Adjoint-Based Error Estimation and Mesh Adaptation for LES of Turbulent Premixed Flames

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1 Introduction and Motivation

Computational Fluid Dynamics (CFD) was developed to reduce the cost of fluid flow experiments whose lifecycle spanning from conception to testing involved numerous design iterations and modifications. The initial applications of CFD focused on aerodynamic and hydrodynamic flows within the engineering industry. At the present time, its role has grown to include a vast spectrum of modern day industries. This is due to the ever-increasing power of computers as predicted by Gordon Moore, namely, that computing power would double approximately every two years. [1]

Since the 1960's, the role of CFD in the aerospace industry has grown to involve more complex design configurations and modelling of physics. Quite naturally, this has been extended to aircraft powerplants: Engine performance software was used to design Compressor maps for the purpose of estimating power outputs; Specialty softwares such as *CHEMKIN, CANTERA* are used to calculate combustion rates and products for given reactants and conditions at the lab level; CFD is being applied to simulate the combustion of fuels in laminar and turbulent conditions.

Turbulent combustion is a very complex physics phenomenon. Up to the 90's, researchers were still working on accurate mathematical models that would be capable of predicting to some extent the interaction and behavior of non-laminar fluid flow regimes. Naturally, computers have been employed as tools to simulate these models and results are validated against experiments.

Because of the huge discrepancy in scales when it comes to turbulence, ranging from the Integral scales to the Kolmogorov scales, vast computational resources would be required to model the entire turbulent regime. This high-fidelity branch of CFD is known as Direct Numerical Simulation (DNS), and is only achievable on Supercomputers, such as was recently demonstrated by Kaneda and Ishihara. [2] DNS remains very expensive in terms of computational and time resources: in reality, complex simulations are impossible, some requiring solution time on the order of 10^8 years.

Large Eddy Simulation(LES) is a branch of CFD has been successfully applied to combustion simulation in the last two decades. It serves as a compromise to model Turbulent scales up to a given specific scale (which we call the filter size): any scale smaller than this is modelled.

Within a Gas Turbine combustion chamber, heat release and pressure are a coupled phenomenon, and any sporadic fluctuations in heat release or pressure will affect the other. This is the field of study for *Thermoacoustics*. Higher temperatures within the combustion chamber raise the pressure which in turn increase the temperature even further, leading to a cycle where heat feeds off pressure and vice versa. It often results in structural damage to components within the combustion chamber and the turbine blades, and these pose huge safety risks and result in very high maintenance costs.

Notice the several stages at which innacuracies can be introduced into the simulation: one is at the algorithm level due to both the meshing of the geometry and the discretization of the governing equations, and the other at the modelling level due to the selection of turbulence models and filter sizes.

2 Scope of Research

The present work intends to address a two-pronged technique to reduce the computational error arising from discretization and meshing. The technique will involve implementation of the adjoint-based error estimation method to be implemented for mesh refinement. Adjoints will be used for sensitivity analysis, namely, monitoring the computational cells to which the functional outputs of the CFD analysis are most sensitive.

The second part involves the use of high-order finite volume discretization of the governing equations: Favre-Averaged Navier Stokes (FANS). The higher the order of discretization, the higher the accuracy of the solution. This minimizes error and is often desired since for a coarser level of mesh refinement, a higher solution accuracy can be achieved, thus this can be viewed as reducing the computational cost.

As discussed in section 1, it is the intention to ensure that the modifications to the CFFC algorithm will be remain parallelizable, taking advantage of the multiprocessing resources that exist at SCINET. Parallelization is achieved by domain decomposition, such that processors can compute smaller sections of the mesh with the corresponding governing equations all the while communicating and linking to each other through the Message Parsing Interface (MPI). Parallelization is the modern-day approach to increase speed while allowing computationally complex simulations.

The present work will focus on implementing adjoint-based error estimation for mesh refinement and high-order finite volume discretization and attempt to address thermoacoustic phenomenon within turbulent premixed combustion

3 Proposed Adaptive Mesh Refinement Strategy

We will preview some of

3.1 The Finite Volume Method

3.2 The High-Order Centrally Essentially Non-Oscillatory (CENO) Scheme

3.3 Explicit Filtering and Commutation Errors

3.4 Block-Based Adaptive Mesh Refinement (AMR)

3.4.1 Isotropic AMR

3.4.2 Anisotropic AMR

4 Adjoint-Based Method for Error Estimation

4.1 Introduction

4.1.1 Steady Adjoints

4.1.2 Unsteady Adjoints

4.2 Derivation

4.3 Solution of Linear Systems

4.4 Use of Solution Error Estimates in Mesh Adaptation

4.5 Implementing Isotropic Mesh Refinement

5 Poisson Solver

5.1 Model Problem

6 LES of a Turbulent Premixed Methane Flame

6.1 Model Problem

7 Summary of Progress to Date and Future Work

7.1 Progress to Date

Task	Completion Date
Literature Review	September-October 2014
Trelis Meshing Software	November 2014
CFFC Group Code Flux Jacobian Analysis	December 2014
Trilinos Package solution for example Poisson Problem in serial and parallel configurations	December 2014
Running a current-state LES case of a Turbulent Premixed Methane Flame using PCM-FPI to get a threshold estimation of solution run time	January 2015

7.2 Future Work

Task	Completion Date
Implementing the approximate Adjoint Derivative to the Flux Jacobians testing on Euler Equations	April 2015
Extension to Mesh adaptation	May 2015
Application of Adjoint Problem to Navier Stokes	June 2015
Explicit Filters for High Order FVM implementation	October 2015
Conference Paper I draft	November 2015
Coupling of High Order method with Adjoint-based AMR	December 2015
CFD simulation of Cold Flow	January 2016
CFD simulation of Laminar Non-Premixed Flame	February 2016
CFD simulation of Laminar Diffusion Flame	February 2016
Journal Paper I	April 2016
Conference Paper II draft	April 2016
CFD simulation of Turbulent Non-Premixed Flame	May 2016
Journal Paper II	July 2016
Conference Paper I Presentation	July 2016
Conference Paper II draft	October 2016
Journal Paper III	October 2016
CFD simulation of Full Thermo-coupling	October 2016
Conference Paper III draft	November 2016
Thesis write-up	September 2017

References

[1] "Excerpts from A Conversation with Gordon Moore: Moore's Law," Video Transcript 0305/TSM/LAI/XX/PDF 306959-001US, Intel Corporation, September 2005.

[2] Kaneda, Y. and Ishihara, T., "High-Resolution Direct Numerical Simulation of Turbulence," *Journal of Turbulence*, Vol. 7, No. 20, 2006.