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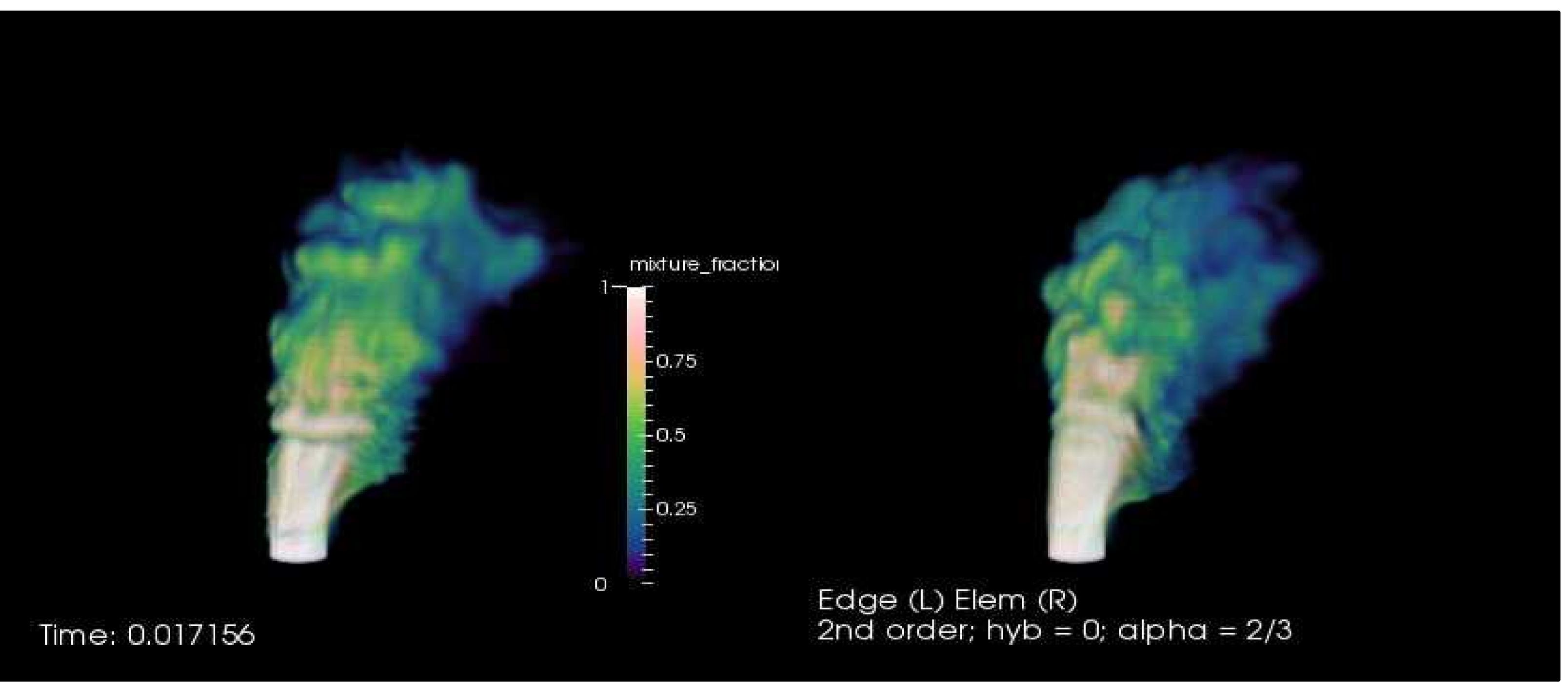

