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

Christopher Ngigi
Ph.D. Candidate

Supervisor: Prof. C. P. T. Groth

Doctoral Examination Committee
Meeting I
University of Toronto, Institute for Aerospace Studies

April 6, 2015

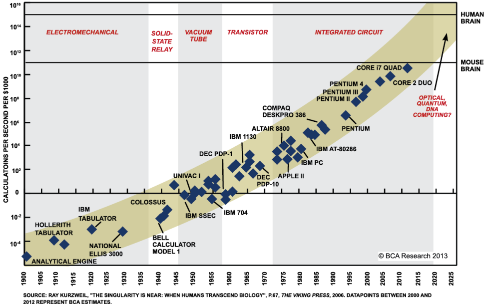
Introduction

(a) Computational Fluid Dynamics (CFD): help reduce time & cost of prototype design for engineering systems

(b) Corresponding experiments: can be expensive (time, resources) to conduct

(c) CFD: developed to capture complex phenomena to varying extents of accuracy

(d) Computing power $\approx$ doubles per 2 years. Costs less to do more?



(a) Moore's Law over the years [BCA Blog] [1]]

Turbulent combustion - Example flame

[Köhler 2006] [2, 3]

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.

- Dimensions: nozzle diameter = 2.0 mm; co-flow air annulus diameter = 140 mm
- Exit fuel Reynolds number: 10×10^3

Turbulent combustion: practical reactive flows almost always involve turbulence.

Simulation techniques:

(a) DNS resolves all the scales

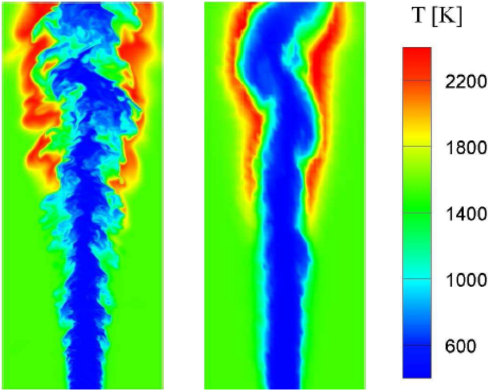
(b) LES models sub-filter scales (SFS) while resolving larger scales

(c) RANS models all turbulent scales

Large eddy simulation (LES): higher accuracy than Reynolds averaged Navier Stokes (RANS) → lower cost (time, resources) than direct numerical simulation (DNS).

Turbulent combustion - LES & DNS comparison

Comparison of DNS and LES by Yang, Pope and Chen [2013][4]: turbulent Ethylene jet flame in co-flow



(a) temperature in x-y plane: DNS (L), LES/PDF (R)

Turbulent combustion - LES & DNS comparison cont'd

Numerical setup of Yang, Pope and Chen [2013]:

$H = 2$ mm is the jet width, computational domain = cuboid

DNS:

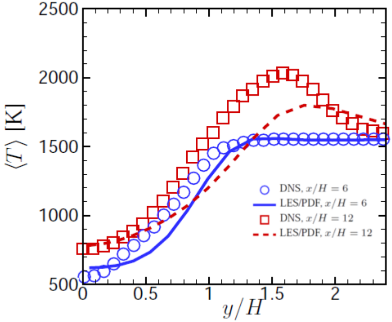
(1) Grid points $= 1.3 \times 10^9$.

(2) Computational cost $\approx 14 \times 10^6$ CPU hours. (10^6 hrs = 114 years)

LES:

(1) Grid points $\approx 8.3 \times 10^3$.

(2) Cost not specified - expected to be several orders of magnitude *lower*.



(a) Mean temperature: DNS and LES

Mean temperature results:

(a) agreement between LES and DNS at $x = 6H$.

(b) LES values lower than DNS for $x = 12H$.

