Adjoint-Based Error Estimation and Mesh Adaptation for Problems with Output Constraints

Marco Ceze
NASA - ORAU

Ben Rothacker and Krzysztof Fidkowski
University of Michigan

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Context and Motivation

Output-based error estimation and mesh adaptation

- Demonstrated applicability to a wide range of aerospace engineering problems.
- Present in production-level codes, *e.g.*: Cart3D, FUN3D.
- Many challenges have been addressed: turbulence modeling, unsteady flows, mesh optimization, *hp*-adaptation, and complex geometries.

Constrained problems are ubiquitous

- Output prediction under trimmed conditions, *e.g.:* DPW.
- Current multi-output adaptive strategies consider static combinations of outputs.
- Various outputs have different domains of dependence.
- Most interesting optimization problems are constrained – how to incorporate constraint errors in the objective function?

Outline of this work

- Discontinuous Galerkin spatial discretization.
- CPTC nonlinear solver with relaxed line-search.
- Exact Jacobian with element-line-Jacobi preconditioner and GMRES linear solver.
- Roe solver for inviscid flux and BR2 for viscous discretization.
- MPI parallelization node-edge weighted mesh partitioning.
- ICCFD7 version of the SA turbulence model.
- ALE mesh deformation for trimming.

In this talk

- Derive an error correction procedure for output-constrained problems.
- Demonstrate adaptive benefits of including constraint-related error.

Problem Statement

Solve the residual equation:

$$\mathbf{R}(\mathbf{U}, \boldsymbol{\alpha}) \quad = \quad \mathbf{0},$$

where:

- $\mathbf{R} \in \mathbb{R}^N$: vector of N residuals that must be driven to zero
- $\mathbf{U} \in \mathbb{R}^N$: state vector that encodes the flow state
- $\boldsymbol{\alpha} \in \mathbb{R}^{N_\alpha}$: trimming parameter vector (trimming "knobs")
- $J^{\text{adapt}}(\mathbf{U}, \boldsymbol{\alpha})$: scalar output on which we want to adapt
- $\mathbf{J}^{\text{trim}}(\mathbf{U}, \boldsymbol{\alpha}) \in \mathbb{R}^{N_\alpha}$: vector of outputs used to define trimming constraints

We want to predict $J^{\text{adapt}}(\mathbf{U}, \boldsymbol{\alpha})$ to $\varepsilon^{\text{adapt}}$ accuracy, subject to flow equations and the following N_α constraints:

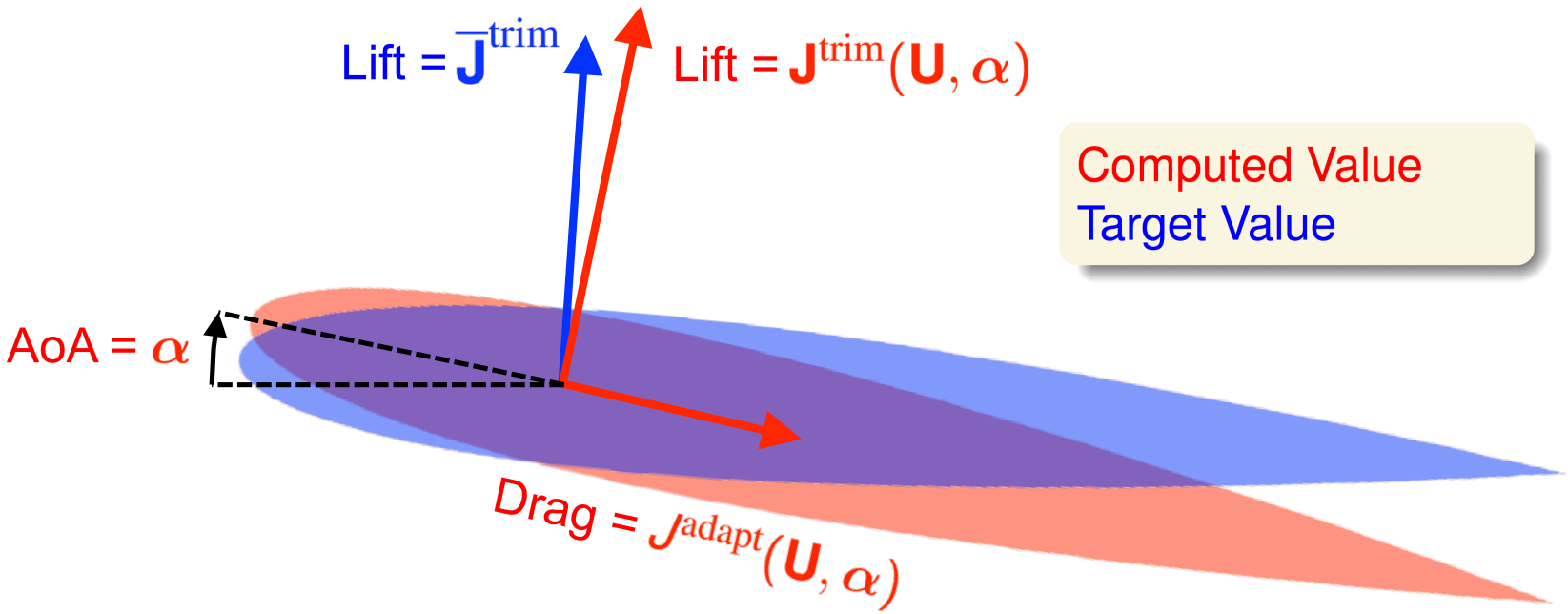
$$\mathbf{J}^{\text{trim}}(\mathbf{U}, \boldsymbol{\alpha}) - \overline{\mathbf{J}}^{\text{trim}} = \mathbf{0}$$

$\overline{\mathbf{J}}^{\text{trim}} \in \mathbb{R}^{N_\alpha}$ is a set of user-specified trim outputs/constraints.

Problem Statement: Example

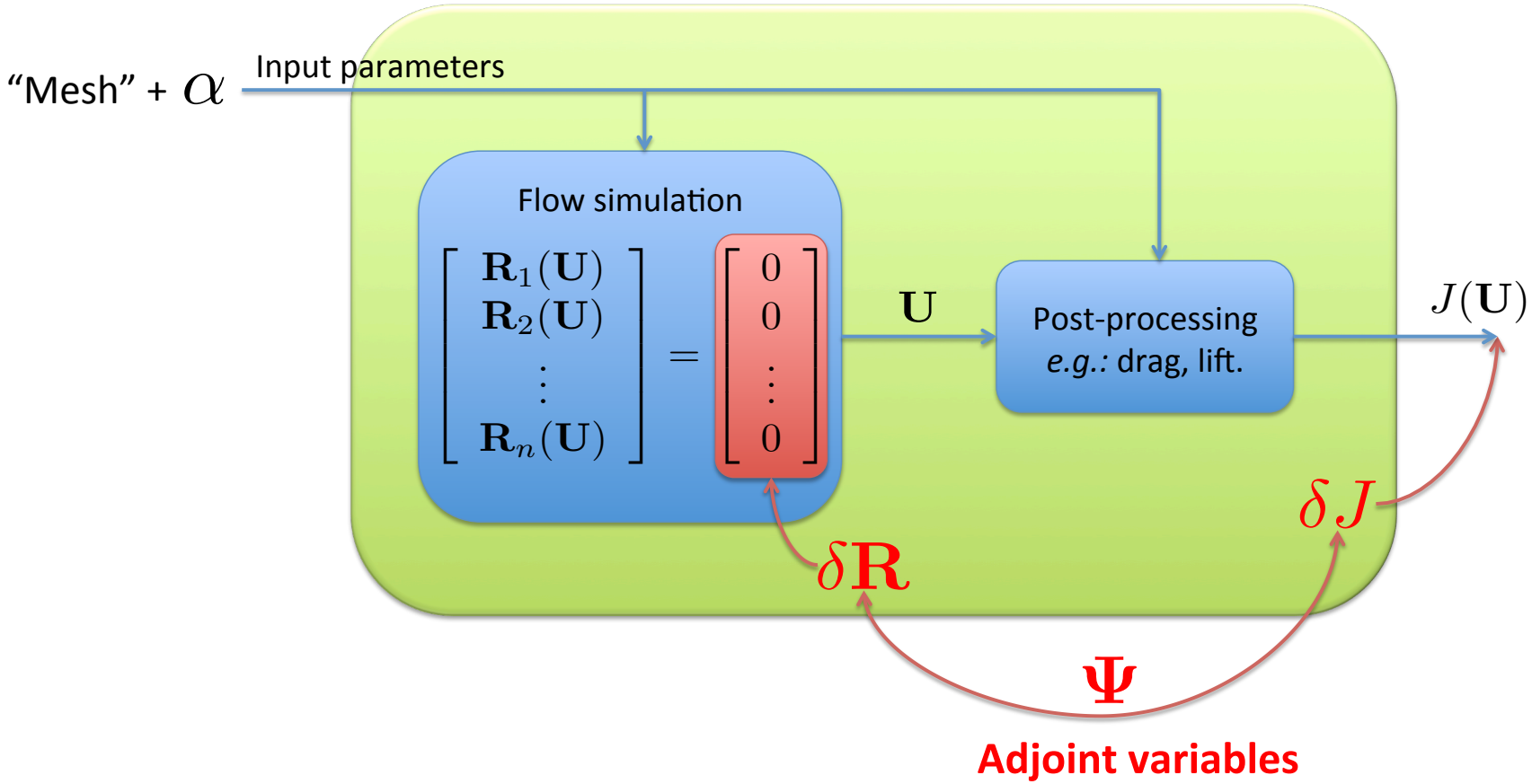
Consider drag prediction under fixed lift:

- $N_\alpha = 1$
- α: single trimming parameter (angle of attack, for example)



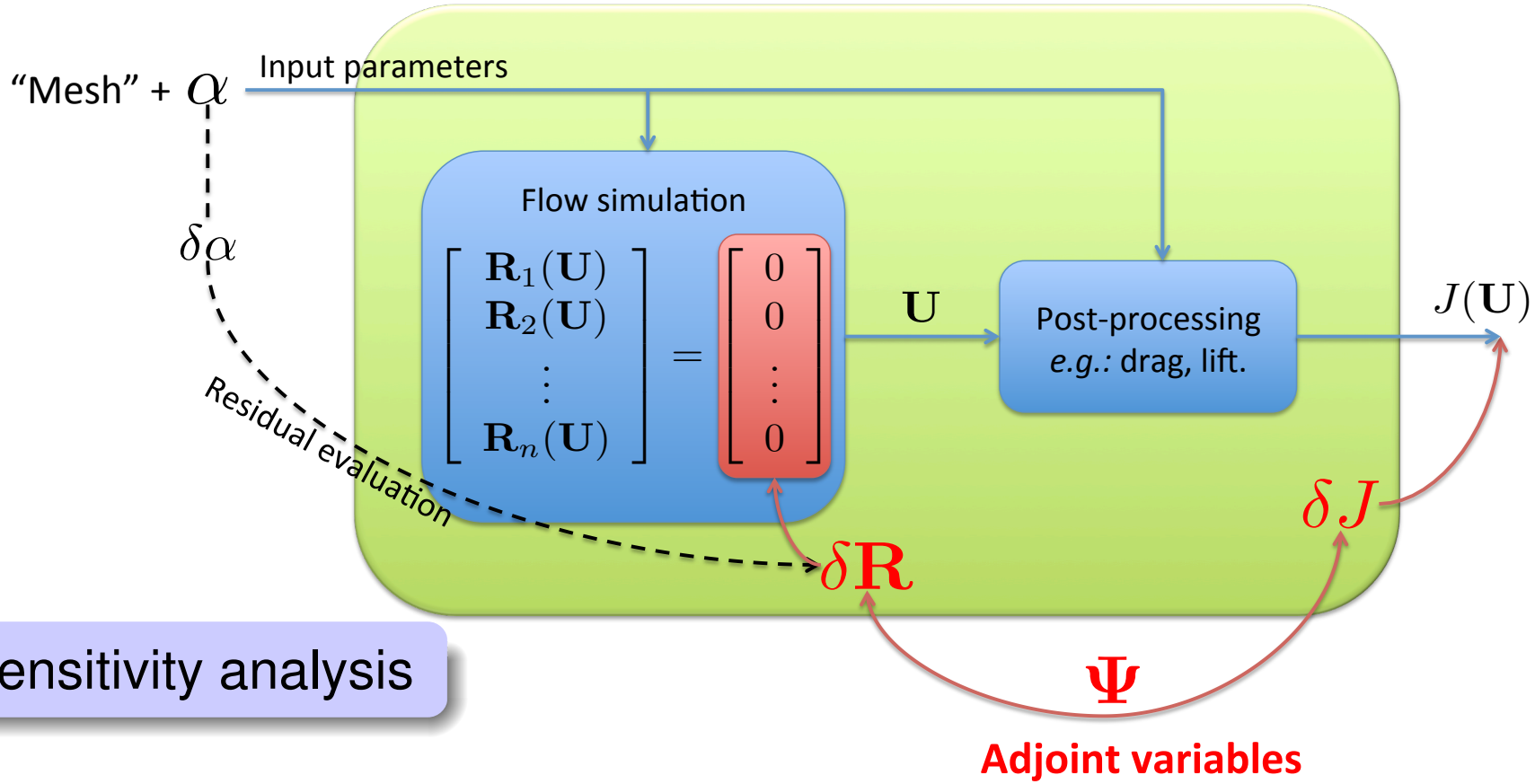
Key ingredient: an adjoint

- Sensitivity of the output w.r.t. residuals in the physics.
- Input perturbations are converted into residual perturbations.
- **Advantage:** residuals are generally cheap to compute.



