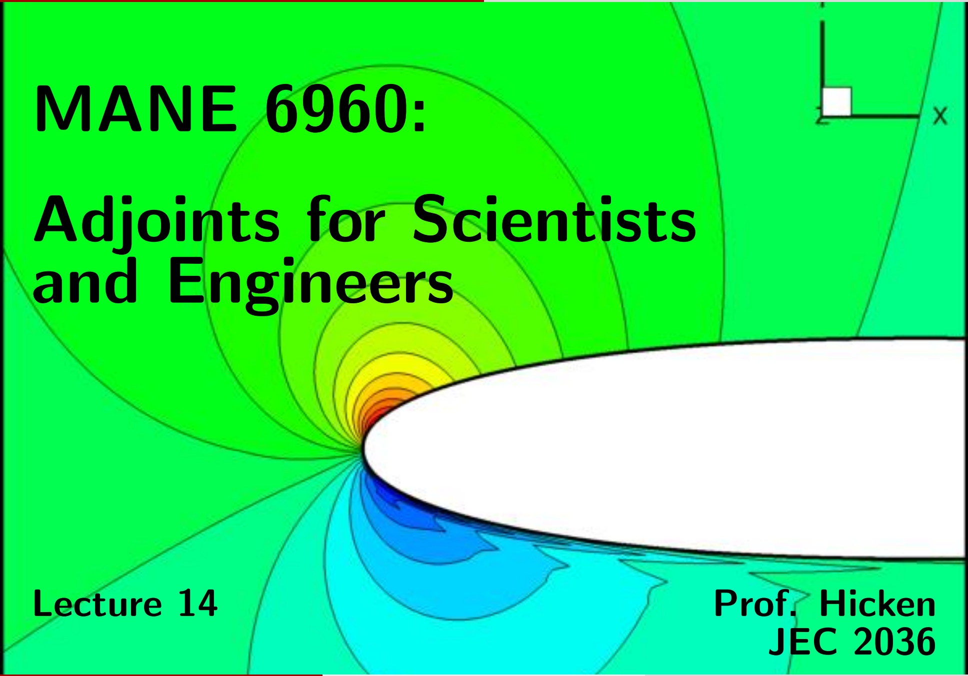
MANE 6960:

Adjoints for Scientists and Engineers



Lecture 14

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JEC 2036

Motivation

Last class I introduced the adjoint-weighted residual (AWR) method in the context of linear BVPs and linear functionals.

In this lecture, I will first generalize the AWR method to nonlinear problems. Subsequently, I will describe various approximations that are used to make the method useful in practice.

AWR Method for Nonlinear Problems

Problem Statement

Let $R_H : \mathbb{R}^S \to \mathbb{R}^S$ be the residual corresponding to the discretization of a nonlinear BVP on a mesh of nominal size H. Furthermore, let $u_H \in \mathbb{R}^S$ be the solution to

$$R_H(u_H) = 0.$$

Our goal is to estimate the functional error

$$\delta J_H = J_H(u_H) - J(u),$$

where $J(u)$ is the exact (nonlinear) functional value based on the exact solution of the nonlinear BVP, and $J_H(u_H)$ is the discretized functional value based on the discrete solution.

Averaged derivatives

Proceeding as in the linear case, we have

$$\delta J_H \approx J_H(u_H) - J_h(u_h),$$

where $u_h \in \mathbb{R}^s$ is the solution to $R_h(u_h) = 0$, the discretized BVP on a fine mesh with nominal element size h.

For the subsequent analysis, we define

$$\delta u_h \equiv u_h^H - u_h,$$

where, as before, $u_h^H \equiv I_h^H u_H$ is the coarse solution represented on the fine mesh/space.

Averaged derivatives (cont.)