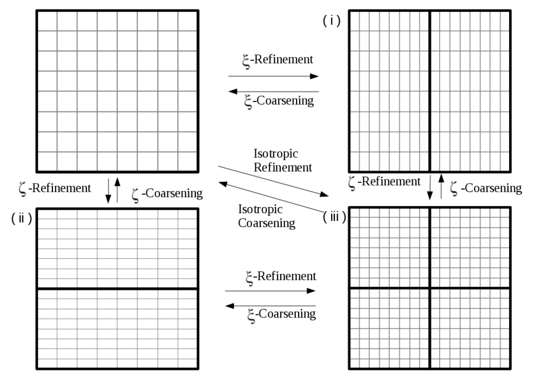
(c) Anticipate improvement for increased LES mesh resolution.

Adaptive mesh refinement (AMR)

Key characteristics of AMR

[Groth et al 1999, 2005, 2011, 2013, 2015]
[Berger et al 1984, 1986, 1989]
[Aftosmis et al 1998, 2000, 2004]

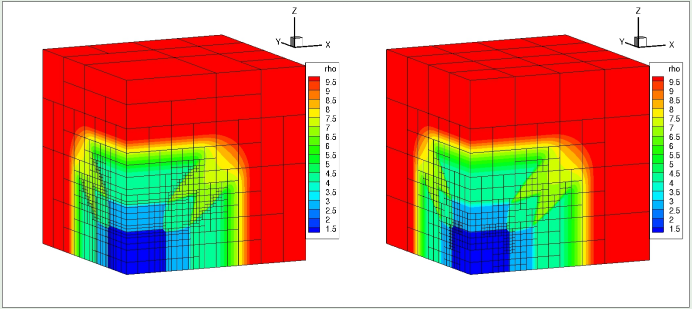
- localized refinement, large variation of scales, easily automatable
- Benefits of AMR: overall large computational cell count savings



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

Benefits: anisotropic vs isotropic AMR

Key characteristics



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

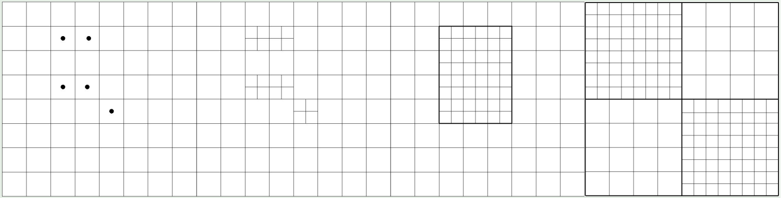
(b) With isotropic AMR. 7036 (8x8x8) blocks [Freret 2015]

- For the above shockcube cases, cell count ratio of anisotropic : isotropic $\approx$ 0.72 thus reflecting approximately 28% reduction in number of cells
- Williamschen [2013] previously obtained savings of up to 85% reduction in cell count for 3D meshes for inviscid flows

Common AMR strategies

Key characteristics

[Northrup 2013]



(a) flagged cells (b) Cell-based refinement (c) Patch-based refinement (d) Block-based refinement

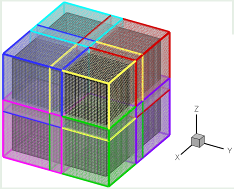
- Cell based: [Powell et al, 1993] [Berger and Leveque, 1989] [Aftosmis et al, 1998]
  Cells refined individually, hierarchy stored in a (very dense) tree
- Patch based: [Berger and Collela, 1989]
  Cells are organized into collections of rectangular patches
- Block based: [Groth and co-workers, 1999, 2005, 2011, 2013, 2015] [Berger, 1994]
  Entire blocks get refined, much lighter tree structure, efficient domain decomposition

Block-based AMR

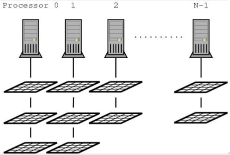
Key characteristics

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

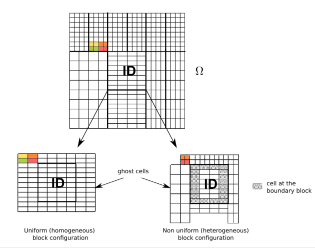
- Entire block gets refined, along with all its cells.
- This approach is much cheaper than individual cell refinement, having a lighter tree structure.
- How the block-based technique works; ghost cells for intercommunication
- Parallelizable, low memory and storage requirements
- New non-uniform approach [Freret 2015]