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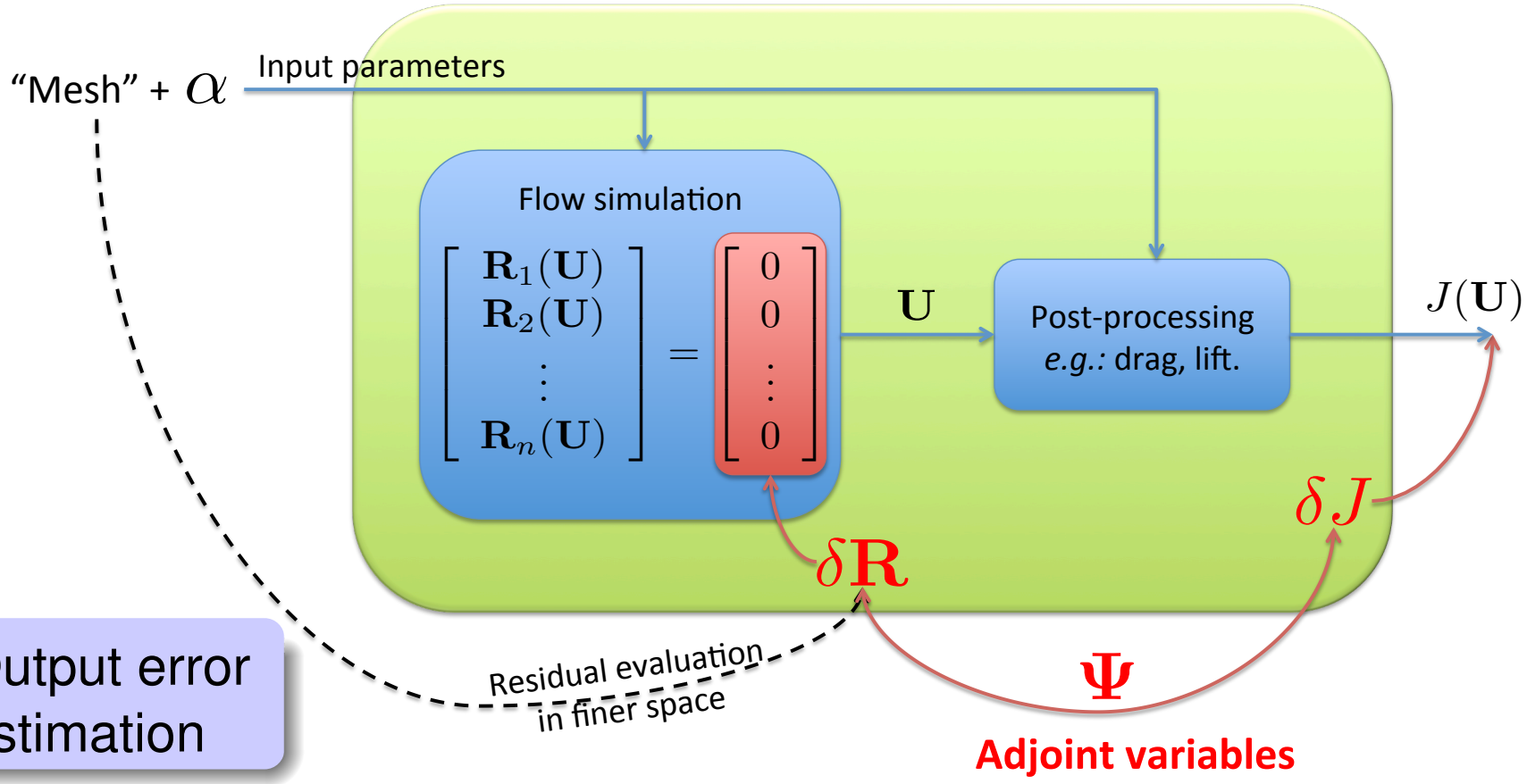
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Sensitivity analysis

Key ingredient: an adjoint

- Sensitivity of the output w.r.t. residuals in the physics.
- Input perturbations are converted into residual perturbations.
- **Advantage:** residuals are generally cheap to compute.



A derivation of the adjoint equation

- Consider an output $\mathcal{J}((\boldsymbol{\alpha}), \mathbf{u})$ where $\mathbf{u}$ satisfies $\mathcal{R}((\boldsymbol{\alpha}), \mathbf{u}) = 0$ for a fixed input parameter set $\boldsymbol{\alpha}$.
- We form a Lagrangian $\mathcal{L}((\boldsymbol{\alpha}), \mathbf{u}, \boldsymbol{\psi})$ to incorporate the constraint:

$$\mathcal{L}((\boldsymbol{\alpha}), \mathbf{u}, \boldsymbol{\psi}) = \mathcal{J}(\mathbf{u}) + \boldsymbol{\psi}^T \mathcal{R}((\boldsymbol{\alpha}), \mathbf{u}).$$

- We take the variation of the Lagrangian assuming $\mathcal{R}((\boldsymbol{\alpha}), \mathbf{u}) = 0$:

$$\delta\mathcal{L}((\boldsymbol{\alpha}), \mathbf{u}, \boldsymbol{\psi}) = \underbrace{\left(\frac{\partial \mathcal{J}}{\partial \mathbf{u}}^T + \boldsymbol{\psi}^T \frac{\partial \mathcal{R}}{\partial \mathbf{u}}\right)}_{=0} \delta\mathbf{u} + \underbrace{\left(\frac{\partial \mathcal{J}}{\partial \boldsymbol{\alpha}}^T + \boldsymbol{\psi}^T \frac{\partial \mathcal{R}}{\partial \boldsymbol{\alpha}}\right)}_{=0} \delta\boldsymbol{\alpha}.$$

Adjoint equation

Linear equation!

Making $\delta\mathcal{L} = 0$ selects only ***realizable*** $\delta\mathcal{J}$'s.

Single output error estimation and adaptation

- $\mathbf{u}^{H,p}$ will generally not satisfy the original PDE: $\mathbb{R}(\mathbf{u}^{H,p}, \mathbf{w}) \neq 0$
  Instead, it satisfies the weak form:

$$\mathbb{R}(\mathbf{u}, \mathbf{w}) + \delta\mathbb{R}(\mathbf{w}) = 0 \quad \text{where} \quad \delta\mathbb{R}(\mathbf{w}) = -\mathbb{R}(\mathbf{u}^{H,p}, \mathbf{w}).$$

- $\psi \in \mathcal{V}$ relates the residual perturbation to an output perturbation:

$$\delta J = J(\mathbf{u}^{H,p}) - J(\mathbf{u}) \approx -\mathbb{R}(\mathbf{u}^{H,p}, \psi)$$

- We approximate ψ in a higher order space $\mathcal{V}^{H,p+1} \supset \mathcal{V}^{H,p}$ and estimate the error as:

$$\delta J \approx -\sum_{\kappa^H \in T^H} \mathbb{R}_{\kappa^H}(\mathbf{u}^{H,p}, \psi^{H,p+1} - \psi^{H,p}),$$

- We assign an adaptive indicator to κ^H based on its contribution to the error estimate:

$$\eta_{\kappa^H} = \left|\mathbb{R}_{\kappa^H}(\mathbf{u}^{H,p}, \psi^{H,p+1} - \psi^{H,p})\right|.$$

Coupled flow-trim solve

- In an output-constrained run we solve:

$$\begin{cases} \mathbf{R}(\mathbf{U},\alpha) & = & \mathbf{0} & \leftarrow & N \text{ flow equations} \\ \mathbf{R}^{\text{trim}}(\mathbf{U},\alpha) & = & \mathbf{0} & \leftarrow & N_\alpha \text{ trim conditions} \end{cases}$$

  where $\mathbf{R}^{\text{trim}}(\mathbf{U},\alpha) = \mathbf{J}^{\text{trim}}(\mathbf{U},\alpha) - \overline{\mathbf{J}}^{\text{trim}}$.

- We seek variations of J^{adapt} that satisfy the constraints above, so:

$$\delta\mathcal{L} = \delta J^{\text{adapt}} + \underbrace{\psi^T \delta\mathbf{R}}_{\text{(a)}} + \underbrace{\phi^T \delta\mathbf{R}^{\text{trim}}}_{\text{(b)}} = 0.$$

- "a" is the output error estimate for fixed α, "b" is the influence of the trim error in the output error due to *inexact* constraint satisfaction.

Coupled adjoint solution

We have an adjoint contribution from both the flow and trimming residuals:

$$\begin{bmatrix} \frac{\partial \mathbf{R}}{\partial \mathbf{U}}^T & \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{U}}^T \\ \frac{\partial \mathbf{R}}{\partial \boldsymbol{\alpha}}^T & \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \boldsymbol{\alpha}}^T \end{bmatrix} \begin{bmatrix} \boldsymbol{\psi} \\ \boldsymbol{\phi} \end{bmatrix} + \begin{bmatrix} \frac{\partial J^{\text{adapt}}}{\partial \mathbf{U}}^T \\ \frac{\partial J^{\text{adapt}}}{\partial \boldsymbol{\alpha}}^T \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

$$\begin{aligned} \boldsymbol{\psi} &= -\left(\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right)^{-T} \left[\frac{\partial J^{\text{adapt}}}{\partial \mathbf{U}}^T + \frac{\partial \mathbf{R}^{\text{trim}}}{\partial \mathbf{U}}^T \boldsymbol{\phi}\right] \\ &= \underbrace{-\left(\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right)^{-T} \frac{\partial J^{\text{adapt}}}{\partial \mathbf{U}}^T}_{\boldsymbol{\psi}^{\text{adapt}}} \underbrace{-\left(\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right)^{-T} \frac{\partial \mathbf{J}^{\text{trim}}}{\partial \mathbf{U}}^T}_{\boldsymbol{\Psi}^{\text{trim}}} \boldsymbol{\phi} \\ &= \boldsymbol{\psi}^{\text{adapt}} + \boldsymbol{\Psi}^{\text{trim}} \boldsymbol{\phi} \end{aligned}$$

Finally, the sensitivity of J^{adapt} to trim residuals is:

$$\boldsymbol{\phi} = -\left[\frac{d\mathbf{J}^{\text{trim}}}{d\boldsymbol{\alpha}}\right]^{-T} \frac{dJ^{\text{adapt}}}{d\boldsymbol{\alpha}}^T = -\left[\frac{dJ^{\text{adapt}}}{d\boldsymbol{\alpha}} \left(\frac{d\mathbf{J}^{\text{trim}}}{d\boldsymbol{\alpha}}\right)^{-1}\right]^T$$

Constrained error estimate and adapt indicator

We get the output error estimate for the constrained case via a change to the total adjoint:

$$\delta J \approx -\left[\psi_h^{\text{adapt}} + \Psi_h^{\text{trim}}\phi\right]^T \mathbf{R}_h(\mathbf{U}_h^H, \alpha_H) = \delta J^{\text{adapt}} + \phi^T \delta \mathbf{J}^{\text{trim}}$$

and the modified adaptive indicator is given by:

