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

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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:

\[ R(U, \alpha) = 0, \]

where:

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

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

\[ J^{\text{trim}}(U, \alpha) - \bar{J}^{\text{trim}} = 0 \]

\( \bar{J}^{\text{trim}} \in \mathbb{R}^{N_\alpha} \) is a set of user-specified trim outputs/constraints.
Consider drag prediction under fixed lift:

- \( N_{\alpha} = 1 \)
- \( \alpha \): 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.

![Diagram of adjoint variables and flow simulation](image)

- Input parameters
- Flow simulation
- Post-processing e.g.: drag, lift.
- Adjoint variables
- \( J(U) \)
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**Flow simulation**

\[
\begin{bmatrix}
R_1(U) \\
R_2(U) \\
\vdots \\
R_n(U)
\end{bmatrix} =
\begin{bmatrix}
0 \\
0 \\
\vdots \\
0
\end{bmatrix}
\]

**Post-processing**

\( J(U) \)

**Sensitivity analysis**

**Adjoint variables**

\( \Psi \)

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\[
\begin{bmatrix}
R_1(U) \\
R_2(U) \\
\vdots \\
R_n(U)
\end{bmatrix}
= \begin{bmatrix} 0 & 0 & \cdots & 0 \end{bmatrix}
\]

Flow simulation

Post-processing e.g.: drag, lift.

Output error estimation

Residual evaluation in finer space

Adjoint variables
A derivation of the adjoint equation

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

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

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

  $$\delta \mathcal{L}(\alpha, u, \psi) = 0$$

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

  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: $R(\mathbf{u}^{H,p}, w) \neq 0$
  Instead, it satisfies the weak form:

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

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

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

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

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

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

$$\eta_{\kappa^H} = \left| R_{\kappa^H}(\mathbf{u}^{H,p}, \psi^{H,p+1} - \psi^{H,p}) \right|.$$
Coupled flow-trim solve

- In an output-constrained run we solve:

\[
\begin{align*}
R(U, \alpha) &= 0 \quad \leftarrow \quad N \text{ flow equations} \\
R^{\text{trim}}(U, \alpha) &= 0 \quad \leftarrow \quad N_{\alpha} \text{ trim conditions}
\end{align*}
\]

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

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

\[
\delta \mathcal{L} = \delta J^{\text{adapt}} + \psi^T \delta R + \phi^T \delta R^{\text{trim}} = 0.
\]

  - “a” is the output error estimate for fixed \( \alpha \), “b” is the influence of the trim error in the output error due to \textit{inexact} constraint satisfaction.
Coupled adjoint solution

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

\[
\begin{bmatrix}
\frac{\partial R}{\partial U}^T & \frac{\partial R_{\text{trim}}}{\partial U}^T \\
\frac{\partial R}{\partial \alpha}^T & \frac{\partial R_{\text{trim}}}{\partial \alpha}^T
\end{bmatrix}
\begin{bmatrix}
\psi \\
\phi
\end{bmatrix}
+ \begin{bmatrix}
\frac{\partial J_{\text{adapt}}}{\partial U}^T \\
\frac{\partial J_{\text{adapt}}}{\partial \alpha}^T
\end{bmatrix} = \begin{bmatrix}
0 \\
0
\end{bmatrix}
\]

\[
\psi = - \left( \frac{\partial R}{\partial U} \right)^{-T} \begin{bmatrix}
\frac{\partial J_{\text{adapt}}}{\partial U}^T \\
\frac{\partial J_{\text{adapt}}}{\partial \alpha}^T
\end{bmatrix} + \frac{\partial R_{\text{trim}}}{\partial U}^T \phi
\]

\[
= - \left( \frac{\partial R}{\partial U} \right)^{-T} \frac{\partial J_{\text{adapt}}}{\partial U}^T \underbrace{\psi_{\text{adapt}}}_{\Psi_{\text{adapt}}} + \frac{\partial R_{\text{trim}}}{\partial U}^T \underbrace{\phi}_{\Psi_{\text{trim}}}
\]

Finally, the sensitivity of \( J_{\text{adapt}} \) to trim residuals is:

\[
\phi = - \left[ \frac{dJ_{\text{trim}}}{d\alpha} \right]^{-T} \frac{dJ_{\text{adapt}}}{d\alpha}^T = - \left[ \frac{dJ_{\text{adapt}}}{d\alpha} \left( \frac{dJ_{\text{trim}}}{d\alpha} \right)^{-1} \right]^T
\]
Constrained error estimate and adapt indicator

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

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

and the modified adaptive indicator is given by:

$$\eta_k = \eta_k^{\text{adapt}} + |\phi|^T \eta_k^{\text{trim}}$$

"Unconstrained" - adaptation uses $\eta_k = \eta_k^{\text{adapt}}$

"Constrained" - adaptation uses $\eta_k = \eta_k^{\text{adapt}} + |\phi|^T \eta_k^{\text{trim}}$
Trim-constraint solver

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

Trimming implementation

Current mesh
Current state, $U$
Current $\alpha$
Trim tolerance, $\varepsilon^{\text{trim}}$

1. Solve for $N_\alpha$ adjoints:
   \[ \frac{\partial R}{\partial U}^T \psi_i^{\text{trim}} + \frac{\partial J_i^{\text{trim}}}{\partial U} = 0 \]

2. Compute $N_\alpha$ residual linearizations:
   \[ \frac{\partial R}{\partial \alpha} \quad \text{(cheap finite differences)} \]

3. Form sensitivity matrix:
   \[ \frac{d J_i^{\text{trim}}}{d \alpha} = \left( \psi_i^{\text{trim}} \right)^T \frac{\partial R}{\partial \alpha} + \frac{\partial J_i^{\text{trim}}}{\partial \alpha} \]

One can also solve flow and trimming equations simultaneously.
Mesh adaptation mechanics

- Select a fraction $f_{\text{frac}}$ 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.
Supersonic biplane

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

![Graphs showing angle of attack and drag convergence for unconstrained and constrained cases.](image)
Supersonic biplane

- Trim and adapt outputs have different domains of dependence.
- Unconstrained adaptation does not target the upper airfoil.
NACA 0012

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

**Strategy**

- Compute "exact" lift at $\alpha = 1^\circ$  
  \[ c_{\ell}^{\text{exact}} = 0.018250. \]
- Set $c_{\ell}^{\text{target}} = 0.018250$.
- Use $c_{\ell}^{\text{exact}}$ and $c_d^{\text{exact}}$ to evaluate constrained vs. unconstrained adaptation.
Trimming parameter converges faster for constrained adaptation.
Unconstrained adaptation lags behind constrained adaptation.
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.
- \( M_\infty = 0.2, \; Re_{C_W} = 9 \times 10^6 \) 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, \( C_t = 0.3 \times C_W \)
- Separation = 4.0 \times C_W
High-lift configuration

Flow/trim solve for first adaptive iteration:

Note: trimming succeeds despite flow solution stall.
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.

6th adapted mesh (155661 elements).
DPW5 case

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

![Graph showing lift coefficient and angle of attack against work units.](image)
DPW5 case

Initial Mach contours

Final Mach contours
DPW5 case

Initial Mach contours

Final Mach contours
DPW5 case

- Including the constraint error smooths 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!