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



(b) Parallelization [Northrup 2013]



(c) Non-uniform approach [Freret 2015]

High order FVM and CENO

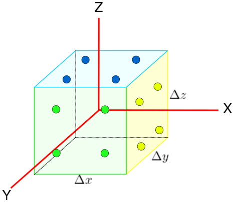
Integral Form of the Governing Equations

$$\frac{\mathrm{d}\bar{\mathbf{U}}}{\mathrm{d}t} = -\frac{1}{V}\oiint_{A}\left(\vec{\mathcal{F}}^{\mathrm{I}} - \vec{\mathcal{F}}^{\mathrm{V}}\right)\cdot\hat{n}\mathrm{d}\mathcal{A} + \bar{\mathbf{S}}$$

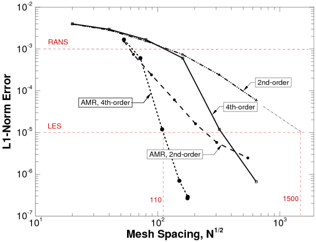
Using a two-dimensional Gauss-Legendre quadrature integration rule:

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

1. High order: $> 2^{nd}$ order. Error (Governing equations : discretized formulations) ↓, (N_G, N_F ↑, more ω)
2. Quadrature rules → reference elements → computational elements via mapping functions



(a) Example of quadrature points on the cell faces



(b) L1 error norm, unsteady advection equation. N = total mesh count

High order FVM and CENO cont'd

3. Discretized scheme expressed in matrix-vector form.
4. Evaluate the inviscid and viscous fluxes: apply weights to quadrature points
5. Evaluate source vector, which adds effects of turbulence and chemistry in reacting flows
6. Apply appropriate time-marching, e.g. RK4 suitable to high order methods.
7. Other groups researching high order methods in LES: Ihme (Stanford) and Poinsot (CERFACS)

Central essentially non-oscillatory (CENO) scheme implementation: [Ivan and Groth 2011, 2012]

- Reconstruction: FVM technique is cell centered. May need state values on faces (flux evaluations), quadrature points (high-order)
- CENO uses fixed stencil for reconstruction
- CENO eliminates oscillations typical of shocks & discontinuities
- smoothness indicators used to select between high order (p) or piecewise linear reconstruction

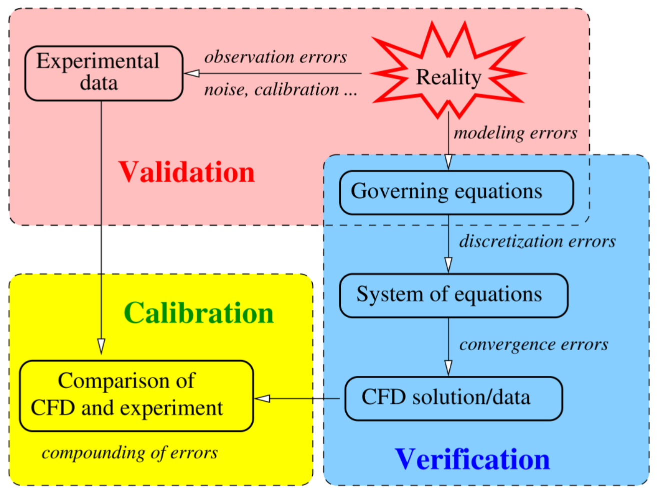
Large Eddy Simulation (LES)

[Piomelli 1999][Ghosal and Moin 1999]

1. LES utilizes a spatial filtering of a given width, $\bar{\Delta}$.
2. Any scales smaller than $\bar{\Delta}$ are modeled $\rightarrow$ sub-filter scales (SFS) [Smagorinsky 1963][Germano 1991][Piomelli 1991][Ghosal and Moin 1999][Lilly 1992]
3. Scales larger than $\bar{\Delta}$ are fully resolved.
4. Need appropriate balance for accuracy, $\rightarrow$ modeling error.
5. Types of filters broadly categorized into:
   (a) **Implicit filtering** [Aspden et al 2008]
      - Filter width not fixed: inherently related to grid resolution
      - Difficult to compare results of adapted/refined meshes and control aliasing and commutation errors
   (b) **Explicit filtering** [Vasilyev et al, 1998] [Deconinck, 2008]
      - Define $\bar{\Delta}$ to fixed for the entire mesh: easily comparable for different meshes
      - Order of truncation errors can be controllable to same order of commutation errors
      - Allows control of aliasing errors

