Output-Based Error Estimation and Mesh Adaptation in Computational Fluid Dynamics: Overview and Recent Results

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Outline

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Introduction

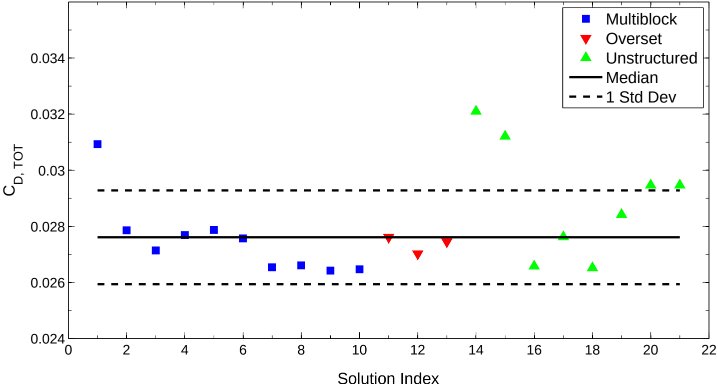
Complex CFD simulations made possible by

- Increasing computational power
- Improvements in numerical algorithms

New liability: ensuring accuracy of computations

- Management by expert practitioners is not feasible for increasingly-complex flowfields
- Reliance on best-practice guidelines is an open-loop solution: numerical error unchecked for novel configurations
- Output calculations are not yet sufficiently robust, even on relatively standard simulations

AIAA Drag Prediction Workshop III

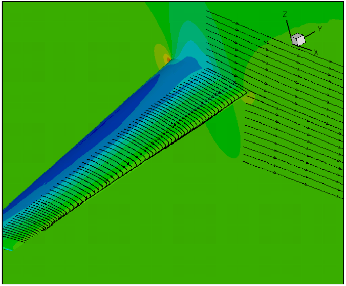


Drag coefficient predictions for the DLR-F6 wing-body at $M = 0.75$, $C_L = 0.5$, $Re = 5 \times 10^6$.

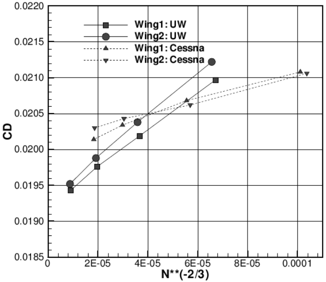
- Variation of 25 drag counts: 1 drag count $\approx$ 4 passengers for a large transport aircraft
- Only slight improvement over results from previous two workshops

"Mesh Convergence" Comparison

Same code run on independently-generated meshes of two wing-only geometries [Mavriplis, 2007]



A DPW wing-alone test case



Drag convergence with uniform refinement

- Highly-disparate length scales in this flow are not adequately resolved using current meshes
- Improvements in computational power alone will be insufficient to decrease numerical error to acceptable levels in the near future

Improving CFD Robustness

Error estimation

- “Error bars” on outputs of interest are necessary for confidence in CFD results
- Mathematical theory exists for obtaining such error bars
- Recent works demonstrate the success of this theory for aerospace applications

Mesh adaptation

- Error estimation alone is not enough
- Engineering accuracy for complex aerospace simulations demands mesh adaptation to control numerical error
- Automated adaptation improves robustness by closing the loop in CFD analysis

Goals of this Work

1. Review the theory behind output-based error estimation
2. Identify similarities between discrete and variational approaches
3. Present existing and new strategies for mesh adaptation
4. Showcase recent work in aerospace applications
5. Identify key challenges and areas for further research

Outline

Discrete Adjoint Definition

Consider N_h algebraic equations and an output,

$$\mathbf{R}_h(\mathbf{u}_h) = 0, \qquad J_h = J_h(\mathbf{u}_h)$$

- $\mathbf{u}_h \in \mathbb{R}^{N_h}$ is the vector of unknowns
- $\mathbf{R}_h \in \mathbb{R}^{N_h}$ is the vector of residuals
- $J_h(\mathbf{u}_h)$ is a *scalar* output of interest

The discrete output adjoint vector, $\psi_h \in \mathbb{R}^{N_h}$, is the sensitivity of J_h to an infinitesimal residual perturbation, $\delta\mathbf{R}_h \in \mathbb{R}^{N_h}$,

$$\delta J_h \equiv \psi_h^T \delta\mathbf{R}_h$$

Discrete Adjoint Equation

The linearized perturbed equations are:

$$\frac{\partial \mathbf{R}_h}{\partial \mathbf{u}_h} \delta \mathbf{u}_h + \delta \mathbf{R}_h = 0,$$

