SIMULATION OF BLUFF BODY STABILIZED FLAMES WITH PELEC: ADAPTIVELY RESOLVING TURBULENCE–COMBUSTION INTERACTIONS IN REAL-WORLD ENGINEERING PROBLEMS

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EXECUTIVE SUMMARY

Gas turbine engines are widely used for propulsion and load-leveling applications, the latter being critical for incorporating intermittent renewable energy sources such as wind on the electrical grid. While efficiency, emissions, and flame stability are central to advances in turbine design, the extreme level of complexity continues to limit the accuracy of high-fidelity models and the control of gas turbine systems. This project uses the state-of-the-art high-performance computing (HPC) resources provided by Blue Waters to perform high-fidelity direct numerical simulations of turbulent premixed flames stabilized on bluff bodies. (By definition, bluff bodies are those that, because of their shape, have separated flow over a substantial part of their surface.) By studying the dynamics of stabilized flames, the researcher analyzed how high-fidelity models should be adapted to strongly turbulent compressible flows with complex chemistry in the presence of strong shear layers and examine mechanisms for enhancing flame stabilization while maintaining high efficiency and low emissions.

RESEARCH CHALLENGE

As researchers and engineers work to improve the understanding and control of gas-engine systems, the complexity and extreme conditions found in these systems pose a significant challenge for computational approaches. To understand the challenges that engineers face and to better understand the interactions among turbulence, combustion, and recirculation-zone dynamics that impact stability, the project poses two important questions:

- How should large-eddy simulation (LES) modeling be adapted to highly turbulent compressible flows with complex chemistry in the presence of strong shear layers, where key physics can be left unresolved by the grid?
- What new mechanisms can be applied to better stabilize flames and prevent blowout while maintaining high efficiency and low emissions?

The first question is motivated by the current inability to model gas turbines in a physically accurate yet computationally efficient manner, while the second is central to turbine design and operation. In this project, these questions are addressed by performing high-fidelity direct numerical simulations (DNS) of turbulent premixed flames stabilized on bluff bodies. In particular, data produced by the high-resolution DNS are being used to analyze key dynamics associated with turbulence–flame interactions in bluff body configurations that are not well captured in high-fidelity LES, that also must be included in future low-fidelity models for practical turbine design, and that lead to instability and flame blowout.

METHODS AND CODES

The researcher has adapted the next-generation compressible reacting flow solver PeleC to the Blue Waters HPC architecture. PeleC, under development at Lawrence Berkeley National Laboratory and the National Renewable Energy Laboratory, scales well, is fully parallelizable, and can be run using both the Message Passing Interface and OpenMP paradigms. The PeleC code uses built-in embedded boundary capabilities for structural modeling, which enables accurate implementation of different bluff body configurations for this work. Furthermore, PeleC incorporates Adaptive Mesh Refinement (AMR) via the AMReX suite, allowing different regions of the simulation domain to be resolved at different levels of fidelity. This permits the addition of local refinement on areas of physical interest, fully resolving flame dynamics and turbulence–combustion interactions. Fig. 1 shows an example of AMReX and AMR at work, with refinement on vorticity. This dynamic refinement results in high-resolution simulations running at reduced computational cost when compared with traditional static meshes. This is particularly true for highly dynamical systems such as engines and turbines where the location of flames and vortex structures is often unpredictable and intermittent in time. The research also incorporates multistep chemistry through Chemkin-type inputs in order to model chemical kinetic effects without loss of fidelity.

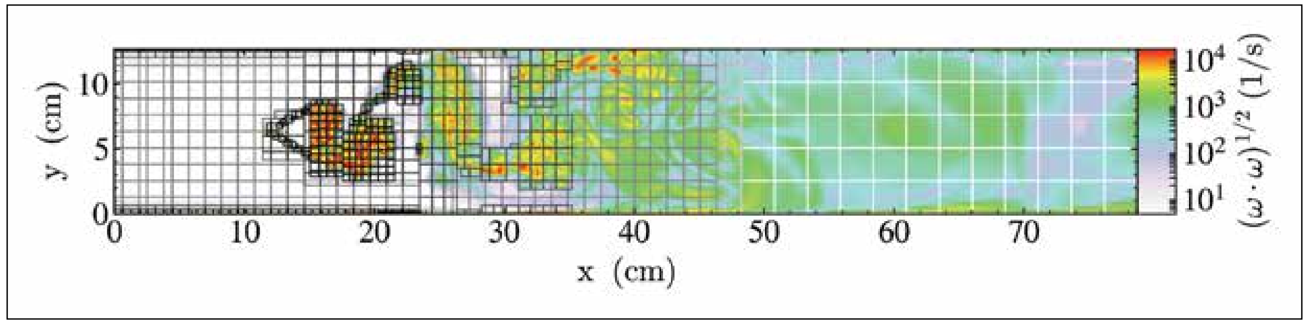

Figure 1: Flow around a triangular prism bluff body, with high-vorticity regions in red. Adaptive meshing provides localized refinement based on the vorticity. Here, each grayscale box shows three-dimensional grids that are between eight and 32 cells on each side. This localized refinement results in higher-resolution simulations at reduced computational cost.

RESULTS & IMPACT

This work used the PeleC exascale combustion code to simulate bluff body flow and successfully produced high-resolution simulations of nonreacting bluff body flow using AMR to provide localized resolution in the near-wake region of the bluff body. Localized refinement allows the simulations to physically resolve the recirculation zone dynamics of the target experimental case at a level not previously examined. These simulations help to determine necessary parameters for computational modeling of this bluff body configuration, including simulation domain, boundary conditions, and resolution criteria necessary for accurate and efficient performance. The lessons learned have been used to design and instantiate reacting-flow simulations and, with these, to explore chemistry model performance and stability within the PeleC simulations running on Blue Waters.

WHY BLUE WATERS

Blue Waters has been both formative and essential for this research. The allocation has allowed the researcher to begin using the highly scalable, adaptive PeleC code to tackle engineering challenges that would not otherwise be able to be considered: questions that are directly applicable to power generation, aviation, and the broader community. The staff have been both attentive and responsive, and ultimately were invaluable in getting the PeleC code up and running, helping with system-specific questions and advice for avoiding potential roadblocks along the way.

Samuel Whitman is a third-year Ph.D. candidate in mechanical engineering at the University of Colorado, Boulder. He expects to receive his degree in 2020 and has been working under the direction of Peter Hamlington and James G. Brasseur.