MANE 6960:

Adjoints for Scientists and Engineers

Lecture 18

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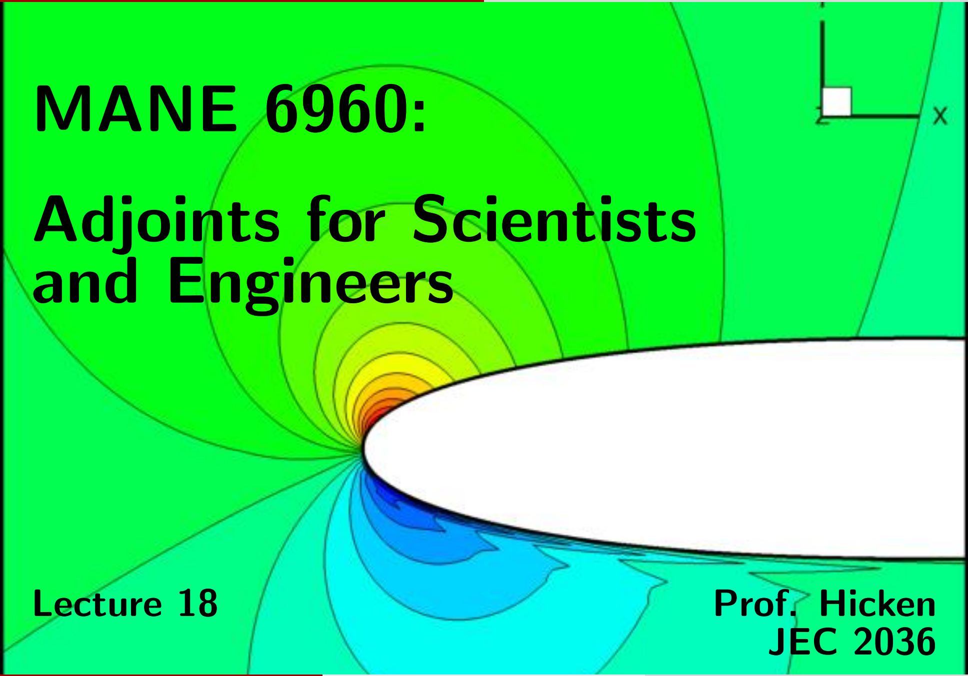
JEC 2036



Motivation

Adjoint-based error estimation and adaptation provides a rigorous framework for controlling output errors.

Nevertheless, the method does have some disadvantages:

- In some cases it is not clear which output should be targeted by the adaptation.
- If multiple outputs are considered, we need multiple adjoint solutions (on the fine space), which can be computationally expensive.
- Most PDE analysis software does not have adjoint capabilities.

Motivation (cont.)

Ideally, we could use the adjoint-based framework, but

- make it more computationally affordable; and
- make it applicable to a wide range of outputs.

In this lecture, I will describe an adjoint-based approach in which we do not need to solve any adjoint problem, at least explicitly.

- The idea, which is described in [FR10], involves the entropy.

Entropy Adjoint for Mesh Adaptation

Review of Entropy

We begin by considering first-order conservation laws (e.g. Euler equations) of the form

$$\frac{\partial F_i(q)}{\partial x_i} = 0. \tag{$\star$}$$

- sum over repeated indices, $i = 1, 2, \ldots, d$.
- $q \in [\mathcal{V}]^q$ are the state variables.
- $F_i : \mathbb{R}^q \to \mathbb{R}^q$ is the conservative flux in the i direction.

Review of Entropy (cont.)

Definition: Entropy Function and Variables [Tad84]

An entropy function, $S : \mathbb{R}^q \rightarrow \mathbb{R}$, is a smooth convex mapping augmented with entropy fluxes, $f_i : \mathbb{R}^q \rightarrow \mathbb{R}$, such that

$$\underbrace{\frac{\partial S}{\partial q}}_{w^T} \frac{\partial F_i}{\partial q} = \frac{\partial f_i}{\partial q}.$$

Scalar

Furthermore, the entropy variables are defined by

$$w = \left(\frac{\partial S}{\partial q}\right)^T$$

Review of Entropy (cont.)

If we assume that the solution q is smooth, and we left multiply the conservation law ($\star$) by w^T, then

$$\frac{\partial S}{\partial q} \underbrace{\frac{\partial F_i}{\partial x_i}}_{=0} = \left(\frac{\partial S}{\partial q} \frac{\partial F_i}{\partial q}\right)\frac{\partial q}{\partial x_i} = \frac{\partial f_i}{\partial q}\frac{\partial q}{\partial x_i}$$

$$= \frac{\partial f_i}{\partial x_i} = 0$$

- Thus, entropy S is conserved in a smooth flow
- More generally, e.g. flows with shocks, S is monotonically decreasing in time.