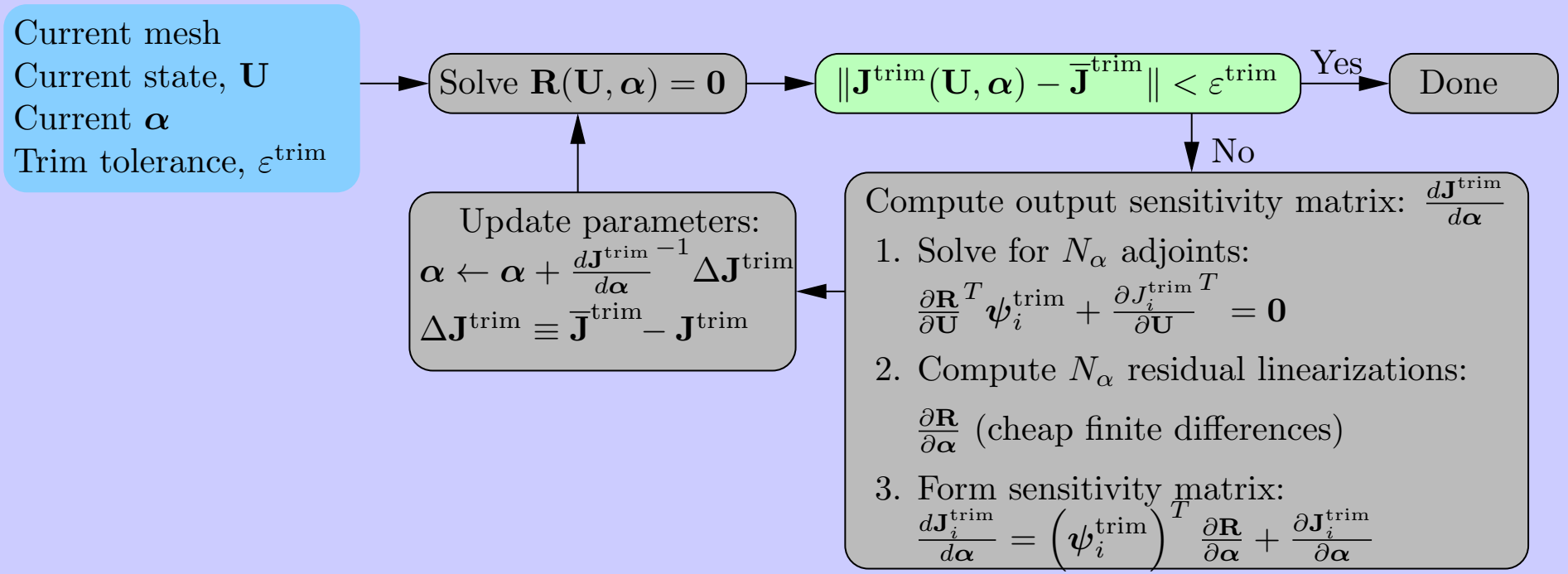
$$\eta_\kappa = \underbrace{\underbrace{\eta_\kappa^{\text{adapt}}}_{\text{Unconstrained}} + |\phi|^T \boldsymbol{\eta}_\kappa^{\text{trim}}}_{\text{Constrained}}$$

- "Unconstrained" - adaptation uses $\eta_k = \eta_k^{\text{adapt}}$
- "Constrained" - adaptation uses $\eta_k = \eta_k^{\text{adapt}} + |\phi|^T \boldsymbol{\eta}_k^{\text{trim}}$

Trim-constraint solver

At each adaptation iteration, we trim parameters to satisfy constraints:

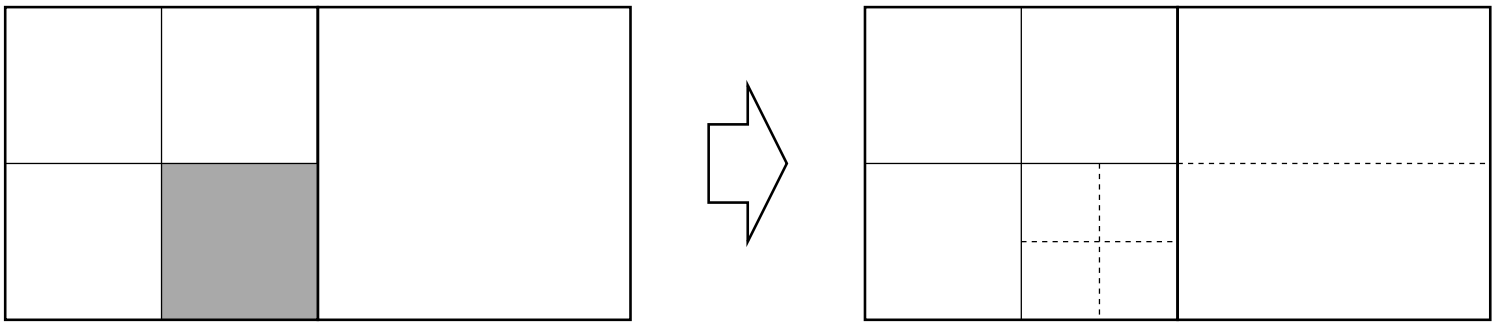
Trimming implementation



One can also solve flow and trimming equations simultaneously

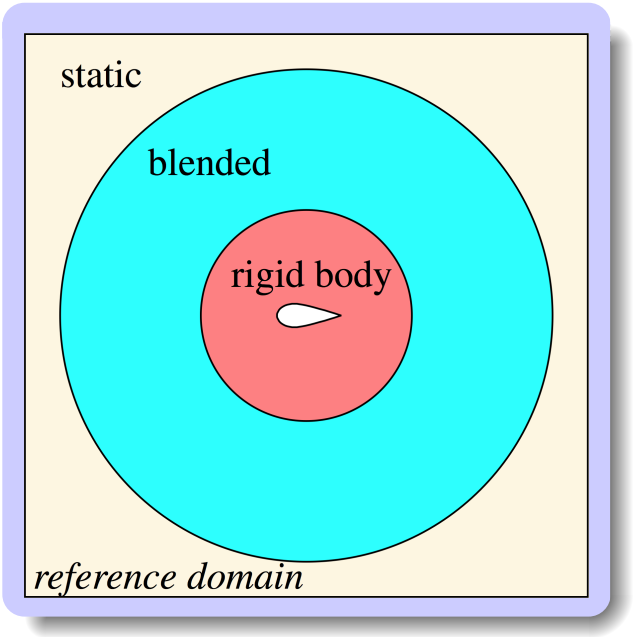
Mesh adaptation mechanics

- Select a fraction f^{frac} of elements with largest error indicators for adaptation.
- Isotropic refinement performed in reference space.
- New boundary nodes are projected to the geometry.
- One level of refinement is kept between adjacent cells.



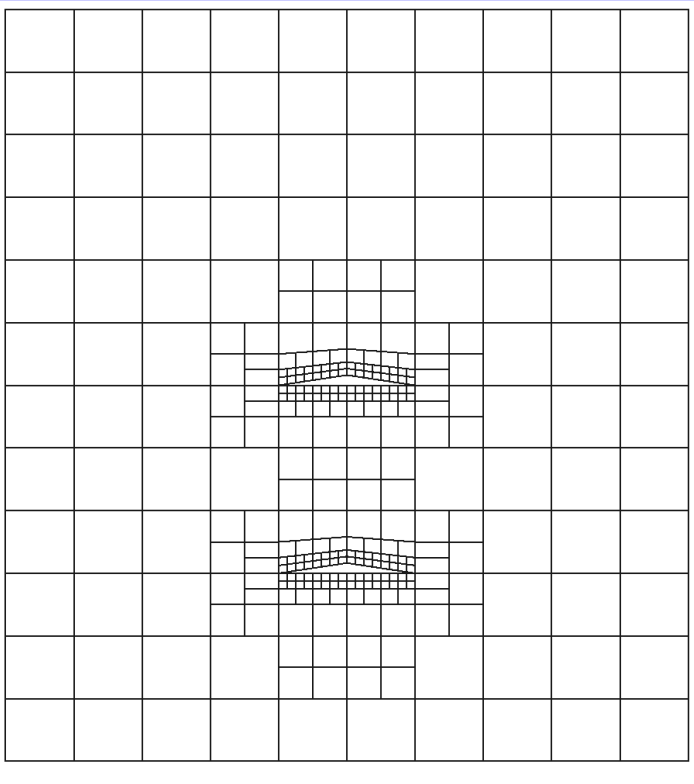
Arbitrary Lagrangian-Eulerian mapping

- We consider geometric parameters.
- Solve transformed PDE on an undeformed reference domain.
- Near-field rigid body motion blended into static farfield mesh.
- Quintic polynomial (in radial coordinate) blending functions.

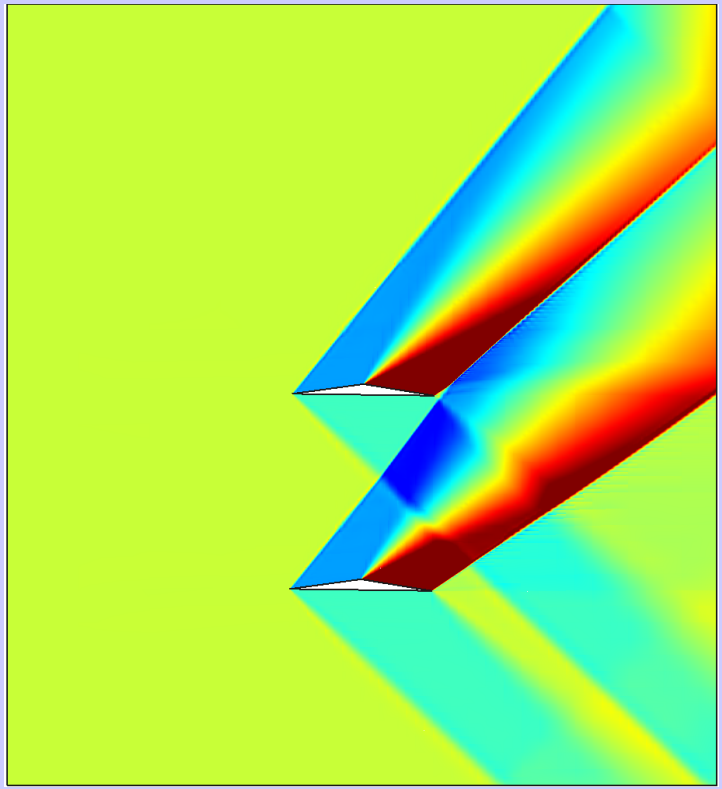


Supersonic biplane

- Trim on total biplane lift via changes to global angle of attack.
- Output of interest is drag on lower airfoil.
- Inviscid flow at $M_\infty = 1.5$ with $p = 2$ approximation order.



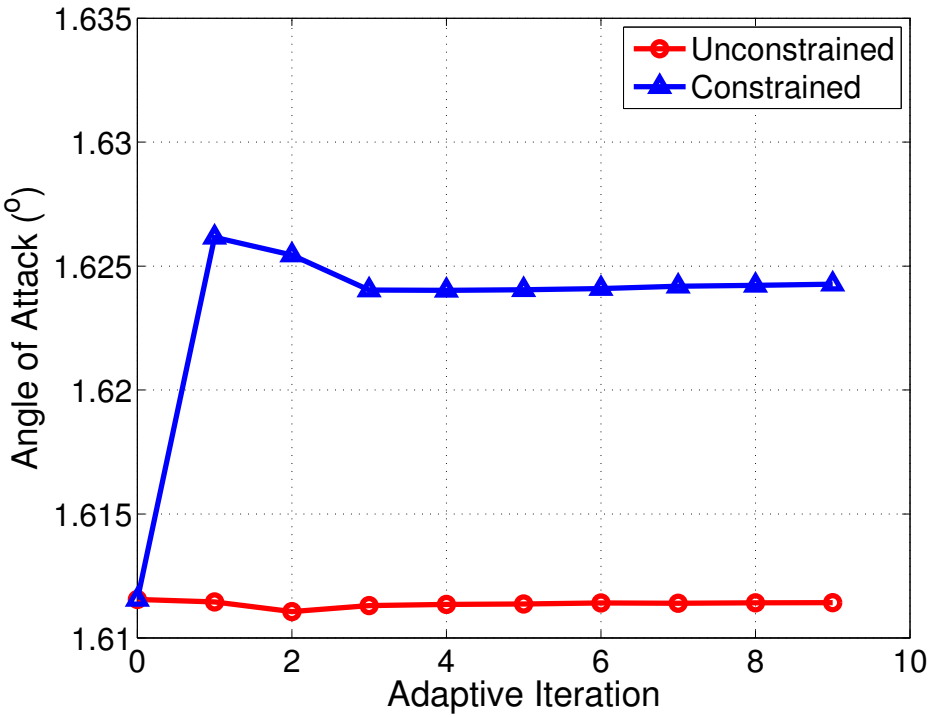
Initial mesh



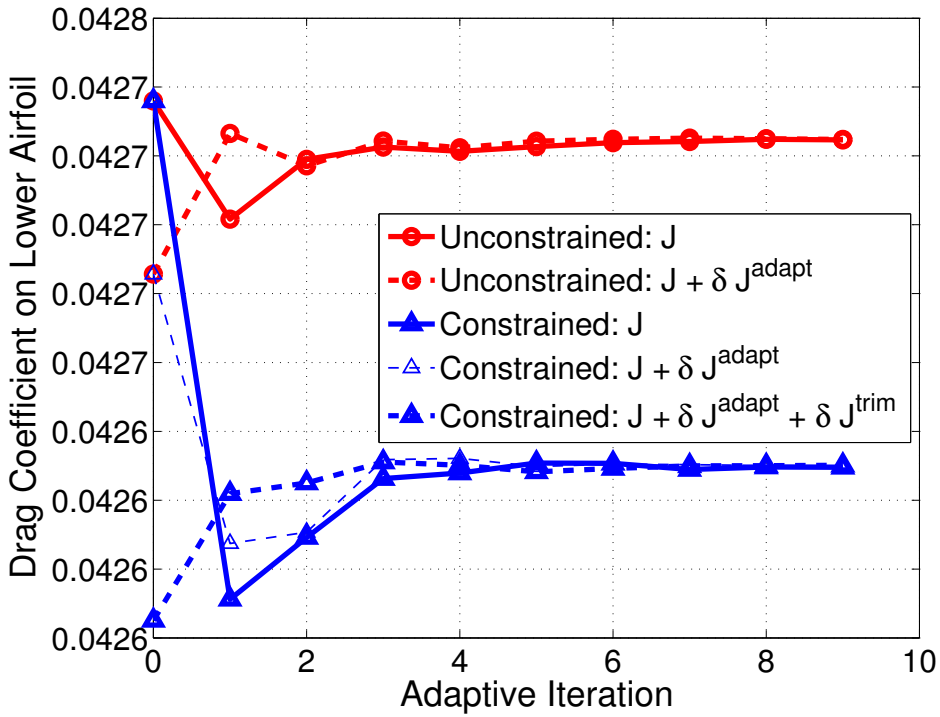
Mach contours

Supersonic biplane

- $c_{\ell,total} = 0.25$ trimming constraint.
- $c_{d,lower}$ adapt output.
- Different converged outputs.



