ParCFD'2020
32^{nd} International Conference on Parallel Computational Fluid Dynamics
May-11-13 2020, Nice FRANCE

PARALLEL DATA-ASSIMILATION CFD MODELING OF TURBULENT COMBUSTION

Xinfeng GAO and Yijun WANG and Stephen M. GUZIK

CFD and Propulsion Laboratory
Colorado State University
Fort Collins, Colorado, USA
e-mail: Xinfeng.Gao@colostate.edu, Yijun.Wang@colostate.edu and
Stephen.Guzik@colostate.edu, web page: http://cfdlab.colostate.edu

Key words: Data-driven CFD, Data assimilation, Maximum likelihood ensemble filter, Data assimilation for turbulent combustion

Abstract. A parallel high-order adaptive finite-volume algorithm is enhanced by data assimilation to further improve our understanding of uncertainties in the predictions of turbulent combusting flows, and thus increase the predictability of fluid and flame dynamics. By assimilating data from high resolution simulations and physical experiments into the present CFD model, the maximum likelihood ensemble filter is employed to correct potential errors in the initial and boundary conditions, physical models, or parameters used in the governing equations. This study applies the parallel data-assimilation CFD algorithm to turbulent premixed flames in a 3D complex geometry and signifies the impact of data assimilation on improving the predicability of turbulent combustion.

1 INTRODUCTION

In CFD modeling of highly-turbulent combustion, the difficult question to answer is how the approximate solution of the Navier-Stokes equations augmented with chemical reactions is related to the *true* solution over *long intervals of time*? This is difficult because the problem in hand is unstable and chaotic. That is, for example, if the exact solution converges to an unstable stationary solution, it is most *unlikely* the numerical solution would converge to an approximation of this unstable stationary solution [4]. While the projection error from a continuous system to a finite dimensional system due to the numerical methods is directly responsible for this, many other sources also contribute to the solution inaccuracy, including the use of physical models in the mathematical equations governing the turbulent combustion process to approximate the unresolved (subgrid) scales, turbulence-combustion interactions, and chemical reactions, and the existence of uncertainties in the parameters of these closure models and in the flow conditions (e.g., initial and boundary conditions, operating conditions, etc). When extracting information from a simulation, interpreting potential physical features, or developing insights for models, one must exercise the caution — a simulation can only be as good as the CFD model used for the simulation, particularly, for highly turbulent combusting flows. Naturally, it is valuable to develop a methodology that helps estimate the uncertainties of the dynamical system, determine what would be a *valid time window* before the simulation deviates from the *true* trajectory, and correct the simulation if that happens.

In this study, we enhance the CFD modeling with data assimilation (DA) to obtain a more accurate simulation of the dynamical system by using available data. The maximum likelihood ensemble filter (MLEF) [5], an ensemble-based DA method, is used to estimate the uncertainties of the dynamical system of the turbulent flames and obtain optimal states whenever/wherever data is assimilated. This is demonstrated using a bluffbody stabilized turbulent methane flame, and the preliminary results signify the potential of DA in enhancing the predictability of CFD modeling of turbulent combustion.

2 PRELIMINARY RESULTS

The DA-enhanced CFD algorithm consists of two main components, a forward CFD model and a DA algorithm, along with a feedback/interface mechanism of the two. Chord [1, 2, 3], a fourth-order finite-volume code, is the forward model to advance the simulation while the data assimilation is achieved by the MLEF algorithm [5]. Figure 1 illustrates the DA-CFD solution process. Each member $(1, \cdots, N_e)$ in the ensemble along with a control case is first propagated by the forward CFD model to the time when data is available and the forecast error covariance, $\mathbf{P}_f$, is evaluated at that time. Then, an observation operator is employed to map the states $(\hat{\mathbf{Q}}^f)$ to the data space $(\mathbf{O})$ for the evaluation of the observation increment (the difference between "truth" and prediction). The MLEF DA algorithm takes these information to optimize a cost function derived from the Bayesian theorem for an optimal deterministic state $(\hat{\mathbf{Q}}^a)$ along with the statistics $(\mathbf{P}^{a,1/2})$. All members are then updated with the $\mathbf{P}^{a,1/2}$ and $\hat{\mathbf{Q}}^a$, which (re-)initialize the next step.

