Recent Advances in Discretization Error Estimation using Error Transport Equations

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Discretization Error (DE) is often a major source of error and uncertainty in Computational Fluid Dynamics predictions

• Adjoint methods have become the method of choice for estimating DE and allowing targeted DE reduction in functionals
  – Provide an error estimate in a single solution functional (e.g., drag)
  – Allow for solution adaptation to reduce DE in a single functional
  – Requires full implicit Jacobian and one additional (linear) solve

• Advantages of Error Transport Equations (ETE) vs. adjoints
  – Provides DE estimates in all functionals simultaneously
  – Provides DE estimates in all field variables (e.g., pressure and velocity over the domain)
  – If the full implicit Jacobian is available, requires one linear solve
Residual Methods and Truncation Error

• At the heart of residual-based error estimation is the ability to accurately quantify the truncation error

• Truncation error can be defined, using the Generalized Truncation Error Expression (GTEE), as the difference between the discrete and continuous governing equations:

  \[ L_h(I^h u) = I^h L(u) + \tau_h(u) \]

  Discrete Governing Equations: \( L_h(\cdot) \)  
  General Continuous Function: \( u \)
  Continuous Governing Equations: \( L(\cdot) \)  
  Restriction/Prolongation Operator: \( I^h / I_h \)
  Truncation Error: \( \tau_h(\cdot) \)

• Truncation error represents higher order terms which are lost during the discretization process
Functional Error Estimation via Adjoints

• For error estimation, adjoints can be thought of as a constrained optimization problem for the functional error, subject to satisfying the discrete (or continuous) governing equations

• Consider a Taylor Series expansion of $L_h(I^h\tilde{u})$ about the discrete solution, $u_h$:

$$L_h(I^h\tilde{u}) = L_h(u_h) - \frac{\partial L_h}{\partial u} \bigg|_{u_h} \varepsilon_h + \frac{\partial^2 L_h}{\partial u^2} \bigg|_{u_h} \frac{\varepsilon_h^2}{2} + O(\varepsilon_h^3)$$

  – Local Discretization Error: $\varepsilon_h = u_h - I^h\tilde{u}$
  – LHS is the truncation error (needs the exact solution)
  – We estimate the truncation error by taking the numerical solution, reconstructing it to a chosen order, then inserting it into the original governing equation: $\tau_h \approx L(I_h u_h)$
Likewise, consider a Taylor Series expansion of a discrete solution functional, $J_h(\cdot)$, about the exact discrete solution, $u_h$:  

$$J_h(I^h \tilde{u}) = J_h(u_h) - \frac{\partial J_h}{\partial u} \bigg|_{u_h} \varepsilon_h + \frac{\partial^2 J_h}{\partial u^2} \bigg|_{u_h} \frac{\varepsilon_h^2}{2} + O(\varepsilon_h^3)$$

Combining in a Lagrangian by noting the discrete equations are exactly satisfied, $L_h(u_h) = 0$:

$$J_h(I^h \tilde{u}) = \left[ J_h(u_h) - \frac{\partial J_h}{\partial u} \bigg|_{u_h} \varepsilon_h + \frac{\partial^2 J_h}{\partial u^2} \bigg|_{u_h} \frac{\varepsilon_h^2}{2} + O(\varepsilon_h^3) \right]$$

$$+ \lambda^T \left[ L_h(I^h \tilde{u}) + \frac{\partial L_h}{\partial u} \bigg|_{u_h} \varepsilon_h - \frac{\partial^2 L_h}{\partial u^2} \bigg|_{u_h} \frac{\varepsilon_h^2}{2} + O(\varepsilon_h^3) \right]$$

$L_h(u_h) = 0$
Background: Adjoint Methods

Functional Error Estimation via Adjoints

- Rearranging, neglecting higher order terms, and inserting the definition of truncation error:

\[
\varepsilon_{J_h} = J_h(u_h) - J_h(I^h \tilde{u}) \approx -\lambda^T \tau_h(\tilde{u}) + \left[ \frac{\partial J_h}{\partial u} \bigg|_{u_h} - \lambda^T \frac{\partial L_h}{\partial u} \bigg|_{u_h} \right] \varepsilon_h + \left[ -\frac{\partial^2 J_h}{\partial u^2} \bigg|_{u_h} + \lambda^T \frac{\partial^2 L_h}{\partial u^2} \bigg|_{u_h} \right] \frac{\varepsilon_h^2}{2}
\]

- The adjoint variables, \( \lambda \), can be computed by requiring the adjoint problem be identically zero such that:

\[
\left[ \frac{\partial L_h}{\partial u} \bigg|_{u_h} \right]^T \lambda = \left[ \frac{\partial J_h}{\partial u} \bigg|_{u_h} \right]^T
\]

- Primal Solution Residual Jacobian: \( \frac{\partial L_h}{\partial u} \bigg|_{u_h} \)

- Linearization of Functional w.r.t. Primal Solution: \( \frac{\partial J_h}{\partial u} \bigg|_{u_h} \)
Error Transport Equation (ETE)

- We seek an efficient alternative to adjoints for functional error estimation which also provides local error estimates.
- This is accomplished by deriving an ETE for the local discretization error everywhere in the domain.