Also linearizing the output we have,

$$\delta J_h = \underbrace{\frac{\partial J_h}{\partial \mathbf{u}_h} \delta \mathbf{u}_h = \overbrace{\psi_h^T \delta \mathbf{R}_h}^{\text{linearized equations}}}_{\text{adjoint definition}} \overbrace{= -\psi_h^T \frac{\partial \mathbf{R}_h}{\partial \mathbf{u}_h} \delta \mathbf{u}_h}$$

Requiring the above to hold for arbitrary perturbations yields the linear *discrete adjoint equation*

$$\left(\frac{\partial \mathbf{R}_h}{\partial \mathbf{u}_h} \right)^T \psi_h + \left(\frac{\partial J_h}{\partial \mathbf{u}_h} \right)^T = 0$$

Variational Adjoint Definition

Galerkin weighted residual statement: determine $\mathbf{u}_h \in \mathcal{V}_h$ such that

$$\mathcal{R}_h(\mathbf{u}_h, \mathbf{v}_h) = 0, \qquad \forall \mathbf{v}_h \in \mathcal{V}_h$$

- $\mathcal{V}_h$ is a finite-dimensional space of functions
- $\mathcal{R}_h(\cdot,\cdot) : \mathcal{V}_h \times \mathcal{V}_h \to \mathbb{R}$ is a semilinear form
- $\mathcal{J}_h(\mathbf{u}_h) : \mathcal{V}_h \to \mathbb{R}$ is a scalar output

The output adjoint is now a function, $\psi_h \in \mathcal{V}_h$, that is the sensitivity of $\mathcal{J}_h$ to a residual perturbation, $\delta\mathbf{r}$:

$$\delta\mathcal{J}_h \equiv (\delta\mathbf{r}_h, \psi_h)$$

where $(\cdot,\cdot) : \mathcal{V}_h \times \mathcal{V}_h \to \mathbb{R}$ is a suitable inner product

Variational Adjoint Statement

The Fréchét-linearized equations are:

$$\mathcal{R}_h'[\mathbf{u}_h](\delta\mathbf{u}_h, \mathbf{v}_h) + (\delta\mathbf{r}_h, \mathbf{v}_h) = 0, \qquad \forall \mathbf{v}_h \in \mathcal{V}_h,$$

Also linearizing the output we have,

$$\delta\mathcal{J}_h = \underbrace{\mathcal{J}_h'[\mathbf{u}_h](\delta\mathbf{u}_h) = (\delta\mathbf{r}_h, \psi_h)}_{\text{adjoint definition}} \overbrace{(\delta\mathbf{r}_h, \psi_h) = -\mathcal{R}_h'[\mathbf{u}_h](\delta\mathbf{u}_h, \psi_h)}^{\text{linearized equations}}$$

Requiring the above to hold for arbitrary perturbations yields the linear *variational adjoint statement*: find $\psi_h \in \mathcal{V}_h$ such that

$$\mathcal{R}_h'[\mathbf{u}_h](\mathbf{v}_h, \psi_h) + \mathcal{J}_h'[\mathbf{u}_h](\mathbf{v}_h) = 0, \qquad \forall \mathbf{v}_h \in \mathcal{V}_h$$

Continuous Adjoint

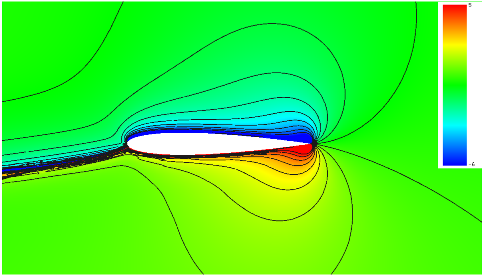
The continuous primal solution, $\mathbf{u} \in \mathcal{V}$, satisfies

$$\mathcal{R}(\mathbf{u}, \mathbf{v}) = 0, \qquad \forall \mathbf{v} \in \mathcal{V},$$

The continuous adjoint solution, $\psi \in \mathcal{V}$, satisfies

$$\mathcal{R}'[\mathbf{u}](\mathbf{v}, \psi) + \mathcal{J}'[\mathbf{u}](\mathbf{v}) = 0, \qquad \forall \mathbf{v} \in \mathcal{V}$$

- $\mathcal{V}$ is an infinite-dimensional space
- ψ is a Green's function relating source residuals to output perturbations [Giles and Pierce, 1997]



x-momentum lift adjoint, $M_\infty = 0.4$, $\alpha = 5^o$

Consistency

- *Primal consistency* requires that the continuous solution $\mathbf{u}$ satisfies the discrete variational statement,

$$\mathcal{R}_h(\mathbf{u}, \mathbf{v}_h) = 0, \qquad \forall \mathbf{v}_h \in \mathcal{V}_h$$

