

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

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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

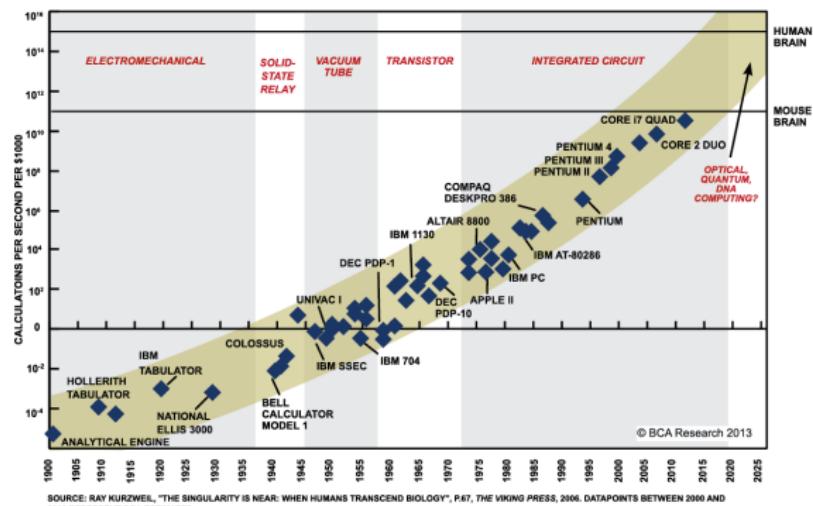


Figure: Moore's Law over the years [BCA Blog] [1]]



Turbulent combustion - experimental

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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]



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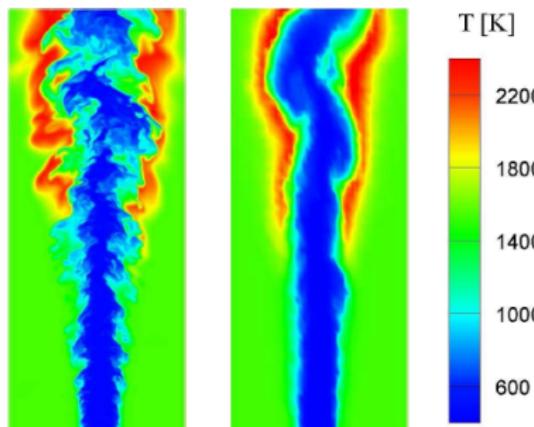
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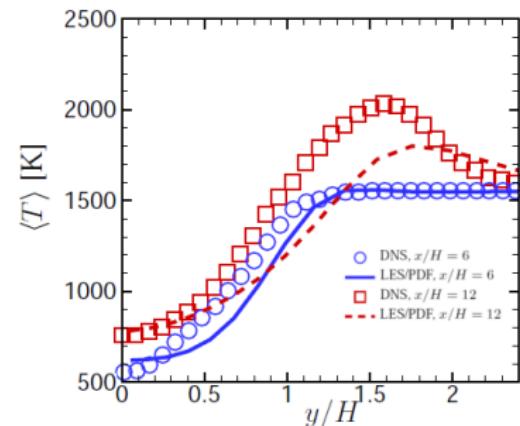
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Considering that DNS resolves all the scales, LES models sub-filter scales (SFS) while resolving the larger scales, and that RANS models all the scales, then we can expect the most accurate to be DNS, then LES, then RANS. Computational results that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



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Their numerical setup:

- DNS

- Grid points = 1.3×10^9 .
- 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.



Adaptive mesh refinement (AMR)

