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

University of Manchester

EngD

Stuart Russant

Supervisors: D. Laurence, H. Iacovides

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

Contents

- Motivation for research into error analysis
- Goals of the research
- Previous work
- The proposed novel method
- Test cases
- Conclusions

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 $\underline{u}$

$$\underline{u} \cdot (\underline{u} \cdot \nabla \underline{u}) - \nu \underline{u} \cdot (\nabla^2 \underline{u}) = \underline{u} \cdot \underline{F}$$

Previous Work
Moment Error Residual Method

- Rearrangement of these produces the second moment equation which is a transport equation for the squared variable:

<u>Scalar</u>

$$\underline{u} \cdot \nabla \frac{f^2}{2} - \nu \nabla^2 \frac{f^2}{2} + \nu \nabla f \cdot \nabla f = fS$$

or

$$\underline{u} \cdot \nabla q - \nu \nabla^2 q = -\nu \nabla f \cdot \nabla f + fS$$

Previous Work
Moment Error Residual Method

- Rearrangement of these produces the second moment equation which is a transport equation for the squared variable:

<u>Vector</u>

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

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.

$$\underline{u}\cdot\nabla\frac{f_{num}^2}{2}-\nu\nabla^2\frac{f_{num}^2}{2}+\nu\nabla f_{num}\cdot\nabla f_{num}-f_{num}S\neq 0$$

- Substituting it into this leaves a residual.

$$Rp=\underline{u}\cdot\nabla\frac{f_{num}^2}{2}-\nu\nabla^2\frac{f_{num}^2}{2}+\nu\nabla f_{num}\cdot\nabla f_{num}-f_{num}S$$

- Rp is rescaled and becomes the error estimate.

Proposed Method: Solving for the Variable and its Square

$$\underline{u} \cdot \nabla q - \nu \nabla^2 q = -\nu \nabla f \cdot \nabla f + f S$$

- 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.

MANCHESTER 1824

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

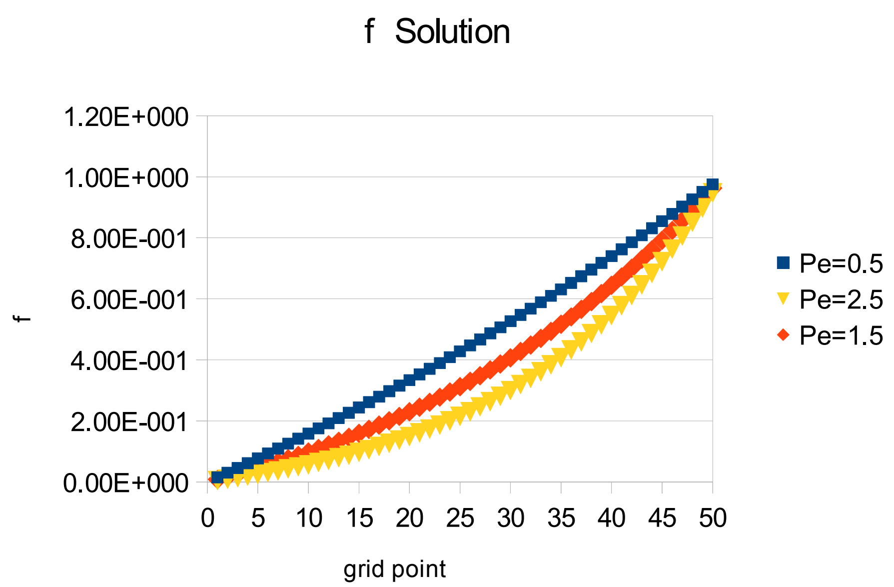
- A simplification of the scalar transport equation in 1D with no source. Boundary conditions $f=0$ at $x=0$, $f=1$ at $x=1$