- Similarly, the combination of $\mathcal{R}_h$ and $\mathcal{J}_h$ is *adjoint consistent* if

$$\mathcal{R}_h'[\mathbf{u}](\mathbf{v}_h, \psi) + \mathcal{J}_h'[\mathbf{u}](\mathbf{v}_h) = 0, \qquad \forall \mathbf{v}_h \in \mathcal{V}_h$$

[Arnold *et al* , 2002; Lu, 2005; Hartmann, 2007; Oliver, 2008]

- *Asymptotic adjoint consistency* is a weaker requirement that the above holds in the limit $h \to 0$, over suitably normalized $\mathbf{v}_h \in \mathcal{V}_h$.
- An adjoint-inconsistent discretization can
  - pollute the error estimate with noise
  - lead to adaptation in incorrect areas

Finite Perturbations

- Above adjoints are valid for infinitesimal residual perturbations
- Finite perturbations can be considered through mean-value linearizations:

$$\delta J_h = (\psi_h^{\mathrm{mv}})^T \delta \mathbf{R}_h, \qquad \delta \mathcal{J}_h = (\delta \mathbf{r}_h, \psi_h^{\mathrm{mv}})$$

  where ψ_h^{mv} is the adjoint obtained when mean-value linearizations are used
  [Pierce and Giles, 2000; Becker and Rannacher, 2001; Barth and Larson, 2002; Hartmann and Houston, 2002]

- In practice, mean-value linearizations are not typically implemented and the equations become approximations:

$$\delta J_h \approx \psi_h^T \delta \mathbf{R}_h, \qquad \delta \mathcal{J}_h \approx (\delta \mathbf{r}_h, \psi_h)$$

Adjoint Implementation

- The discrete adjoint, ψ_h, is obtained by solving a linear system
- This system involves linearizations about the primal solution, $\mathbf{u}_h$, which is generally obtained first
- When the full Jacobian matrix, $\frac{\partial \mathbf{R}_h}{\partial \mathbf{u}_h}$, and an associated linear solver are available, the transpose linear solve is straightforward
- When the Jacobian matrix is not stored, the discrete adjoint solve is more involved: all operations in the primal solve must be linearized, transposed, and applied in reverse order [Giles *et al* , 2003; Nielsen *et al* , 2004]
- In unsteady discretizations, the adjoint must be marched backward in time from the final to the initial state

Outline

Forms of Error Estimation

Local choices

1. **Discretization error**: difference between the discrete solution and the exact, continuous solution
2. **Residual error**: result of substituting the approximate solution into the underlying PDE – nonzero residuals indicate where the equations are not strongly satisfied

These are generally sufficient for driving adaptation in elliptic problems, such as elasticity or low-speed flows. [Verfurth, 1994]

However, in **hyperbolic problems** (i.e. aerospace CFD applications),

- Local residuals may not always be large in certain crucial areas that significantly affect the solution downstream
- Error estimates based on local residual or discretization errors fail to capture these *propagation effects* [Houston and Süli, 2002]

Output Error Estimation

Output error: difference between an output computed with the discrete system solution and that computed with the exact solution

Output error estimation techniques

- Identify all areas of the domain that are important for the accurate prediction of an output
- Account for propagation effects
- Require solution of an adjoint equation

Output error estimates can be used to:

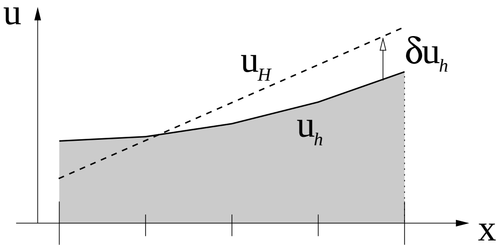
- Ascribe confidence levels to engineering outputs in the presence of numerical errors
- Drive an adaptive method to reduce the output error below a user-specified tolerance

Two Discretization Levels

In practice, cannot solve on an infinite-dimensional space, $\mathcal{V}$

Consider two discretization spaces:

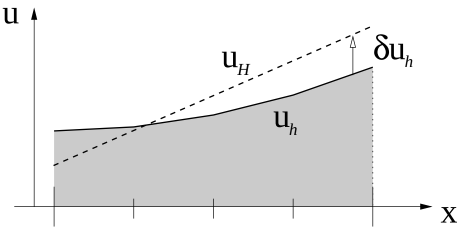
- A coarse one, $\mathcal{V}_H$, with N_H degrees of freedom
- A fine one, $\mathcal{V}_h$, with N_h degrees of freedom



The "fine" discretization (h) is obtained from the coarse discretization (H) by using a smaller mesh size or increased interpolation order