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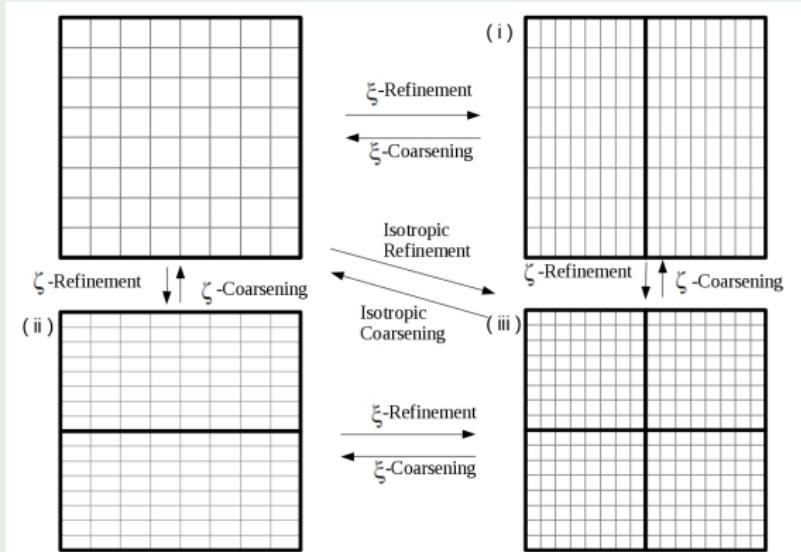
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Key characteristics

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

- localized refinement, large variation of scales, easily automatable



(a) Cell refinement strategies on a reference uniform mesh[Zhang 2011]

- Benefits of AMR: overall large computational cell count savings



Common AMR strategies

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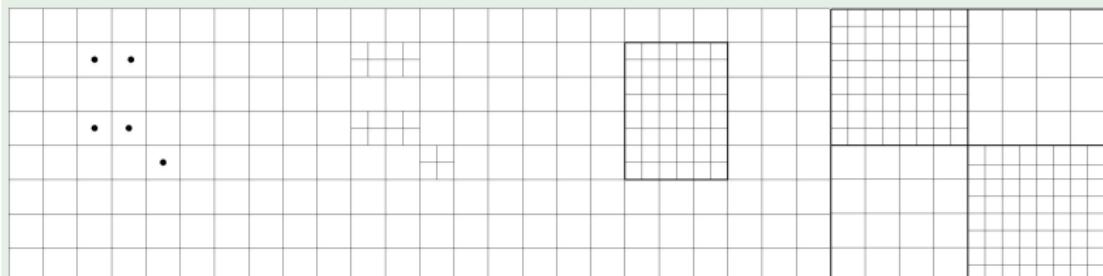
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Key characteristics

[Northrup 2013]



(b) flagged cells

(c) Cell-based refinement

(d) Patch-based refinement (e) Block-based refinement

- Cell based: [Powell et al, 1993] [Berger and Leveque, 1989] [Aftosmis et al, 1998]
Cells refined individually, hierarchy stored in a (very dense) tree
- Patch based: [Berger and Collela, 1989]
Cells are organized into collections of rectangular patches
- Block based: [Groth and co-workers, 1999] [Berger, 1994]
Entire blocks get refined, much lighter tree structure, efficient domain decomposition



Block based AMR

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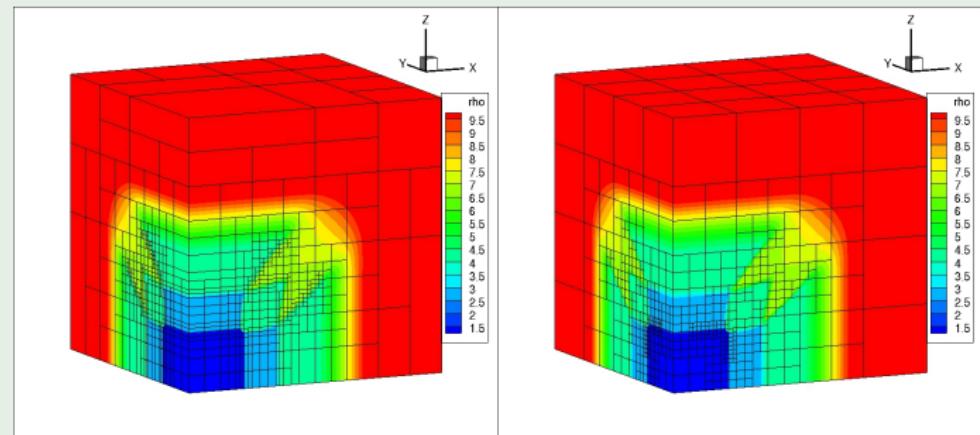
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Block-based AMR: [Groth and co-workers 1999, 2005, 2006, 2010, 2011, 2012]

Entire block gets refined, along with all its cells. This approach is much cheaper than individual cell refinement, having a lighter tree structure.