$$u\frac{\partial f}{\partial x} - \nu \frac{\partial^2 f}{\partial x^2} = 0$$

- The solution is

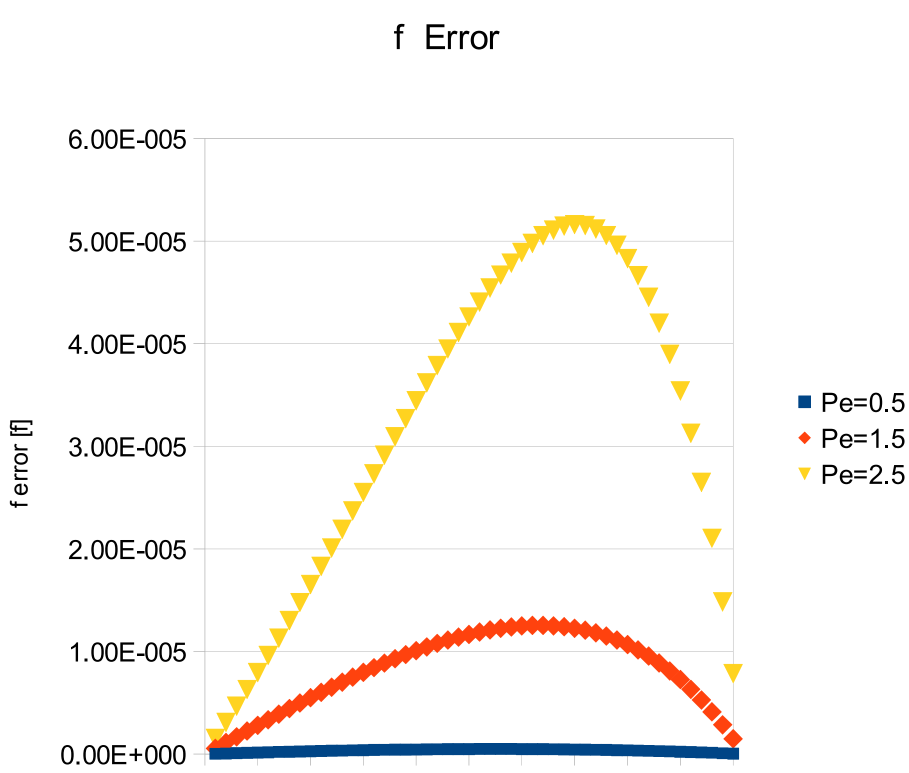
$$f = \frac{e^{\frac{xPe}{L}} - 1}{e^{Pe} - 1}$$

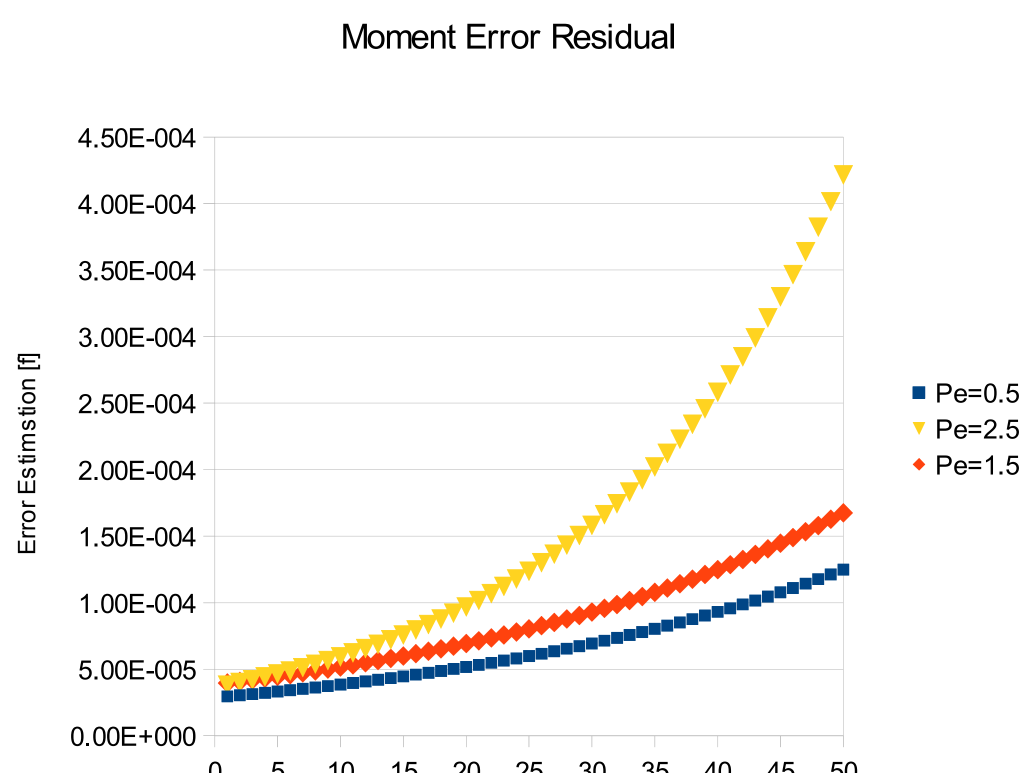
where Pe is the Peclet number and L is the length of the geometry