Thus, we have

$$\begin{aligned} J_H(u_H) - J_h(u_h) &= J_h(u_h^H) - J_h(u_h) \\ &= J_h(u_h + \delta u_h) - J_h(u_h). \end{aligned}$$

Unlike the linear case, we cannot express this functional difference as a functional of the difference. However, notice that

$$\begin{aligned} J_h(u_h + \delta u_h) - J(u_h) &= \int_0^1 \frac{d}{ds} J_h(u_h + s\,\delta u_h)\, ds \\ &= \int_0^1 J_h'[u_h + s\,\delta u_h]^T \delta u_h\, ds \\ &= \left(\int_0^1 J_h'[u_h + s\,\delta u_h]\, ds \right)^T \delta u_h \end{aligned}$$

Averaged derivatives (cont.)

Consequently, the functional difference is equal to an averaged derivative times δu_h.

$$(g_h, \delta u_h)_h = g_h^T \delta u_h \qquad \rightarrow \qquad \left(\int_0^1 J_h'[u_h + s\delta u_h]\, ds \right)^T \delta u_h.$$

Linear case Non linear case

This suggests that we define the adjoint in a slightly different way from the linear case...

Definition: Mean-value Adjoint [FD11]

The (discrete) mean-value adjoint is denoted by $\overline{\psi}_h$ and satisfies the linear equation

$$\left(\overline{R}_h[u_h, u_h^H]\right)^T \overline{\psi}_h = \left(\overline{J}_h[u_h, u_h^H]\right)^T,$$

where the averaged Jacobian and gradient are, respectively,

$$\overline{R}_h[u_h, u_h^H] \equiv \int_0^1 R_h'[u_h + s\delta u_h]\, ds$$

$$\overline{J}_h[u_h, u_h^H] \equiv \int_0^1 J_h'[u_h + s\delta u_h]\, ds.$$

Mean-value Adjoint

Notice that we have the following identities:

$$\overline{R}_h[u_h, u_h^H]\delta u_h = \int_0^1 R_h'[u_h + s\,\delta u_h]\,\delta u_h\,ds$$

$$= \int_0^1 \frac{d}{ds} R_h(u_h + s\,\delta u_h)\,ds$$

$$= R_h(u_h + \delta u_h) - R_h(u_h) \qquad (1)$$

Similarly

$$\overline{J}_h[u_h, u_h^H]\delta u_h = J_h(u_h + \delta u_h) - J_h(u_h) \qquad (2)$$

Mean-value Adjoint (cont.)

Using the above identities, as well as the definition of the mean-value adjoint, we find that

$$J_h(u_h + \delta u_h) - J_h(u_h) = \bar{J}_h[u_h, u_h^H]\,\delta u_h \quad , \quad \text{by } (2)$$

$$= \bar{\Psi}_h^T \bar{R}_h[u_h, u_h^H]\,\delta u_h \quad , \quad \text{by def}^n\ \bar{\Psi}_h$$

$$= \bar{\Psi}_h^T \left(R_h(u_h + \delta u_h) - \cancelto{0}{R_h(u_h)} \right) \quad , \quad \text{by } (1)$$

$$= \bar{\Psi}_h^T R_h(u_h^H)$$

Mean-value Adjoint (cont.)

Theorem: AWR for nonlinear problems

Let u_H denote the solution to $R_H(u_H) = 0$, which corresponds to a discretized BVP on a coarse space. Analogously, let u_h denote the solution of $R_h(u_h) = 0$, the fine-space discretization of the same BVP. Then the difference

$$J_H(u_H) - J_h(u_h) = \overline{\psi}_h^T R_h(u_h^H),$$

where $\overline{\psi}_h$ is the solution to the mean-value adjoint equation on the fine-space.

AWR Approximations

Problems with the AWR Method

There is a significant computational cost when applying the AWR method to nonlinear problems: the mean-value adjoint.

- The mean-value adjoint requires the integral of potentially expensive derivatives.

The AWR method, whether it is used on linear or nonlinear problems, has another drawback.

- The adjoint, ψ_h or $\overline{\psi}_h$, is needed on the fine mesh/space.

Let's consider the approximations used to mitigate these costs.