(f) With Anisotropic AMR. 5522 (8x8x8) blocks (g) With isotropic AMR. 7036 (8x8x8) blocks
[Freret 2015] [Freret 2015]

- For the above shockcube cases, cell ratio of isotropic : anisotropic ≈ 0.78 thus reflecting approximately 22% reduction in number of cells
- Williamschen [2013] have previously obtained savings of up to 85% reduction in cell count in 3D [Williamschen 2013]



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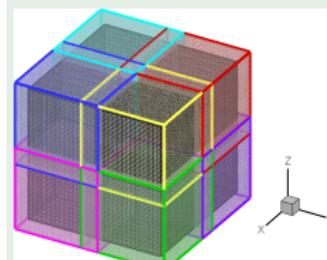
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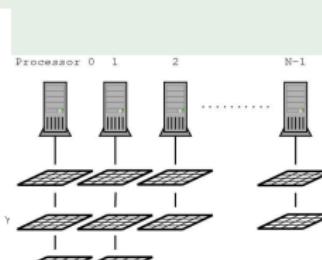
Key characteristics

[Groth and co-workers 1999, 2005, 2006, 2010, 2011, 2012, 2013]:

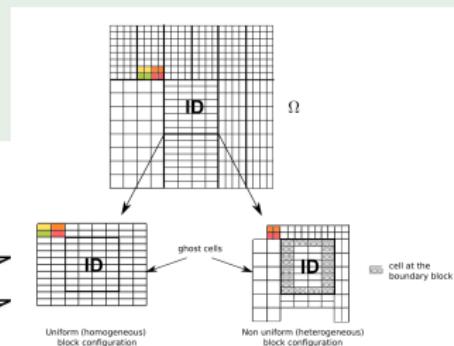
- How the block-based technique works; ghost cells for intercommunication
- Parallelizable, low memory and storage requirements
- New non-uniform approach [Freret 2015]



(h) Ghost cells on 8 blocks
[Rashad 2009]



(i) Parallelization [Northrup 2013]



(j) Non-uniform approach [Freret 2015]



High order finite volume method

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Error reduction via p

High order methods generally $> 2^{nd}$ order accuracy.

Integral Form of the Governing Equations

$$\frac{d\bar{\mathbf{U}}}{dt} = -\frac{1}{V} \iint_A (\vec{\mathcal{F}}^I - \vec{\mathcal{F}}^V) \cdot \hat{n} dA + \bar{\mathbf{S}}$$

Using a two-dimensional Gauss quadrature integration rule:

$$\frac{d\bar{\mathbf{U}}_{ijk}}{dt} = \frac{1}{V_{ijk}} \sum_{l=1}^{N_f} \sum_{m=1}^{N_{GF}} \left(\omega \left(\vec{\mathcal{F}}^I - \vec{\mathcal{F}}^V \right) \cdot \hat{n} A \right)_{ijk,l,m} + \sum_{n=1}^{N_{GV}} (\omega_n \mathbf{S})_{i,j,k,n} = \bar{\mathbf{R}}_{ijk} (\bar{\mathbf{U}})$$

The discretized scheme is then expressed in matrix-vector form. [Northrup 2013] GMRES. The higher the order p of the scheme, the more the quadrature points (N_G) which have their own corresponding weights ω .

- Gauss-Legendre quadrature rules are defined on reference cartesian cubic elements, and mapped onto 3D hexahedral elements via mapping functions
- High-order schemes reduces numerical error by increasing the accuracy of approximation between the actual governing equations (PDE form) and the discretized value.
- Other groups researching this: Ihme (Stanford) and Poinsot (CERFACS)