1D Convection Diffusion Solution Error and Previous Error Estimation

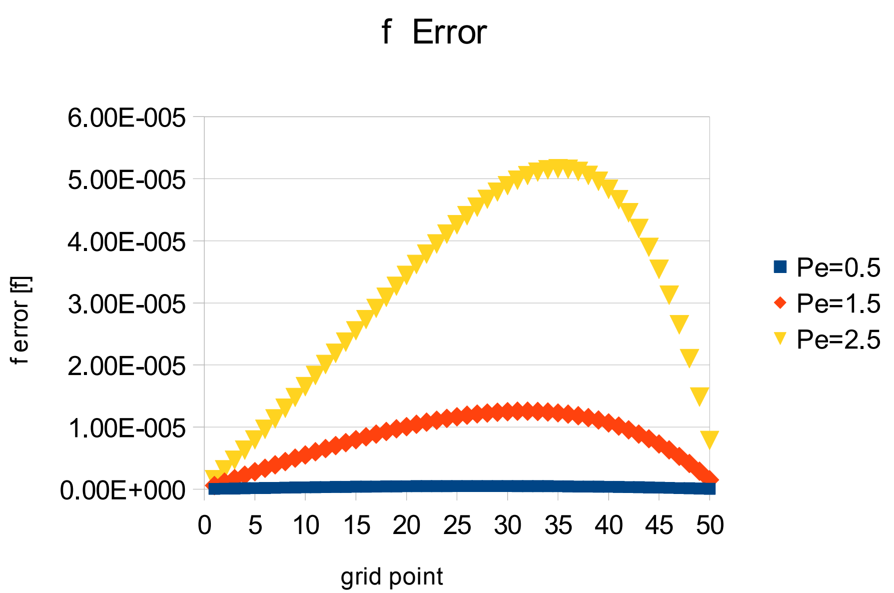
- The solution error
- The moment error residual method prediction



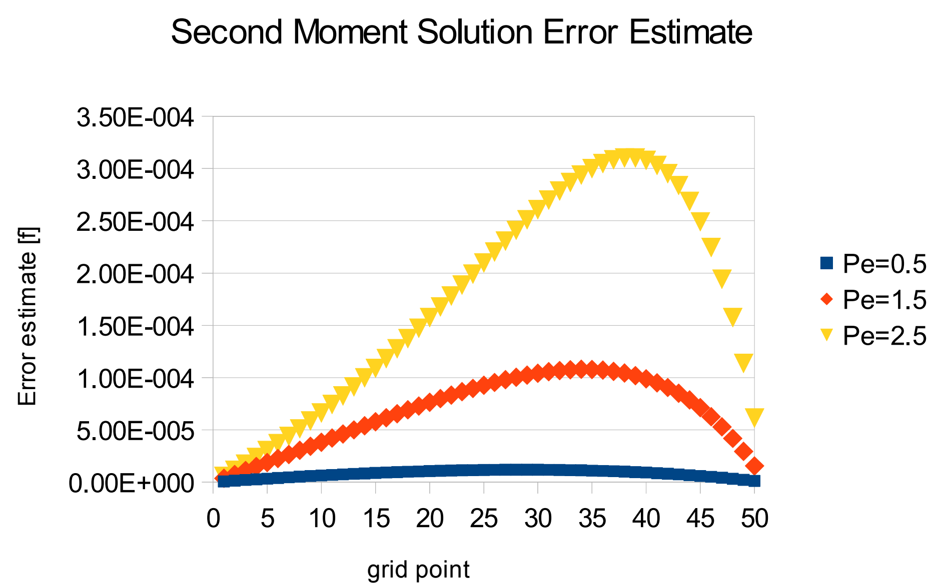


1D Convection Diffusion New Method Error Estimation

- The numerical error



- The second moment solution error estimation

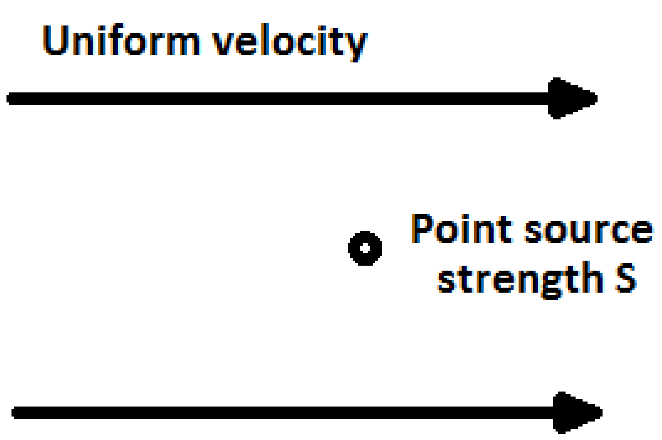


Point Source of a Scalar in a Crossflow in 3D

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

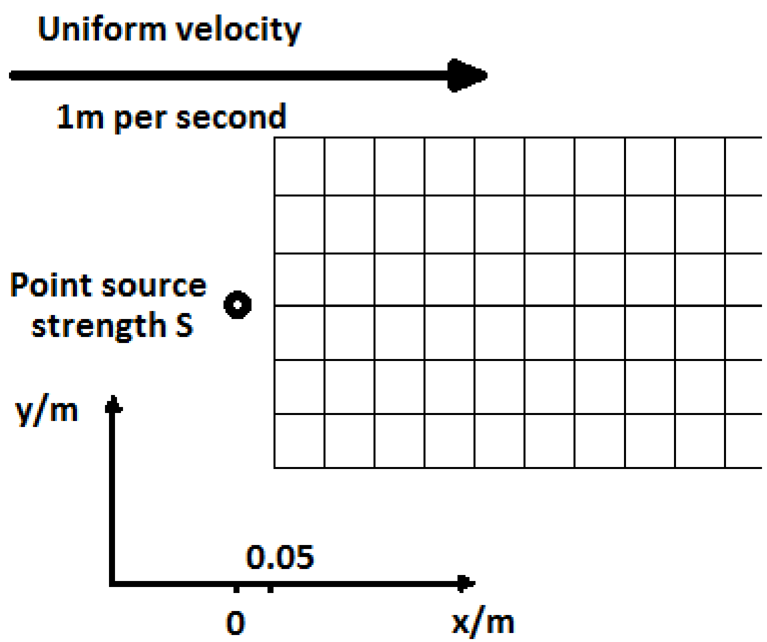
- Scalar transport equation is
$$\underline{u}\cdot\nabla f - \nu\nabla^2 f = S$$