Review of Entropy (cont.)

Another important result, in the present context, is that performing a change of variables to w symmetrizes the conservation law.

To see this, we need the following two results; see, e.g., [Tad84].

1. The inverse Hessian

$$\frac{\partial q}{\partial w} = \left(\frac{\partial w}{\partial q}\right)^{-1} = \left(\frac{\partial^2 S}{\partial q^2}\right)^{-1},$$

Note:

$\frac{\partial}{\partial q}(q) = I$

$\frac{\partial q}{\partial w}\frac{\partial w}{\partial q} = I$

is symmetric positive definite.

S is convex

2. $\dfrac{\partial F_i}{\partial q}\dfrac{\partial q}{\partial w}$ is symmetric

Review of Entropy (cont.)

Using these results, we have

$$0 = \frac{\partial F_i}{\partial x_i} = \frac{\partial F_i}{\partial q} \frac{\partial q}{\partial x_i}$$

$$= \left(\frac{\partial F_i}{\partial q} \frac{\partial q}{\partial w}\right)^T \frac{\partial w}{\partial x_i} \qquad \because \left(\frac{\partial F_i}{\partial q} \frac{\partial q}{\partial w}\right) \text{ is sym}$$

$$= \underbrace{\left(\frac{\partial q}{\partial w}\right)^T}\left[\left(\frac{\partial F_i}{\partial q}\right)^T \frac{\partial w}{\partial x_i}\right] = 0$$

This is $\frac{\partial^2 S}{\partial q^2}$, an invertable matrix (Why?)

Connection to Adjoints

We see that the entropy variables w satisfy the equation

$$\left(\frac{\partial F_i}{\partial q}\right)^T \frac{\partial w}{\partial x_i} = 0,$$

which suggests that they can be interpreted as adjoint variables.

If so, what is the output corresponding to these adjoint variables?

Connection to Adjoints (cont.)

Let $J(q)$ denote the (as yet) unknown functional and form the Lagrangian

$$L(q,\psi) = J(q) + \int_{\Omega} \psi^T \frac{\partial F_i}{\partial x_i}\, d\Omega.$$

Next, we take directional derivative of L with respect to q in the (arbitrary) direction v and set the result to zero: (this gives adj eq'n)

$$L'[q]v = J'[q]v + \int_{\Omega} \psi^T \frac{\partial}{\partial x_i}\left(\frac{\partial F_i}{\partial q} v\right) d\Omega = 0 \quad \forall\, v \in \mathcal{V}$$

$$= J'[q]v - \int_{\Omega} v^T \left(\frac{\partial F_i}{\partial q}\right)^T \frac{\partial \psi}{\partial x_i}\, d\Omega$$

$$+ \int_{\partial\Omega} v^T \left(\frac{\partial F_i}{\partial q}\right)^T \psi\, n_i\, d\Gamma = 0, \quad \forall\, v \in \mathcal{V}$$

Connection to Adjoints (cont.)

Next, we replace ψ with w to find that

$$L'[q]v = J'[q]v - \int_{\Omega} v^T \cancelto{0}{\left[\left(\frac{\partial F_i}{\partial q} \right)^T \frac{\partial w}{\partial x_i} \right]} d\Omega$$

$$+ \int_{\partial\Omega} v^T \left(\frac{\partial F_i}{\partial q} \right)^T w \, n_i \, d\Gamma = 0, \quad \forall v \in \mathcal{V}$$

But $\left(\frac{\partial F_i}{\partial q}\right)^T \frac{\partial w}{\partial x_i} = 0$; thus, rearranging gives

$$J'[q]v = - \int_{\partial\Omega} \underbrace{\overbrace{\frac{\partial S}{\partial q}}^{w^T} \frac{\partial F_i}{\partial q}}_{= \frac{\partial f_i}{\partial q}} v \, n_i \, d\Gamma$$

$$= D_v \underbrace{\left[- \int_{\partial\Omega} f_i(q) \, n_i \, d\Gamma \right]}_{J}$$

Connection to Adjoints (cont.)