Central essentially non-oscillatory (CENO) scheme implementation

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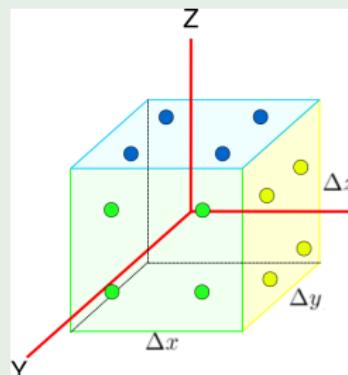
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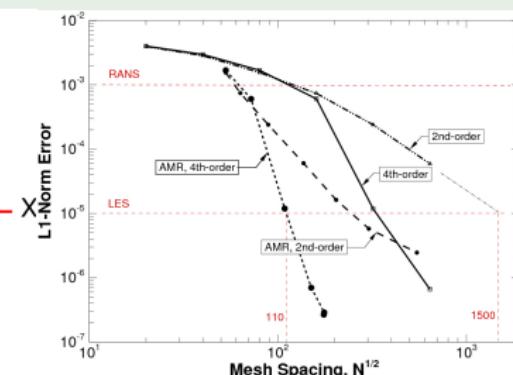
Error reduction via p

[Ivan and Groth 2011, 2012]

- CENO eliminates oscillations that are typical of discontinuities
- Reconstruction: FVM technique is cell centered. We may at times need state values on faces (flux evaluations) or at quadrature points (high-order)
- CENO uses fixed stencil for reconstruction
- smoothness indicators are used to select if a high order (p) reconstruction is to be carried out, or just a piecewise linear reconstruction



(k) Example of quadrature points on the cell faces



(l) L1 error norm in the solution for an unsteady advection equation having a quantity distribution gaussian profile. N = total mesh count



Large Eddy Simulation (LES)

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[Piomelli 1999][Ghosal and Moin 1999]

1. The accuracy of LES lies between the very accurate DNS and RANS.
2. DNS is mostly impractical and very expensive
3. RANS has fully modelled turbulence. Only the largest scales are resolved
4. LES utilizes a spatial filtering of a given width, $\bar{\Delta}$. Any scales below this will be modelled → sub-filter scales (SFS) [Smagorinsky 1963][Germano 1991][Piomelli 1991][Ghosal and Moin 1999][Lilly 1992]
5. while scales larger than $\bar{\Delta}$ will be fully resolved.
6. Hence in LES an appropriate balance is sought for accuracy, since too much reliance on modeling can be a source of error. Broadly categorized into:

(a) *Implicit filtering* [Aspden et al 2008]

- The filter width is not explicitly defined
- Inherently related to grid resolution
- Main disadvantage - difficult to compare results of adapted/refined meshes
- Difficult to control aliasing and commutation errors

(b) *Explicit filtering* [Vasilyev et al, 1998] [Deconinck, 2008]

- Define $\bar{\Delta}$ to be fixed for the entire mesh: top-hat, Gaussian, etc.
- Results easily comparable since $\bar{\Delta}$ does not change for different meshes
- Order of truncation errors (discretized scheme) can be controlled to be the same order of the commutation errors
- Allows control of aliasing errors