- The exact solution is
$$f = \frac{S}{4\pi|\underline{x}|\nu} e^{\frac{-u(|\underline{x}|-x)}{2\nu}}$$

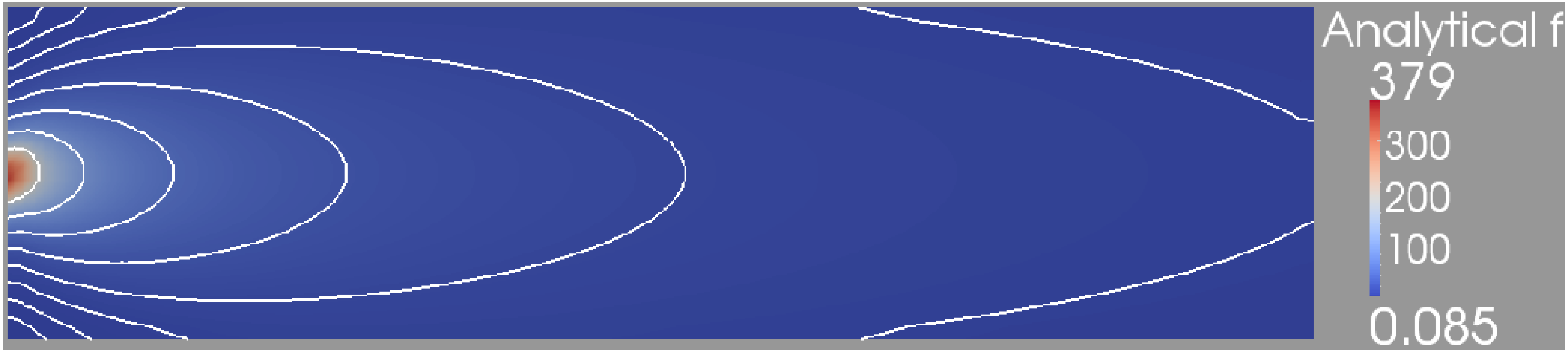


Point Source of a Scalar in a Crossflow in 3D

- A rectangle mesh begins at x=0.05m to avoid the singularity.
- Boundary conditions: $u_x = 1\text{m/s}$, $f = f_{exact}$ and $q = q_{exact}$ at the inlet and walls.



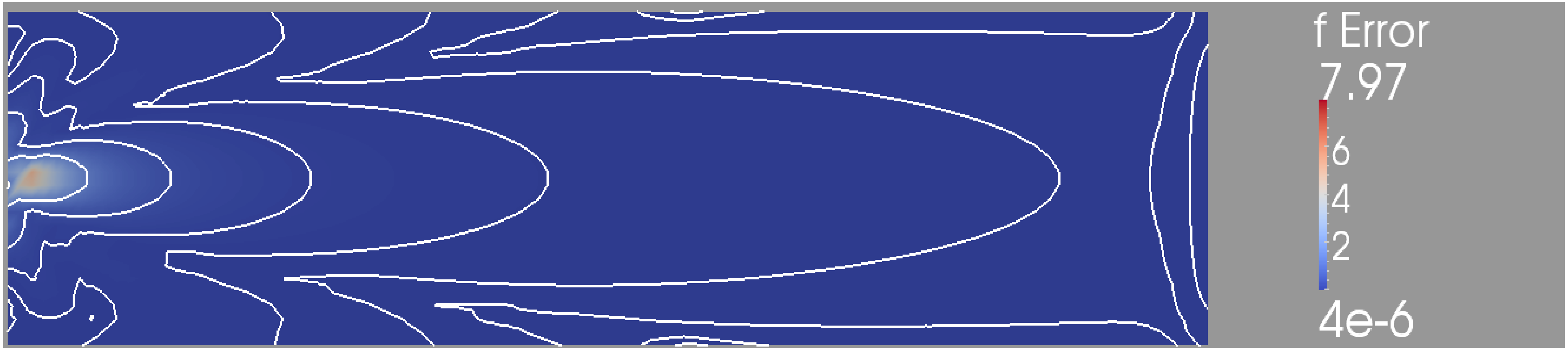
Point Source of a Scalar in a Crossflow Analytical Solution