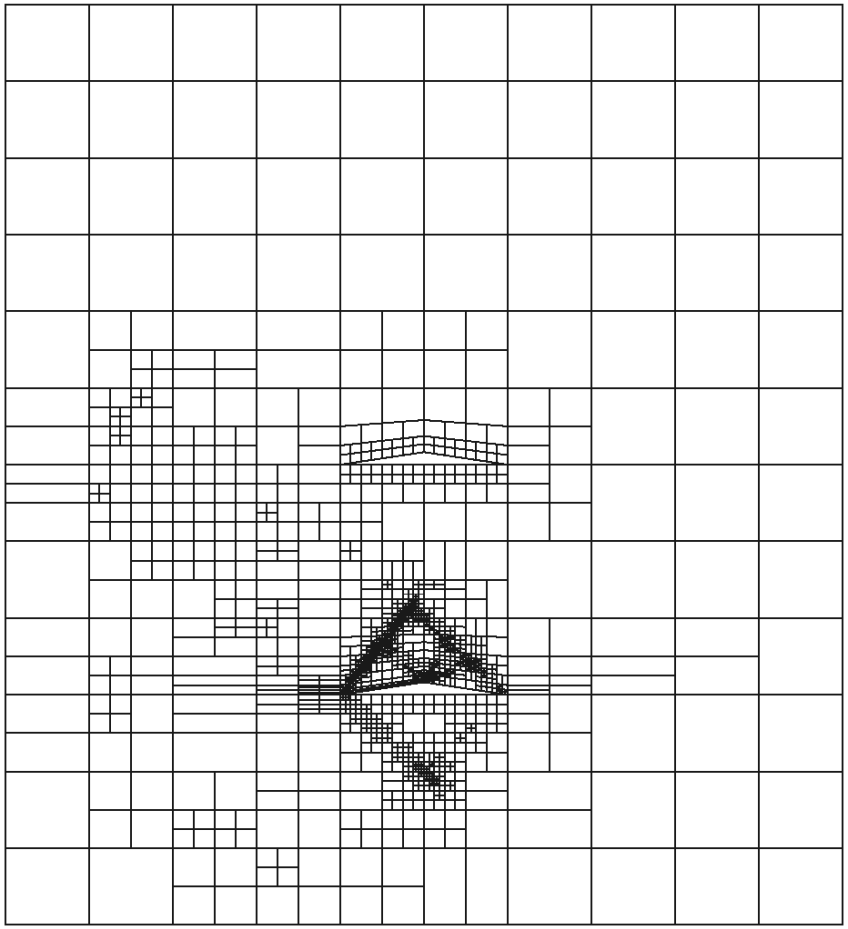
Angle of Attack Convergence



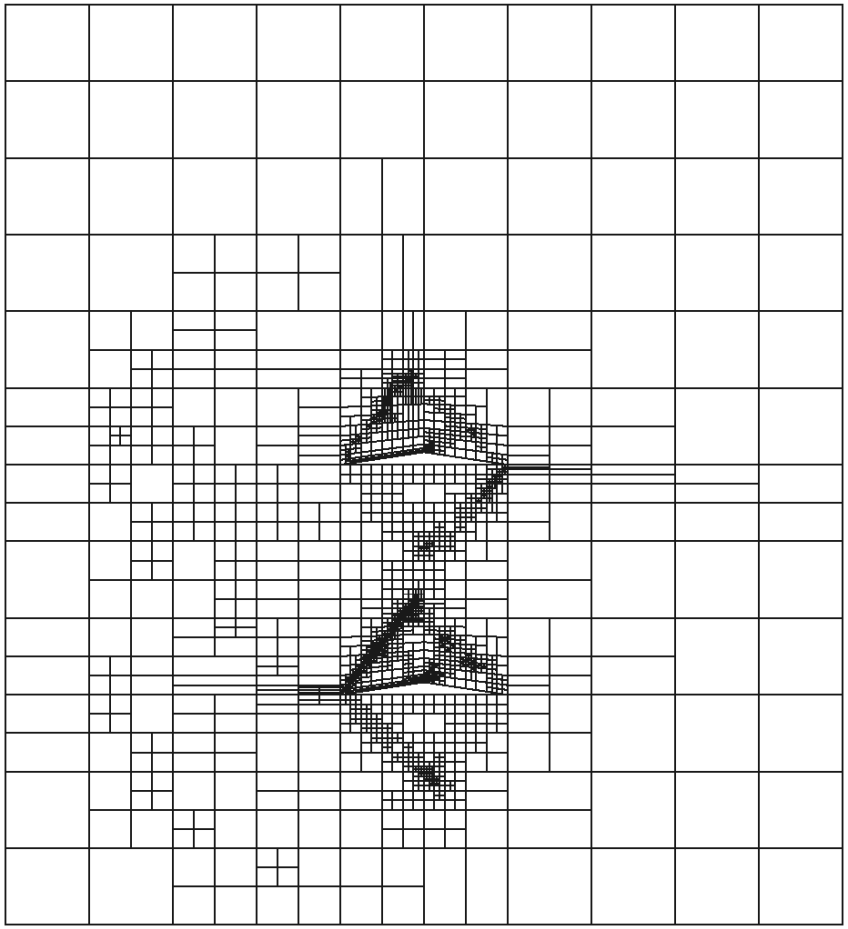
Drag Convergence

Supersonic biplane

- Trim and adapt outputs have different domains of dependence.
- Unconstrained adaptation does not target the upper airfoil.



Unconstrained adaptation



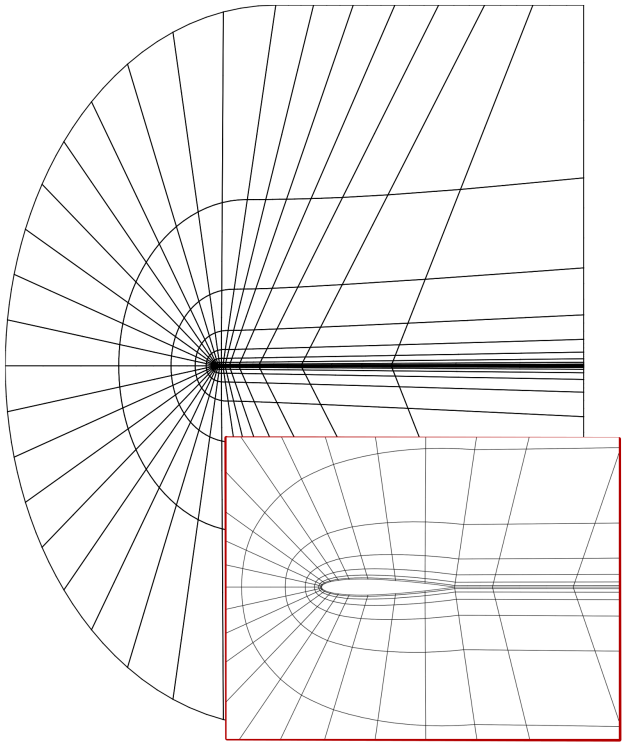
Constrained adaptation

NACA 0012

- $M_\infty = 0.5$, $Re = 5000$, $p = 1$.
- Lift-constrained drag prediction.
- Trimming parameter is the angle of attack.

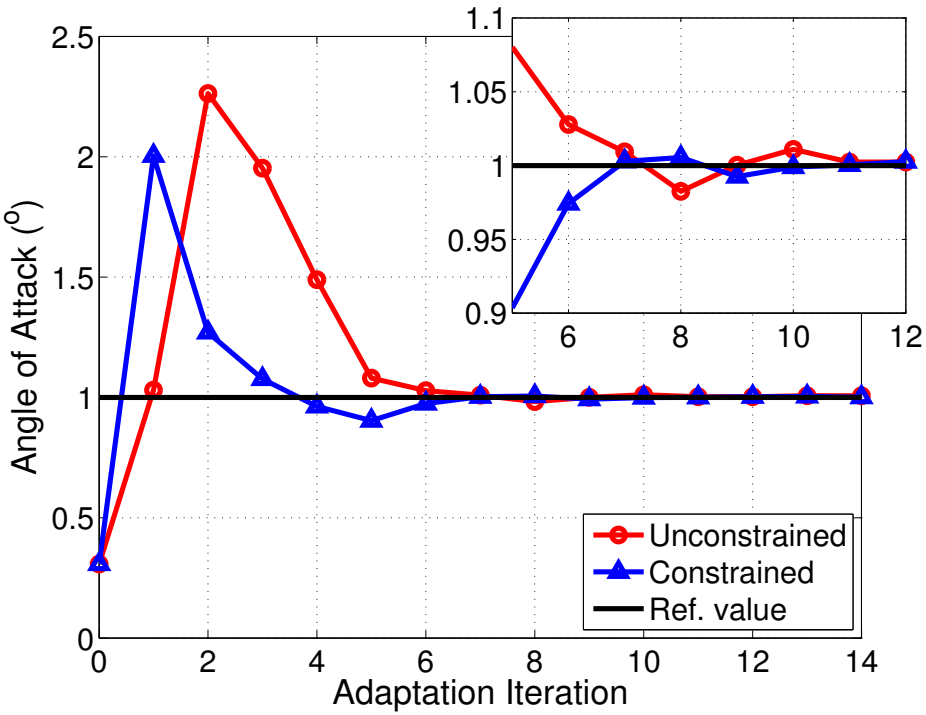
Strategy

- Compute "exact" lift at $\alpha = 1°$ $\Rightarrow c_\ell^{\text{exact}} = 0.018250$.
- Set $c_\ell^{\text{target}} = 0.018250$.
- Use c_ℓ^{exact} and c_d^{exact} to evaluate constrained vs. unconstrained adaptation.

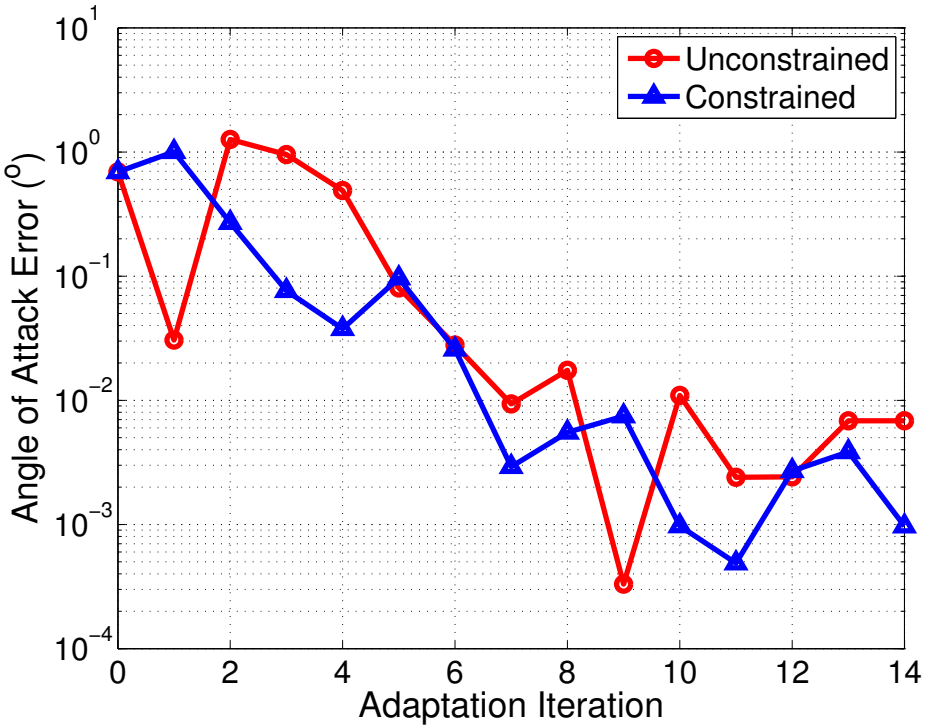


NACA 0012

Trimming history:



