Entropy-Based Mesh Refinement, I: The Entropy Adjoint Approach

2009 AIAA CFD Conference

Krzysztof J. Fidkowski and Philip L. Roe

Department of Aerospace Engineering
University of Michigan

June 23, 2009

Outline

1. Introduction
2. Output-Based Error Estimation
3. The Entropy Adjoint Connection
4. Implementation and Results
5. Conclusions

Introduction

Increasing interest in solution-based adaptive methods in CFD

- Complex problems often exhibit a wide range of length scales whose distribution is not known *a priori*
- Questions of robustness and solution accuracy persist even "routine" calculations

Variety of adaptive indicators available

- **Heuristic:** generally cheap but not robust
- **Rigorous:** robust but often expensive

We propose an **entropy adjoint** indicator that is somewhat of a compromise between heuristics and theory

Output Error Estimation

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

$$\delta J = J_H(\mathbf{u}_H) - J(\mathbf{u})$$

$$\mathbf{u}_H \in \mathcal{V}_H = \text{approximate solution}, \qquad \mathbf{u} \in \mathcal{V} = \text{exact solution}$$

Adjoint-based output error estimation techniques

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

The Continuous Adjoint

Primal equation

$$\mathbf{r}(\mathbf{u}) = 0, \ \text{on } \Omega$$

The continuous adjoint, ψ, is a Lagrange multiplier for

$$\mathcal{L} = J(\mathbf{u}) - \int_\Omega \psi^T \mathbf{r}(\mathbf{u}) d\Omega$$

Requiring a stationary Lagrangian for permissible state variations, $\delta\mathbf{u} \in \mathcal{V}^{\text{perm}}$, yields (in weak form) the

Adjoint equation

$$J'[\mathbf{u}](\delta\mathbf{u}) - \int_\Omega \psi^T \mathbf{r}'[\mathbf{u}](\delta\mathbf{u}) d\Omega = 0, \quad \forall \delta\mathbf{u} \in \mathcal{V}^{\text{perm}}$$

Example: First-Order Conservation Laws

Consider a system of conservation laws in quasi-linear form,

$$\mathbf{r}(\mathbf{u}) = \mathbf{A}_i \partial_i \mathbf{u} = 0$$

The adjoint equation is, after an integration by parts,

$$J'[\mathbf{u}](\delta\mathbf{u}) + \int_\Omega \partial_i \psi^T \mathbf{A}_i \delta\mathbf{u} d\Omega - \int_{\partial\Omega} \psi^T \mathbf{A}_i \delta\mathbf{u}\, n_i ds = 0, \quad \forall \delta\mathbf{u} \in \mathcal{V}^{\text{perm}}$$

If $J(\mathbf{u})$ is an integral on $\partial\Omega$, ψ must satisfy

$$\mathbf{A}_i^T \partial_i \psi = 0, \quad \text{in } \Omega,$$

subject to the boundary conditions

$$J'[\mathbf{u}](\delta\mathbf{u}) - \int_{\partial\Omega} \psi^T \mathbf{A}_i \delta\mathbf{u}\, n_i ds = 0, \quad \forall \delta\mathbf{u} \in \mathcal{V}^{\text{perm}}$$

Output Error Estimation with Adjoints

1. $\mathbf{u}_H \in \mathcal{V}_H$ will generally not satisfy the analytical PDE: $\mathbf{r}(\mathbf{u}_H) \neq 0$
2. If $\delta\mathbf{u} \equiv \mathbf{u}_H - \mathbf{u}$ is small, we can write

$$\mathbf{r}(\mathbf{u}_H) = \mathbf{r}(\mathbf{u} + \delta\mathbf{u}) \approx \mathbf{r}'[\mathbf{u}](\delta\mathbf{u})$$

3. Using the adjoint equation we have

$$\delta J \approx J'[\mathbf{u}](\delta\mathbf{u}) = \int_\Omega \psi^T \mathbf{r}'[\mathbf{u}](\delta\mathbf{u}) \approx \int_\Omega \psi^T \mathbf{r}(\mathbf{u}_H)$$