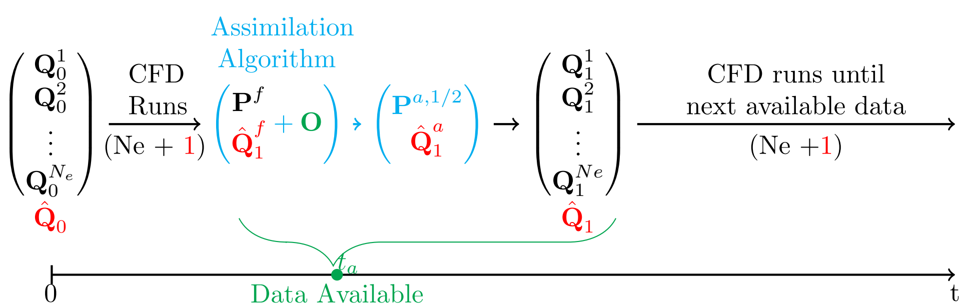


Figure 1: Three major steps in the data assimilation enhanced CFD algorithm.

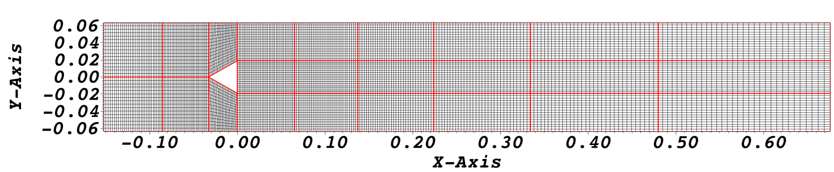
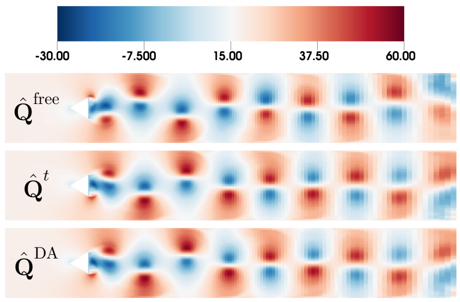
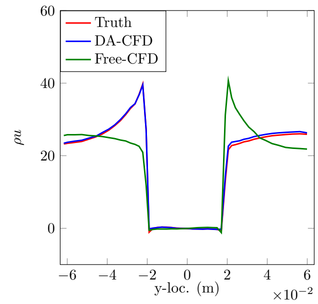


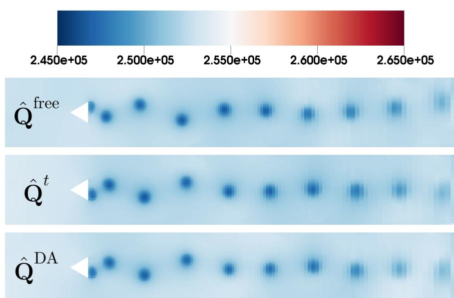
Figure 2: A center plane grid showing the equilateral triangle cross section of the bluff body.



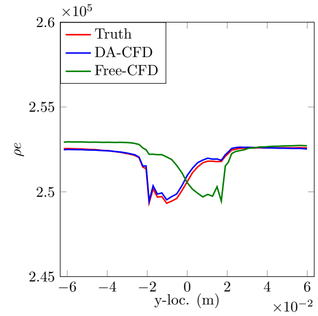
(a) ρu contour



(c) y-profile of ρu at x =0.0005m

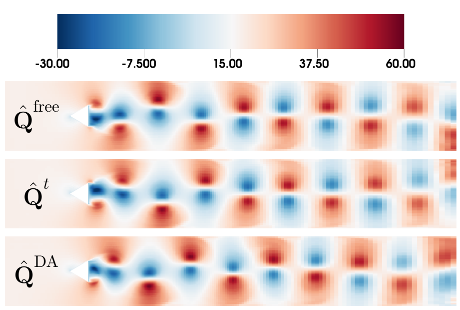


(b) ρe contour

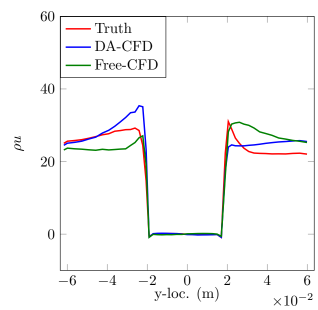


(d) y-profile of ρe at x =0.0005m

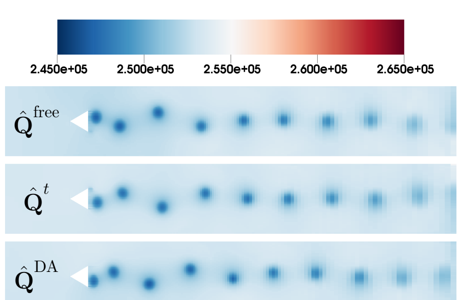
Figure 3: Comparison of the DA-CFD solution ($\hat{\mathbf{Q}}^{\mathrm{DA}}$) of the x-momentum and total energy from the center plane to the "truth"($\hat{\mathbf{Q}}^{t}$) and the free CFD simulation($\hat{\mathbf{Q}}^{\mathrm{free}}$) at the 5th DA cycle.



