Proceedings of the Fourth Model Validation for Propulsion (MVP 4) Workshop

2020 AIAA Science and Technology (SciTech) Forum and Exposition
January 7 & 9, 2020
Orlando, Florida

Adam Comer, Matthias Ihme, Chiping Li, Christopher Lietz, Joseph Oefelein,
Brent Rankin, Venkateswaran Sankaran

Abstract

The purpose of this report is to document the Proceedings of the Fourth Model Validation for Propulsion (MVP) Workshop which was held at the 2020 AIAA SciTech Forum on January 7th and 9th at Orlando, Florida. The Model Validation for Propulsion Workshop is an open forum bringing together researchers and modelers to help improve our understanding and capabilities of modeling turbulent reacting flows in relevant aerospace propulsion systems. The main MVP 4 Workshop session was held on Tuesday, January 7, 2020, and was attended by approximately 20 researchers. There were five technical presentations during this session representing contributions from four organizations. This session focused on the Volvo and AFRL bluff-body premixed flame validation cases. An invited panel session on a new rotational detonation engine test case to be featured in the Fifth MVP Workshop was conducted on Thursday, January 9, 2020. These proceedings summarize the objectives, final program, discussion topics, and conclusions for the MVP 4 Workshop. These proceedings and further information are available on the MVP Workshop website: https://community.apan.org/wg/afrlcg/mvpws

TABLE OF CONTENTS

INTRODUCTION

Objectives of MVP Workshop Series

The Model Validation for Propulsion Workshop is an open forum bringing together researchers and modelers to help improve our understanding and capabilities of modeling turbulent reacting flows in relevant aerospace propulsion systems. The objectives of the MVP Workshop series include the following:

- Define and evaluate procedures/metrics for grid convergence for reacting LES and quantify numerical error.
- Evaluate performance of physics models for combustion, turbulence and turbulent combustion closures.
- Identify the requisite data for validation of reacting LES.
- Identify fundamental gaps in current knowledge of reacting LES models to inform basic research programs.
- Use data and comparisons to guide the development of improved models.

Organizing Committee for the MVP Workshop Series

The organizing committee for the MVP Workshop series consists of the following members:

- Adam Comer, University of Michigan
- Matthias Ihme, Stanford University
- Chiping Li, Air Force Office of Scientific Research
- Christopher Lietz, Sierra Lobo Inc.
- Joseph Oefelein, Georgia Institute of Technology
- Brent Rankin, Air Force Research Laboratory
- Venkateswaran Sankaran, Air Force Research Laboratory

Objectives of MVP 4 Workshop

Technical presentations featuring simulations of the AFRL bluff-body test case were solicited. To advance the workshop comparisons beyond first and second moment statistics and to prepare for comparisons with high repetition-rate laser diagnostic data, the focus of the workshop was the application of unsteady metrics. The application of these metrics was advocated for use in the following types of studies:

- Grid Convergence – Participants were encouraged to pursue novel methods for producing grid independent results and required to show some quantification of the sensitivity of the results to grid resolution.
- Explicit Filtering – The application and development of explicit filtering to separate physical model errors from numerical errors and to enable more definitive statements about model accuracy were requested.
- Sensitivity Analyses – To aid in the identification of the largest sources of error and to guide potential future experiments, sensitivity studies of the boundary conditions and modeling approaches were suggested as useful technical paper topics.

An invited panel session featured presentations and discussions on experimental and computational efforts involving the future MVP 5 Workshop test case, a rotating detonation rocket engine.

Planning for MVP 5 Workshop

MVP 5 will focus on a new test case. Specifically, a rotating detonation rocket engine experiment currently being evaluated at three universities has been selected. Simulations of this test case have been performed at the Air Force Research Laboratory and are in progress at multiple universities. Bluff-body flame efforts are expected to continue at MVP 6 in parallel with the rotating detonation rocket engine. Exact MVP 5 dates and validation case guidance will be provided in the spring of 2020, and the workshop will continue to be held in conjunction with AIAA SciTech.