The output error is given by an adjoint-weighted residual

- Above is only an estimate when the output or equations are nonlinear and the perturbations are finite
- The estimate can be localized to yield an adaptive indicator

Entropy Adjoint Connection

Two disadvantages of adjoint-based output error estimation

1. Adjoint solution is required for each output
2. Only requested outputs are targeted

We seek a *general purpose* adaptive indicator that

- does not require solution of an adjoint problem
- produces an "overall good" solution

One promising approach makes use of the **entropy variables**

Starting point (first-order conservation laws):

$$\underbrace{\mathbf{r}(\mathbf{u}) = \mathbf{A}_i \partial_i \mathbf{u} = 0}_{\text{primal equation}}, \qquad \underbrace{\partial_i F_i = 0}_{\text{entropy conservation}}$$

$F_i(\mathbf{u})$ is the entropy flux associated with an entropy function $U(\mathbf{u})$

Entropy Adjoint Connection (ctd.)

- The entropy pair $(U(\mathbf{u}), F_i(\mathbf{u}))$ must satisfy $U_{\mathbf{u}}\mathbf{A}_i = (F_i)_{\mathbf{u}}$
- The **entropy variables** are defined by

$$\mathbf{v} \equiv U_{\mathbf{u}}^T$$

The entropy variables symmetrize the equations in the sense that

1. $\mathbf{u}_{\mathbf{v}}$ is symmetric, positive definite
2. $\mathbf{A}_i\mathbf{u}_{\mathbf{v}}$ is symmetric

Using these symmetry properties, we have

$$0 = \mathbf{A}_i\partial_i\mathbf{u} = \mathbf{A}_i\mathbf{u}_{\mathbf{v}}\partial_i\mathbf{v} = \mathbf{u}_{\mathbf{v}}\mathbf{A}_i^T\partial_i\mathbf{v} \quad \Rightarrow \quad \mathbf{A}_i^T\partial_i\mathbf{v} = 0$$

The entropy variables satisfy the adjoint equation! (BCs too)

Entropy Adjoint Connection (ctd.)

We examine the adjoint-weighted residual to deduce the output:

$$
\begin{aligned}
\delta J &= \int_\Omega \mathbf{v}^T \delta \mathbf{r}\, d\Omega = \int_\Omega \mathbf{v}^T \mathbf{A}_i \partial_i \delta \mathbf{u}\, d\Omega \\
&= -\int_\Omega \underbrace{\partial_i \mathbf{v}^T \mathbf{A}_i}_{=0} \delta \mathbf{u}\, d\Omega + \int_{\partial\Omega} \underbrace{\mathbf{v}^T \mathbf{A}_i}_{(F_i)_\mathbf{u}} \delta \mathbf{u}\, n_i ds \\
&= \int_{\partial\Omega} (F_i)_\mathbf{u} \delta \mathbf{u}\, n_i ds = \delta \left[\underbrace{\int_{\partial\Omega} F_i n_i ds}_{J} \right]
\end{aligned}
$$

J measures the net entropy flow out of the domain

Primal equation:

$$\mathbf{r}(\mathbf{u}) = \mathbf{A}_i \partial_i \mathbf{u} - \partial_i (\mathbf{K}_{ij} \partial_j \mathbf{u}) = 0$$

- Viscous dissipation is a source term in the adjoint equation for $\mathbf{v}$

The entropy variables serve as an "adjoint" solution for

$$J = \underbrace{\int_{\partial\Omega} F_i n_i ds}_{\text{outflow of } U} + \underbrace{\int_{\Omega} \partial_i \mathbf{v}^T \widetilde{\mathbf{K}}_{ij} \partial_j \mathbf{v}\, d\Omega}_{\text{generation of } U} - \underbrace{\int_{\partial\Omega} \mathbf{v}^T \widetilde{\mathbf{K}}_{ij} \partial_j \mathbf{v}\, n_i ds}_{\text{diffusion of } U}$$

where $\widetilde{\mathbf{K}}_{ij} \equiv \mathbf{K}_{ij} \mathbf{u}_{\mathbf{v}}$ is symmetrized in the sense that $\widetilde{\mathbf{K}}_{ij} = \widetilde{\mathbf{K}}_{ji}^T$