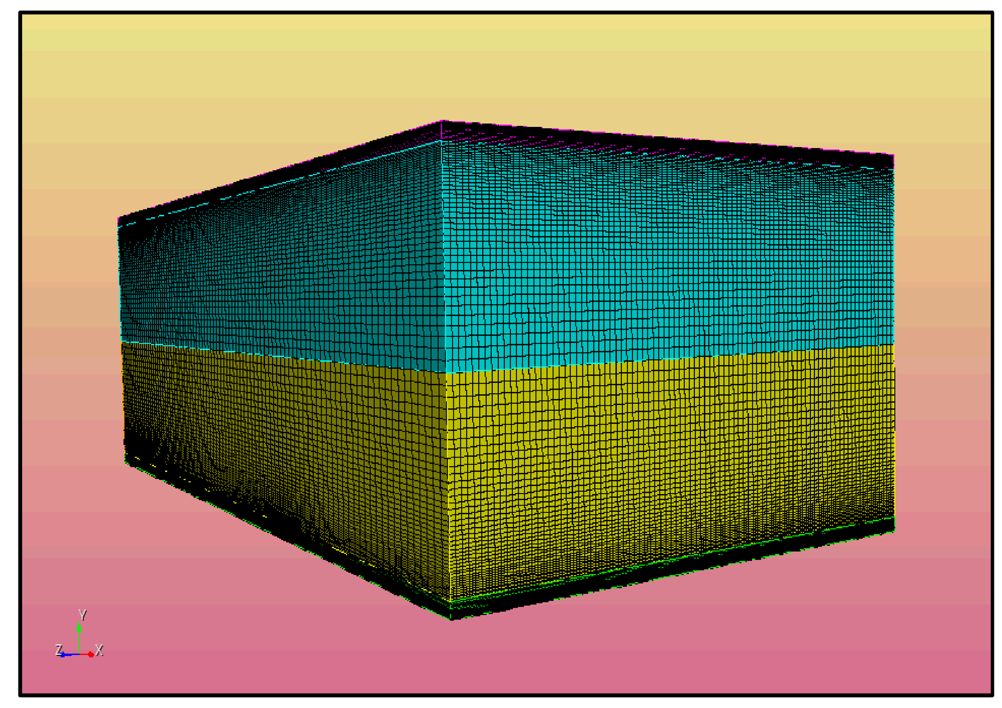

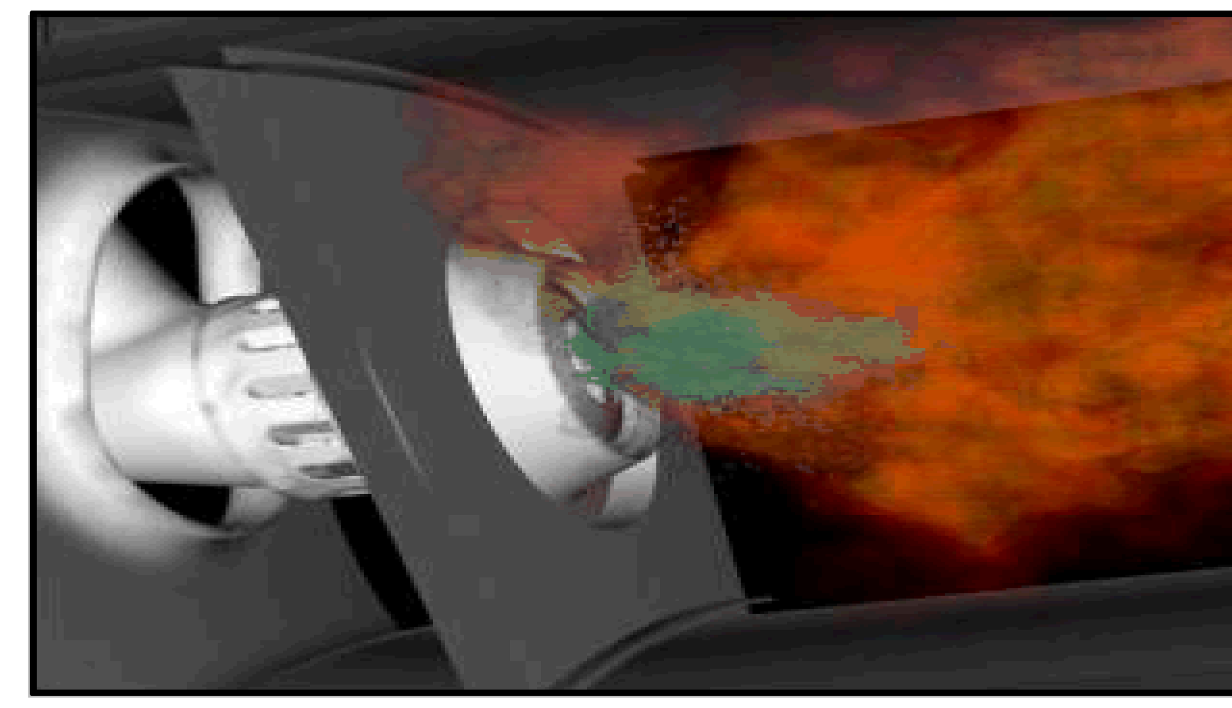

Performing Uncertainty Quantification on Large Eddy Simulations of Turbulent Flows

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Motivation

Optimizing combustion efficiency and reducing pollutants are key goals in combustion research today. By quantifying uncertainties in large eddy simulations (LES) of turbulent flows, LES can be better utilized to help accomplish such objectives.

Barriers Addressed:
A common hurdle that must be faced when performing any study that requires a large quantity of cases to be run computationally for multiple days/weeks is finding a method to mass submit, maintain, post-process, and troubleshoot the multitude of runs. Over the course of the summer, I have been in development of a solution to this problem that is robust, elegant, and can be easily utilized to assist with our current and future uncertainty quantification (UQ) work for LES of other turbulent flows.