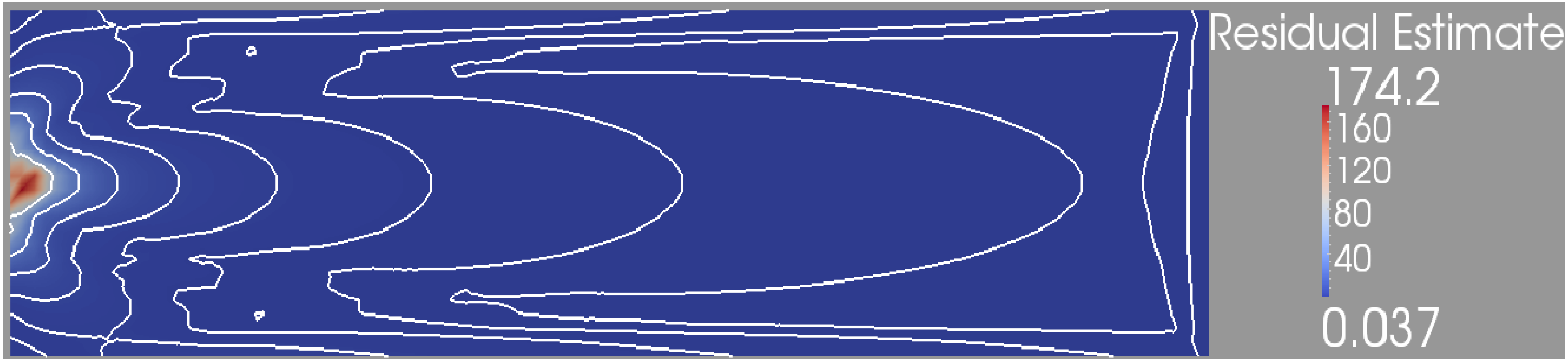
The analytical solution shown on a cut through the mesh with 10 contours on a log scale across the range.

Point Source of a Scalar in a Crossflow Results

The difference between the numerical and analytical solution.

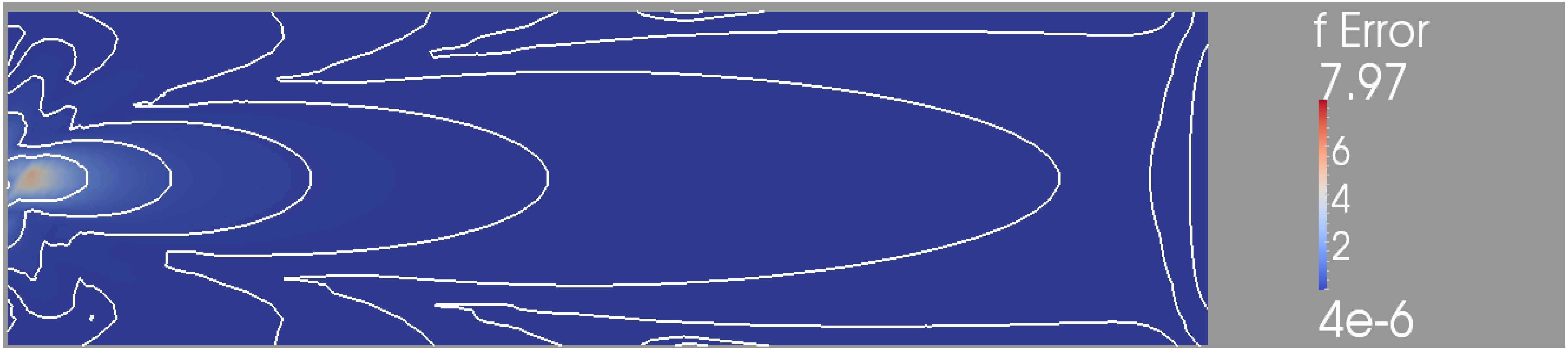


The second moment residual error estimate.