Adjoint-Weighted Residual Method

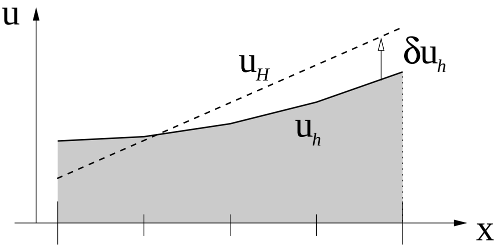
Goal: Calculate $\mathcal{J}_H(\mathbf{u}_H) - \mathcal{J}_h(\mathbf{u}_h)$ = output error *estimate*



- Could solve for $\mathbf{u}_h$ and recompute the output – expensive and not directly useful for adaptation
- Idea: $\mathbf{u}_H$ generally does not satisfy the fine-level equations. That is, $\mathcal{R}_h(\mathbf{u}_H, \mathbf{v}_h) \neq 0$. Instead, $\mathbf{u}_H$ solves: find $\mathbf{u}'_h \in \mathcal{V}_h$ such that

$$\mathcal{R}_h(\mathbf{u}'_h, \mathbf{v}_h) - \mathcal{R}_h(\mathbf{u}_H, \mathbf{v}_h) = 0 \quad \forall \mathbf{v}_h \in \mathcal{V}_h$$

Adjoint-Weighted Residual Method (ctd.)



- $-\mathcal{R}_h(\mathbf{u}_H, \mathbf{v}_h)$ is a residual perturbation on the fine discretization
- Suppose we have an adjoint solution on the fine mesh: $\psi_h \in \mathcal{V}_h$
- The adjoint lets us calculate the output perturbation from the point of view of the fine discretization:

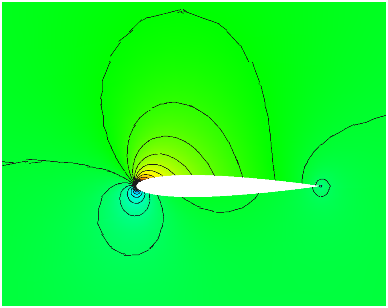
$$\delta \mathcal{J}_h = \mathcal{J}_h(\mathbf{u}_H) - \mathcal{J}_h(\mathbf{u}_h) \approx -\mathcal{R}_h(\mathbf{u}_H, \psi_h)$$

[Becker and Rannacher, 1996; Giles *et al* , 1997]

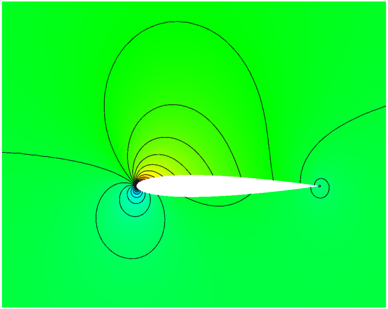
Adjoint-Weighted Residual Example

NACA 0012, $M_\infty = 0.5$, $\alpha = 5^o$

Interested in lift error in a $p = 1$ DG solution. Using $p = 2$ for fine space, $\mathcal{V}_h$



$p = 1$ Mach contours



$p = 2$ Mach contours

- Adjoint-based error estimate: $-\mathcal{R}_h(\mathbf{u}_H, \psi_h) = -.001097$
- Actual difference between $p = 2$ and $p = 1$ solution outputs is $\delta\mathcal{J}_h = -0.001099$

Approximating ψ_h

How do we calculate ψ_h = the adjoint on the fine discretization?

Options:

1. Solve for $\mathbf{u}_h$ and then ψ_h – expensive! Potentially still useful to drive adaptation. [Solín and Demkowicz, 2004]
2. Solve for $\psi_H \in \mathcal{V}_H$ = the adjoint on the coarse discretization:

$$\mathcal{R}'_H[\mathbf{u}_H](\mathbf{v}_H, \psi_H) + \mathcal{J}'_H[\mathbf{u}_H](\mathbf{v}_H) = 0, \qquad \forall \mathbf{v}_H \in \mathcal{V}_H,$$