- Expanding $L_h(I^h\tilde{u})$ about the discrete solution, $u_h$:

$$L_h(I^h\tilde{u}) = L_h(u_h) - \frac{\partial L_h}{\partial u} \bigg|_{u_h} \varepsilon_h + O(\varepsilon_h^2)$$

- By inserting the truncation error, $L_h(I^h\tilde{u}) = \tau_h(\tilde{u})$, and neglecting higher order terms, an estimate of the local error can be obtained by solving the following (linear) ETE:

$$\frac{\partial L_h}{\partial u} \bigg|_{u_h} \varepsilon_h \approx -\tau_h(\tilde{u})$$
Error Estimation

Adjoint / ETE Equivalence

• To illustrate the connection between the ETE and functional error estimation, the adjoint problem is used to rewrite the functional error estimate (minus higher order remaining error) as:

\[
\mathcal{E}_J \approx -\mathcal{L} \mathcal{H} \\
\mathcal{H} \approx \frac{\partial J_h}{\partial u} \left|_{u_h} \left[ \frac{\partial L_h}{\partial u} \right]_{u_h} \right|^{-1} \tau_h(\mathcal{H})
\]

• Therefore, the functional error estimate can be viewed as either:
  – Inner product of the adjoint solution with the truncation error
  – Inner product of the ETE solution with the functional linearization
Application

Quasi-1D Nozzle

- **Computational Domain:**
  \[ x \in [-1, 1] \]

- **Area Distribution:**
  \[ A(x) = 1 - 0.8 e^{-12.5x^2} \]

- **Inflow Conditions:**
  - \( p_0 = 300 \text{ kPa} \)
  - \( T_0 = 600 \text{ K} \)

- **Outflow Conditions:**
  - \( p_{\text{back}} = 297.485 \text{ kPa} \)

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Adjoint / ETE Equivalence for Solution Functionals

Adjoint / ETE Equivalence

• Functional of Interest:
  \[ J_h(u_h) = \sum_{i=1}^{N_{\text{cells}}} p_i \Delta x_i \]

• Primal Case:
  – Subsonic-Subsonic

• Truncation Error:
  – Exact TE

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Higher-Order Primal Solutions

Recent Advances in Discretization Error Estimation using Error Transport Equations
## Higher-Order Primal Solutions

### Runtime Comparison: LO + ETE vs. HO

#### Subsonic-Subsonic

<table>
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<tr>
<th>Grid Size (cells)</th>
<th>2(^{nd}) Order + ETE</th>
<th>4(^{th}) Order</th>
<th>Speedup</th>
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#### Subsonic-Supersonic

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<th>4(^{th}) Order</th>
<th>Speedup</th>
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</table>

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Effect of Lower Order Jacobian

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Global Error Estimation on Perturbed Grids

Variable: Pressure
Primal Solution: Subsonic-Supersonic
Reconstruction Order: $k = 2$

Functional: Integral of Pressure
Primal Solution: Subsonic-Supersonic
Reconstruction Order: $k = 2$

Pressure Discretization Error

Integral of Pressure

Reconstruction Order: $k = 2$

Recent Advances in Discretization Error Estimation using Error Transport Equations
Global Error Estimation on Perturbed Grids

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Local Error Estimation on Perturbed Grids

Recent Advances in Discretization Error Estimation using Error Transport Equations

Pressure Discretization Error

Energy Truncation Error

Grid Perturbation: $\Delta = 0.00$
Local Error Estimation on Perturbed Grids

Pressure Discretization Error

Energy Truncation Error

Grid Perturbation: $\Delta = 0.05$
Local Error Estimation on Perturbed Grids

Pressure Discretization Error

Energy Truncation Error

Grid Perturbation: $\Delta = 0.20$

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Conclusions

- Error transport equations (ETE) were shown to be mathematically equivalent to adjoint methods when using the same linearization and truncation error.
- ETE provide error estimates in all functionals simultaneously, as well as all local (field) quantities.
- The error estimates from ETE can be used to provide higher order functionals and local (field) quantities.
- Use of a lower order Jacobian reduces the order of the correction by one (generally from 4\textsuperscript{th} order to 3\textsuperscript{rd} order).
- Error estimation on perturbed (i.e., unstructured) grids is more challenging but can still provide good error estimates.
Thank You