Avoiding the Mean-value Adjoint

We can avoid the mean-value adjoint by replacing the integrated Jacobian and gradient with point derivatives as follows:

$$J_h(u_h + \delta u_h) - J_h(u_h) = \int_0^1 J_h'[u + s\,\delta u_h]\,\delta u_h\,ds$$

$$= \cancel{J_h(u_h)} + J_h'[u_h]\,\delta u_h + O(\|\delta u_h\|^2) - \cancel{J_h(u_h)}$$

$$\doteq J_h'[u_h]\,\delta u_h + O(\|\delta u_h\|^2)$$

Avoiding the Mean-value Adjoint (cont.)

Based on the above approximation, we can use the adjoint corresponding to the linearization about u_h:

$$(R'_h[u_h])^T \psi_h = J'_h[u_h].$$

no averaged derivatives

Thus,

$$J_h(u_h + \delta u_h) - J_h(u_h) = J_h'[u_h]\,\delta u_h + O(\|\delta u_h\|^2)$$

$$= \psi_h^T R_h'[u_h]\,\delta u_h + O(\|\delta u_h\|^2)$$

$$= \psi_h^T \left(R_h(u_h + \delta u_h) - \cancel{R_h(u_h)}^{\,0} \right) + O(\|\delta u_h\|^2)$$

$$= \psi_h^T R_h(u_h^H) + O(\|\delta u_h\|^2)$$

Avoiding the Mean-value Adjoint (cont.)

The above approximation for the mean-value adjoint is frequently used in the practice.

- The approximation is justified provided δu_h is sufficiently small.
- If the problem is highly nonlinear (e.g. shocks), then δu_h may become large.

Avoiding Fine-space Solutions

The second problem with the exact AWR is the need for ψ_h, which implies the solution of

$$(R'_h[u_h])^T \psi_h = J'_h[u_h].$$

This is problematic for two reasons:

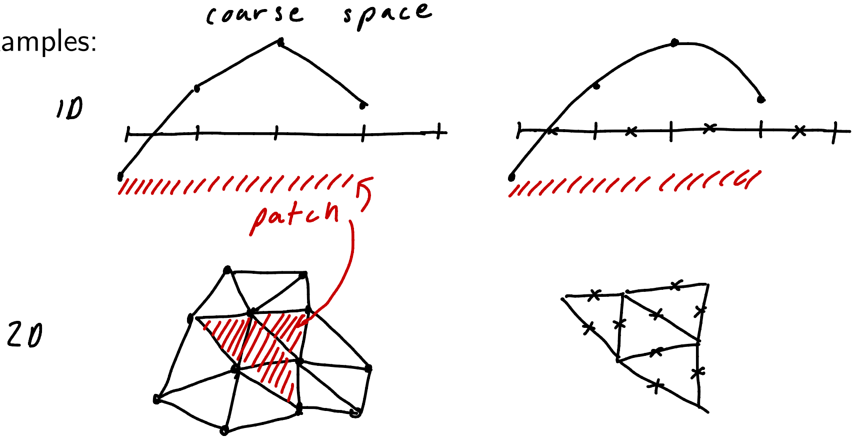
- The linear system for ψ_h may be significantly larger than the baseline problem for u_H.
- The Jacobian and gradient are linearized about u_h, which we do not have.

nonlinear case only

Avoiding Fine-space Solutions (cont.)

One common approach to approximate ψ_h (and u_h), is to use a patch-based reconstruction, in which ψ_H is interpolated onto the fine space using a larger stencil.

Examples:



Avoiding Fine-space Solutions (cont.)

A disadvantage of the reconstruction approach, especially in the case of u_h, is that it does not account for the physics of the problem.

- A high-order interpolation is not justified near a discontinuity, such as a shock.

Avoiding Fine-space Solutions (cont.)

Consequently, a second common approach is to approximately solve for ψ_h using a few iterations of an iterative method.

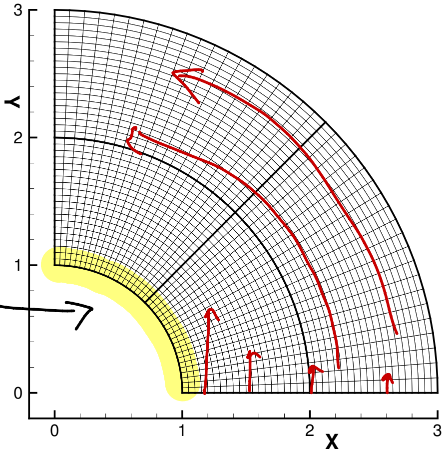
- This is justified, since the difference $\psi_h^H - \psi_h$ is likely to contain mostly high-frequency terms that can be eliminated rapidly using a suitable stationary iterative method (i.e. a smoother).