Purpose:
The purpose of this poster is to present any initial findings from our current UQ work, give some insight into the development and current functionality of the toolkit created, and to discuss the tasks we aim to complete as the summer comes to conclusion.

Research Goals

LES is a numerical model that directly resolves the larger eddies and implicitly models the small scales. By quantifying the uncertainty in large eddy simulations (LES) of turbulent flows, we can understand how parametric and structural uncertainty in our turbulence model can impact the model's outputs. My goal for this summer was to assist my mentors in their efforts to quantify the uncertainty in LES of low-Mach-number, turbulent, wall-modeled channel flow and jet-in-crossflow.

The two **questions** that we hope to answer by the end of this summer are:

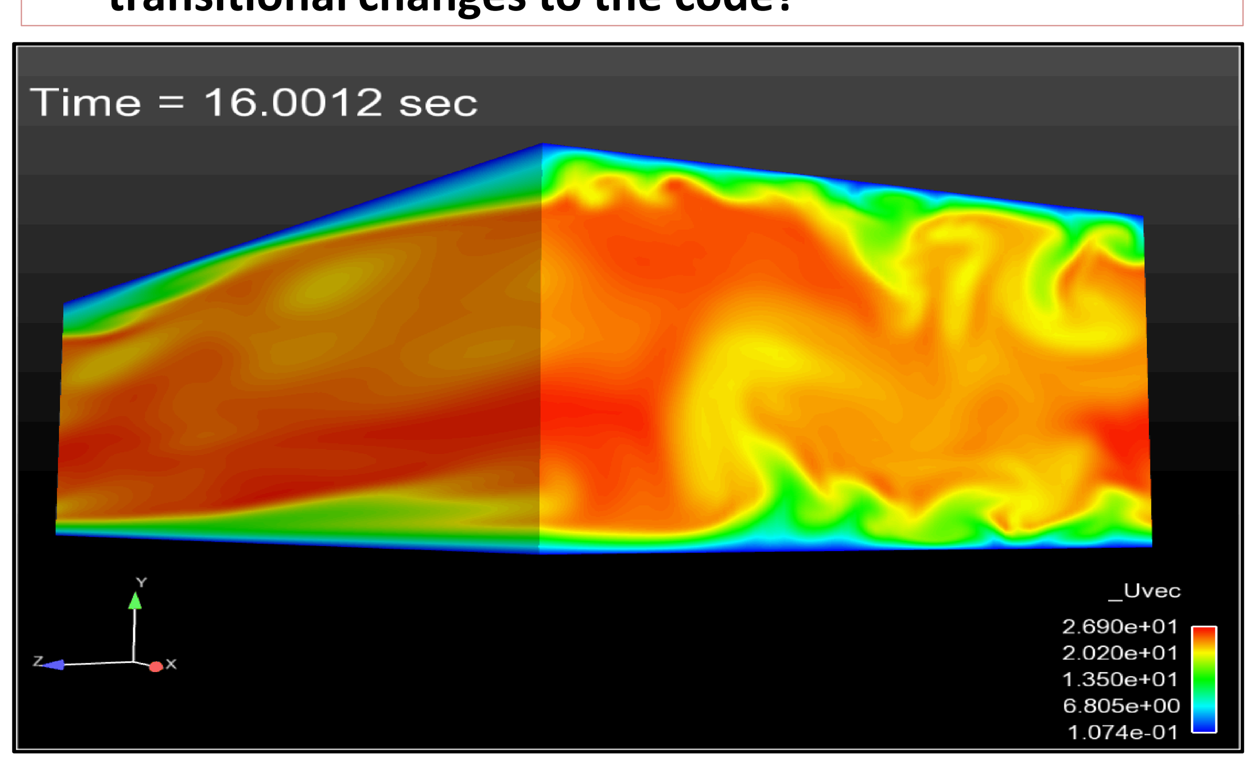
(1) Can the input parameters we chose allow us quantify the uncertainty in our model? And,