- The expression for J is an entropy balance statement: $J(\mathbf{u}) = 0$
- The terms in J do not necessarily balance for $\mathbf{u}_H$

Using the Entropy Variables

The entropy variables are readily computable from **u**,

$$\mathbf{v} = U_{\mathbf{u}}^T = \left[\frac{\gamma - S}{\gamma - 1} - \frac{1}{2}\frac{\rho V^2}{p}, \quad \frac{\rho u_i}{p}, \quad -\frac{\rho}{p}\right]^T,$$

where the entropy function U is

$$U = -\rho S/(\gamma - 1), \quad S = \ln p - \gamma \ln \rho,$$

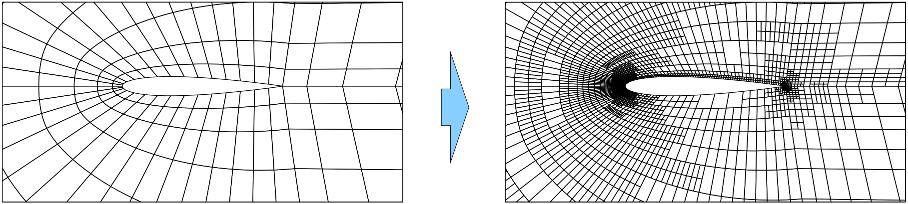
Approach

Use **v** as an adjoint solution in output error estimation

- Targeted areas are those where **entropy generation** or **entropy transport** is not predicted well
- Similar to adapting on residual of entropy transport equation
- *Separate adjoint solve is not required*

Implementation

- Discontinuous Galerkin (DG) finite element discretization
- Discrete adjoint solution
- Error estimation performed on order $p + 1$ space (same mesh)
- Fixed-fraction, isotropic, hanging-node adaptation
- Curved, body-fitted quadrilateral and hexahedral meshes

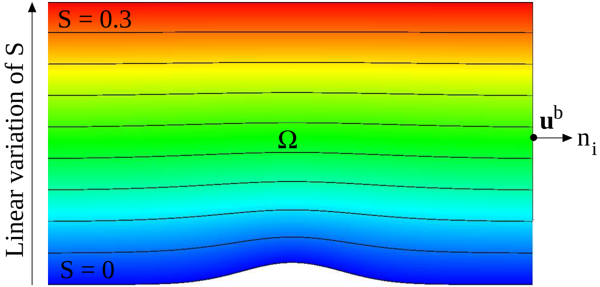


Sample initial mesh   Sample adapted mesh

Verification of the Entropy Adjoint Connection

Compare the entropy variables, $\mathbf{v}_h$, to the discrete adjoint, ψ_h, for

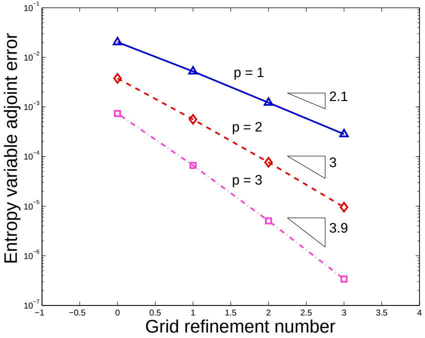
$$J_h = \int_{\partial\Omega} F_i(\mathbf{u}_h^b)\, n_i ds$$