Overview of error

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Likely sources of error

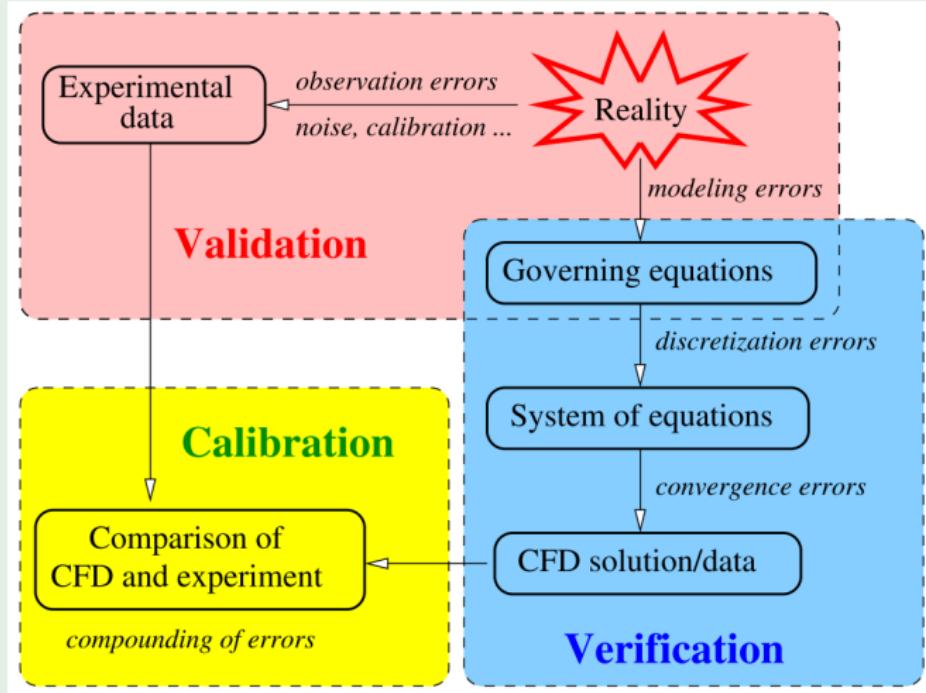


Figure: Some sources of error [Fidkowski 2012]



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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



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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:

1. **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.
2. **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:

- (a) gradient-based : [Bibb et al, 2006] [Giles and Pierce, 2000]
- (b) 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.

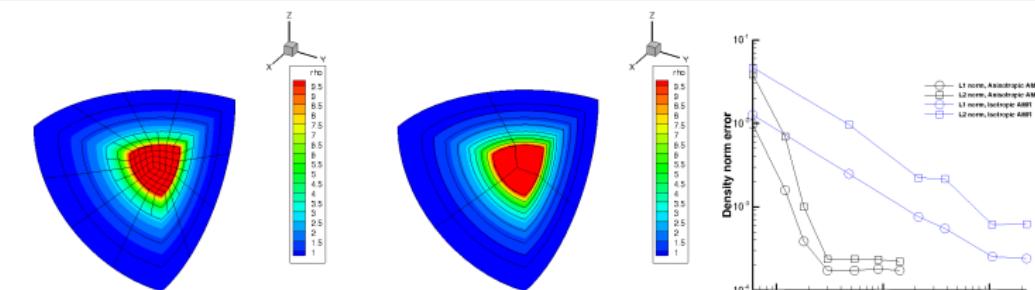
- (a) The reasoning behind this is to have enough cells to capture the changes as *smoothly* as possible.
- (b) Once refinement is completed, the solution is re-run and the gradients re-evaluated. Changes made as necessary. Error can be compared to a higher discretization (h or p) solution.
- (c) This is the present utility in the anisotropic and isotropic AMR functionality of the CFFC code used by the CFD and Propulsion group.
- (d) 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

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



(a) With isotropic AMR

(b) With anisotropic AMR

(c) 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

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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. (It is a function of the residual, but the residual is in turn a function of both the input and the state).

The adjoint has two main formulations [Giles and Pierce: 1997, 2001][Jameson, 2001][Venditti and Darmofal, 2000, 2002] [Becker and Rannacher: 2001, 2003]:

(a) 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.

(b) 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.



Scope and methodology within framework

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1. Reducing numerical error: using high order CENO and adjoint based error estimation : $\mathcal{O}(h^p) \rightarrow h$ and p adaptation
2. Combustion modeling:
 - PCM-FPI: allowing detailed chemical kinetics via tabulation of precomputed laminar premixed flames [H. Perez 2011]
3. Favre averaged Navier Stokes governing equations
4. Large Eddy Simulation:
 - Explicit Filtering [Deconinck 2008]
 - Sub-filter scale (SFS) modeling [H-Perez 2011]
5. High-order finite volume methods: CENO technique - benefits of higher accuracy on a coarse mesh [Groth and Ivan 2013][Ivan 2010][Rashad 2009]
6. AMR
 - Block-based AMR: speed and parallelization [Groth et al 1999]
 - Anisotropic vs Isotropic: how cell count (computational cost) can be reduced [Zhang 2011][Williamschen 2013][Freret 2015]
 - Now the non-uniform vs the uniform block modification [Freret 2015]
7. Solver: [Northrup 2013] implemented an implicit time marching GMRES method that improves the capability of the CFFC code
8. Creating a framework for the adjoint based error estimation method



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

Discrete Adjoint

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

yielding a linear system of equations:

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

where:

- \mathbf{J} = the functional
- \mathbf{R} = the residual
- $\boldsymbol{\Psi}$ = the adjoint vector

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

1. Finite differencing - perturbing the state \mathbf{U} to evaluate \mathbf{R}
2. Automated differentiation - tools that evaluate the differential [Bischof et al: 1992, 1996, 2008]
3. Approximate method - using the inbuilt functions within CFFC code [Northrup, 2013]
4. Complex step [Martins, Alonso and Sturdza: 2003]



Error estimation indicators

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[Venditti and Darmofal 2000][Fidkowski and Darmofal 2011]

(a) Our goal is to reduce discretization errors based on the mesh resolution.

