Development of h-p Adjoint-based error estimation for LES of reactive flows

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Meeting I
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April 6, 2015

Outline:

Introduction

Cost of experiment vs numerical simulation

- Computational Fluid Dynamics (CFD) developed to reduce the time and cost of prototypes in fluid flow experiments.
- Complexities may be expensive to set up in experimental modeling
- CFD methods and models have been developed to capture this phenomenon to varying extents of accuracy

Moore's law: Computing power $\approx$ doubles every 2 years

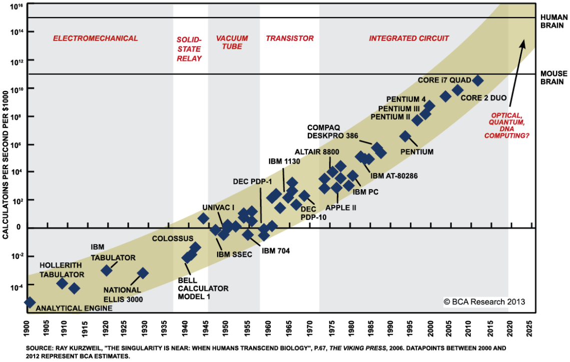


Figure 1: Moore's Law over the years [BCA Blog] [1]]

Turbulent combustion - experimental

Turbulent combustion: real fluid flows almost always involve turbulence. Large eddy simulation (LES) - technique to achieve higher accuracy than Reynolds' averaged Navier Stokes (RANS) at lower computational cost (time, resources) than direct numerical simulation (DNS).

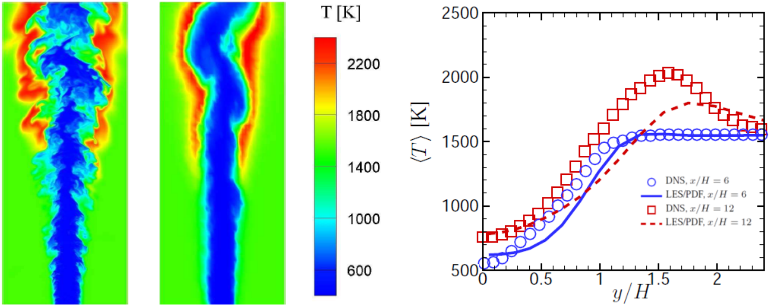
Lifted turbulent Ethylene (C_2H_4) jet flame issuing into a concentric co-flow of air. Zone between flame-base and nozzle may have partial premixing. Fuel and air temperature, pressure near standard [Köhler 2006] [2]

- Dimensions: Nozzle diameter = 2.0 mm; Co-flow air annulus diameter = 140 mm
- Exit Reynolds number: 10000
- Air mass flow: 320 g/min
- Mean fuel jet velocity: 44 m/s

[Köhler 2006] [3]

Turbulent combustion - simulation example

Considering that DNS resolves all the scales, LES models sub-filter scales (SFS) while resolving the larger scales, and that RANS models all the scales, then we can expect the most accurate to be DNS, then LES, then RANS. Computational results that Yang, Pope and Chen obtained are:



(a) temperature in x-y plane: DNS (l), LES/PDF (r)

(b) Mean temperature :DNS and LES

Figure 2: DNS and LES results for a turbulent Ethylene jet flame in hot co-flow, [Yang et al, 2013 [4]]

Turbulent combustion - simulation example cont'd

Their numerical setup:

- DNS
  - Grid points $= 1.3 \times 10^9$.
  - Computational cost $=\approx 14 \times 10^6$ CPU hours.
  - Computational domain $= 3D$ cuboid $L_x \times L_y \times L_z = 15H \times 20H \times 3H$ in the streamwise x-, transverse y-, and spanwise z-directions, where H = 2 mm is the jet width. Boundary conditions (BCs) are inflow/outflow in x and y, while periodic in z.
- LES
  - Grid points $\approx 8.3 \times 10^3$.
  - Computational cost = not specified - expected to be several orders of magnitude *lower*.
  - Computational domain $= 3D$ cuboid $L_x \times L_y \times L_z = 15H \times 30H \times 3H$. (larger y to move the transverse boundary away from the central turbulent jet, which can avoid the artifact of the Dirichlet boundary condition on entrainment near the jet.)

The results they obtained for mean temperature reveal good agreement between LES and DNS at x/H = 6, with lower-than-predicted values at x/H = 12. They anticipate mean temperature prediction to improve with finer mesh resolution in the LES grid.

Scope of research

- Reducing numerical error
- High Order ... CENO
- Explicit filtering
- Adjoint based error estimation
- Using h and p adapatation

Methodology

- Favre Averaged Governing Equations
- Large Eddy Simulation:
  - Explicit Filtering
  - Some LES errors: Aliasing, Commutation
  - Sub-filter scale (SFS) modeling
- High-order finite volume methods: CENO technique - benefits of higher accuracy on a coarse mesh
- AMR
  - Block-based AMR: speed and parallelization
  - Anisotropic vs Isotropic: how cell count (computational cost) can be reduced
  - Now the non-uniform vs the uniform block modification
  - Mesh geometry: CFFC can deal with cartesian or curvilinear coordinates - is this via using mapping functions for reference elements?

