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

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Outline

1. Introduction
2. Output-Based Error Estimation
3. The Entropy Adjoint Connection
4. Implementation and Results
5. Conclusions
Increasing interest in solution-based adaptive methods in CFD

- Complex problems often exhibit a wide range of length scales whose distribution is not known \textit{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

\[ \delta J = J_H(u_H) - J(u) \]

- \( u_H \in \mathcal{V}_H = \) approximate solution,
- \( u \in \mathcal{V} = \) exact solution

**Adjoints-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

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The Continuous Adjoint

Primal equation

\[ r(u) = 0, \text{ on } \Omega \]

The continuous adjoint, \( \psi \), is a Lagrange multiplier for

\[ L = J(u) - \int_{\Omega} \psi^T r(u) d\Omega \]

Requiring a stationary Lagrangian for permissible state variations, \( \delta u \in V_{\text{perm}} \), yields (in weak form) the

\[ J'[u](\delta u) - \int_{\Omega} \psi^T r'[u](\delta u) d\Omega = 0, \quad \forall \delta u \in V_{\text{perm}} \]
Example: First-Order Conservation Laws

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

\[ r(u) = A_i \partial_i u = 0 \]

The adjoint equation is, after an integration by parts,

\[ J'[u](\delta u) + \int_\Omega \partial_i \psi^T A_i \delta u d\Omega - \int_{\partial \Omega} \psi^T A_i \delta u n_i ds = 0, \quad \forall \delta u \in V_{\text{perm}} \]

If \( J(u) \) is an integral on \( \partial \Omega \), \( \psi \) must satisfy

\[ A_i^T \partial_i \psi = 0, \quad \text{in } \Omega, \]

subject to the boundary conditions

\[ J'[u](\delta u) - \int_{\partial \Omega} \psi^T A_i \delta u n_i ds = 0, \quad \forall \delta u \in V_{\text{perm}} \]
Output Error Estimation with Adjoints

1. \( u_H \in \mathcal{V}_H \) will generally not satisfy the analytical PDE: \( r(u_H) \neq 0 \)

2. If \( \delta u \equiv u_H - u \) is small, we can write

\[
 r(u_H) = r(u + \delta u) \approx r'[u](\delta u)
\]

3. Using the adjoint equation we have

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

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
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):

\[
\begin{align*}
\mathbf{r}(\mathbf{u}) &= \mathbf{A}_i \partial_i \mathbf{u} = 0, \\
\partial_i F_i &= 0
\end{align*}
\]

- Primal equation
- Entropy conservation

\(F_i(\mathbf{u})\) is the entropy flux associated with an entropy function \(U(\mathbf{u})\)
The entropy pair \((U(u), F_i(u))\) must satisfy \(U_u A_i = (F_i)u\)

- **The entropy variables** are defined by

\[
v \equiv U^T_u
\]

The entropy variables symmetrize the equations in the sense that

1. \(u_v\) is symmetric, positive definite
2. \(A_i u_v\) is symmetric

Using these symmetry properties, we have

\[
0 = A_i \partial_i u = A_i u_v \partial_i v = u_v A_i^T \partial_i v \implies A_i^T \partial_i v = 0
\]

The entropy variables satisfy the adjoint equation! (BCs too)
We examine the adjoint-weighted residual to deduce the output:

\[ \delta J = \int_{\Omega} \mathbf{v}^T \delta \mathbf{r} \, d\Omega = \int_{\Omega} \mathbf{v}^T \mathbf{A}_i \partial_i \delta \mathbf{u} \, d\Omega = -\int_{\Omega} \partial_i \mathbf{v}^T \mathbf{A}_i \delta \mathbf{u} \, d\Omega + \int_{\partial \Omega} \mathbf{v}^T \mathbf{A}_i \delta \mathbf{u} \, n_i ds \]

\[ = \int_{\partial \Omega} (F_i) u \delta \mathbf{u} \, n_i ds = \delta \left[ \int_{\partial \Omega} F_i n_i ds \right] \]

\[ J \text{ measures the net entropy flow out of the domain} \]
Second-Order Conservation Laws

Primal equation:

\[ r(u) = A_i \partial_i u - \partial_i (K_{ij} \partial_j u) = 0 \]

- Viscous dissipation is a source term in the adjoint equation for \( v \)

The entropy variables serve as an “adjoint” solution for

\[
J = \int_{\partial \Omega} F_i n_i ds + \int_{\Omega} \partial_i v^T \tilde{K}_{ij} \partial_j v d\Omega - \int_{\partial \Omega} v^T \tilde{K}_{ij} \partial_j v n_i ds
\]

where \( \tilde{K}_{ij} \equiv K_{ij} u_v \) is symmetrized in the sense that \( \tilde{K}_{ij} = \tilde{K}_{ji}^T \)

- The expression for \( J \) is an entropy balance statement: \( J(u) = 0 \)
- The terms in \( J \) do not necessarily balance for \( u_H \)
Using the Entropy Variables

The entropy variables are readily computable from $\mathbf{u}$,

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

where the entropy function $U$ is

$$U = -\frac{\rho S}{(\gamma - 1)}, \quad S = \ln p - \gamma \ln \rho,$$

**Approach**

Use $\mathbf{v}$ 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
Verification of the Entropy Adjoint Connection

Compare the entropy variables, $v_h$, to the discrete adjoint, $\psi_h$, for

$$J_h = \int_{\partial \Omega} F_i(u_h^b) n_i ds$$

Linear variation of $S$

Compute: \( (\text{Entropy variable adjoint error})^2 = \int_{\Omega} ||\psi_h - v_h||^2 d\Omega \)
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

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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
Degree of freedom (DOF) versus output error for $p = 2$

Entropy adjoint performance is comparable to output adjoints
NACA 0012, $M = 0.4$, $\alpha = 5^\circ$, Final Meshes

Drag Adjoint

Entropy Adjoint

Lift Adjoint

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

- 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**

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Degree of freedom (DOF) versus output error for $p = 2$
Entropy adjoint performance is comparable to output adjoints
NACA 0012, $M = 0.8, \alpha = 1.25^\circ$

- 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
Degree of freedom (DOF) versus output error for $p = 2$

More noise in results – entropy adjoint still performs well
NACA 0012, $M = 0.8$, $\alpha = 1.25^\circ$, 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
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