- Consider 2 levels of mesh resolution: coarse (H) and fine (h). We calculate the state (\mathbf{U}_H) and functional ($\mathbf{J}_H(\mathbf{U}_H)$) on the coarse space. Residual, $\mathbf{R}_H(\mathbf{U}_H) = 0$
- We would like to evaluate the functional on the fine space, $\mathbf{J}_h(\mathbf{U}_h)$ (expensive). Thus we use a prolongation operator ($\mathbf{U}_h^H = I_h^H \mathbf{U}_H$) to inject the fine space state onto the coarse space state.
- The output error, $\delta \mathbf{J} \equiv \mathbf{J}_H(\mathbf{U}_H) - \mathbf{J}_h(\mathbf{U}_h) \neq 0$
- Expect the new residual, $\mathbf{R}_h(\mathbf{U}_h^H) \neq 0$
- The injected coarse state solves: $\mathbf{R}_h(\mathbf{U}_h') - \mathbf{R}_h(\mathbf{U}_h^H) = 0 \rightarrow (\mathbf{U}_h') = (\mathbf{U}_h^H)$
- $\delta \mathbf{J} \approx \mathbf{J}_h(\mathbf{U}_h^H) - \mathbf{J}_h(\mathbf{U}_h) = \boldsymbol{\Psi}_h^T \delta \mathbf{R}_h = -\boldsymbol{\Psi}_h^T \mathbf{R}_h(\mathbf{U}_h^H)$, using the definition of the fine space adjoint, $\boldsymbol{\Psi}_h$
- Error estimate is the value of $\delta \mathbf{J}$, and does not need evaluation of \mathbf{U}_h , primal solution on the fine space. We can use this error estimate as a flag for refinement, given some threshold value

(b) Steady vs unsteady adjoints: for unsteady, march forward in time, evaluating ψ , then march backwards in time. Now have all the sensitivities. Use this to refine the mesh at those time levels. Check set tolerance and repeat until convergence.

(c) Expected benefits of adjoint vs gradient based methods: the adjoint technique is a one time calculation for the sensitivity of a single output to several inputs.



Adjoint as basis of mesh refinement: $\mathcal{O}(h)$

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Some of the groups using adjoint with AMR

1. Becker and Rannacher [2001] - An Optimal Control Approach to a Posteriori Error Estimation in Finite Element Methods
2. Fidkowski and Darmofal [2011] - Review of Output-Based Error Estimation and Mesh Adaptation in Computational Fluid Dynamics
3. Hartmann [2006] - Error Estimation and Adjoint-based Adaptation in Aerodynamics
4. Nemeć and Aftosmis [2007] - Adjoint Error Estimation and Adaptive Refinement for Embedded-Boundary Cartesian Meshes
5. Nemeć, Aftosmis, and Wintzer [2008] - Adjoint-Based Adaptive Mesh Refinement for Complex Geometries
6. Hartmann, Held and Leicht [2010] - Adjoint-based error estimation and adaptive mesh refinement for the RANS and k- turbulence model equations
7. Woopen, May and Schütz [2013] - Adjoint-Based Error Estimation and Mesh Adaptation for Hybridized Discontinuous Galerkin Methods
8. Li, Allaneau and Jameson [2011] - Continuous Adjoint Approach for Adaptive Mesh Refinement
9. Diskin and Yamaelev [2011] - Grid Adaptation Using Adjoint-Based Error Minimization