Important Note Regarding Use of Workshop Proceedings Material

Results in the MVP Workshop proceedings are contributed in the spirit of open collaboration. Some results represent completed work, and other results represent work in progress. Readers should keep this in mind when reviewing these materials. It is inappropriate to quote or reference specific results from these proceedings without first checking with the individual author(s) for permission and for the most recent information and references.

FINAL PROGRAM FOR MVP 4 WORKSHOP

Main MVP Workshop Session on Bluff-Body Premixed Flames

Tuesday, January 7, 2020, 6:00PM-9:00PM

Introduction to MVP 4 Workshop

- **A. Comer**, “Introduction and MVP Overview.”

Computational Results and Discussion

- **D. Lindblad**, “LES and DMD Analysis of a Bluff-Body Stabilized Premixed Propane-Air Flame.”
- **Z. Jozefik**, “Grid Characteristics Study of a Bluff-Body Stabilized Turbulent Premixed Flame.”
- **X. Gao**, “Enhanced CFD modeling with Data Assimilation of Flows in Bluff-Body Combustors.”
- **S. Guzik**, “Adaptive Mesh Refinement for LES of Combustion Stabilized with Bluff-Body Geometry.”
- **T. Gallagher**, “Untangling Numerics and Modeling: Explicit Filtering for Reacting LES.”

Experimental Results and Discussion

- **B. Rankin**, “AFRL Bluff-Body Stabilized Turbulent Premixed Flame Validation Case.”

Future Directions for Bluff-Body Flame Model Validation,
Discussion led by Venkateswaran Sankaran

Invited Panel Session and Workshop Discussion on Rotating Detonation Rocket Engines

Thursday, January 9, 2020, 9:30AM-12:00PM

Introduction to MVP 4 Workshop

- **C. Lietz**

Experimental Results

- **C. Knowlen**
- **K. Ahmed**
- **C. Slabaugh**

Computational Results

- **G. Candler**
- **V. Raman**
- **J. Oefelein**

Future Directions for Rotating Detonation Rocket Engine Model Validation,
Discussion led by Venkateswaran Sankaran

SUMMARY OF MVP 4 WORKSHOP

Bluff-Body Premixed Flame Validation Cases

The most significant observations and conclusions from the five presentations on the bluff-body test case are summarized in this section.

- **Experiment Update** – Experimental data from the AFRL bluff-body test case were presented, highlighting the collection of simultaneous 10kHz CH_2O planar laser induced fluorescence (PLIF), OH PLIF, and particle image velocimetry (PIV) data. This dataset presents an opportunity to extend current validation efforts into a more direct comparison of unsteady dynamics. Boundary and operating conditions have been characterized, and imaging measurements are ongoing. Spanwise non-uniformities behind the bluff-body were reported for the reacting case and are caused by large-scale corner vortex structures located between the ends of the bluff-body and the adjoining walls. These non-uniformities are not present in the non-reacting case, which is consistent with studies by other research groups. Future computational efforts focusing on comparison with experimental data should consider eliminating the spanwise periodicity assumption and including all of the walls.
- **Explicit Filtering** – A summary of explicit filtering findings from MVP and interactions outside of the workshop was presented. An external explicit filtering workshop established a consensus that the strong sensitivity of implicitly filtered reacting LES solutions to grid resolution and numerics is a significant obstacle that needs to be addressed. Due to these issues, observations and model assessments obtained from results with one code may not hold for another code, hindering general and rigorous closure model development. It appears that the importance of this issue in reacting flows exceeds that of non-reacting flows, since the flame scales produce dramatic changes in the thermochemical state and flowfield and often exist at the sub-filter scale. Explicit filtering, error estimation, and dynamical systems formulations for LES closure were presented as potential solutions, but no consensus exists for the best approach. Advances in explicit filtering, including computationally efficient procedures and high-order filtering, have enabled grid convergence at a fixed filter width for the reacting bluff-body test case. Unfortunately, explicit filtering has been demonstrated by one group with only one code for this workshop.