Angle of Attack Convergence

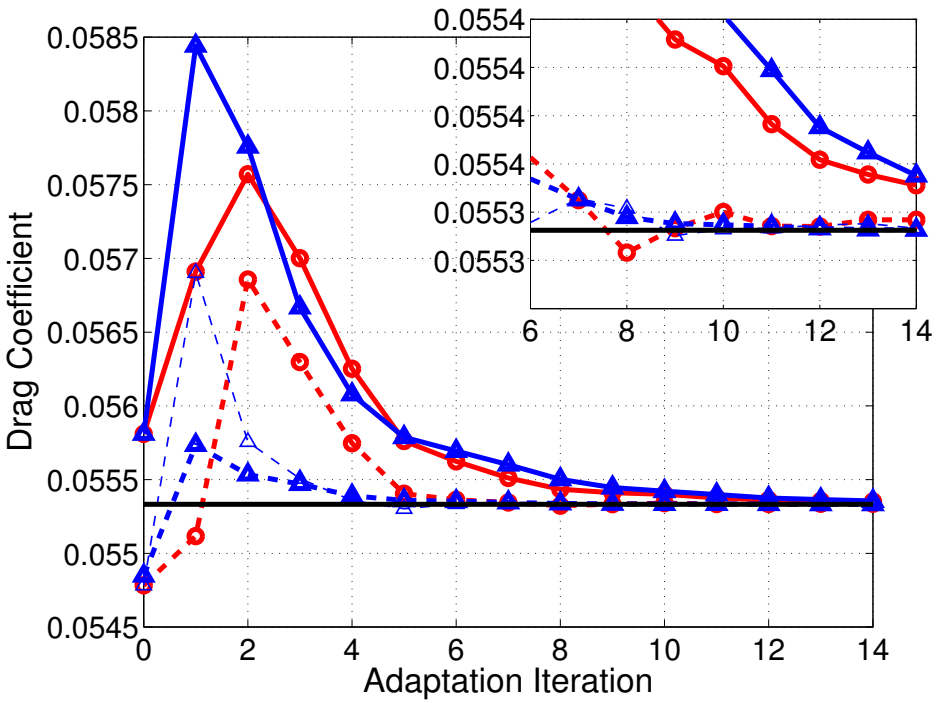


Angle of Attack Error

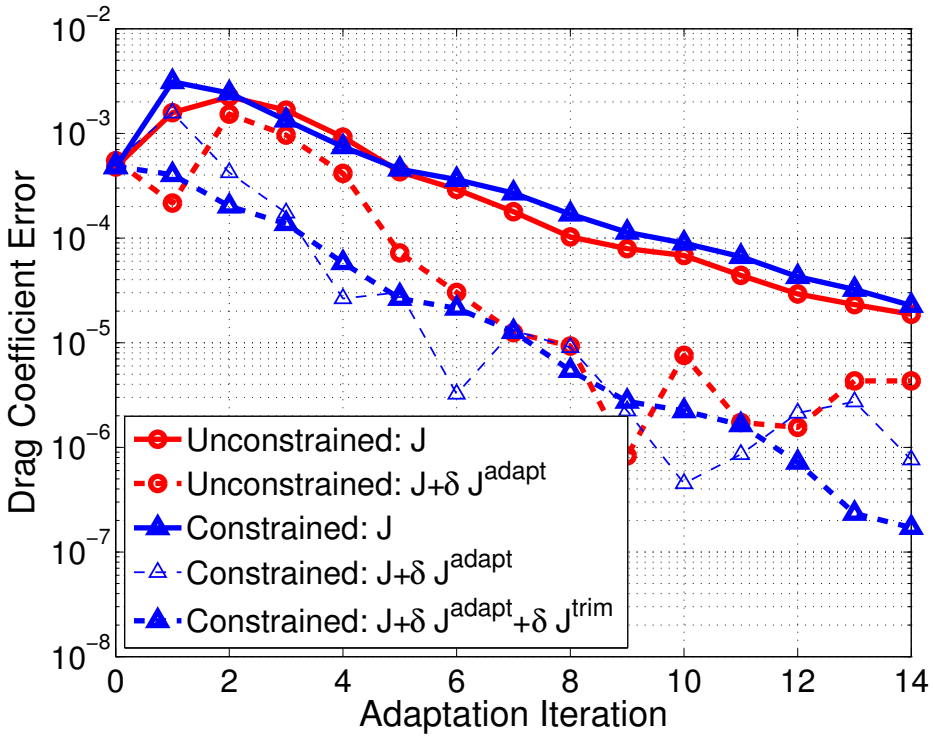
Trimming parameter converges faster for constrained adaptation.

NACA 0012

Output history:



Drag Convergence

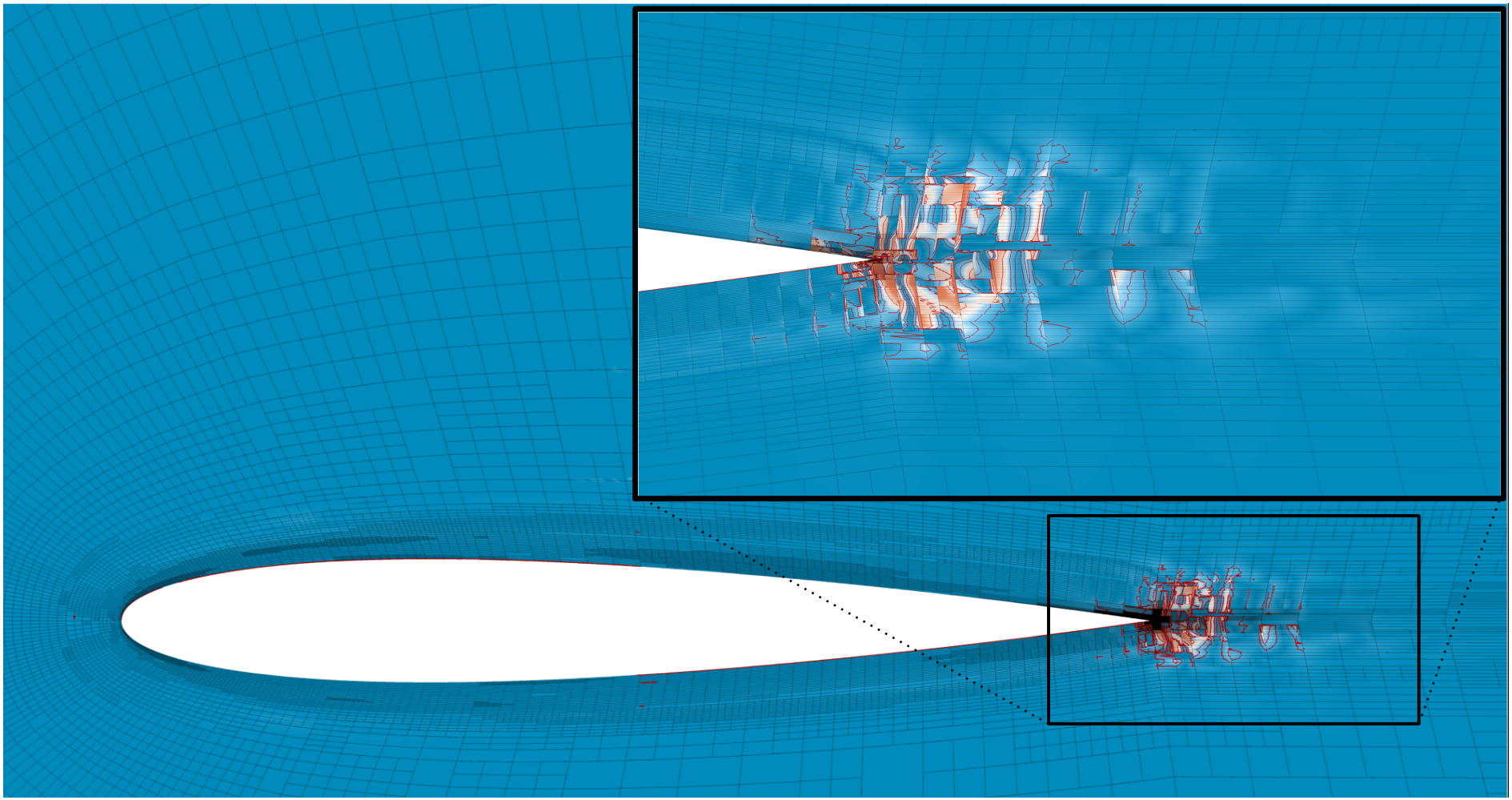


Drag Error

Unconstrained adaptation lags behind constrained adaptation.

NACA 0012

Difference in the final lift adjoints between constrained and unconstrained:



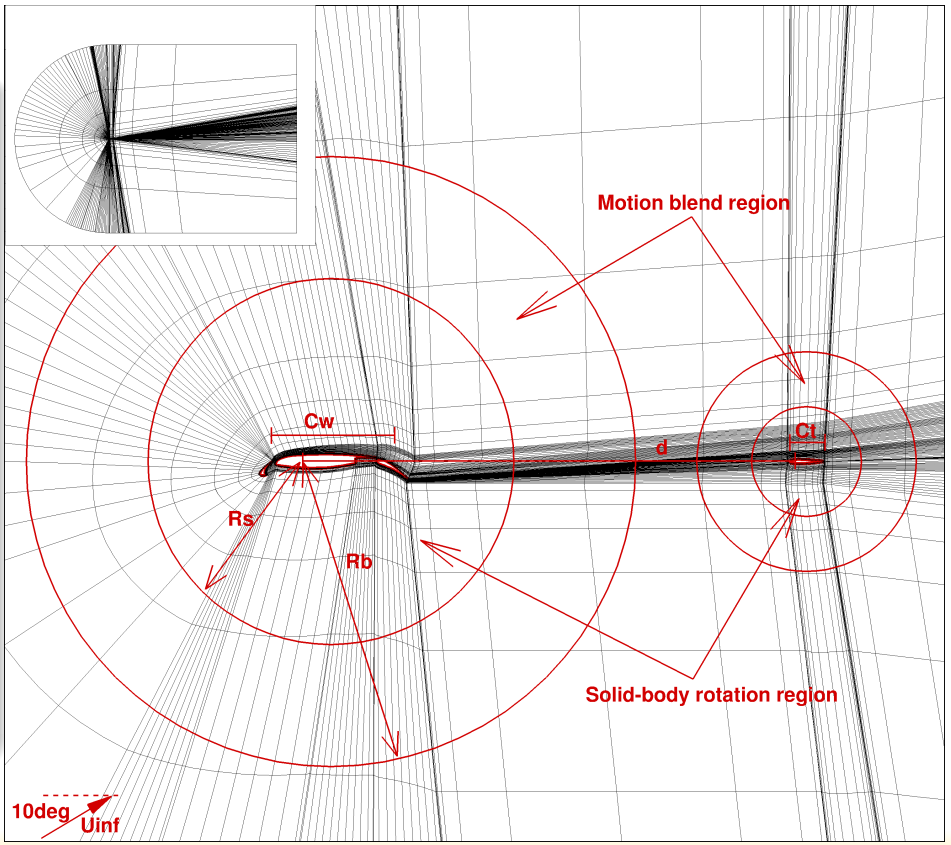
Density component of lift adjoint

High-lift configuration

- MDA 30P-30N main airfoil with NACA 0012 elevator.
- $M_\infty = 0.2$, $Re_{C_w} = 9x10^6$ with $p = 1$.
- Freestream at 10°.
- $c_\ell^{\text{target}} = 3.0$, $c_m^{\text{target}} = 0.0$