AWR Examples: Euler Equations

Vortex Flow [Hic12]

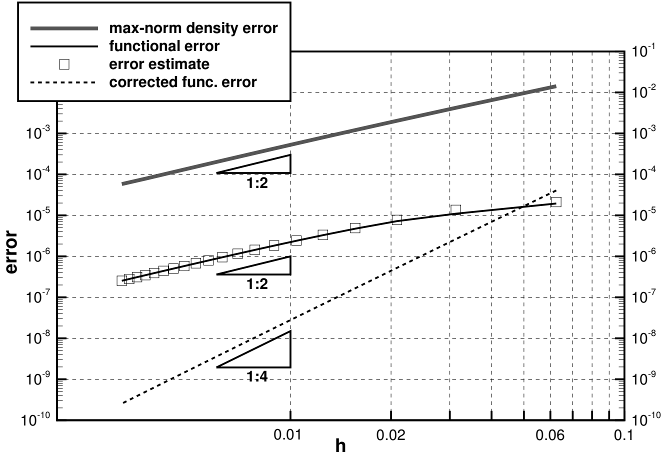
Isentropic Vortex flow:

- streamlines are concentric circles
- smooth solution (ideal case)
- functional is force in x-direction over inner radius.



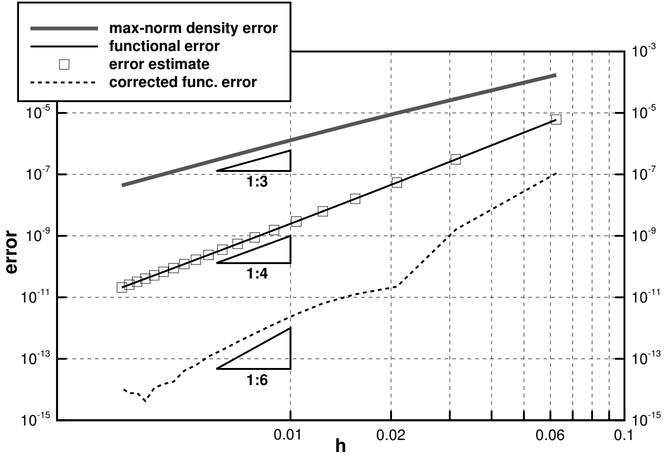
Vortex Flow [Hic12] (cont.)

2nd-order coarse space; 3rd-order fine space



Vortex Flow [Hic12] (cont.)

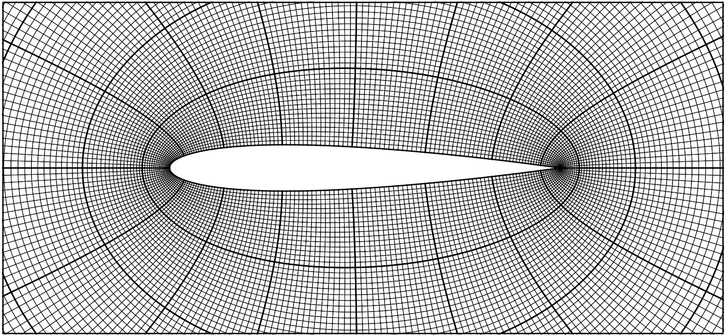
3rd-order coarse space; 4th-order fine space



Subsonic Airfoil [Hic12]