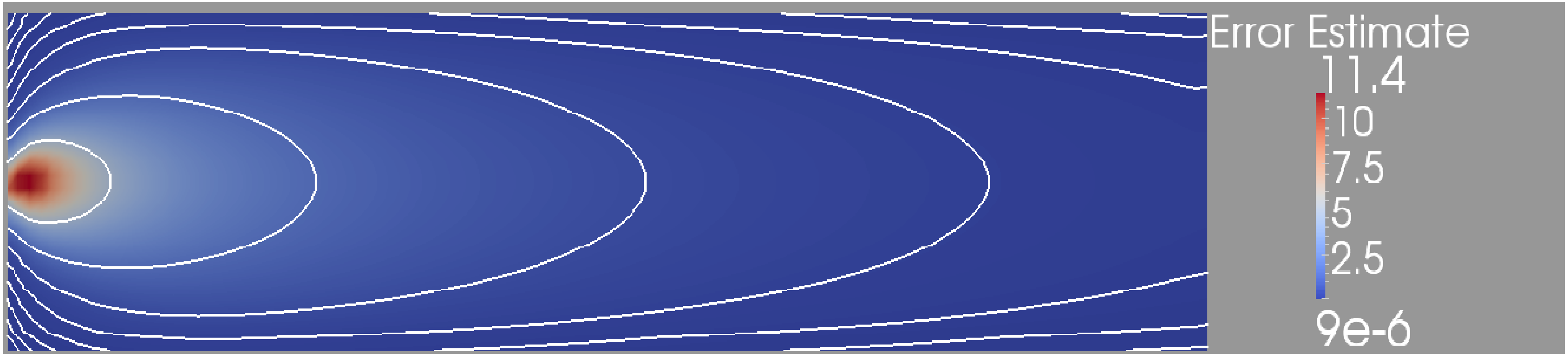


Point Source of a Scalar in a Crossflow Results

The difference between the numerical and analytical solution.



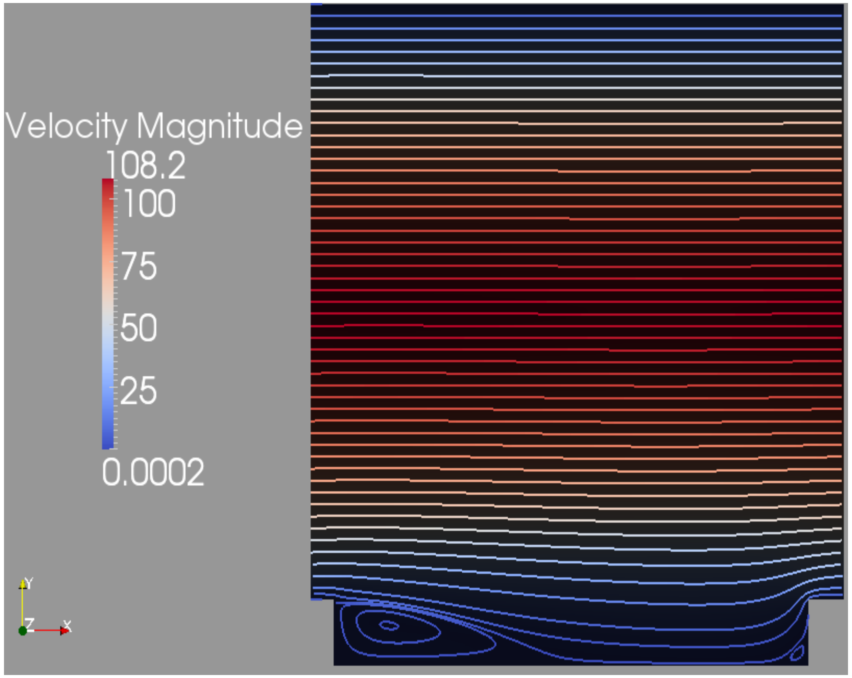
The second moment solution error estimate.



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

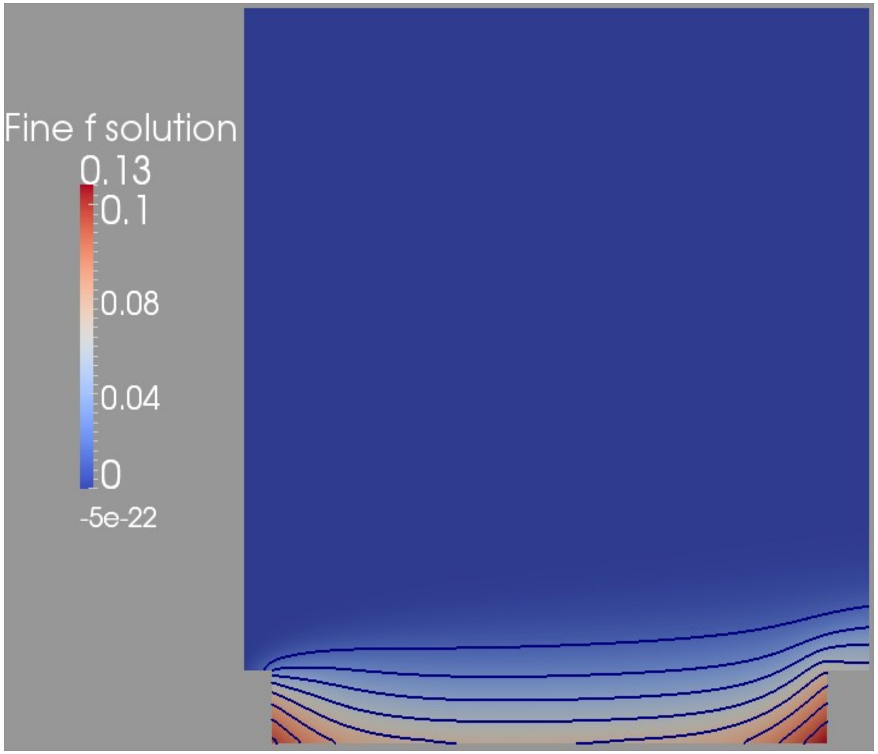


Constant Flux of a Scalar Through the Walls of a Ribbed Channel Flow

- The boundary conditions for the squared and unsquared scalar variables were constant flux through the walls.