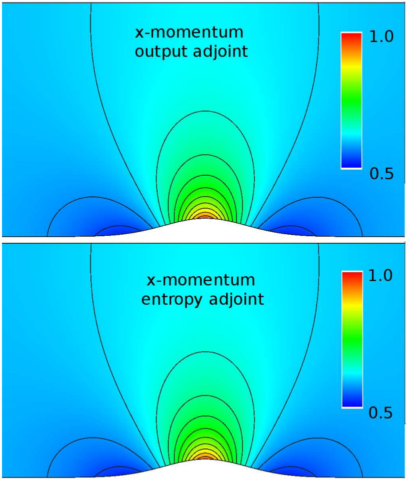


Compute: $\quad$ (Entropy variable adjoint error)$^2 = \int_{\Omega} ||\psi_h - \mathbf{v}_h||_2^2 d\Omega$

Verification of the Entropy Adjoint Connection (ctd.)

Behavior of entropy variable adjoint error under uniform refinement





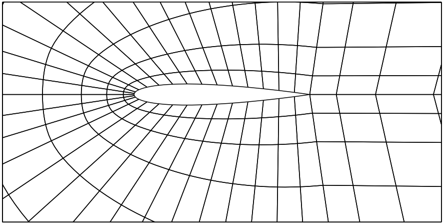
- Error decreases at $O(h^{p+1})$
- The entropy variables are indeed adjoint solutions

NACA 0012, $M = 0.4, \alpha = 5^o$

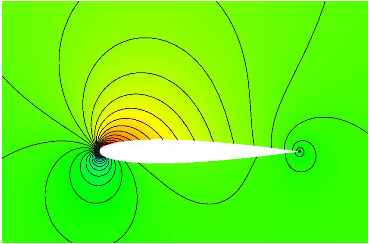
- Hanging-node adaptation
- fixed fraction: 10%
- $q = 5$ geometry representation
- Quadrilateral meshes
- $p = 2$ solution interpolation
- Measured lift and drag

Indicators

1. Drag adjoint
2. Lift adjoint
3. Moment adjoint
4. Entropy adjoint
5. Residual



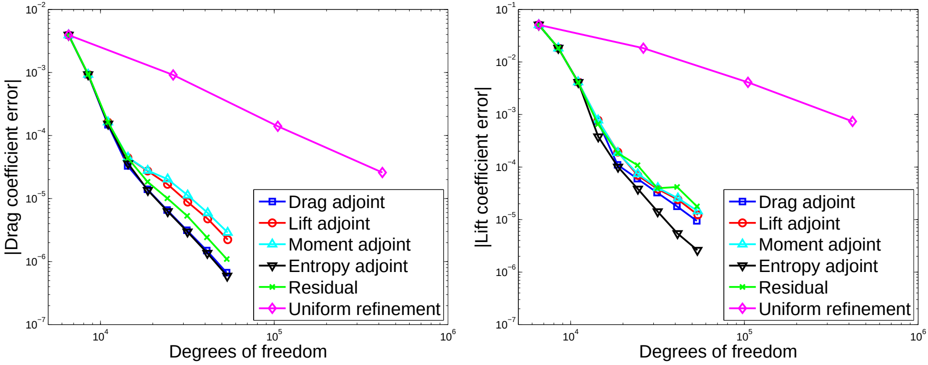
Initial mesh



Mach contours

NACA 0012, $M = 0.4, \alpha = 5^o$

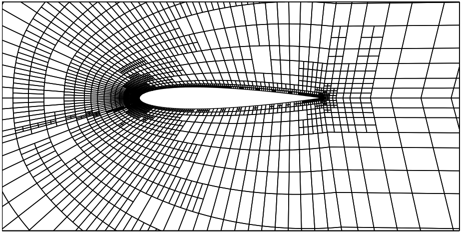
- Degree of freedom (DOF) versus output error for $p = 2$
- Entropy adjoint performance is comparable to output adjoints



