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

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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 ≈ doubles every 2 years

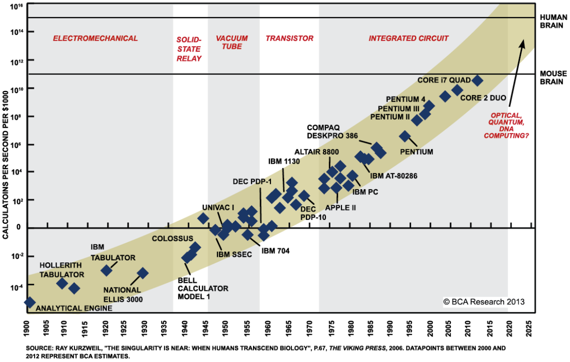


Figure 1: Moore's Law over the years [BCA Blog] [1]]

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).

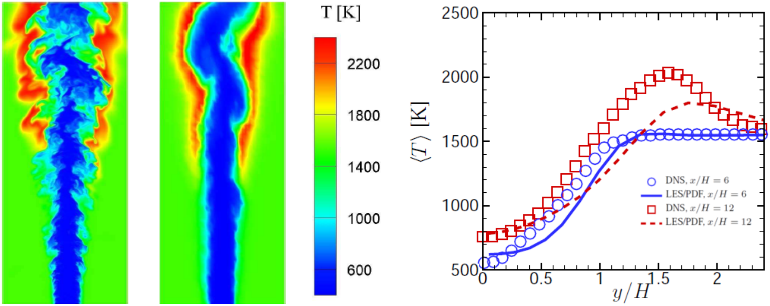
Lifted turbulent Ethylene (C_2H_4) jet flame issuing into a concentric co-flow of air. Zone between flame-base and nozzle may have partial premixing. Fuel and air temperature, pressure near standard [Köhler 2006] [2]

- 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
- Initial adjoint analysis done by Martin for the advection equations

Overview of error

Likely sources of error

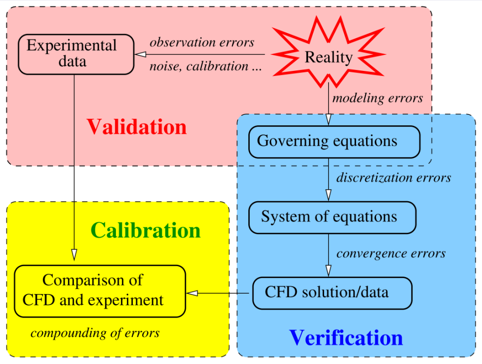


Figure 3: Some sources of error [Fidkowski 2012]

Types of error

We can broadly classify the two key sources of error in CFD as follows:

1. Numerical error:
   a. Solution error - that between the exact solution value and the CFD obtained value
   b. Truncation error - exists between the actual governing equations and the discretized PDEs for the numerical scheme
   c. Convergence error - arising due to nature of the iterative technique used
2. Modeling error:
   a. Pertaining to LES:
      - Sub-filter scale turbulence model: inappropriate model selected
      - Combustion and chemistry model
      - Filtering:
        aliasing errors - decomposed nonlinear terms in FANS = feedback of frequencies beyond filter bandwidth, = 'fake' stresses
        commutation errors - exist between filtering and differential operations
   b. Errors in geometry definition
   c. Errors in types of mesh cells - selection of the mesh refinement, types of cells, configuration to bulk flow direction

Adaptive mesh refinement (AMR)

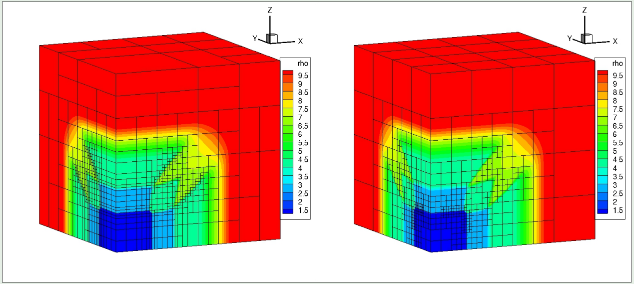
Key characteristics

AMR: [Berger et al 1984, 1986, 1989] [Aftomis et al 1998, 2000, 2004]

- localized refinement, large variation of scales, easily automatable

Block-based AMR: [Groth and co-workers 1999, 2005, 2006, 2010, 2011, 2012]

- Parallelizable, low memory and storage requirements



(a) With Anisotropic AMR. 5522 (8x8x8) blocks [Freret 2015]

(b) With isotropic AMR. 7036 (8x8x8) blocks [Freret 2015]

- Benefits of AMR: overall large computational cell count savings
- Isotropic vs anisotropic: up to 85% savings in cell count in 3D [Williamschen 2013]
- How the block-based technique works
- Ghost cells for intercommunication

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

Central essentially non-oscillatory (CENO) scheme

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

Large Eddy Simulation

Give an overview
Explicit filtering. [Deconinck, 2008]

- one point about explicit vs implicit filtering
- another point about the filtering