The following risks associated with this limited experience were highlighted during the workshop discussions:

- It remains to be demonstrated that explicit filtering produces the same grid-converged solution for a fixed filter width when used with different numerical methods (i.e., do variations in time-stepping, flux computation, limiters, etc. influence the explicitly-filtered, grid-converged solution).
- Many variants of explicit filtering exist. It is not clear that they will all give the same grid-converged solutions, even when the filter widths are matched. If these methods produce significantly different results, then explicit filtering may be an ineffective approach to eliminating code-to-code variations in solutions, as the implementations and algorithms for explicit filtering will likely be unique for every code.

To address these risks and to work towards answering some of the questions that they pose, the following suggestions for future workshops were provided and received a positive response:

- As a preliminary step, the existing explicit filtering implementation should be tested with different numerical methods offered by the associated code. This effort would provide confidence in the approach's capacity to minimize code-to-code solution variation.
- Enforce explicit filtering as a requirement for any future bluff-body simulation efforts.
- Every group should vary its numerical schemes and attempt to show that the same grid-converged solution is obtained for a fixed filter width, in spite of differences in numerical methods.

- **New Metrics for Comparison** – A sparsity-promoting dynamic mode decomposition (DMD) algorithm was applied to bluff-body simulation results. The algorithm revealed that a symmetrical mode corresponding to shear-layer roll-up was the dominant mode for a domain that was five bluff-body dimensions in length starting from the trailing edge. The mode shape and its clear symmetry were encouraging, as they suggest that the algorithm is sufficient to identify physically relevant modes with definitive characterizations in terms of symmetry. Additionally, enstrophy budgets conditioned on progress variable were used by one group to examine grid resolution effects. This group examined the variation in the magnitude of the enstrophy equation terms as the grid was refined. The results were produced using a laminar combustion assumption (closure of species production source terms with resolved scale quantities only) and showed significant changes in baroclinic torque as the grid was refined. This approach provides more insights into grid sensitivity than typical statistical comparisons since it highlights the physical processes most affected by lack of resolution.

- **Grid Sensitivity –** Results were presented with a dual-mesh solver, featuring a second-order solver near walls and a fifth-order Cartesian solver away from the walls. Since the results employed laminar combustion closure, an approach that is known to be sensitive to grid resolution based on previous workshops, multiple profile statistics did not appear to be converged, even at high resolution.

- **Boundary Condition Sensitivity –** Exit boundary condition sensitivity has been observed by multiple groups in previous workshops. During this workshop, one group noted severe instabilities when trying to use a grid with an extended outlet that enables simulation of exit flow outside the combustion chamber. Similar instabilities were observed by another group in a previous workshop for this boundary condition setup, whereas other codes appear to produce stable behavior with meshed exit domains. It remains unclear why certain solvers suffer from stability issues with this particular boundary condition approach.

- **Data Assimilation** – Updating the predicted flowfield by assimilating data from experiments offers improvements in simulation fidelity, synchronization of computational and experimental datasets, and improved resolved scale dynamics for embedded DNS approaches. A statistical state estimation approach has been successfully applied to the non-reacting bluff-body case. Well-resolved non-reacting simulation results were used as the truth, and the data assimilation approach was applied to coarse-grid simulations. The coarse solution with data assimilation showed nearly exact, time-accurate agreement with the high-resolution results, whereas the free-running solution with no assimilation produced significant errors. Preliminary testing for reacting flows has been performed on a model partial differential equation with less complexity than the reacting Navier-Stokes equations, and beyond these preliminary assessments, the reacting bluff-body flow is the intended application.

- **Adaptive Mesh Refinement (AMR)** – An AMR framework with multiple grid levels offers the capacity to compute model terms at the coarse grid level and interpolate those values onto finer grid solutions for the closure of the Navier-Stokes equations. Since the entire model term is computed on the coarse grid, this approach differs from simply fixing the filter width in the model terms. This method was shown to improve grid convergence of kinetic energy statistics for a non-reacting unit physics case (Taylor-Green vortex) using fifth-order numerics. The capacity of this approach to handle the more complex and numerous closures in reacting flows is unknown.