The output corresponding to the entropy adjoint for first-order conservation laws is the flux of entropy into the domain:

$$J(q) = -\int_{\partial\Omega} f_i(q) n_i \, d\Gamma.$$

Second-order Conservation Laws

Next, we consider second-order conservation laws of the form

$$\frac{\partial F_i}{\partial x_i} - \frac{\partial}{\partial x_i}\left(K_{ij} \frac{\partial q}{\partial x_j} \right) = 0. \tag{$\dagger$}$$

- In addition to the previous requirements on the entropy, we now also require that w symmetrize K_{ij}:

$$\tilde{K}_{ij} = K_{ij} \frac{\partial q}{\partial w}, \qquad \text{with} \qquad (\tilde{K}_{ij})^T = \tilde{K}_{ij}.$$

Second-order Conservation Laws (cont.)

In this case, the entropy variables do not satisfy the adjoint form of (†), i.e. adjoint PDE without source terms.

Nevertheless, the entropy variables still represent the sensitivity to residual perturbations of a specific output.

Second-order Conservation Laws (cont.)

The analysis shows that [FR10]

$$J(q) = \underbrace{-\int_{\partial\Omega} f_i(q) n_i \, d\Gamma}_{1} \underbrace{- \int_{\Omega} \frac{\partial w^T}{\partial x_i} K_{ij} \frac{\partial q}{\partial x_j} \, d\Omega}_{2} + \underbrace{\int_{\partial\Omega} w^T K_{ij} \frac{\partial q}{\partial x_j} n_i \, d\Gamma}_{3}.$$

1. convective inflow of entropy
2. generation of entropy due to viscous dissipation
3. entropy diffusion across boundary

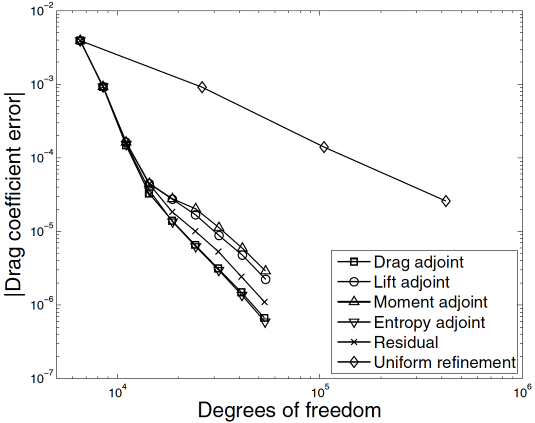
Entropy Adjoint and Mesh Adaptation

The theory above indicates that we can use the entropy variables w as adjoints in the AWR that targets the above functionals:

- No need to solve for adjoint variables, since $w = w(q)$ is explicit.
- For analytical solutions, J should be zero, because the source terms will be balanced by the boundary terms.
- Can show that the AWR in this case is equivalent to adapting on the entropy-transport residual [FR10].

Entropy Adjoint: Example 1

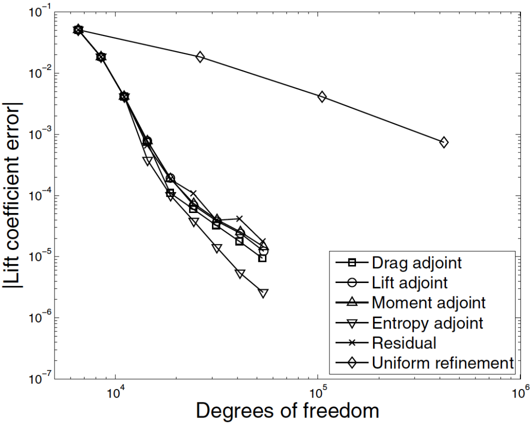
NACA 0012 in inviscid flow, $M_\infty = 0.4$, $\alpha = 5°$.



Error in drag as a function of DOF [FR10]

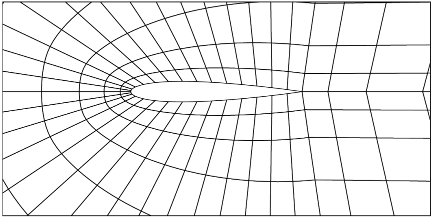
Entropy Adjoint: Example 1 (cont.)

NACA 0012 in inviscid flow, $M_\infty = 0.4$, $\alpha = 5°$.



Error in lift as a function of DOF [FR10]

Entropy Adjoint: Example 1 (cont.)