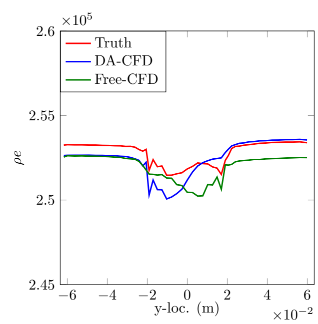
(a) ρu contour



(c) y-profile of ρu at x =0.0005m



(b) ρe contour



(d) y-profile of ρe at x =0.0005m

Figure 4: Comparison of the DA-CFD solution ($\hat{\mathbf{Q}}^{\mathrm{DA}}$) of the x-momentum and total energy from the center plane to the "truth" ($\hat{\mathbf{Q}}^{t}$) and the free CFD simulation ($\hat{\mathbf{Q}}^{\mathrm{free}}$) at the 8th DA cycle.

The parallel DA-CFD algorithm is first applied to the nonreacting flows occurring in the bluffbody configuration (see Fig. 2). At the inflow boundary, a cold methane-air mixture (ϕ=0.65) flows in at 14.9m/s with T=310K. The total pressure at the outflow boundary is 100 KPa. No-slip and adiabatic conditions are applied at solid wall surfaces. The ensemble is created using the lagged forecast method, including 19 members and 1 deterministic control case. Observation data of density and velocity field are synthesized from a reference CFD simulation for a region of $x \times y \in [0, 0.338\text{m}] \times [-0.635\text{m}, 0.635\text{m}]$ and a 1D y-profile at $x = 0.0005\text{m}$ in the region, respectively. The initial conditions (ICs) for the ensemble are artificially made different from that of the reference case, representing uncertainties in ICs, to demonstrate the DA impact on error correction. The assimilation frequency is 1/3 of the flow-through time. A "free" CFD simulation (without using DA) starting from the same ICs as the control case is run for comparison. Figures 3 and 4 demonstrate the assimilation solutions from using data from the 2D region and the 1D profile, respectively. Figure 3 shows the DA-CFD solution is properly corrected with 5 DA cycles, so are the vortex shedding frequency and phase. Figure 4 shows DA-CFD is pulled close to the truth with 8 DA cycles. Although discrepancies exist in the line plots, all (mass, momentum, vortex shedding frequency and phase) is being properly corrected after a dozen DA cycles. In both cases, the non-observed component (ρe) is also being positively impacted due to the coupling of the physics, which mathematically is realized in the DA algorithm via the error covariance matrix. A perfect correction is not expected, because errors (8-10%) are introduced to the synthesized observations to represent the experimental uncertainty. Consistently, we found that the more high-confidence data are assimilated, the more frequently they are assimilated, the faster the predictions are pulled towards the truth. With a thorough preliminary study, we are currently investigating the reacting flows. At the conference, we will present detailed findings of the DA impact on the predictability of turbulent combustion.

REFERENCES

[1] Gao, X., Owen, L. D., and Guzik, S. M. J. A parallel adaptive numerical method with generalized curvilinear coordinate transformation for compressible Navier-Stokes equations. *Int. J. Numer. Meth. Fluids 82* (2016), 664–688.

[2] Guzik, S. M., Gao, X., and Olschanowsky, C. A high-performance finite-volume algorithm for solving partial differential equations governing compressible viscous flows on structured grids. *Comput. Math Appl. 72* (2016), 2098–2118.

[3] Owen, L. D., Guzik, S. M., and Gao, X. A high-order adaptive algorithm for multispecies gaseous flows on mapped domains. *Comput. Fluids 170* (2018), 249–260.

[4] Titi, E. S. On approximate Inertial Manifolds to the Navier-Stokes equations. *Journal of Mathematical Analysis and Applications 149* (1990), 540–557.

[5] Zupanski, M. Maximum likelihood ensemble filter: Theoretical aspects. *Mon. Wea. Rev. 133* (2005), 1710–1726.