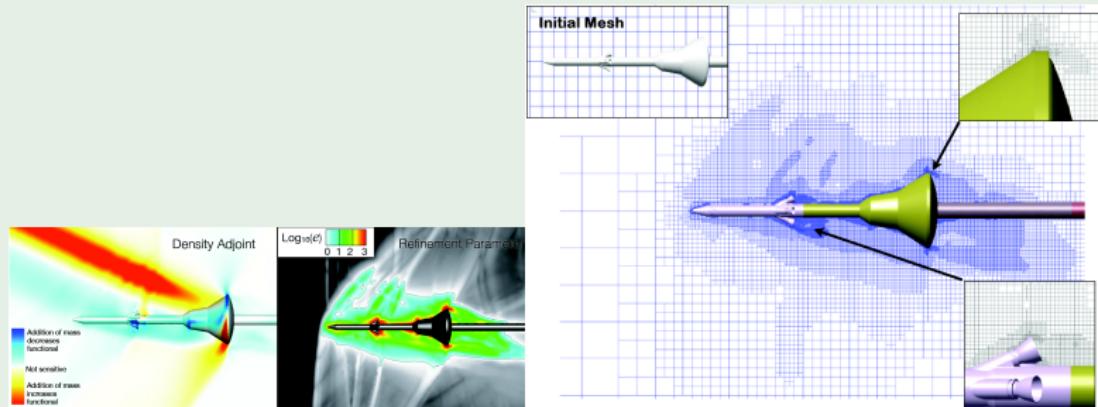
Extension to $\mathcal{O}(h^p)$

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1. h : using error estimates for mesh adaptation. Entire block would be refined.

Launch abort vehicle example, [Nemec et al, 2008]

Functional as a linear combination of normal and axial forces. $M = 1.1$; $\alpha = -25$ deg



(d) Adjoint of density with accompanying error estimate

(e) Final obtained mesh. Initial was 3.7×10^3 cells; final 2×10^6 cells

2. p : using the error estimates to run, locally, on the flagged block, a higher discretization of the numerical scheme. Usually, for high order, $p > 2$.



Poisson problem

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

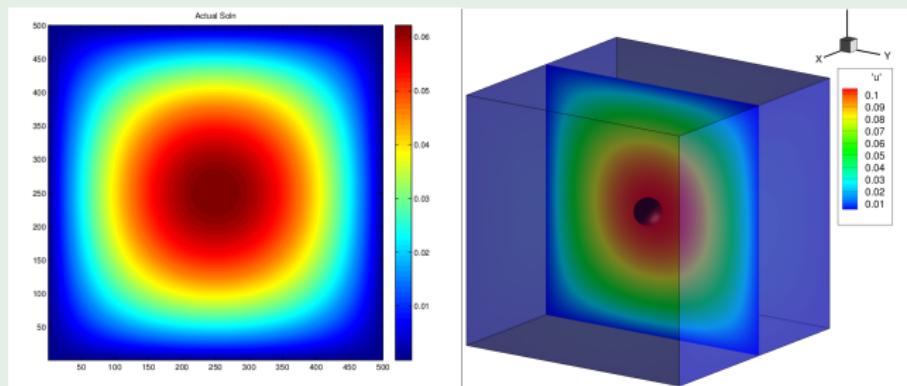


Figure: Solution contours for Poisson problem

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.

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

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:

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

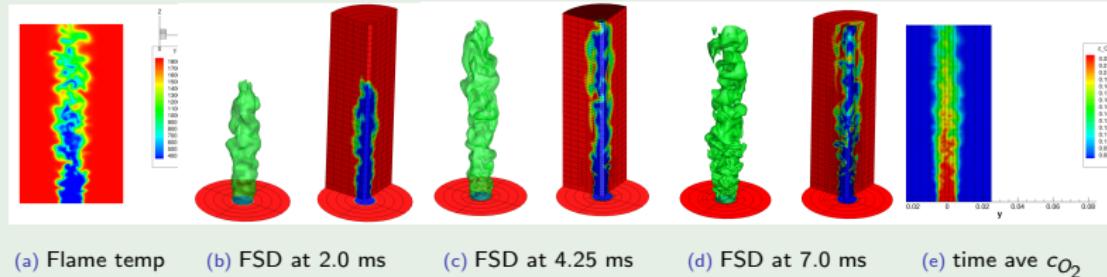


Running already existing LES case on SciNET

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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, $\phi = 0.7$.



*FSD, flame surface density is used to model the flame structure, particularly for turbulent premixed flames.