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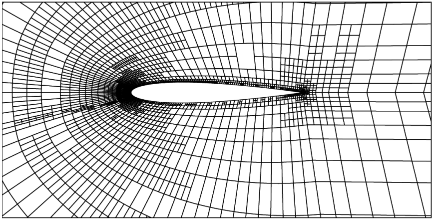
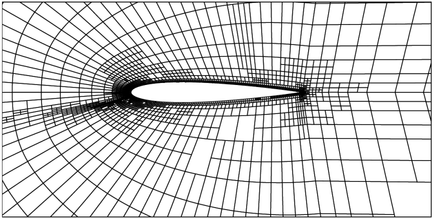
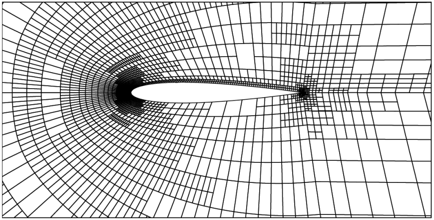


drag



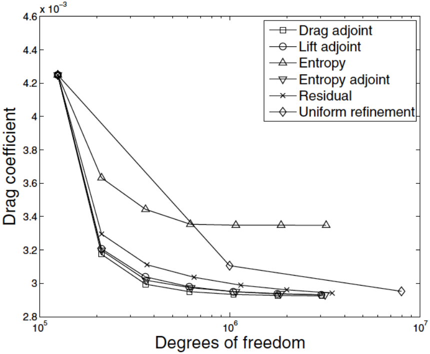
lift



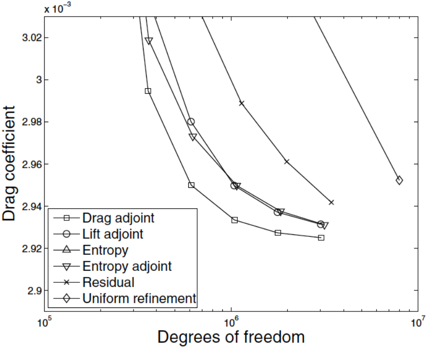
entropy

Entropy Adjoint: Example 2

Rectangular wing in inviscid flow, $M_\infty = 0.4$, $\alpha = 3°$.



drag error

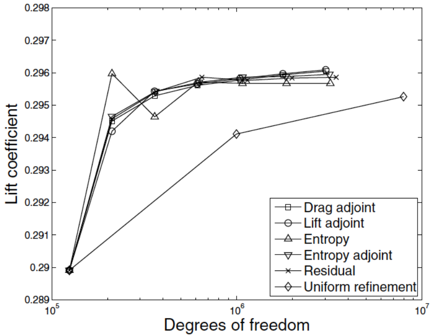


drag error zoom

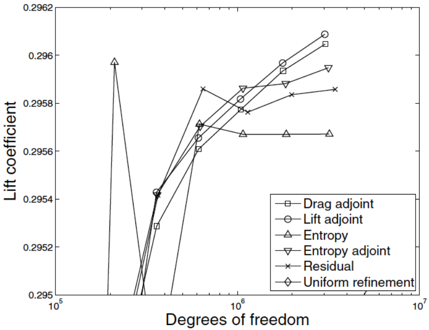
Error in drag as a function of DOF [FR10]

Entropy Adjoint: Example 2 (cont.)

Rectangular wing in inviscid flow, $M_\infty = 0.4$, $\alpha = 3°$.



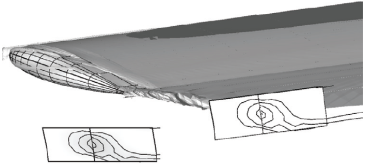
lift error



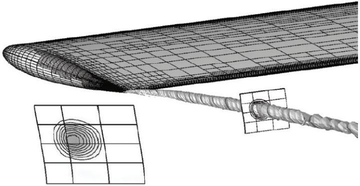
lift error zoom

Error in lift as a function of DOF [FR10]

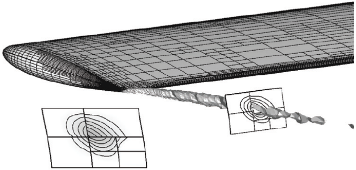
Entropy Adjoint: Example 2 (cont.)



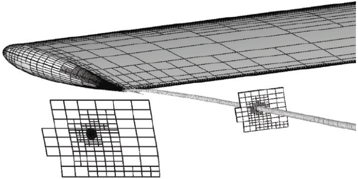
initial



drag



lift



entropy

References

[FR10] Krzysztof J. Fidkowski and Philip L. Roe, *An entropy adjoint approach to mesh refinement*, SIAM Journal on Scientific Computing **32** (2010), no. 3, 1261–1287.

[Tad84] Eitan Tadmor, *Skew-selfadjoint form for systems of conservation laws*, Journal of Mathematical Analysis and Applications **103** (1984), no. 2, 428–442.