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

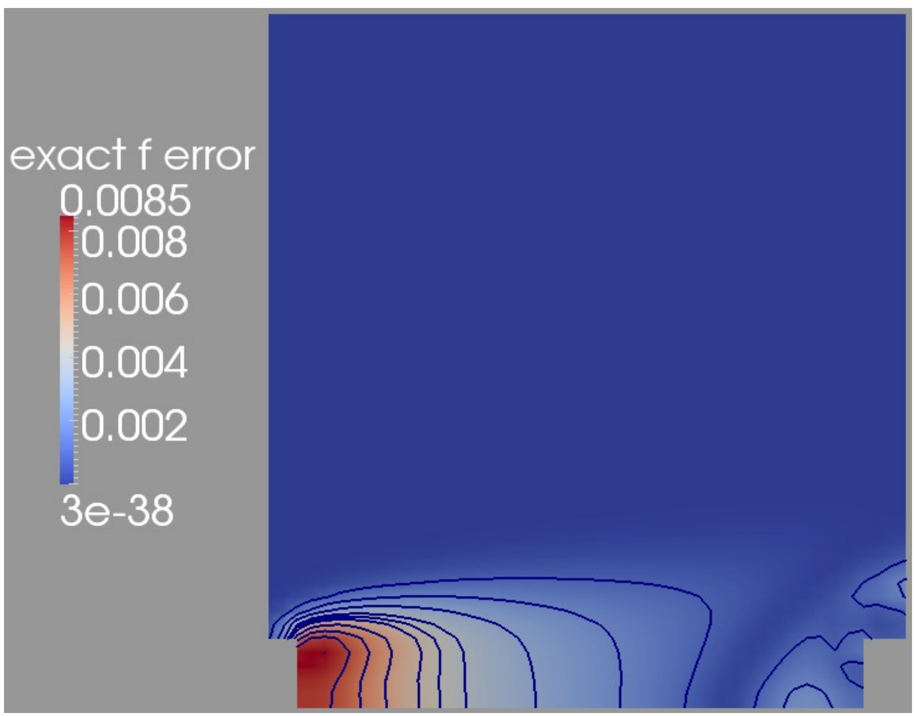
$$\frac{\partial q}{\partial x} = 0.1 f_{wall}\ [f^2 m^{-1}]$$