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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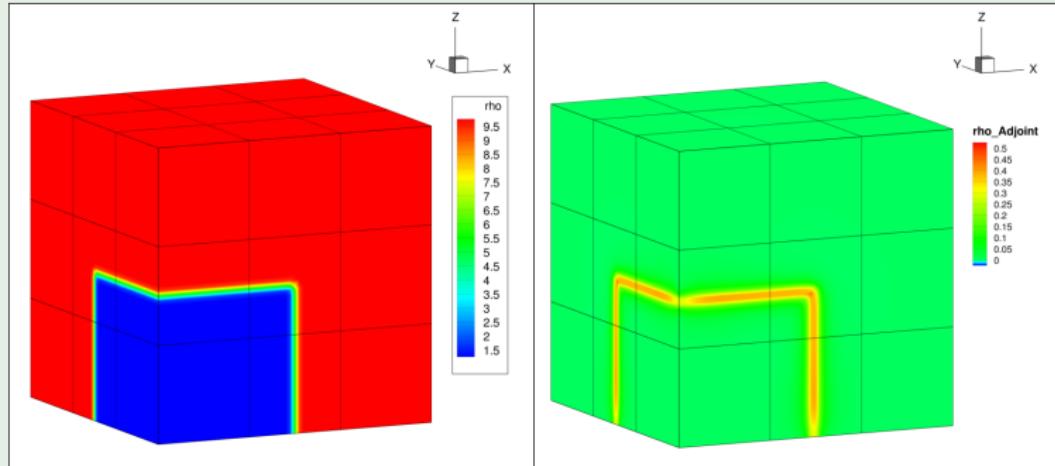
Poisson

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Timeline

Preliminary work with the discrete adjoint - shockcube problem. 8 (20x20x20) blocks



- Initial conditions: $\frac{\rho_L}{\rho_R} = 8$, $\frac{P_R}{P_L} = 10$.
- 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

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Work done 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 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
Implementing the approximate Adjoint Derivative to the Flux Jacobians testing on Euler Equations	March 2015



Future work

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Projected milestones

Task	Completion Date
Extension to Mesh adaptation	May 2015
Application of Adjoint Problem to Navier Stokes	June 2015
Explicit Filters for High Order FVM implementation	October 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
CFD simulation of Turbulent Non-Premixed Flame	May 2016
CFD simulation of Full Thermo-coupling	October 2016
Thesis write-up	September 2017



Questions?

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Thank You For Your Attention!



References

References

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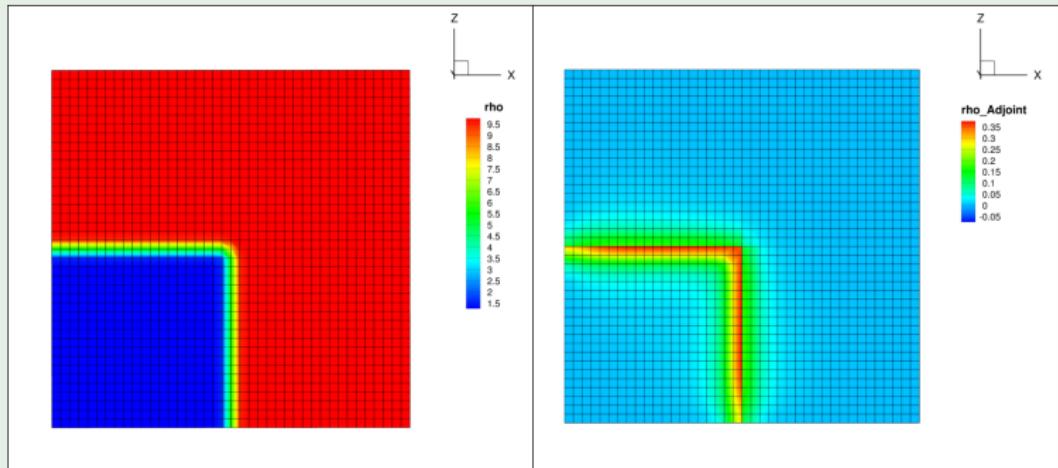
Work on the adjoint: Backup slide

References

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Preliminary work with the discrete adjoint - shockcube problem. 8 (20x20x20) blocks

CFFC = Computational Framework for Fluids and Combustion



(h) ρ at $t = 0$

(i) Ψ_ρ at $t = 0$

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