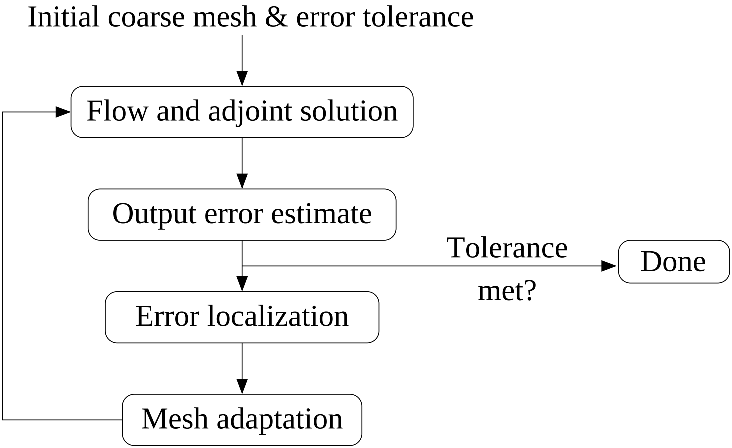
   1. Reconstruct ψ_H on the fine discretization using a higher-accuracy stencil. Smoothness assumption on adjoint. [Rannacher, 2001; Barth and Larson, 2002; Venditti and Darmofal 2002; Lu, 2005; Fidkowski and Darmofal, 2007]
   2. Initialize ψ_h with ψ_H and take a few iterative solution steps on the fine discretization. [Barter and Darmofal, 2008; Oliver and Darmofal, 2008]

Error Estimation Summary

1. Solve the coarse-discretization forward and adjoint problems: $\mathbf{u}_H$ and ψ_H
2. Pick a fine discretization "h" (mesh refinement or order enrichment)
3. Calculate or approximate ψ_h = adjoint on the fine mesh
4. Project $\mathbf{u}_H$ onto the fine discretization and calculate the residual $\mathcal{R}_h(\mathbf{u}_H, \mathbf{v}_h)$
5. Weight the fine-space residual with the fine-space adjoint to obtain the output error estimate
6. **Note**: the computed output error $\mathcal{J}_h(\mathbf{u}_H) - \mathcal{J}_h(\mathbf{u}_h)$ is an estimate of the true error, <u>not a bound</u>

Outline

Mesh Adaptation

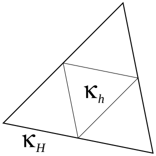


Error Localization

Assuming the coarse and fine spaces are nested, the error estimate can be written as

$$\mathcal{J}_H(\mathbf{u}_H) - \mathcal{J}_h(\mathbf{u}_h) \approx - \sum_{\kappa_H \in T_H} \sum_{\kappa_h \in \kappa_H} \mathcal{R}_h(\mathbf{u}_H, \psi_h|_{\kappa_h}),$$

- T_H is the coarse triangulation
- κ_H/κ_h is an element of the coarse/fine triangulation
- $|_{\kappa_h}$ refers to restriction to element κ_h



Elemental contributions
$\Rightarrow$ **error indicator**:

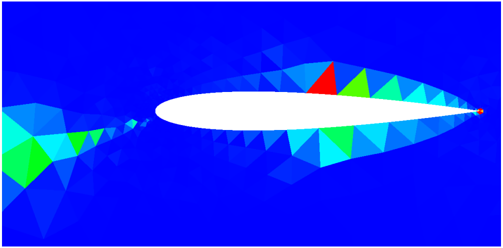
$$\epsilon_{\kappa_H} \equiv \left| \sum_{\kappa_h \in \kappa_H} \mathcal{R}_h(\mathbf{u}_H, \psi_h|_{\kappa_h}) \right|$$

[Becker and Rannacher, 2001]
[Giles and Süli, 2002]
[Hartmann and Houston, 2002]
[Venditti and Darmofal, 2002]

Error Localization (ctd.)

<u>Error indicator</u>

$$\epsilon_{\kappa_H} = \left| \sum_{\kappa_h \in \kappa_H} \mathcal{R}_h(\mathbf{u}_H, \psi_h|_{\kappa_h}) \right|$$



Lift error indicator on a $p = 1$ DG solution

- Continuous FEM discretizations require a more careful bookkeeping of the elemental contributions
- Refinement in areas where ϵ_{κ_H} is large will reduce the residual there and hence improve the output accuracy

Adaptation Mechanics

1. *h*-adaptation: only triangulation is varied
2. *p*-adaptation: only interpolation order is varied

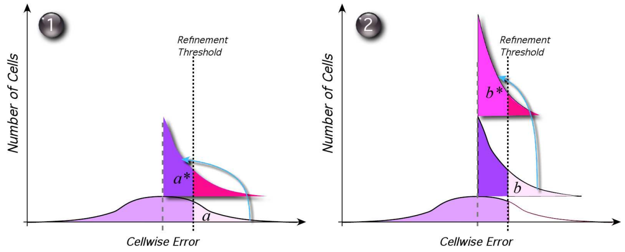
h-adaptation is key in CFD, where solutions often possess localized, singular features. However, *hp*-adaptation is becoming popular with growing popularity of high-order methods.

Given an error indicator, how should the mesh be adapted?