Foundation for error estimation

Basis for selective mesh refinement - we would like to refine the mesh where the cells have a very critical effect on the solution, while coarsening the less critical areas to save on computational cost.
Basically, there are two types of error estimation procedures available:

- a priori error estimators: these predict the long-term behavior of the errors in the discretization. They are not actually designed to approximate the error estimate for a given mesh.
- a posteriori error estimators: these use the simulation results to derive estimates of solution errors. Furthermore, these results are used to guide adaptive schemes:
  - where either the mesh is locally refined (h-version)
  - where the polynomial degree is raised (p-method)

Two main a posteriori approaches are the:

- gradient-based : [Bibb et al, 2006] [Giles and Pierce, 2000]
- adjoint-based : [Giles and Pierce, 2000][Venditti and Darmofal - 2000,2002][Fidkowski and Darmofal, 2011]

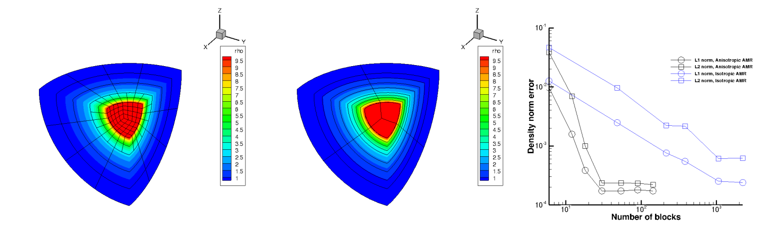
A background on gradient/physics-based refinement

In these simulations, the mesh or discretization order is changed based on the rates of change of (physical) solution variables.
Where the change occurs most rapidly over a few mesh cells, then over this location the mesh resolution can be increased (higher mesh refinement), or the scheme order can be increased, effectively using a higher order discretization over these cells.

- The reasoning behind this is to have enough cells to capture the changes as *smoothly* as possible.
- Once refinement is completed, the solution is re-run and the gradients re-evaluated. Changes made as necessary. Error can be compared to a higher discretization (h or p) solution.
- This is the present utility in the anisotropic and isotropic AMR functionality of the CFFC code used by the CFD and Propulsion group.
- main disadvantages of the gradient based approach [Giles and Pierce, 2000]:
  - for each separate state variable, a separate simulation must be run to evaluate the desired mesh resolution - increases computational time
  - gradient-based approach can only deal with continuous functionals as opposed to discrete optimization functionals
  - inability to deal with functions that have multiple minima. In this latter case, the gradient-based technique will generally converge to the nearest local minima, whose value may not represent overall system minimum.

Example of gradient-based mesh refinement

Physics as criteria for mesh coarsening/refinement - sphere with a bow shock example



(c) With isotropic AMR (d) With anisotropic AMR (e) Error in the density norm

[Freret, 2015] and [Williamschen, 2013]

- The graph reveals the asymptotic behavior of the convergence, yet for increased number of cells, there should be continual reduction in the density error norm

About the adjoint

To make error estimation more relevant to engineering applications: assess the error made in predicting an integral quantity which represents an engineering output. This output is the functional. For example,the output can be the average pressure on a wall.
The adjoint technique is a sensitivity analysis, that measures the rates of change of a design functional to a given change in the input. (It is a function of the residual, but the residual is in turn a function of the input/state).
The adjoint has two main formulations [Venditti and Darmofal, 2000]:

- continuous:
  - An objective function is formed to enforce the flow conditions (i.e. primal nonlinear PDEs).
  - Consider linear perturbations to the primal flow variables: the objective function should remain constant w.r.t the perturbations.
  - Hence obtain analytical adjoint equations. Obtain appropriate boundary conditions, and discretized directly. Primary benefit - offers insight into the nature of the adjoint solution.
- discrete
  - begin with the nonlinear discrete residual equations from the primal problem
  - apply linear perturbations to these.
  - If adjoint consistent (discrete adjoint = continuous adjoint), no need for B.C. specification -automatically incorporated via the primal residual.
  - thus obtain a linear system of equations - only need linear sensitivities of the functional and the Jacobian matrix associated with the primal residual.

Discrete adjoint

For these initial stages, beginning with the discrete formulation of the adjoint

Discrete Adjoint

$$\left(\frac{\partial R}{\partial U}\right)^T \Psi = -\left(\frac{\partial J}{\partial U}\right)^T$$

yielding a linear system of equations:

$$Ax = b$$

Where:

- J = the functional
- R = the residual
- ψ = the adjoint vector

Methods to evaluate the matrix $\frac{\partial R}{\partial U}$ for the discrete adjoint:

- Finite differencing [citations]
- Forward linearization with automated differentiation [citations]
- Adjoint method [citations]
- Complex step [citations]

Usage of the adjoint as a basis of refinement: h and p

Some of the groups using **adjoint with AMR**

- Becker and Rannacher [2001] - An Optimal Control Approach to a Posteriori Error Estimation in Finite Element Methods
- Fidkowski and Darmofal [2011] - Review of Output-Based Error Estimation and Mesh Adaptation in Computational Fluid Dynamics
- Hartmann [2006] - Error Estimation and Adjoint-based Adaptation in Aerodynamics
- Nemec and Aftosmis [2007] - Adjoint Error Estimation and Adaptive Refinement for Embedded-Boundary Cartesian Meshes
- Nemec, Aftosmis, and Wintzer [2008] - Adjoint-Based Adaptive Mesh Refinement for Complex Geometries
- 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