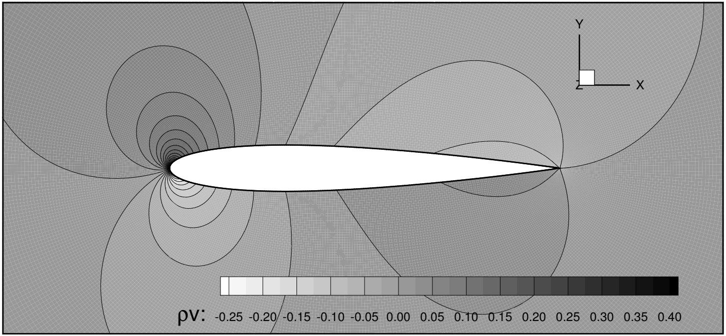
Mach 0.5 flow over NACA 0012

- functional is coefficient of drag
- flow and adjoint fields have singularities at trailing edge



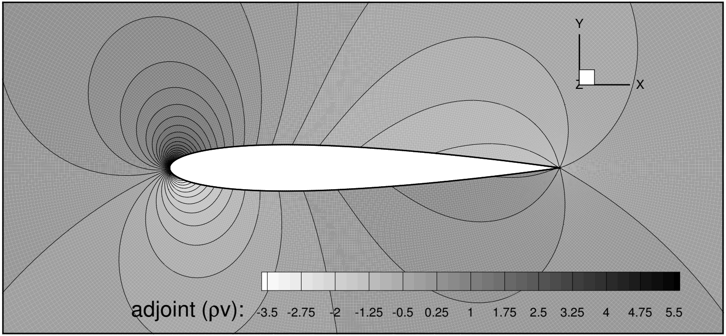
Subsonic Airfoil [Hic12] (cont.)

ρv contours



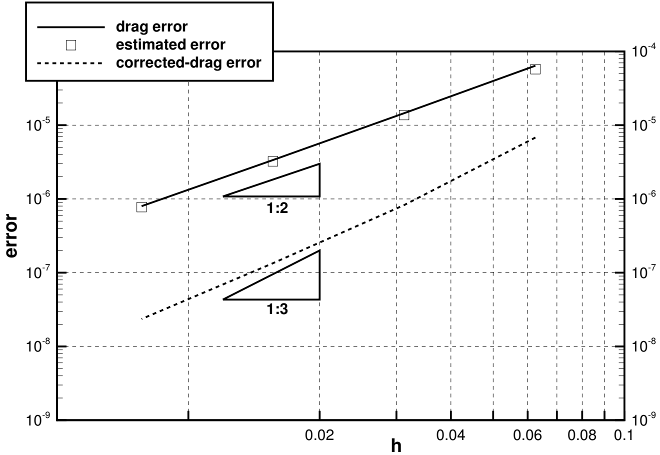
Subsonic Airfoil [Hic12] (cont.)

$\psi_{\rho v}$ contours



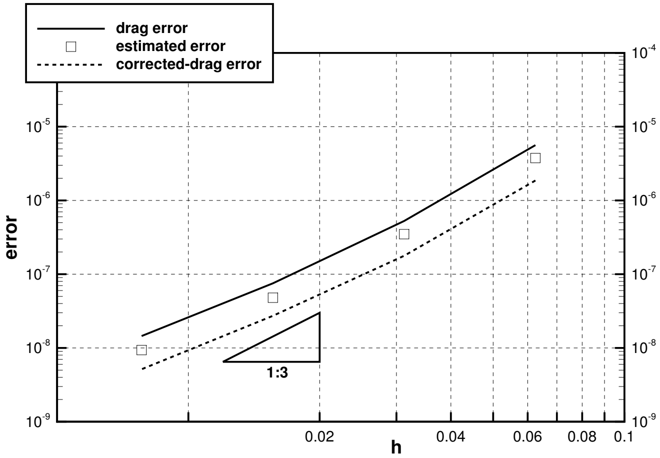
Subsonic Airfoil [Hic12] (cont.)

2nd-order coarse space; 3rd-order fine space



Subsonic Airfoil [Hic12] (cont.)

3rd-order coarse space; 4th-order fine space



References

[FD11] Krzysztof J. Fidkowski and David L. Darmofal, *Review of output-based error estimation and mesh adaptation in computational fluid dynamics*, AIAA Journal **49** (2011), no. 4, 673–694.

[Hic12] Jason E. Hicken, *Output error estimation for summation-by-parts finite-difference schemes*, Journal of Computational Physics **231** (2012), no. 9, 3828–3848.