On the use of a Second Moment Equation for *A Posteriori* Error Estimate in CFD

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Motivations Driving Research into Error Analysis

- Modern computer power has increased and the development of numerical error analysis has been left behind.
- A reliance on computer power provides grid independent results, but information on the nature, location and size of errors is not known.
- To simulate using the mesh refinements required for grid independence is an inefficient use of resources.
- CFD is seen as unreliable in the design process – providing an error analysis on all results would change this.
The Requirements of a CFD Error Analysis method in Industry – Goals of the Research

- To output information about the location of errors.
- To output information about the size of these errors.
- To not increase the time/power requirements of the simulation significantly.
- To be simple to implement by the user.
Previous Work

• A few recent attempts at creating error analysis methods.

• Their use has been to improve automatic mesh refinement.

• For example the moment error residual method (prof. H. Jasak) involves using the second moment equation to calculate an error estimate.
Previous Work
Moment Error Residual Method

- Scalar transport equation for \( f \)
  \[
  \underline{u} \cdot \nabla f - \nu \nabla^2 f = S
  \]
  - Multiply by \( f \)
  \[
  \underline{u} \cdot (f \nabla f) - \nu f \nabla^2 f = f S
  \]

- Vector transport equation for \( \underline{u} \)
  \[
  \underline{u} \cdot \nabla \underline{u} - \nu \nabla^2 \underline{u} = \underline{F}
  \]
  - Take the scalar product with \( \underline{u} \)
  \[
  \underline{u} \cdot (\underline{u} \cdot \nabla \underline{u}) - \nu \underline{u} \cdot (\nabla^2 \underline{u}) = \underline{u} \cdot \underline{F}
  \]
• Rearrangement of these produces the second moment equation which is a transport equation for the squared variable:

**Scalar**

\[ \overline{u} \cdot \nabla \left( \frac{f^2}{2} \right) - \nu \nabla^2 \frac{f^2}{2} + \nu \nabla f \cdot \nabla f = fS \]

or

\[ \overline{u} \cdot \nabla q - \nu \nabla^2 q = -\nu \nabla f \cdot \nabla f + fS \]
Rearrangement of these produces the second moment equation which is a transport equation for the squared variable:

**Vector**

\[
\underline{u} \cdot \nabla \frac{u \cdot u}{2} - \nu \nabla^2 \frac{u \cdot u}{2} + \nu (\nabla u_i \cdot \nabla u_i) = \underline{u} \cdot \underline{F}
\]

or

\[
\underline{u} \cdot \nabla K - \nu \nabla^2 K = -\nu (\nabla u_i \cdot \nabla u_i) + \underline{u} \cdot \underline{F}
\]
Previous Work
Moment Error Residual Method

• The simulation solution is not a solution of this equation.

\[
\mathbf{u} \cdot \nabla \left( \frac{f_{num}^2}{2} \right) - \nu \nabla^2 \left( \frac{f_{num}^2}{2} \right) + \nu \nabla f_{num} \cdot \nabla f_{num} - f_{num} S \neq 0
\]

• Substituting it into this leaves a residual.

\[
R_p = \mathbf{u} \cdot \nabla \left( \frac{f_{num}^2}{2} \right) - \nu \nabla^2 \left( \frac{f_{num}^2}{2} \right) + \nu \nabla f_{num} \cdot \nabla f_{num} - f_{num} S
\]

• \( R_p \) is rescaled and becomes the error estimate.
Proposed Method: Solving for the Variable and its Square

\[ u \cdot \nabla q - \nu \nabla^2 q = -\nu \nabla f \cdot \nabla f + f S \]

- Instead, the second moment equation will be solved to calculate the variable squared.
- Once the scalar (or vector) solution is found, it is used to estimate the source term in the second moment equation.
- In Saturne a user scalar is solved, using the source term as an explicit source, to find the squared variable solution, and can be done simultaneously.
Proposed Method: Using Solutions to Create an Error Estimate

\[ q - \frac{f^2}{2} \]

- These values were found to give good qualitative estimations of the errors.

- It can be shown this combination does not depend linearly on the solution errors.

\[ \sqrt{q} - \frac{f}{\sqrt{2}} \]

- These values were found to give good quantitative estimations of the errors.

- This combination depends linearly on the solution errors.
Proposed Method: Using Solutions to Create an Error Estimate

- The proposed error estimation is a combination of these two sets of values:

\[ \left[ q - \frac{f^2}{2} \right] \frac{\max(\sqrt{q} - \frac{f}{\sqrt{2}})}{\max(q - \frac{f^2}{2})} \]

- The better estimation of the shape has been rescaled by the better estimation of the scale.
1D Convection Diffusion Equation

- A simplification of the scalar transport equation in 1D with no source. Boundary conditions \( f = 0 \) at \( x = 0 \), \( f = 1 \) at \( x = 1 \)

\[
\frac{\partial f}{\partial x} - \nu \frac{\partial^2 f}{\partial x^2} = 0
\]

- The solution is

\[
f = \frac{e^{\frac{x Pe}{L}} - 1}{e^{Pe} - 1}
\]

where \( Pe \) is the Peclet number and \( L \) is the length of the geometry.
1D Convection Diffusion Solution Error and Previous Error Estimation

- The solution error
- The moment error residual method prediction
1D Convection Diffusion New Method Error Estimation

- The numerical error
- The second moment solution error estimation
Point Source of a Scalar in a Crossflow in 3D

- A point source strength $S$ at the origin in a uniform crossflow in the $x$ direction

- Scalar transport equation is
  \[ \mathbf{u} \cdot \nabla f - \nu \nabla^2 f = S \]

- The exact solution is
  \[ f = \frac{S}{4\pi |x| \nu} e^{\frac{-u(|x|-x)}{2\nu}} \]
Point Source of a Scalar in a Crossflow in 3D

- A rectangle mesh begins at $x=0.05\text{m}$ to avoid the singularity.

- Boundary conditions: $u_x = 1\text{m/s}$, $f = f_{\text{exact}}$ and $q = q_{\text{exact}}$ at the inlet and walls.
The analytical solution shown on a cut through the mesh with 10 contours on a log scale across the range.
Point Source of a Scalar in a Crossflow Results

The difference between the numerical and analytical solution.

The second moment residual error estimate.
Point Source of a Scalar in a Crossflow Results

The difference between the numerical and analytical solution.

The second moment solution error estimate.
Constant Flux of a Scalar Through the Walls of a Ribbed Channel Flow

- Simulation of the transfer of a scalar through the walls of a ribbed channel into a fully developed laminar flow.
- A mesh independent velocity solution was used as a frozen velocity on a coarse mesh for a non-periodic calculation.

Fine mesh velocity solution
The boundary conditions for the squared and unsquared scalar variables were constant flux through the walls.

\[
\frac{\partial f}{\partial x} = 0.1[f m^{-1}]
\]

\[
\frac{\partial q}{\partial x} = 0.1 f_{wall} [f^2 m^{-1}]
\]
Ribbed Channel Flow Results

- The $f$ solution errors
- The moment residual prediction
Ribbed Channel Flow Results

- The $f$ solution errors
- The moment solution prediction
Conclusions

- Developments in error analysis are necessary for CFD to become a trusted tool for design.
- The area is underdeveloped, and previous methods have room for improvement.
- The method presented here has shown promise at evaluating both the location and size of solution errors when solving for a scalar transport.
- The vector transport analysis also shows promise.
Thank You for Listening

Any Questions?

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