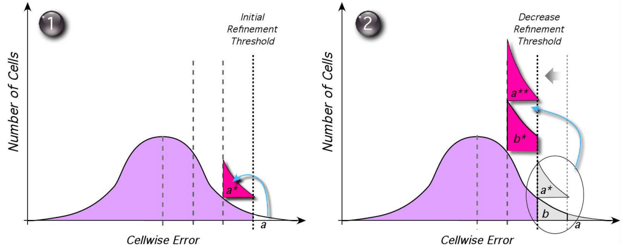
- Refine some/all elements?
- Incorporate anisotropy (stretching)?
- How to handle elements on the geometry?

Keeping in mind that mesh generation is difficult in the first place and that adaptation needs to be automated to enable multiple iterations

Which Elements to Refine? [Nemec *et al* , 2008]

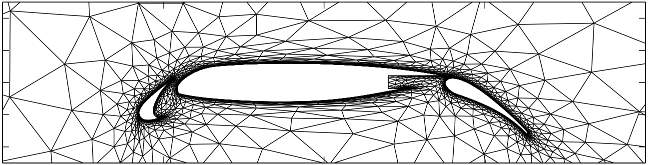


Constant threshold: refine all elements above a constant error indicator

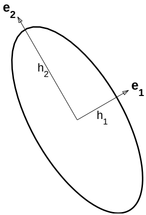


Decreasing threshold: threshold decreases with each iteration

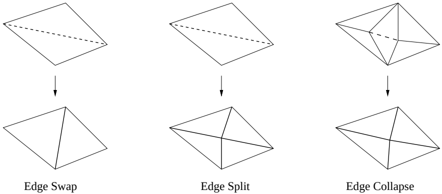
Meshing and Adaptation Strategies



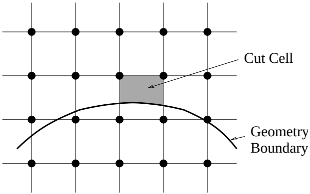
Metric-based anisotropic mesh regeneration (e.g. BAMG software)



Riemannian ellipse



Local mesh operators, and direct optimization

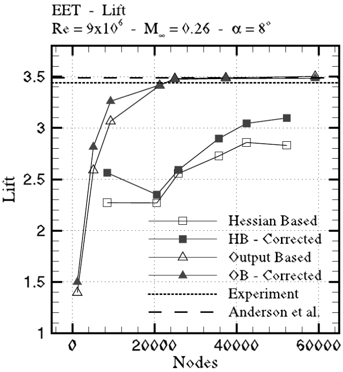


Cut-cell meshes: Cartesian and simplex

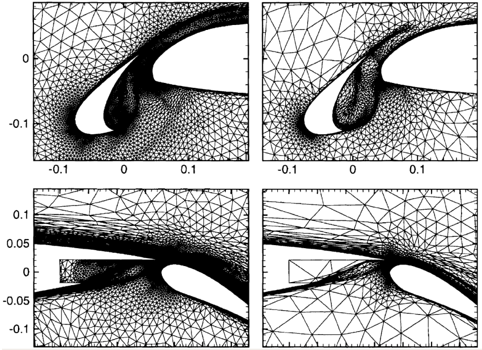
Outline

High-Lift RANS [Venditti and Darmofal, 2002]

Comparison to pure Hessian-based adaptation



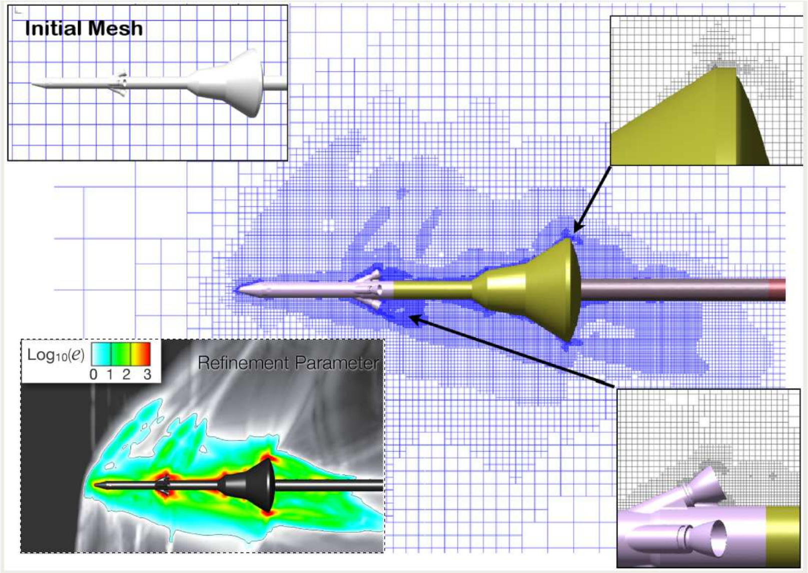
Lift convergence



Output (left) and Hessian (right) adapted meshes

Significantly improved accuracy per degree of freedom when using output adaptation

