participants in the Predictive Methods group for their intellectually stimulating discussions and ideas, which have opened new avenues for advancing the field. Several open challenges emerged from these group discussions. One pressing question is how to effectively assess the performance of WMLES in complex multiphysics scenarios. Addressing this challenge highlights the need for high-quality experimental validation data to ensure accuracy and credibility in these simulations. Another challenge lies in quantifying uncertainties from closure models, gridding strategies, and variable machine precision. Lastly, a fundamental question persists: Can we develop generalizable models for WMLES that are robust against numerical errors? Achieving this goal would mark a major leap forward, enabling more predictive capabilities across diverse applications. Together, these challenges provide the next roadmap for future research and collaboration.

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