Existing framework

- The CFFC code already includes the following required features:
- Block-Based : people, year
- AMR:
- Deconick's research on explicit filters
- High Order FVM with CENO:
- Scott's work/input: Newton iterations and gmres solver
- Lucie's non-uniform approach - improves accuracy of flux evaluations and reduces computational cost for anisotropic
- PCM-FPI combustion modelling: modeled by F. Hernandez-Perez and N. Shahbazian
- Initial adjoint analysis done by Martin for the advection equations

Overview of error

Types of numerical error

- Truncation error
- Solution error Then explain a bit how they arise and how they can be dealt with

Adaptive mesh refinement (AMR)

- Benefits of AMR
- How the block-based technique works
- Ghost cells for intercommunication
- Current stencils
- how the high-order will affect the current stencil
- use radial sphere diags

High order finite volume method

An explanation on h.o FVM. how the high-order works, and how it reduces numerical error. separate slide of other groups researching this: Ihme and Poinssot. show some of their results

CENO

- Lucien's work
- Ramy's work
- Marc Charest's work
- Luiz's work

A background on gradient/physics-based refinement

Describe gradient based techniques

Adjoint-based error estimation

explaining what the adjoint is.
who was the first to use adjoint

- Cite initial work for this: Giles and Pierce, venditti and darmofal, fidkowski, jameson

continuous and discrete adjoint formulations

- continuous adjoint formulation
- discrete adjoint formulation: methods to evaluate the discrete adjoint
  - one
  - two
  - three

Adjoint-based error estimation cont'd

description of the adjoint methods to evaluate psi

- first
- second
- third

Techniques to evaluate dR/dU

- complex step
- finite differencing
- automated differentiation
- approximate method

Error estimation indicators

All about residual weighting (flag for refinement) and a 1D cartoon example, perhaps, of restriction/prolongation

- projecting onto fine space
- restricting onto coarse space
- getting the error in the residual and using this as a flag for refinement

Steady vs unsteady

Lastly: treatment of steady vs unsteady adjoints

Benefits of the adjoint approach

Expected benefits of adjoint vs gradient based methods

Mesh adaptation based on adjoint

This is a separate slide on mesh adaptation as based on the adjoint. Enough diagrams from venditti and darmofal, fidkowski

Basis of refinement: h and p

Show or put some figures with citations. Show what other groups have done. WHO has researched or is using **adjoint with AMR**?

- Fidkowski and Darmofal [2011] - Review of Output-Based Error Estimation and Mesh Adaptation in Computational Fluid Dynamics
- Hartmann, ERROR ESTIMATION AND ADJOINT-BASED ADAPTATION IN AERODYNAMICS, [2006]
- Nemec and Aftosmis [2007] - Adjoint Error Estimation and Adaptive Refinement for Embedded-Boundary Cartesian Meshes
- Hartmann, Held and Leicht [2010] - Adjoint-based error estimation and adaptive mesh refinement for the RANS and k- turbulence model equations
- Woopen, May and Schütz [2013] Adjoint-Based Error Estimation and Mesh Adaptation for Hybridized Discontinuous Galerkin Methods
- Li, Allaneau and Jameson [2011] - Continuous Adjoint Approach for Adaptive Mesh Refinement
- Diskin and Yamaleev [2011] Grid Adaptation Using Adjoint-Based Error Minimization

How we can use this

- using it for mesh refinement - how some previous groups used this
- how we can link mesh adaptation AMR to the adjoint via h
- how we can use p based refinement

Progress to date

- CFFC code familiarization : LES test case - on parallel clusters - SciNET. Job scheduling and post-processing results (tecplot)
- creating and solving linear systems in parallel implementation - trilinos and MPI
  - 2D Poisson problem
  - 3D Poisson problem
- Preliminary work with the discrete adjoint - shockcube problem
  - give the initial states, l and r
  - how the code was modified - multiblock and multiproc for uniform blocks
  - some results
  - work in progress
    - boundary conditions
    - compare with other techniques to get dR/dU

Timeline: April 2015 - January 2016

- Put a table of what you have done till now

Projected milestones

- Put a table of what you will do in the next steps

Thank You For Your Attention!

Questions?

References I

[1] BCA Research Blog,
http://blog.bcaresearch.com/wp-content/uploads/2013/10/Chart-III-8-Moores-Law-Over-199-Years-And-Going-Strong.png,
Accessed 29-03-2015

[2] Köhler, M., Boxx, I., Geigle, K. P., and Meier, W.,
Simultaneous planar measurements of soot structure and velocity fields in a turbulent lifted jet flame at 3-kHz",
Applied Physics B 103 (2), 271-279,
2011

[3] Adelaide international sooting flame (ISF) workshop,
http://www.adelaide.edu.au/cet/isfworkshop/data-sets/turbulent/,
Accessed 29-03-2015

[4] Yang, Y., Pope, S. B., Chen, J. H.,
"An LES/PDF study of a turbulent lifted ethylene jet flame in a heated coflow",
8th US National Combustion Meeting,
2013

Backup Slide

- Important backup slide point.