Overview of error in CFD

Likely sources of error



(a) Some sources of error [Fidkowski 2012]

Types of error in CFD

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

1. Numerical error:
   (a) Solution error - between exact value and the CFD-obtained value
   (b) Truncation error - actual governing equations PDEs and the discretized form of the numerical scheme
   (c) Convergence error - nature of the iterative technique used
2. Modeling error:
   (a) Sub-filter scale turbulence model: inappropriate model selected
   (b) Combustion and chemistry model
   (c) Aliasing errors - decomposed nonlinear terms in FANS = feedback of frequencies beyond filter bandwidth, = 'fake' stresses
   (d) Commutation errors - exist between filtering and differential operations

Foundation for error estimation

Two general types of error estimation:

1. *a priori* error estimators: predict long-term behavior of the errors.
2. *a posteriori* error estimators: use simulation results to derive estimates of solution errors and guide adaptive schemes.

Where calculated error estimates are higher than set threshold:

- Mesh can be locally refined (h-refinement) while coarsening the less critical areas to save on computational cost.
- Degree of polynomial representation can be raised (p-refinement)

Two main *a posteriori* approaches are:

(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]

Gradient/physics-based refinement

Where rates of change of (physical) solution variables are highest, mesh refinement can be applied, or the scheme order can be increased.

(a) Thus have enough cells to capture solution changes $\rightarrow$ represent them as *smoothly* as possible.

(b) Re-iterate solution to establish new gradients. Changes are again made as necessary.

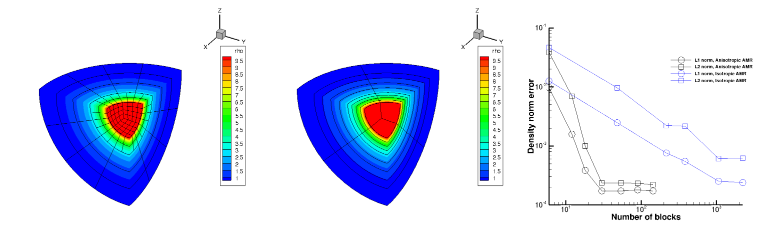
(c) Error can be compared to a higher *h*-refinement solution.

(d) This is the present utility in the anisotropic and isotropic AMR functionality of the CFFC code used by the CFD and Propulsion group.

(e) Main disadvantages of the gradient based approach it the lack of continual reduction of solution error with continued *h*-refinement - see next slide

Limitation of gradient-based mesh refinement

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

Solution adjoint

(a) Make error estimation more relevant for engineering applications

(b) Assess error in predicting an *integral quantity representation* of an engineering output (the functional): e.g. average pressure on a wall.

(c) Adjoint technique is a sensitivity analysis. Measures rates of change of a design functional to a given change in the input.

Solution adjoint formulation

Two main formulations

[Giles and Pierce: 1997,2001][Jameson, 2001][Venditti and Darmofal, 2000, 2002] [Becker and Rannacher: 2001,2003]:

1. *Continuous*:
   - Objective function formed to enforce the flow conditions (i.e. primal nonlinear PDEs).
   - Applying linear perturbations to primal flow variables
   - Then obtains analytical adjoint equations. Apply relevant b.c.s, and discretize
2. *Discrete*:
   - Apply linear perturbations to nonlinear discrete residual equations from primal problem
   - If adjoint consistent (discrete adjoint = continuous adjoint), no need for b.c. specification $\rightarrow$ 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 & proposed methodology within existing framework