- **Workshop Improvements** – In addition to requiring explicit filtering (see Explicit Filtering section), it was proposed that a unit physics case be introduced and that participants be required to demonstrate an accurate solution before moving on to more complicated cases, including the bluff-body and future rotational detonation engine (RDE) case. For the unit physics case, a temporal mixing layer DNS of approximately 100 million cells was proposed as a potential candidate. By choosing a DNS case, the difficulties of matching experimental boundary conditions and data would be eliminated. Furthermore, the unit physics case enables the use of the same grids across multiple codes to ensure consistency in code-to-code comparisons.

Future Rotating Detonation Rocket Engine Validation Case

The most significant observations and conclusions from the presentations on the rotating detonation engine test case are summarized in this section.

- **Experiment Update** – Experimental data from the AFRL RDRE test case was presented by three universities, highlighting the collection of metrics useful in current validation efforts. The measurements include capillary-tube attenuated pressure (CTAP) and high-speed imagery capturing the number and speed of waves inside the chamber. Additional instrumentation installed on some experiments includes high-speed pressure transducers, thermocouples, and thrust stands, with the collection of this information expected in the near future to further support the M&S. The test conditions cover a wide range of equivalence ratios and mass flow rates, from which three representative sets were chosen and supplied to modeling groups. Some discrepancies among the experiments are being investigated to determine their origin, with a focus on the fuel and air plenums.

- **Defining the Computational Domain –** While the inflow parameters are well defined, questions were raised regarding the appropriate extent of the simulation domain. As with the experimental results, the upstream boundary is the primary region of concern. Simulations thus far include only a small portion of the reactant plenums, but some results indicated that a strong plenum response may result from the passing waves which may couple back to the detonations. Consequently, these feed plenums will be examined and increased to more closely reflect the full experiment and mitigate the possibility that the inflow boundary is impacted by pressure waves.
- **Defining the Initial Condition –** While no standardized method of igniting the detonation was required, each participant was encouraged to use a single high-pressure, high-temperature kernel to start the reaction near the injector face. The sensitivity to method of ignition has been explored to some extent, but not in a rigorous way which might be used to establish best practices. In the coming months, fully defining this initialization will be a priority.

CONCLUSIONS FOR MVP 4 WORKSHOP

The most significant outcomes and conclusions from the Fourth Model Validation for Propulsion Workshop are summarized here.

- As an active experiment with reduced uncertainty compared to the Volvo test case, the AFRL case will be the focus of future MVP bluff-body efforts. The AFRL test case presents an opportunity to extend current validation efforts into a more direct comparison of unsteady dynamics via simultaneous high-speed datasets.

- The explicit filtering approach presented in MVP 2 was discussed, and support for enforcing an explicit filtering requirement for workshop participation involving the bluff-body test case was expressed. Some preliminary testing of the current explicit filtering implementation with different numerical schemes would help mitigate risks and garner support for this approach. Given the need for further testing and refined guidance, efforts on the bluff-body test case will not be featured in MVP 5 (2021) and will be continued in MVP 6 (2022).

- Enstrophy budgets provided comparisons of greater fidelity and physical insight than typical statistics. The use of a sparsity-promoting DMD technique was demonstrated and identified a dominant symmetrical mode in one set of results. These findings suggest that DMD is a viable method for quantitatively comparing flame dynamics and flow unsteadiness for the bluff body test case, offering advantages over instantaneous image comparisons.

- The rotating detonation rocket engine validation case will be the focus of MVP 5 (2021). Additional work is needed to understand the influence of the fuel and air plenums on the experimental and computational results, to define the computational domain, and to prescribe the boundary conditions. In order to define the initial conditions, the sensitivity of the computational results to the ignition process should be investigated.