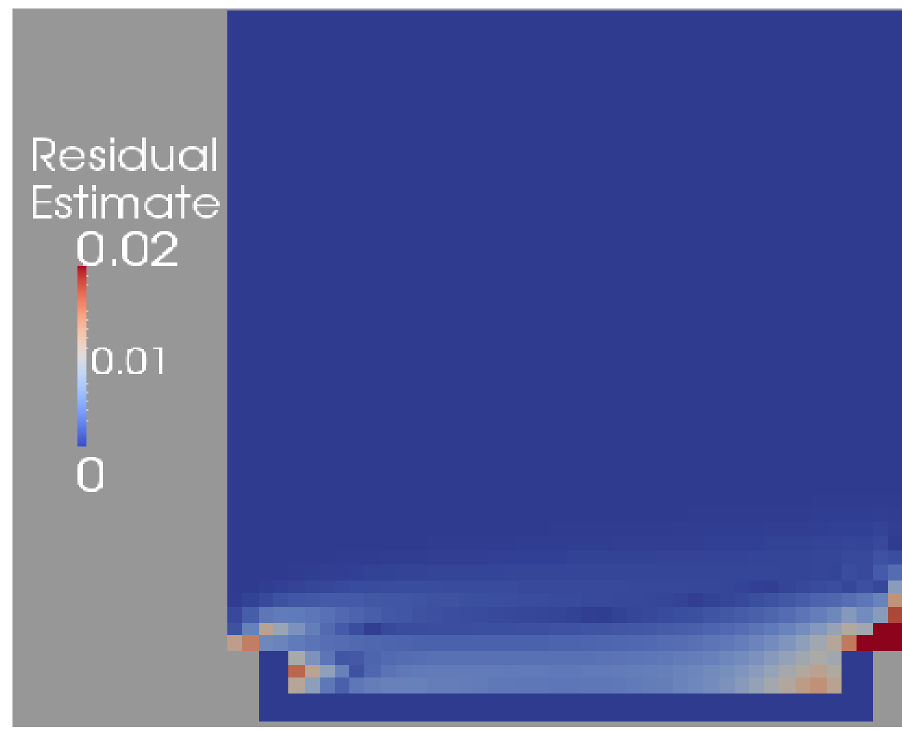
The fine mesh solution

Ribbed Channel Flow Results

- The f solution errors

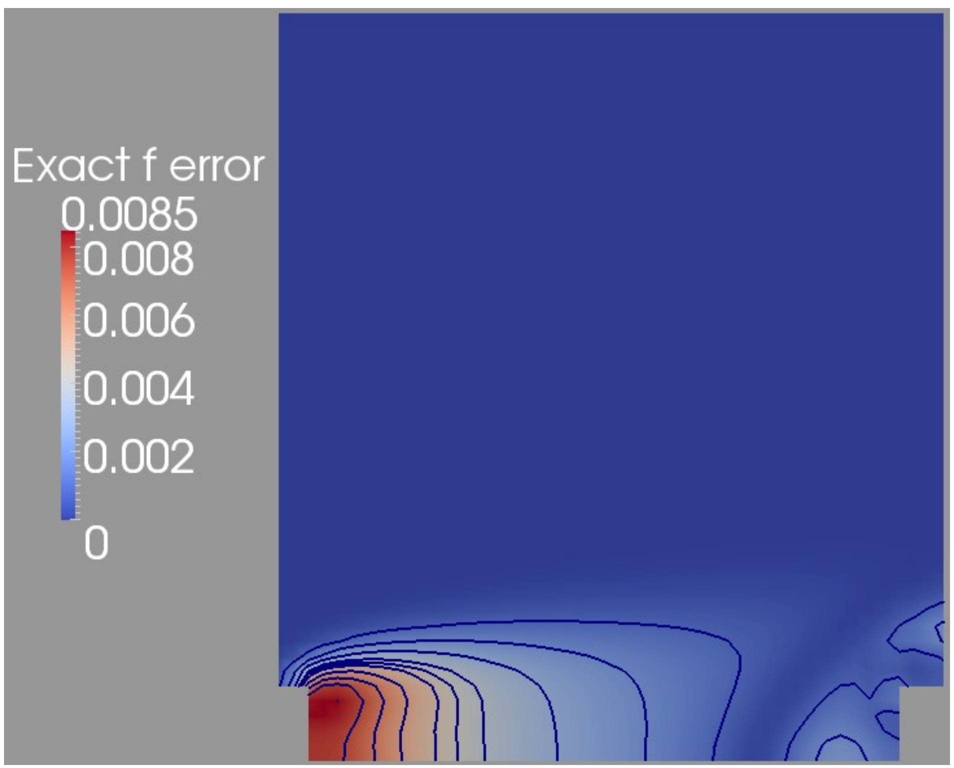


- The moment residual prediction

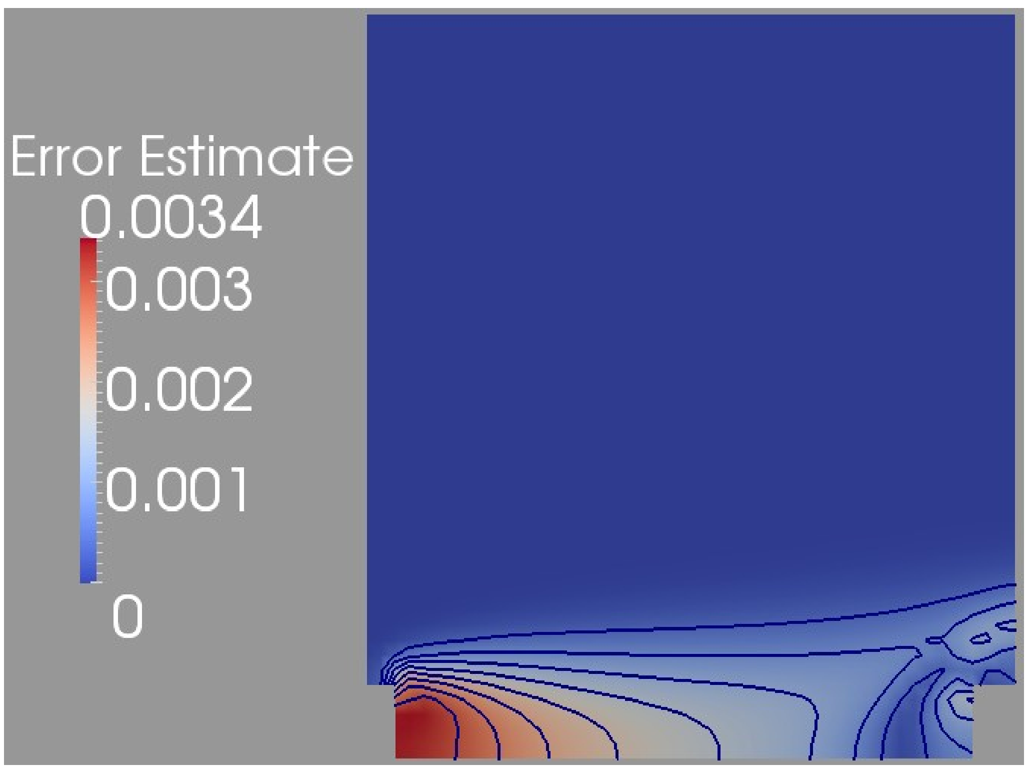


Ribbed Channel Flow Results

- 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?

Stuart Russant