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-filtered 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. Solution method: [Northrup 2013] implemented an implicit time marching GMRES method that improves the capability of the CFFC code
8. Develop a framework for the adjoint based error estimation with h-p AMR and CENO

Discrete adjoint

Discrete Adjoint

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

Linear system of equations in the form:

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

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 U to evaluate 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

A method to reduce discretization errors based on the mesh resolution. [Venditti and Darmofal 2000][Fidkowski and Darmofal 2011]

(a) Consider 2 levels of mesh resolution: coarse (H) and fine (h). Calculate the state ($\mathbf{U}_H$) and functional ($\mathbf{J}_H(\mathbf{U}_H)$) on coarse space. Residual, $\mathbf{R}_H(\mathbf{U}_H) = 0$

(b) To evaluate functional on the fine space, $\mathbf{J}_h(\mathbf{U}_h)$ is expensive. Use prolongation operator ($\mathbf{U}_h^H = I_h^H \mathbf{U}_H$) to inject coarse space state onto fine space state.

(c) Output error, $\delta \mathbf{J} \equiv \mathbf{J}_H(\mathbf{U}_H) - \mathbf{J}_h(\mathbf{U}_h) \neq 0$

(d) Expect new residual, $\mathbf{R}_h(\mathbf{U}_h^H) \neq 0$

(e) Using the definition of the fine space adjoint, the error estimate = $\delta \mathbf{J} \approx \mathbf{J}_h(\mathbf{U}_h^H) - \mathbf{J}_h(U_h) = \mathbf{\Psi}_h^T \delta \mathbf{R}_h = -\mathbf{\Psi}_h^T \mathbf{R}_h(\mathbf{U}_h^H)$

(f) Error estimate is the value of $\delta \mathbf{J}$, and does not need evaluation of U_h, primal solution on the fine space. Can use this error estimate as a flag for refinement, given some threshold value

Introduction
AMR
FVM
LES
Error
Error estimates
Methodology
Discrete adjoint
Ψ with h
Estimation
Other groups
Usage
Progress
Timeline

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

Extensive literature from groups researching **adjoint with AMR**

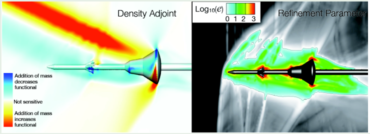
1. Becker and Rannacher [2001] - An Optimal Control Approach to a Posteriori Error Estimation in Finite Element Methods
2. Fidkowski and Darmofal [2011] - Review of Output-Based Error Estimation and Mesh Adaptation in Computational Fluid Dynamics
3. Hartmann [2006] - Error Estimation and Adjoint-based Adaptation in Aerodynamics
4. Nemec and Aftosmis [2007] - Adjoint Error Estimation and Adaptive Refinement for Embedded-Boundary Cartesian Meshes
5. Nemec, 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 Yamaleev [2011] - Grid Adaptation Using Adjoint-Based Error Minimization

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

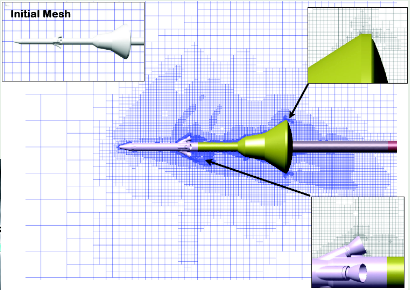
Introduction
AMR
FVM
LES
Error
Error estimates
Methodology
Discrete adjoint
Ψ with h
Usage
Progress
Timeline

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

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



(a) Adjoint of density with accompanying error estimate

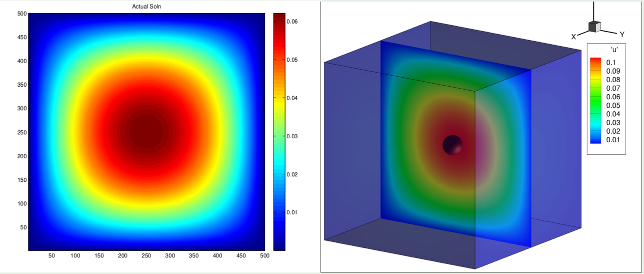


(b) Final obtained mesh. Initial was $3.7x10^3$ cells; final $2x10^6$ cells

For p increment, can use error estimates to locally run a higher discretization of the numerical scheme on flagged block.