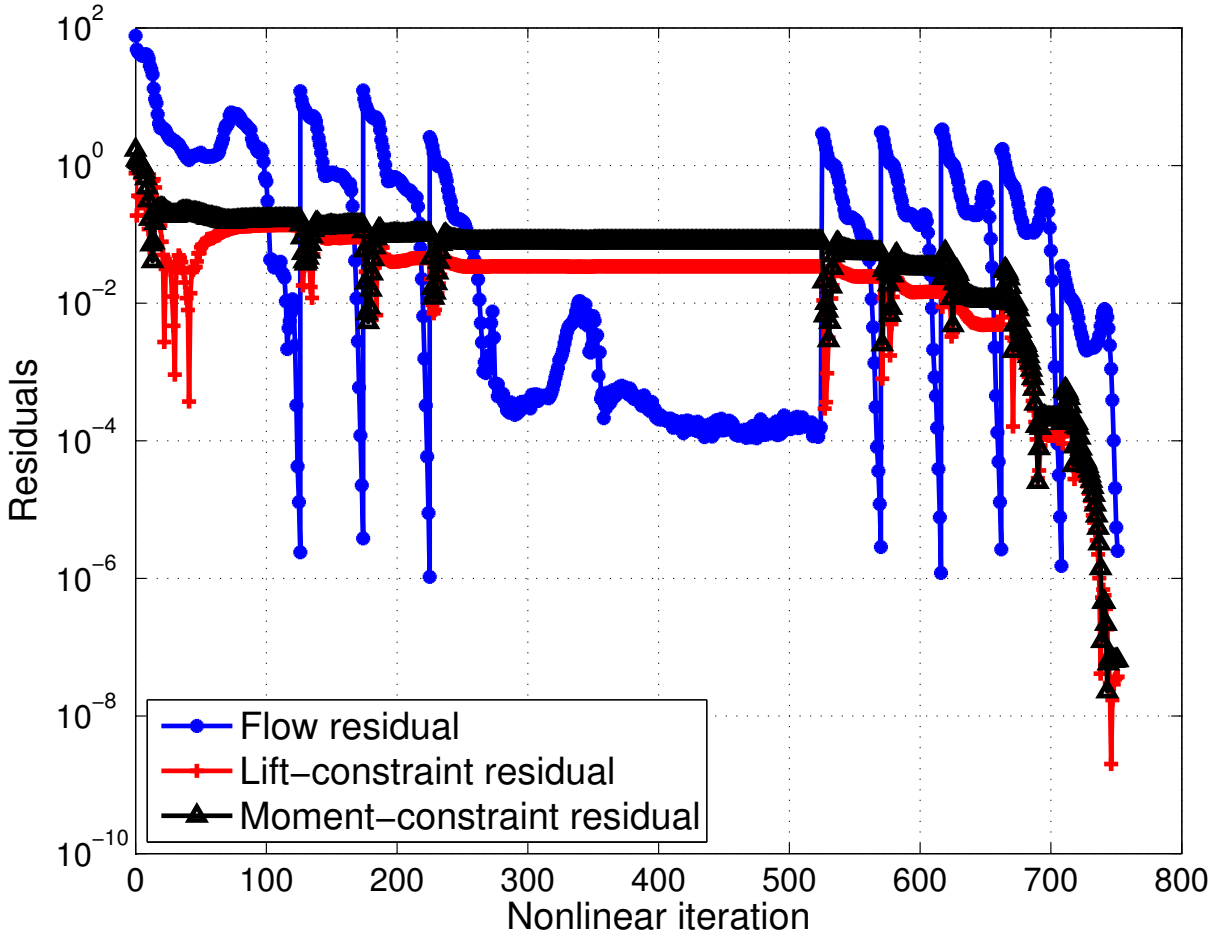
Case Parameters

- Trim lift and moment constraints via changes to angle of attack.
- Output of interest is total drag.
- Wing chord, $C_w = 0.5588$
- Tail chord, $C_t = 0.3 * C_w$
- Separation $= 4.0 * C_w$



High-lift configuration

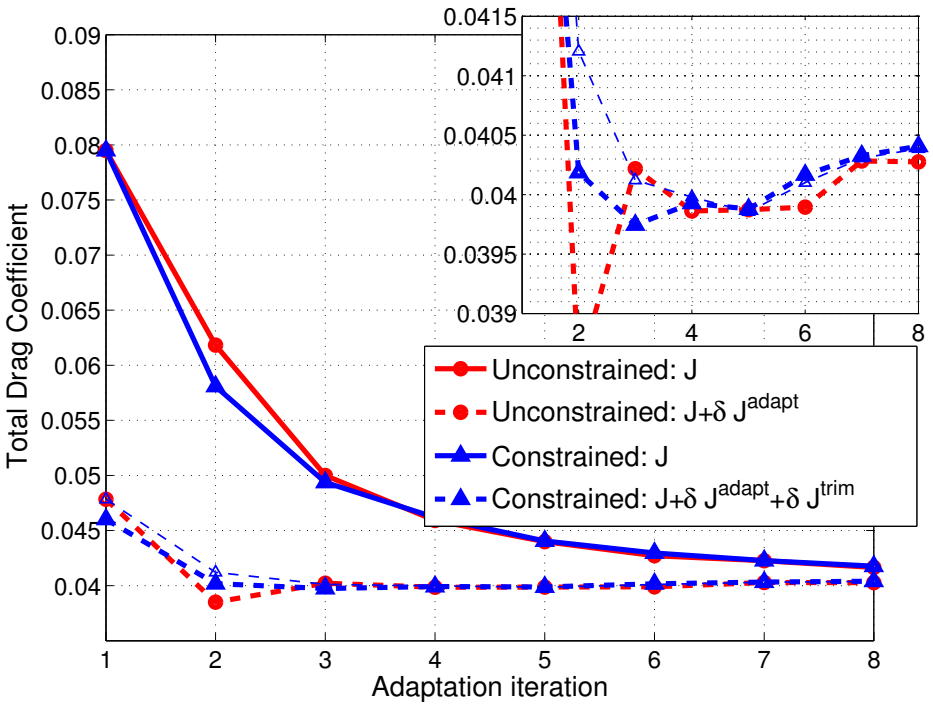
Flow/trim solve for first adaptive iteration:



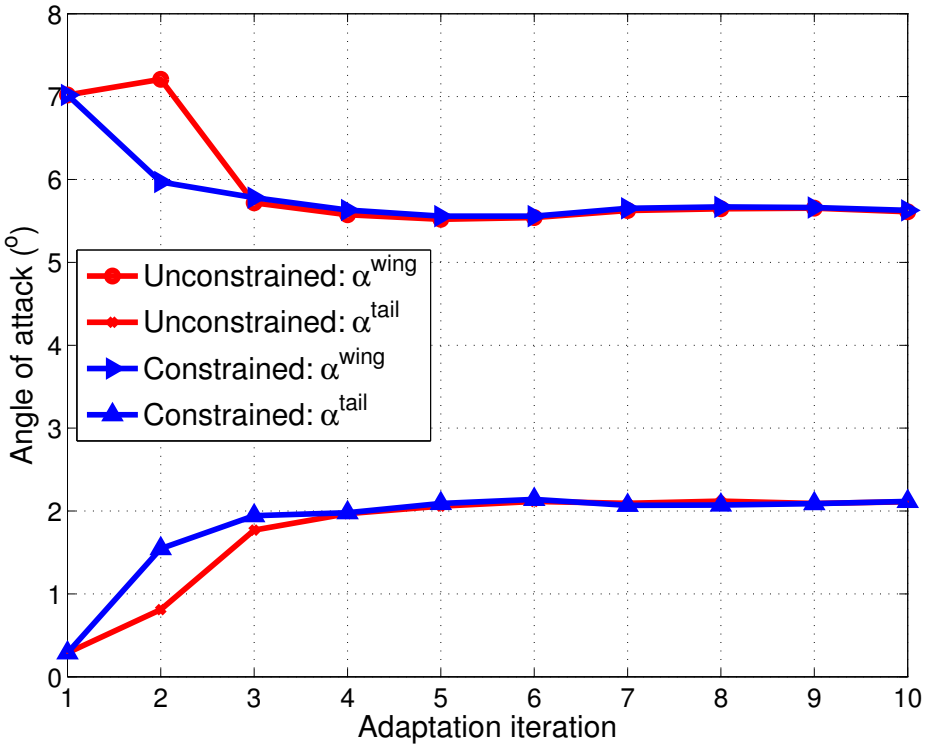
Note: trimming succeeds despite flow solution stall.

High-lift configuration

Output and trimming history:



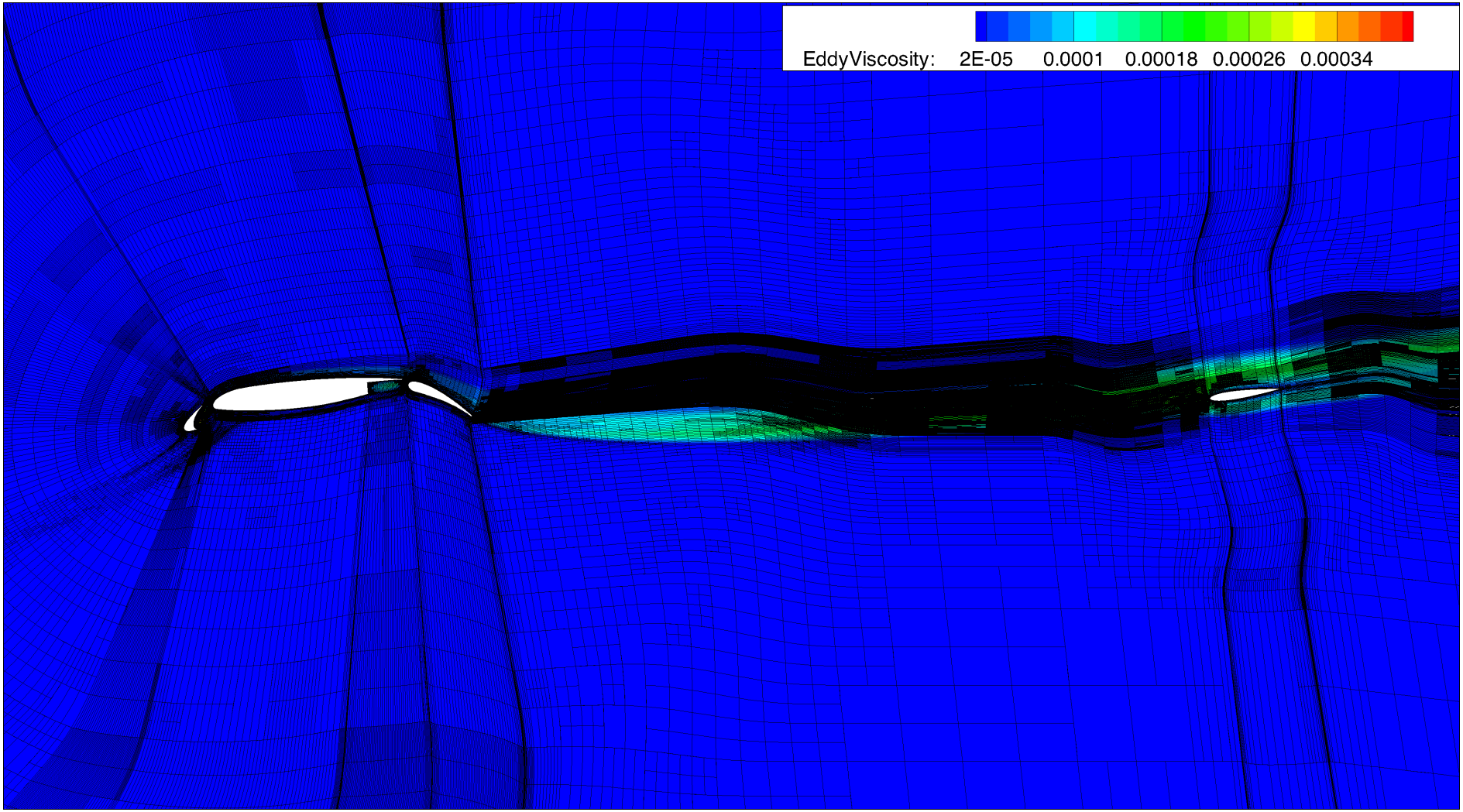
Drag Convergence



Angle of Attack Convergence

High-Lift configuration - why the similarity?

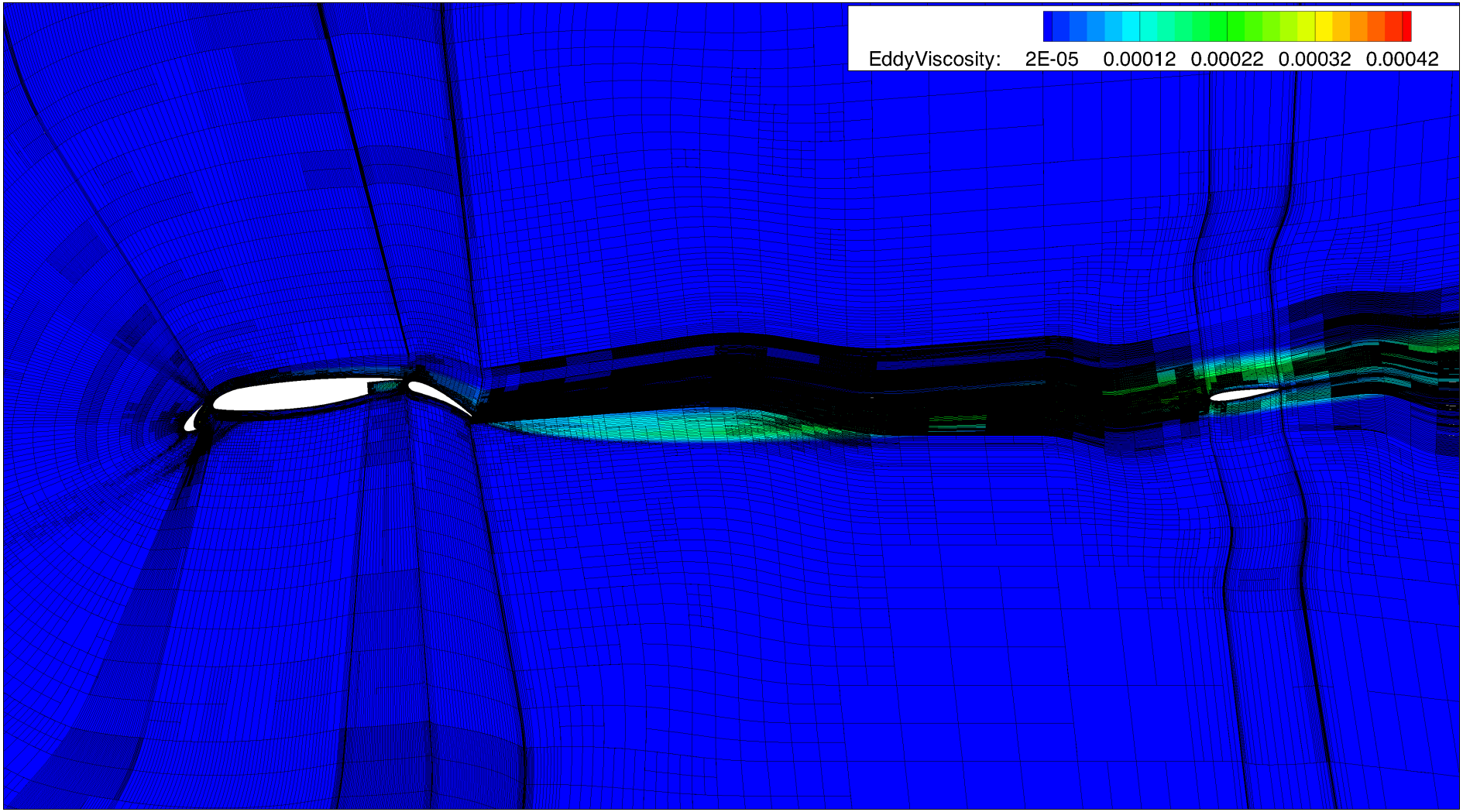
Adaptation targets same area with and without constraint:



Unconstrained Mesh

High-lift configuration - why the similarity?