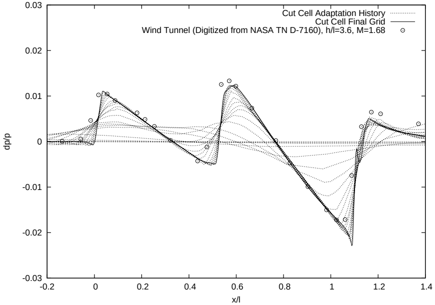
Launch Abort Vehicle [Nemec *et al* , 2008]



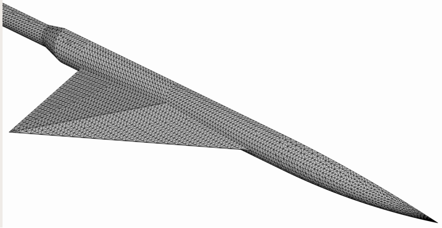
$M_\infty = 1.1, \alpha = -25^o$, two million cells in final mesh

Sonic Boom [Park, 2008]

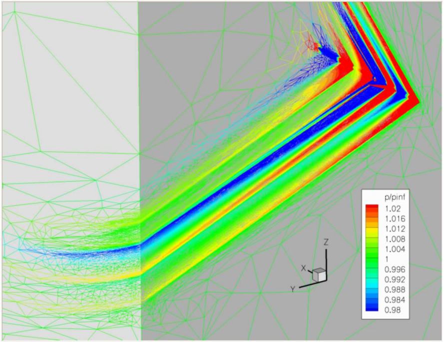
- Tetrahedral cut-cell finite volume discretization
- Direct anisotropic optimization with local operators
- Sonic boom adaptation on pressure signature



Pressure signature



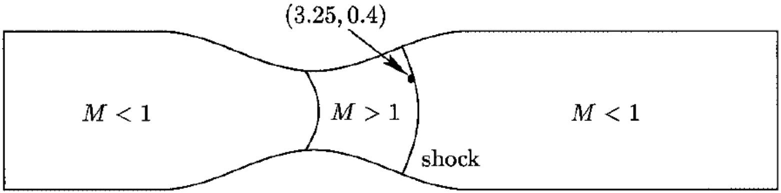
Surface mesh



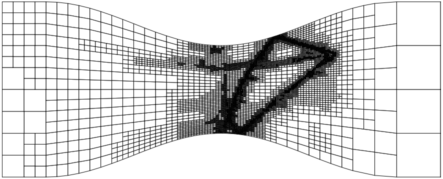
Adapted background mesh

Transonic Nozzle [Hartmann and Houston, 2002]

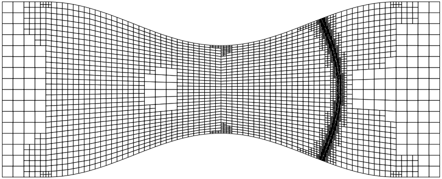
Discontinuous Galerkin, $p = 1$, discretization



The output of interest is the density immediately before the shock



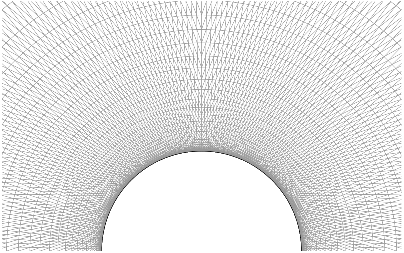
Output-adapted, 172k dof, error = 7×10^{-6}



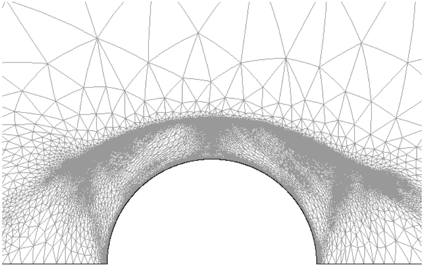
Residual-adapted, 343k dof, error = 3×10^{-5}

Hypersonic Heat Transfer [Barter and Darmofal, 2008]

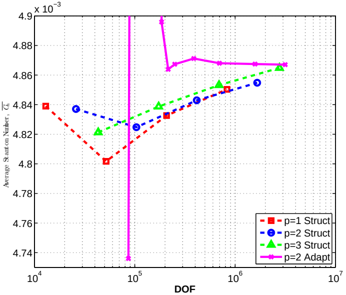
- High-order DG discretization
- PDE-based artificial viscosity for shock stabilization
- $M_\infty = 17.605$, $Re = 376,930$ over a cylinder geometry
- Output = integrated heat flux