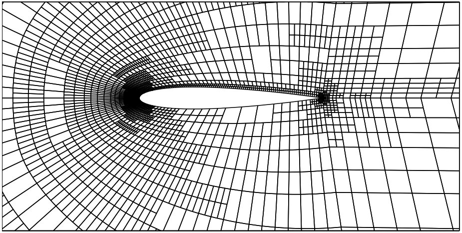
Drag Error

Lift Error

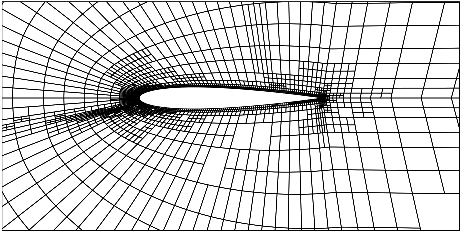
NACA 0012, $M = 0.4, \alpha = 5^o$, Final Meshes



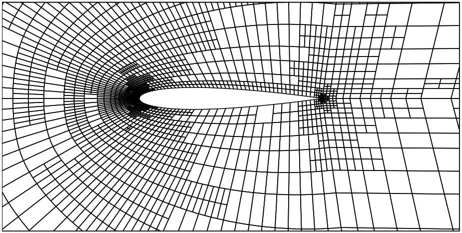
Drag Adjoint



Entropy Adjoint



Lift Adjoint



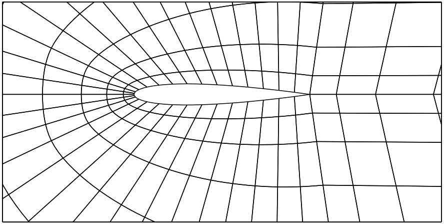
Residual

NACA 0012, $M = 0.5, \alpha = 2^o, Re = 5k$

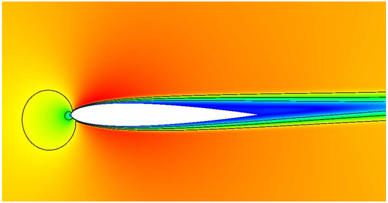
- Hanging-node adaptation
- fixed fraction: 10%
- $q = 3$ geometry representation
- Quadrilateral meshes
- $p = 2$ solution interpolation
- Measured lift and drag

Indicators

1. Drag adjoint
2. Lift adjoint
3. Entropy adjoint
4. Residual
5. Entropy



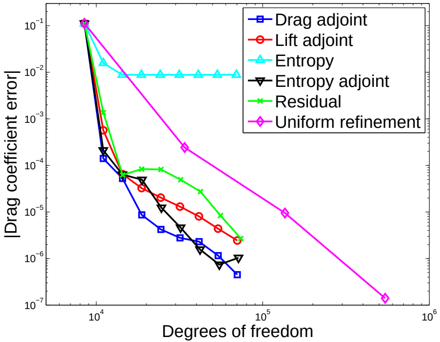
Initial mesh



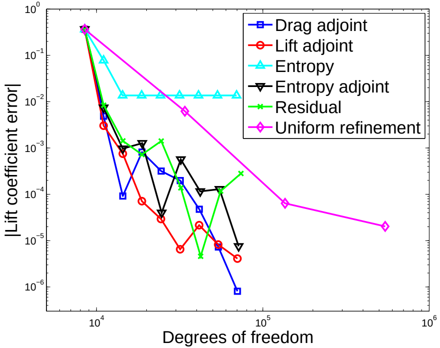
Mach contours

NACA 0012, $M = 0.5, \alpha = 2^o, Re = 5k$

- Degree of freedom (DOF) versus output error for $p = 2$
- Entropy adjoint performance is comparable to output adjoints



Drag Error



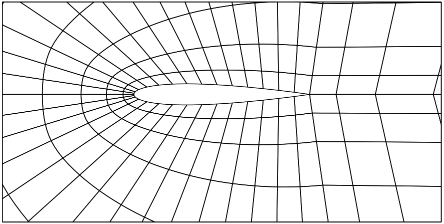
Lift Error

NACA 0012, $M = 0.8, \alpha = 1.25^o$

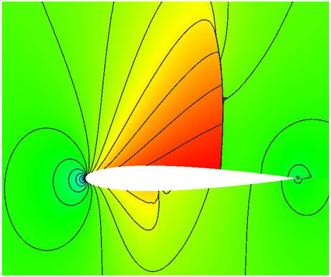
- Hanging-node adaptation
- fixed fraction: 10%
- $q = 3$ geometry representation
- Element-constant artificial viscosity
- $p = 2$ solution interpolation
- Measured lift and drag