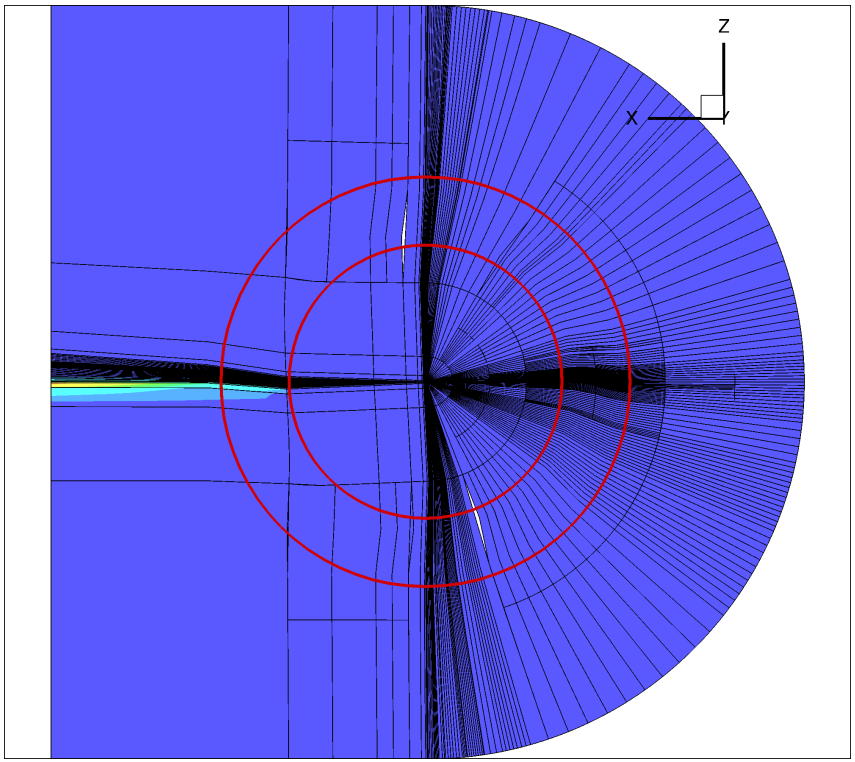
Adaptation targets same area with and without constraint:



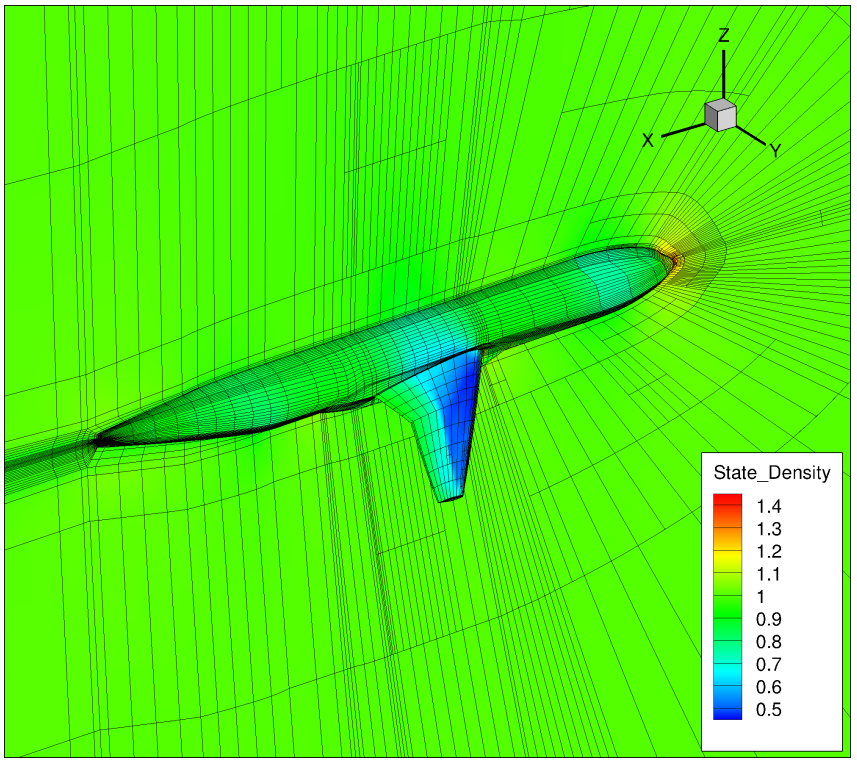
Constrained Mesh

DPW5 case

- No-tail CRM geometry at $M_\infty = 0.85$, $Re = 5 \times 10^6$, and $C_L^{\text{target}} = 0.5$.
- Approximation order is $p = 1$.
- The output of interest is the total drag.
- Initial cubic ($q = 3$) mesh generated by agglomerating 3 linear cells in each direction.



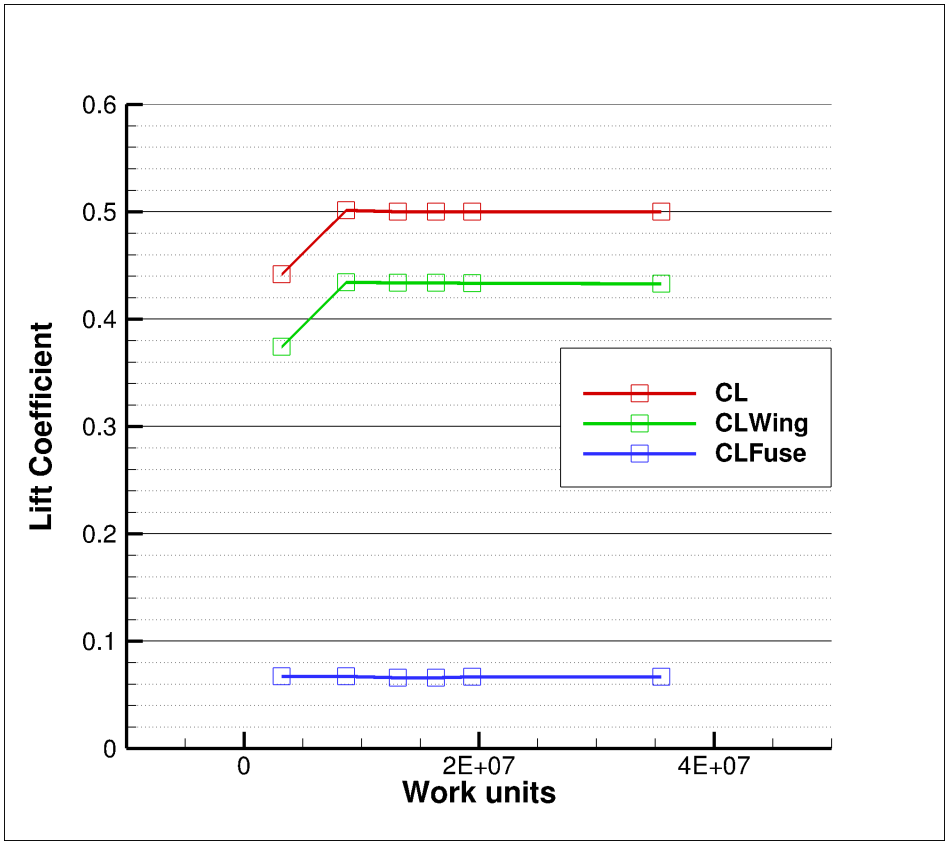
Trimming diagram.

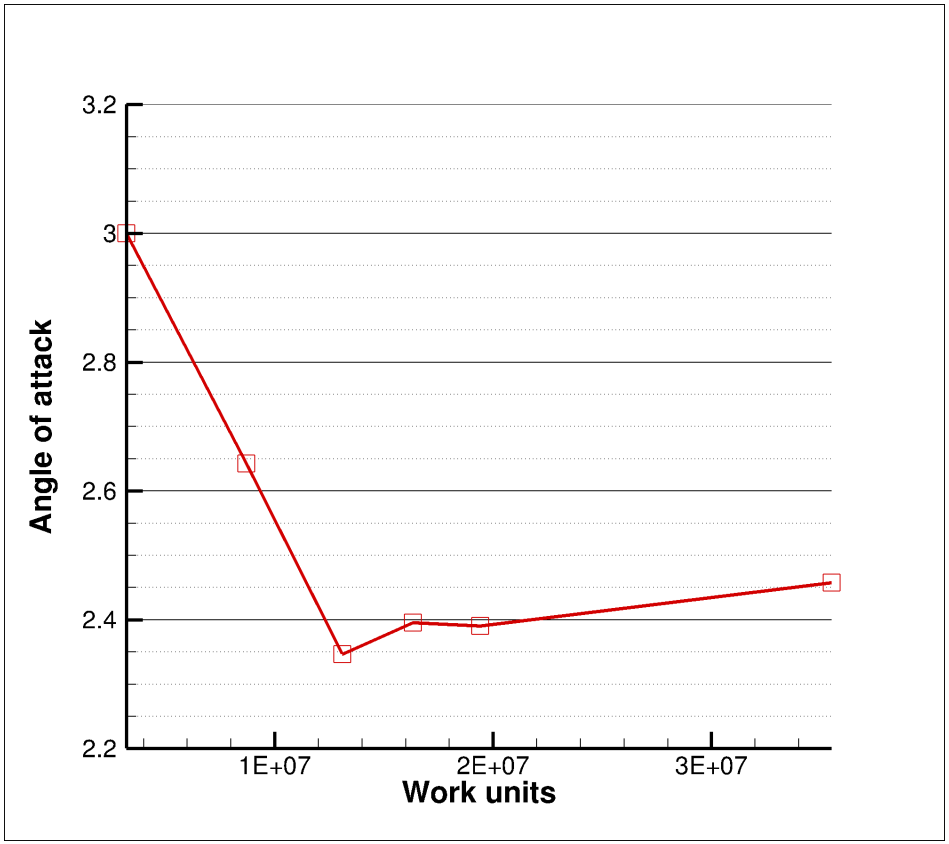


6^{th} adapted mesh (155661 elements).

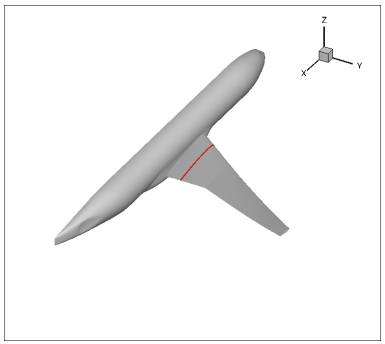
DPW5 case

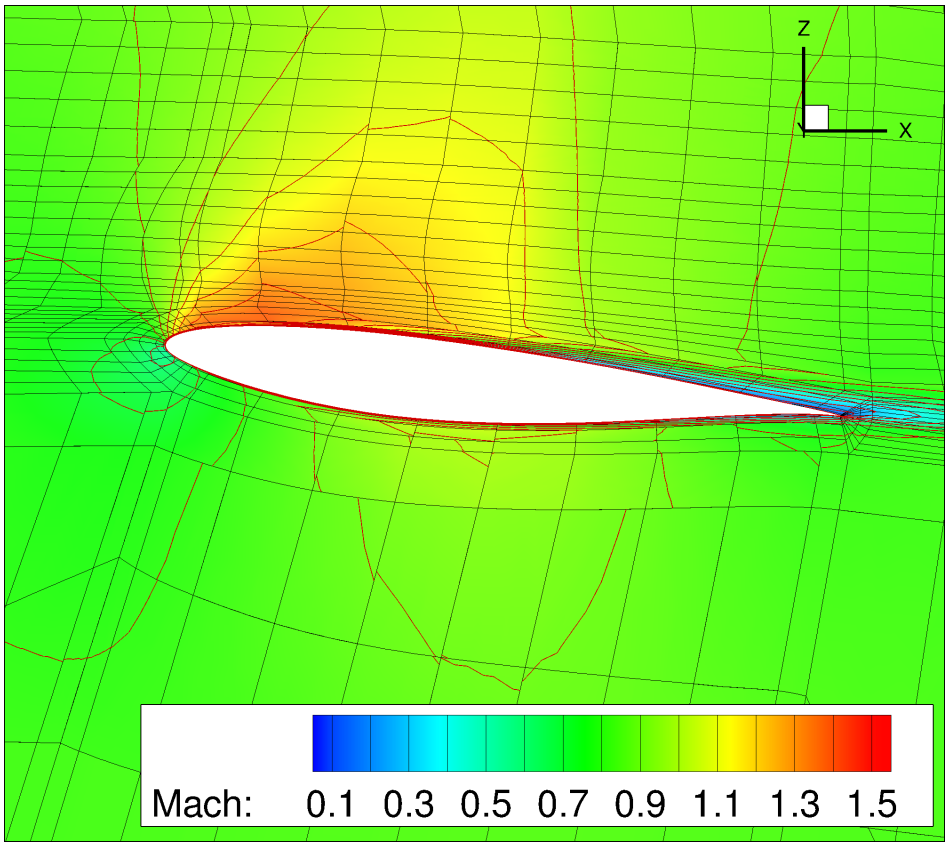
Adaptation proceeds with under-converged constraint residual due to excessively coarse initial mesh.