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 adjoints: Expected benefits of adjoint vs gradient based methods

Mesh adaptation based on adjoint

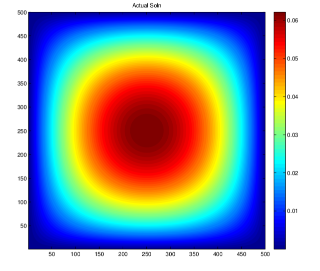
This is a separate slide on mesh adaptation as based on the adjoint. Enough diagrams from venditti and darmofal, fidkowski

How we can use this

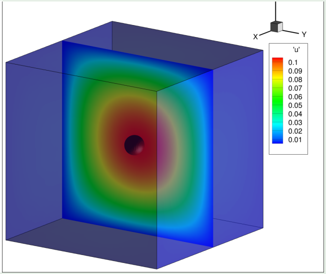
- using it for mesh refinement - how some previous groups used this
- how we can link mesh adaptation AMR to the adjoint via h
- how we can use p based refinement

Poisson problem

Creating and solving linear systems in parallel implementation - trilinos and MPI



(f) 2D case on $N^2 = 200^2$



(g) 3D case on $N^3 = 100^3$

Figure 4: Solution contours for Poisson problem

In 2D:$D = [0,1]^2$, $f(x,y) = 2(x(1-x) + y(1-y))$ is the source term and $u(x,y)$ is the solution to be computed.

Using a 2^{nd} order centered finite difference scheme= $-\dfrac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4 * u_{ij}}{h^2} = f_{ij}$

In 3D:$D = [0,1]^3$, $f(x,y,z) = 3(x(1-x) + y(1-y) + z(1-z))$ is the source term and $u(x,y,z)$ is the solution to be computed.

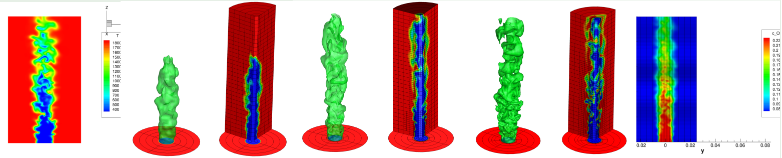
Using a 2^{nd} order centered finite difference scheme:

$$-\frac{u_{i+1,j,k-1} + u_{i-1,j,k-1} + u_{i,j+1,k-1} + u_{i,j-1,k-1} + u_{i+1,j,k+1} + u_{i-1,j,k+1} + u_{i,j+1,k+1} + u_{i,j-1,k+1} - 6u_{ijk}}{h^2} = f_{ijk}$$

Running already existing LES case on SciNET

CFFC code familiarization : LES test case
- on parallel clusters - SciNET. Job scheduling and post-processing results (tecplot)

Turbulent premixed CH_4 flame, $\phi = 0.7$.



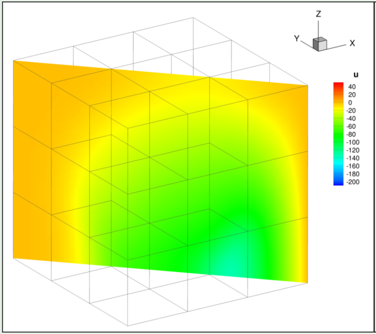
(a) Flame temp (b) FSD at 2.0 ms (c) FSD at 4.25 ms (d) FSD at 7.0 ms (e) time ave c_{O_2}

Computational costs:

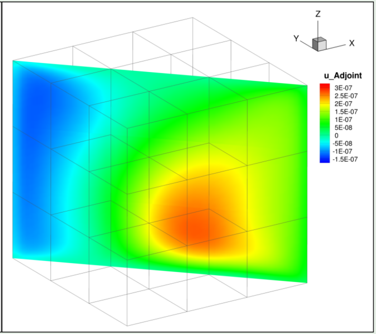
- (a) and (e): 800 procs, 3200 (8x8x8) blocks, 1.64 x10^6 cells, no refinement, 125x10^3 CPU hrs
- (b) 800 (8x8x8) blocks, 410,000 cells, no refinement
- (c) 5595 (8x8x8) blocks, 2.8 million cells, 3 levels of mesh refinement
- (d) 18531 (8x8x8) blocks, 9.5 million cells, 3 levels of mesh refinement

Work on the adjoint

Preliminary work with the discrete adjoint - shockcube problem



(f) $\rho.u$



(g) $\Psi_{rho.u}$

- give the initial states, l and r: Initial conditions: $\frac{\rho_L}{\rho_R} \approx 6$. Adjoint evaluated at t $= 0.035$ sec.
- how the code was modified - multiblock and multiproc for uniform blocks
- Selected as functional the average pressure in the shockcube.

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

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