Initial mesh



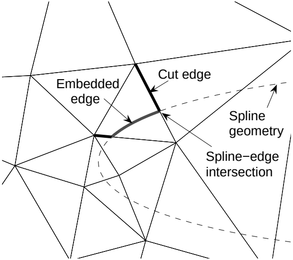
Adapted mesh, $p = 2$

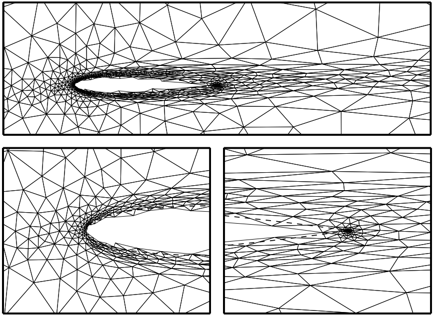


Output convergence

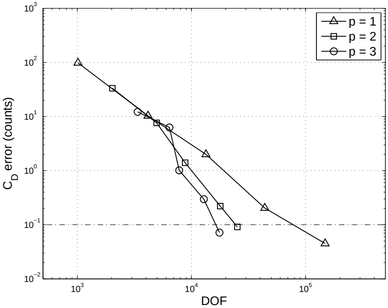
Simplex Cut Cells [Fidkowski and Darmofal, 2007]

- High-order DG discretization
- Cubic spline geometry
- Metric-driven re-meshing with BAMG
- Laminar flow in 2D ($Re = 5,000$)





Drag-adapted mesh, $p = 3$



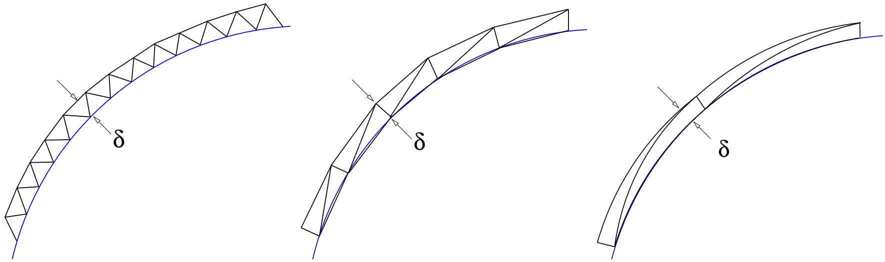
Output convergence

Outline

Robust Mesh Adaptation

- Still a challenge and an area of ongoing research for complex 3D configurations with anisotropic solutions
- Largest barrier limiting the application of output-based adaptation to simple geometries and/or simplified physics

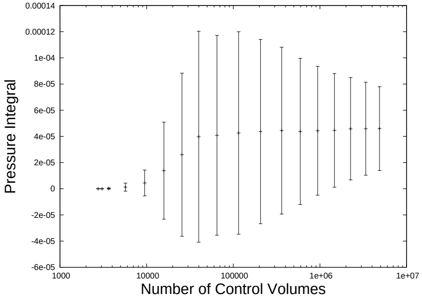
To be practical for aerospace applications, automated adaptation will also need to efficiently resolve curved, anisotropic features:



(a) Isotropic (b) Linear anisotropic (c) Curved anisotropic

Computable Error Bounds

- Example: Park's sonic boom adaptation
- Error is severely under-predicted on the coarse initial meshes
- Estimate improves only as shock is resolved



Output error estimate history

- Research exists on computation of strict, constant-free, output error bounds for certain classes of problems [Peraire *et al* , 1997–2006]
- Additional research necessary to extend to equation sets relevant to aerospace CFD applications

Unsteady Applications

- Unsteadiness arises even for nominally steady applications [Nemec *et al* , 2008]
- Time accurate adjoint solutions require substantial algorithmic and computational overhead
- Unsteady adjoint analyses exist in shape optimization research [Lee *et al* , 2006; Nadarajah and Jameson, 2002–2007; Rumpfkeil and Zingg, 2007]
- Time-step adaptive results have already been demonstrated [Mani and Mavriplis, 2007]
- Future research: combined spatial and temporal adaptation for problems exhibiting non-smooth spatial and temporal features

Concluding Remarks

- Robust CFD analyses of complex configurations require error estimation and mesh adaptation
- Local interpolation or residual-based error estimates are inadequate for the hyperbolic problems common in aerospace applications
- Mathematical theory exists for output error estimation using adjoint solutions and residual evaluations on a refined mesh
- Robust mesh adaptation is one of the largest barriers for the effective implementation of these methods
- Computable error bounds and unsteady extensions are additional areas of ongoing work

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