Poisson problem in 2 and 3 space dimensions

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



(a) 2D case on $N^2 = 500^2 = 250,000$ grid points (b) 3D case on $N^3 = 100^3 = 1,000,000$ grid points

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.

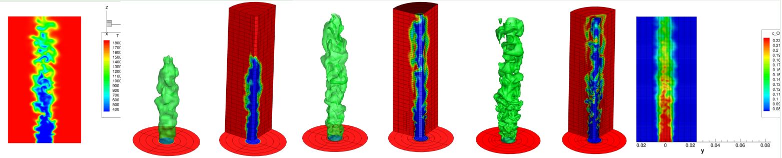
Using a 2^{nd} order centered finite difference scheme:

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

Performing an LES simulation 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 at t=9.0 ms (b) FSD at 2.0 ms (c) FSD at 4.25 ms (d) FSD at 7.0 ms (e) time ave c_{O_2}

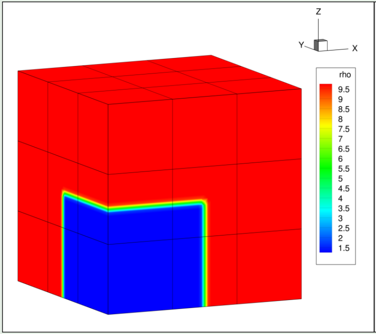
*FSD, flame surface density is used to model the flame structure, particularly for turbulent premixed flames.

Computational costs:

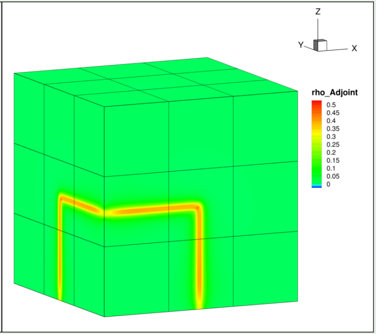
- (a) and (e): 800 procs, 3200 (8x8x8) blocks, 1.64 x10^6 cells, no refinement, 125x10^3 CPU hrs
- (b) 800 (8x8x8) blocks, 410,000 cells, no refinement
- (c) 5595 (8x8x8) blocks, 2.8 million cells, 3 levels of mesh refinement
- (d) 18531 (8x8x8) blocks, 9.5 million cells, 3 levels of mesh refinement

Solution of adjoint problem for the Euler equations

Preliminary work with the discrete adjoint - shockcube problem. 27 (20x20x20) blocks



(a) ρ at t = 0



(b) Ψ_ρ at t = 0

- Adjoint code was written to evaluate Ψ for multiple AMR blocks and multiprocessors
- Shock cube problem: initial conditions $\rightarrow \frac{\rho_R}{\rho_L} = 8,\ \frac{P_R}{P_L} = 10.$
- Selected as functional the average pressure in the shockcube.

Timeline: September 2014 - March 2015

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

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 Premixed Flame	February 2016
CFD simulation of Turbulent Non-Premixed Flame	November 2016
CFD simulation of Turbulent Premixed Flame	March 2017
Thesis write-up	September 2017

Questions?

Thank You For Your Attention!

References

[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

[5] Grätsch, T., Bathe, K. J.,
"A posteriori error estimation techniques in practical finite element analysis", Journal of Computers and Structures 83, 235265 , 2005

[6] Bibb, K., Gnoffo, P. A., Park, M. A., Jones, W. T.,
"Parallel, Gradient-Based Anisotropic Mesh Adaptation for Re-entry Vehicle Configurations", AIAA/ASME Joint Thermophysics and Heat Transfer Conference, AIAA Paper 20063579, 2006