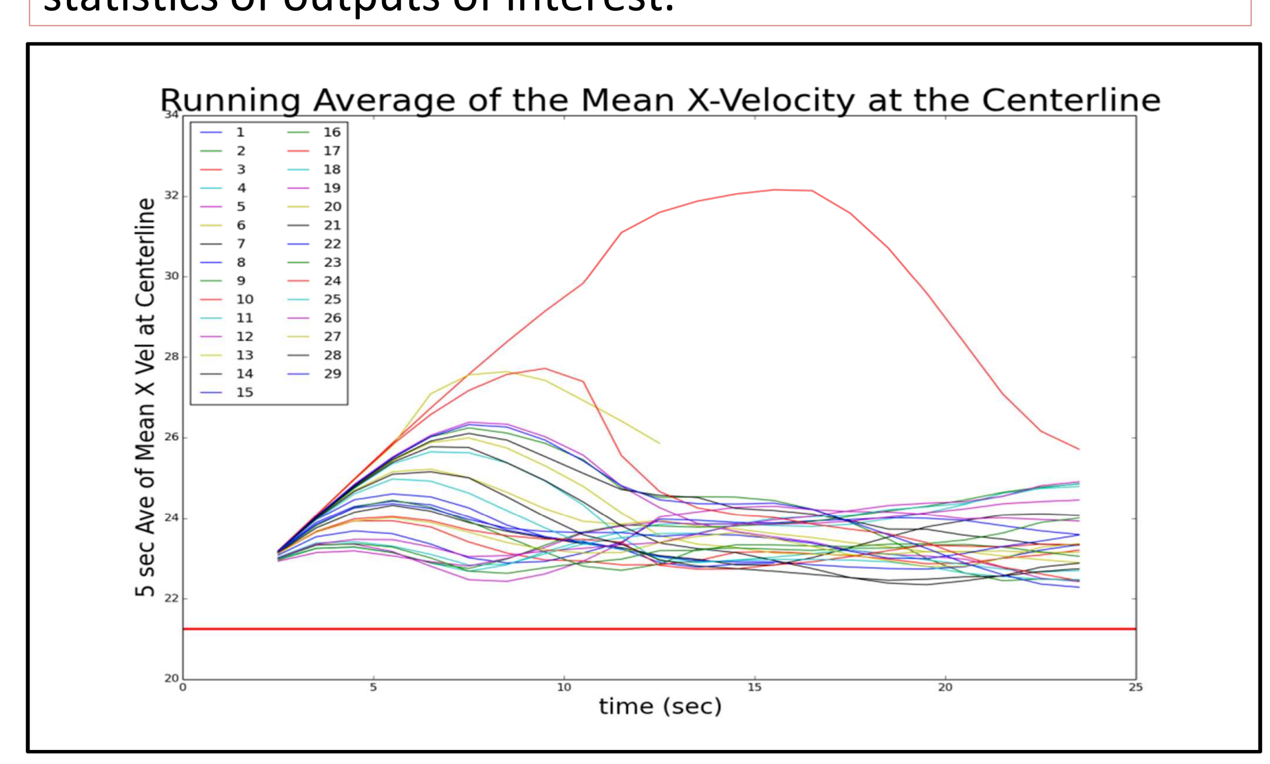
(2) Can we create an efficient toolkit that would allow us to mass submit and maintain these runs, while also being flexible enough to complete instructions specific to each UQ study with minute to no transitional changes to the code?

Method

Through a system of bash and python scripts, I have created an early version of the toolkit that is currently able to complete several crucial steps in deployment and maintenance of UQ sets. By creating some structure in the syntax of the data file, introducing a parameter file layout that allows for input parameters to be dependent on intermediary parameters, and implementing code that allows for compatibility with future UQ work, the toolkit can currently provide several beneficial functions.

We are testing this toolkit to perform UQ for LES of the wall-modeled channel flow. We will have ran 150 cases by the completion of the wall-model UQ study. Each case is being run by one of Sandia's high-performance computers for four days at a time. We are to able to run each case for a maximum of four days and can do multiple such runs to achieve statistical convergence. After the completion of each case in the set, we will analyze the data, computing statistics of outputs of interest.





Results

We have successfully run the first seventy-five case set of the wall-model run and are currently in the process of post-processing the data. Upon completion of the post-processing step, we will be able to answer **question (1)** for the wall-model case. Our next goal is to submit our second case set for the wall-model runs and start the UQ study for jet-in-crossflow.

The toolkit has been beneficial in submitting, maintaining, and post-processing the cases that have and are currently running. Some features of the toolkit include:

- Ability to easily declare input parameters and intermediate parameters.
- Ability to understand user written python code to calculate values for input parameters that are dependent on declared intermediate parameters.
- Creates an organized directory system that makes maintaining and submitting hundreds of runs simple.
- Makes submitting, restarting, status-checking, and post-processing cases straight-forward.
- Much more…

Conclusion & Discussion

Having successfully ran the first set of cases for the turbulent, wall-modeled channel flow, we will be able to assess the uncertainty in our model.

So far, we have completed the first version of the toolkit, testing its features with our first set of wall-model runs.

Here are some features we are currently implementing for the next version of the toolkit:

- Compatibility with various frameworks/solvers (currently supports Fuego and Nalu)
- Ability to handle multiple input decks.
- "Open-ended" design, allowing user to adjust code to fit environment (e.g. non-Sandia computers).
- Possible GUI to make status checking individual cases simpler.
- More robust post-processing and analysis steps.
- Detailed documentation.

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