Indicators

1. Drag adjoint
2. Lift adjoint
3. Entropy adjoint
4. Residual



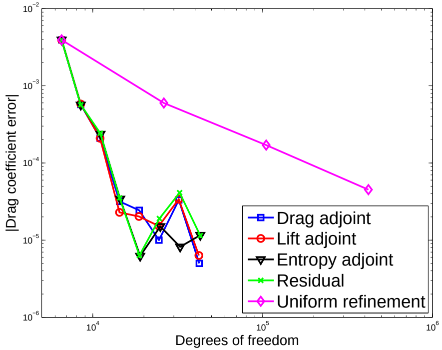
Initial mesh



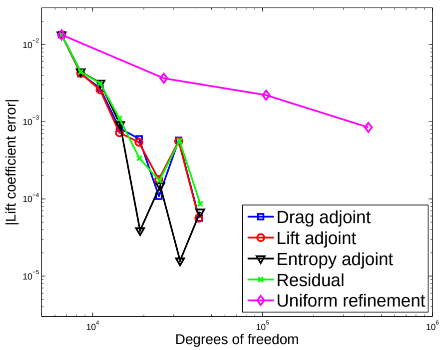
Mach contours

NACA 0012, $M = 0.8, \alpha = 1.25^o$

- Degree of freedom (DOF) versus output error for $p = 2$
- More noise in results – entropy adjoint still performs well

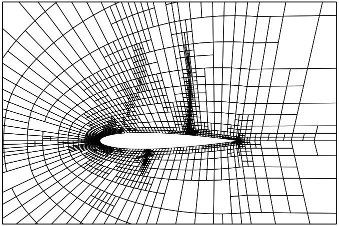


Drag

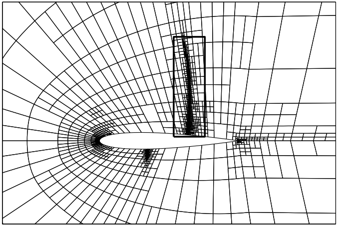


Lift

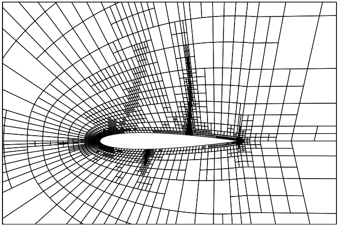
NACA 0012, $M = 0.8, \alpha = 1.25^o$, Final Meshes



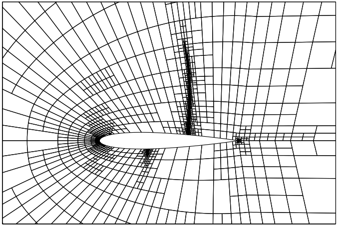
Drag Adjoint (2990)



Entropy Adjoint (2814)



Lift Adjoint (2997)



Residual (2372)

Conclusions

- Output error estimation based on adjoint solutions is a rigorous, but somewhat expensive, approach for targeting select output quantities of interest
- The entropy variables satisfy an adjoint equation; the resulting “entropy adjoint” indicator is cheap to compute and targets errors in entropy generation and transport
- Performance of the entropy adjoint indicator is comparable to standard output adjoints for the flows tested

Ongoing work

- Extension to unsteady flows (entropy adjoint connection holds)
- Application to other conservation laws with an entropy extension
- Relationship to engineering output quantities

Questions?

Acknowledgements

- **P.L. Roe** acknowledges hospitality at the Department of Applied Mathematics and Theoretical Physics, University of Cambridge UK, and the financial support of a William Penney Fellowship from the UK Ministry of Defence
- **K.J. Fidkowski** acknowledges the support of the University of Michigan, Ann Arbor