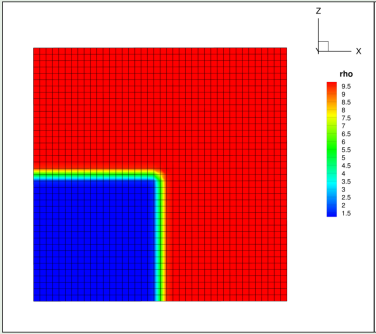
Work on the adjoint: Backup slide

References

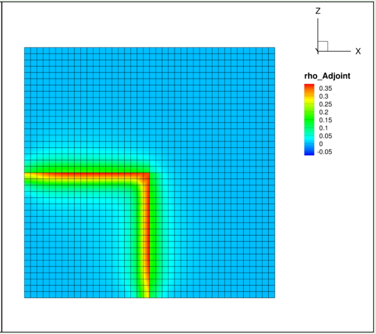
Backup

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

CFFC = Computational Framework for Fluids and Combustion



(a) ρ at t = 0



(b) Ψ_ρ at t = 0

- 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.

Turbulent combustion - LES & DNS comparison cont'd

Numerical setup of Yang, Pope and Chen [2013]:

Boundary conditions (BCs) are inflow/outflow in x and y, while periodic in z.
$H = 2$ mm is the jet width.
Computational domain = cuboid
Streamwise x-, transverse y-, and spanwise z-directions.

- DNS
  1. Grid points $= 1.3 \times 10^9$.
  2. Computational cost $\approx 14 \times 10^6$ CPU hours.
  3. $L_x \times L_y \times L_z = 15H \times 20H \times 3H$
- LES
  1. Grid points $\approx 8.3 \times 10^3$.
  2. Cost not specified - expected to be several orders of magnitude *lower*.
  3. $L_x \times L_y \times L_z = 15H \times 30H \times 3H$.
     (larger y moves the y-boundary away from central turbulent jet, avoiding the artifact of the Dirichlet boundary condition on entrainment near the jet.)

Mean temperature results show agreement between LES and DNS at $\frac{x}{H} = 6$.
LES values lower than DNS for $\frac{x}{H} = 12$.
Anticipate this to improve for increased LES mesh resolution.

References

Backup

Turbulent combustion - Example flame

[Köhler 2006] [2, 3]

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 temp, air temp and pressure near std.
- Dimensions: nozzle diameter = 2.0 mm; co-flow air annulus diameter = 140 mm
- Exit fuel Reynolds number: 10×10^3
- Air mass flow: 320 g/min
- Mean fuel jet velocity: 44 m/s

Turbulent combustion: practical reactive flows almost always involve turbulence.

Simulation techniques:

(a) DNS resolves all the scales

(b) LES models sub-filter scales (SFS) while resolving larger scales

(c) RANS models all turbulent scales

Large eddy simulation (LES): higher accuracy than Reynolds averaged Navier Stokes (RANS) $\rightarrow$ lower cost (time, resources) than direct numerical simulation (DNS).

High order finite volume method

Error reduction via p

Integral Form of the Governing Equations

$$\frac{\mathrm{d}\overline{\mathbf{U}}}{\mathrm{d}t} = -\frac{1}{V}\oiint_{A}\left(\vec{\mathcal{F}}^{\mathrm{I}} - \vec{\mathcal{F}}^{\mathrm{V}}\right)\cdot\hat{n}\mathrm{d}\mathcal{A} + \overline{\mathbf{S}}$$

Using a two-dimensional Gauss quadrature integration rule:

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

(a) High order methods generally $> 2^{nd}$ order accuracy, reduce numerical error between PDE governing equations and discretized formulations.

(b) Discretized scheme expressed in matrix-vector form: [Northrup 2013] GMRES solver.

(c) High $p \rightarrow$ more the quadrature points (N_G with weights ω).

(d) (Gauss-Legendre) quadrature rules $\rightarrow$ reference elements $\rightarrow$ computational elements via mapping functions

(e) Evaluate the inviscid and viscous fluxes: apply weights to quadrature points

(f) Evaluate source vector, which adds effects of turbulence and chemistry in reacting flows

(g) Apply appropriate time-marching, e.g. RK4 suitable to high order methods.

(h) Other groups researching high order methods in LES: Ihme (Stanford) and Poinsot (CERFACS)