

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

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Meeting I

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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

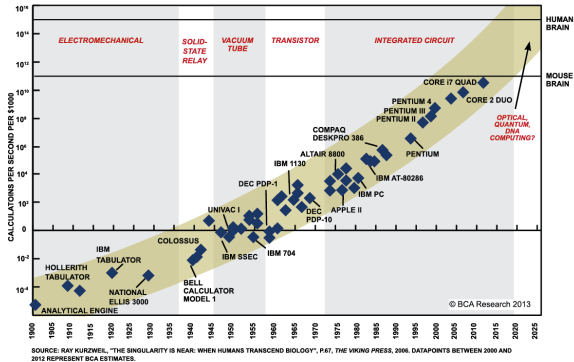


Figure: Moore's Law over the years [BCA Blog] [1]]



Turbulent combustion - experimental

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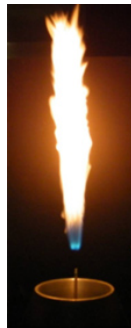
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Turbulent combustion: real fluid flows almost always involve turbulence. Large eddy simulation (LES) - technique to achieve higher accuracy than Reynolds' averaged Navier Stokes (RANS) at lower computational cost (time, resources) than direct numerical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

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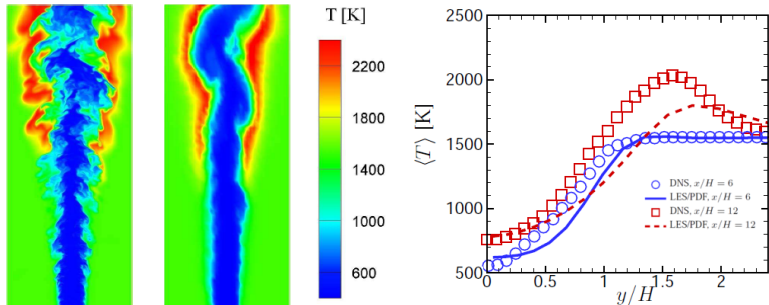
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Considering that DNS resolves all the scales, LES models sub-filter scales (SFS) while resolving the larger scales, and that RANS models all the scales, then we can expect the most accurate to be DNS, then LES, then RANS. Computational results that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



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

(b) Mean temperature :DNS and LES

Figure: 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

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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.



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



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- 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

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- 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

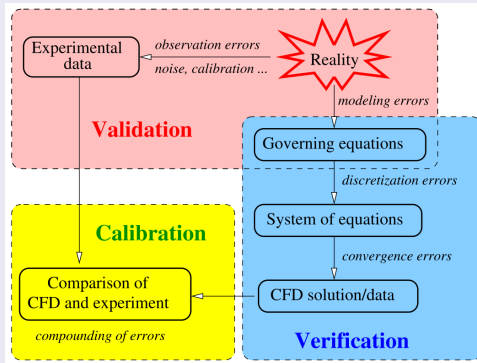


Figure: Some sources of error [Fidkowski 2012]

Modelling error chiefly arises from

- LES: Aliasing error, commutation error

- Mesh: selection of the mesh refinement, types of cells, configuration to bulk flow direction

Discretization error chiefly arises from

- Truncation error - how high order reduces this
- Solution error



Adaptive mesh refinement (AMR)

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- 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

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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

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



Large Eddy Simulation

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Give an overview

Explicit filtering. [Deconinck, 2008]

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



Foundation for error estimation

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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

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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.



About the adjoint

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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. (Well, actually, 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

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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 $\frac{\partial J}{\partial R}$ 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

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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

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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

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



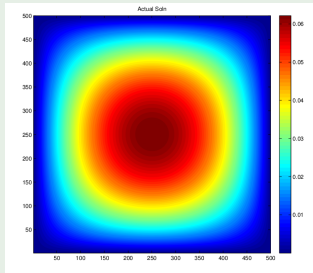
How we can use this

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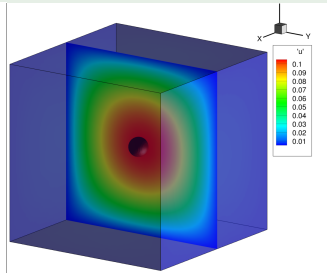
- using it for mesh refinement - how some previous groups used this
- how we can link mesh adaptation AMR to the adjoint via h
- how we can use p based refinement

Poisson problem

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



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



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

Figure: 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.

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

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:

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



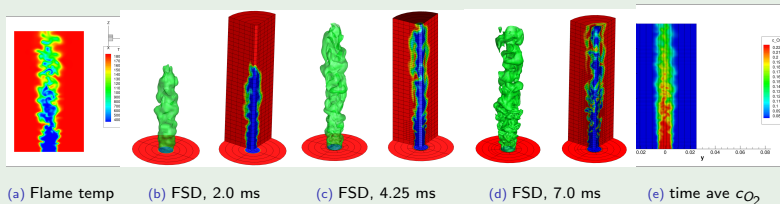
Running already existing LES case on SciNET

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CFFC code familiarization : LES test case

- on parallel clusters - SciNET. Job scheduling and post-processing results (tecplot)

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



Computational costs:

- (a) and (e): 800 procs, 3200 (8x8x8) blocks, 1.64×10^6 cells, no refinement, 125×10^3 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

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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

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- Put a table of what you have done till now



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



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Computations were performed on the GPC supercomputer at the SciNet HPC Consortium. SciNet is funded by: the Canada Foundation for Innovation under the auspices of Compute Canada; the Government of Ontario; Ontario Research Fund - Research Excellence; and the University of Toronto.

Thank You For Your Attention!

Questions?



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Backup Slide

- Important backup slide point.