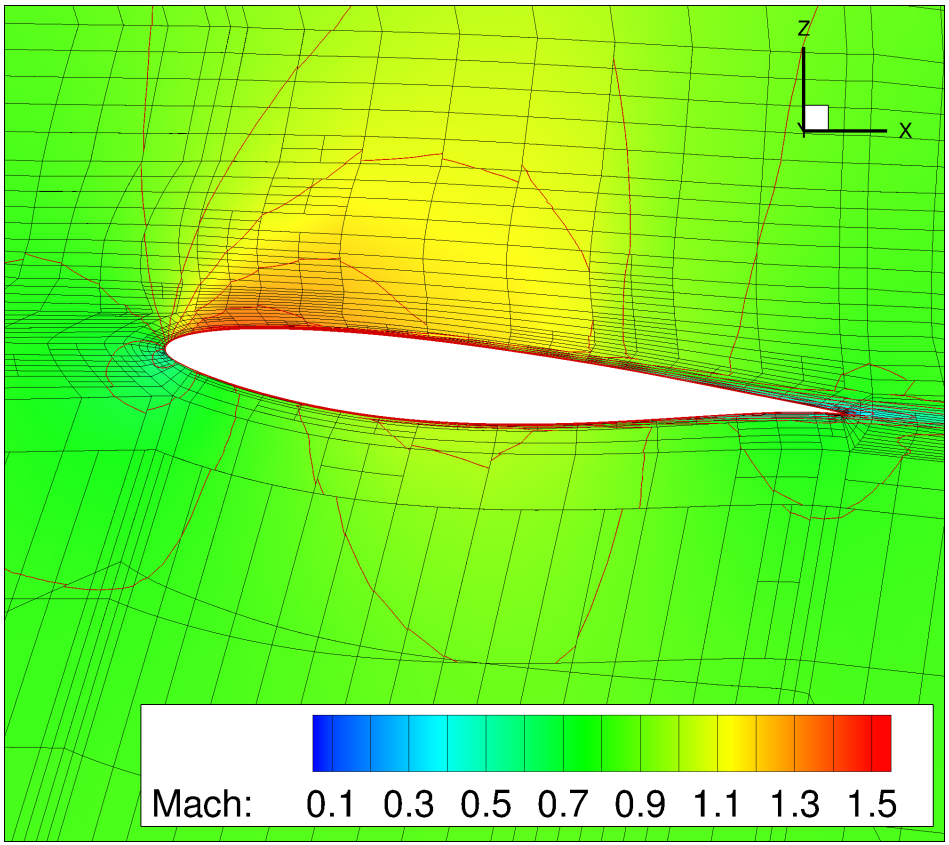


DPW5 case



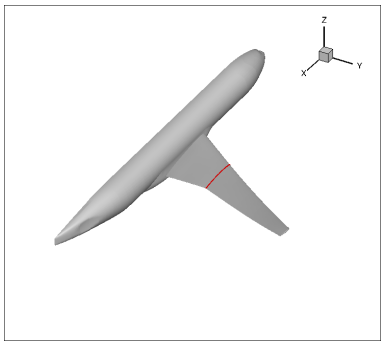


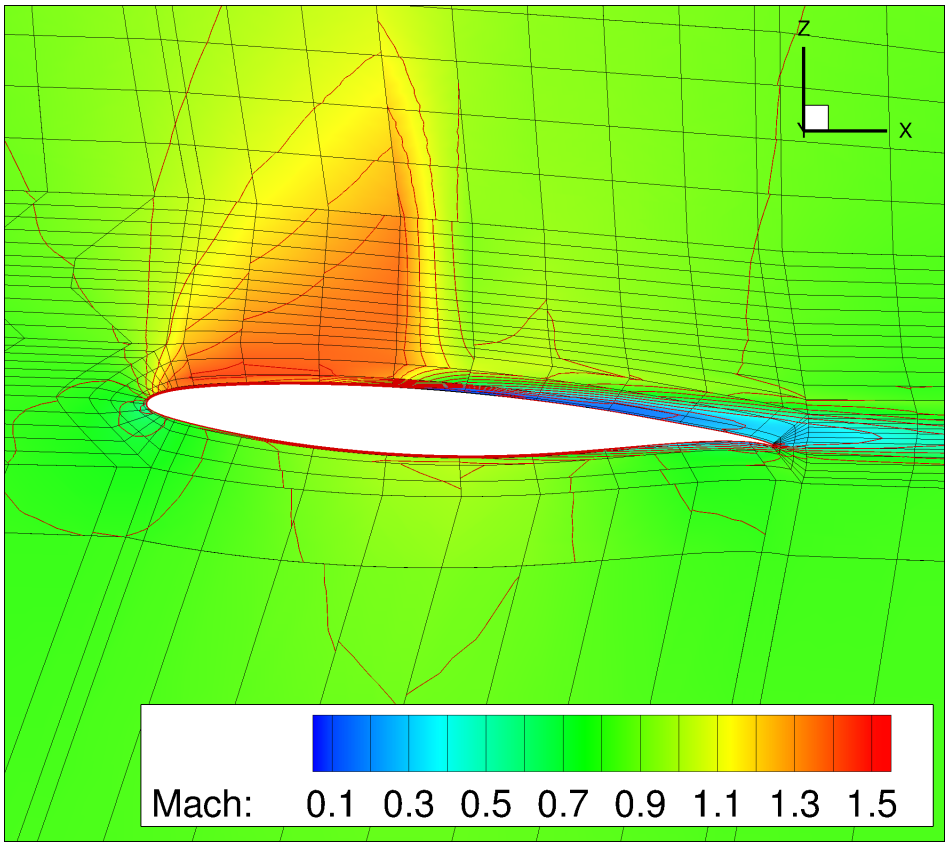
Initial Mach contours



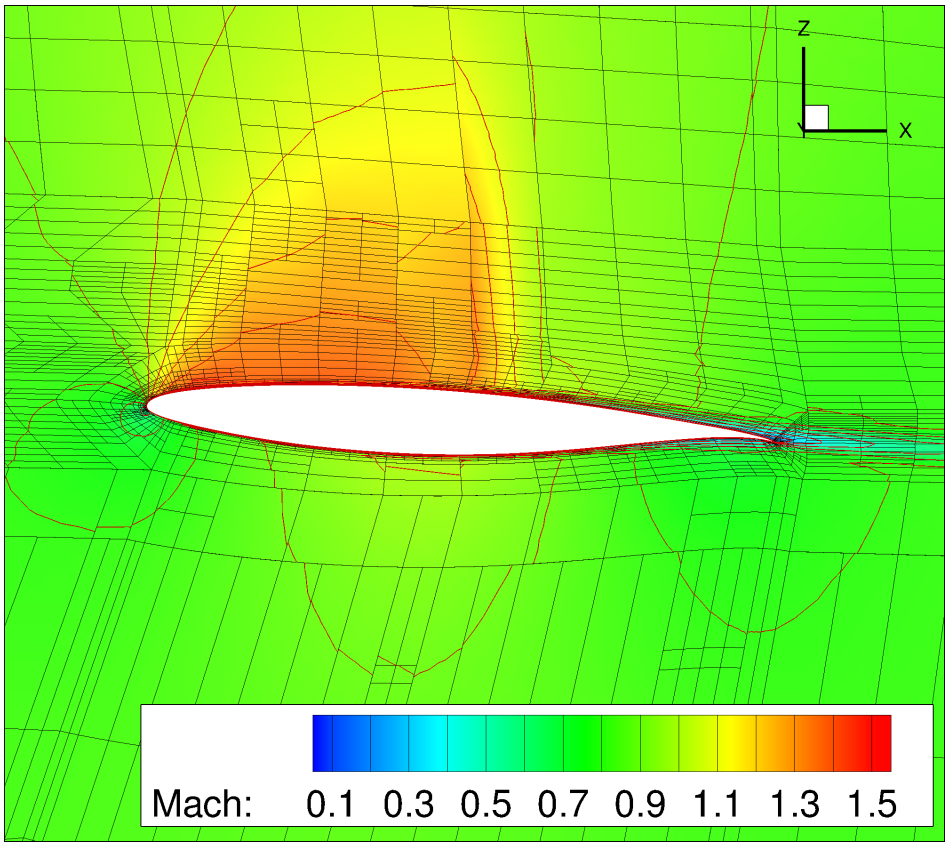
Final Mach contours

DPW5 case





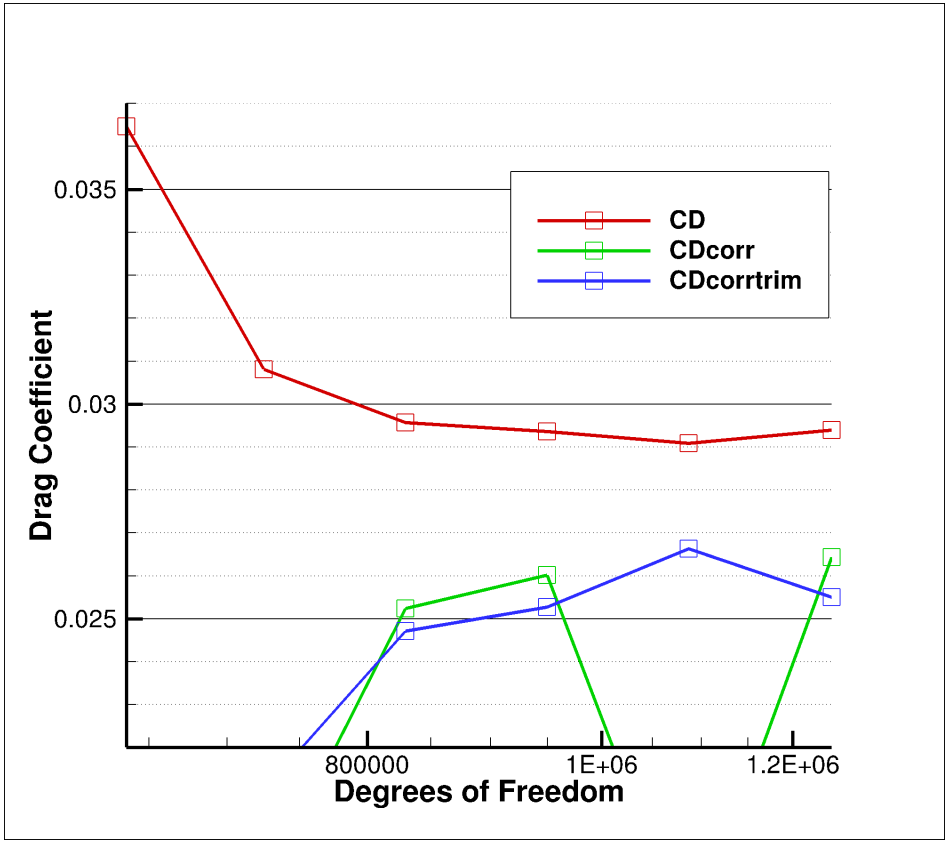
Initial Mach contours



Final Mach contours

DPW5 case

- Including the constraint error smoothes the error correction.
- **Note:** we are not fully solving the fine-space adjoints.



Concluding remarks

- We extended the adjoint-based error estimation method to problems with output constraints.
- We demonstrated this extension in several problems with varying complexity.
- In cases where the domains of dependence largely overlap, the benefits of the constrained adaptation is marginal.
- In cases with disjoint outputs, the constrained adaptation method offers a clear advantage – most evident in the convergence of the trimming parameter.
- Future developments: simultaneous flow-trim solve, extension to error sampling adaptive strategies *e.g.:* optimization-based *hp* (Ceze and Fidkowski) and MOESS (Yano and Darmofal).

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Thank you!