SAND2007-0891C

Use of a Manufactured Solution for Verifying CFD Flux Schemes and BCs

Tuesday, 20 February, 2007

10:45–11:10

SIAM Conference on Computational Science and Engineering

Ryan B. Bond, Curtis C. Ober,
Thomas M. Smith, & Steven W. Bova
Sandia National Laboratories

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.

Verification

- Code verification deals with identifying:
  - Programming mistakes that cause the governing equations to be solved incorrectly, or
  - Shortcomings of formulations or algorithms that cause undesirable behavior in certain situations.
- Code verification involves comparing code output with known solutions.
- Solution verification deals with quantifying numerical errors in a given solution.

Order Verification

- One thing to verify is consistency: does the discrete solution converge to the continuum solution as the mesh is systematically refined?
- A more thorough analysis includes order verification: does the observed order of accuracy match the expected order of accuracy?
- Order verification can be performed via
  - the method of exact solutions, for equation sets having classical exact solutions or
  - the method of manufactured solutions (MMS), also known as order verification via the manufactured solution procedure (OVMSP).

Sandia National Laboratories

Comparison to Exact Solutions

1. An exact solution to the governing equations is obtained for a given domain and set of initial/boundary conditions.
2. Numerical solutions are produced using a series of systematically refined spatial and/or time discretizations.
3. The error norms of these numerical solutions are compared to determine the spatial and/or temporal order of accuracy.

Shortcomings of Using Classical Exact Solutions

- A classical exact solution may not exist for a given equation set.
- Classical exact solutions which do exist may lack generality and therefore fail to test all of the terms in the governing equations.
- Testing the full suite of boundary conditions may not be possible using classical exact solutions.
- Classical exact solutions which do exist may be difficult to accurately implement (*e.g.,* solutions obtained by Laplace transforms).

Sandia National Laboratories

The Method of Manufactured Solutions

1. Generate (*i.e.,* manufacture) a solution on the domain of interest: it need not satisfy the governing equations, but it needs to satisfy certain constraints (Knupp & Salari, 2003).
2. Operate on this manufactured solution with the differential operator found in the governing equation set.
3. Add the resulting expression to the governing equation set as a source term.
4. Provide this source term to the code, and then proceed with order verification.

Example

1) Consider Laplace's Equation :

$$\nabla^2 u = 0.$$

2) Manufacture a solution u^*.

3) Operate (analytically) on u^* with ∇^2 :

$$\nabla^2 u^* = f^*.$$

4) Provide the source term f^* to the code.

5) Run the code with the additional source term to obtain numerical solutions on a series of systematically refined grids.

6) Compare the numerical solutions with u^* to determine the spatial order of accuracy for the code.

Boundary Condition Issues

- For general boundary conditions (Dirichlet, Neumann, *etc*.), code input can be derived from the conditions satisfied by u^* on the boundary.
- For specialized boundary conditions (a.k.a. hardwired boundary conditions) one way to perform a test is to have u^* satisfy the boundary conditions in order to test their implementation.
- For hyperbolic and parabolic equation sets, only constraints corresponding to incoming characteristics need to be satisfied.

Sandia National Laboratories

Premo

premo (Latin) – to squeeze (compress)

Develop simulation capabilities to perform compressible flow calculations.

- **Compressible subsonic through hypersonic**
- **Laminar through turbulent regimes**
- **Inviscid and viscous flows**
- **Steady state and transient**

- **Finite Volume**
- **Node centered**
- **Edge Based**
- **Unstructured Mesh**

Sandia National Laboratories

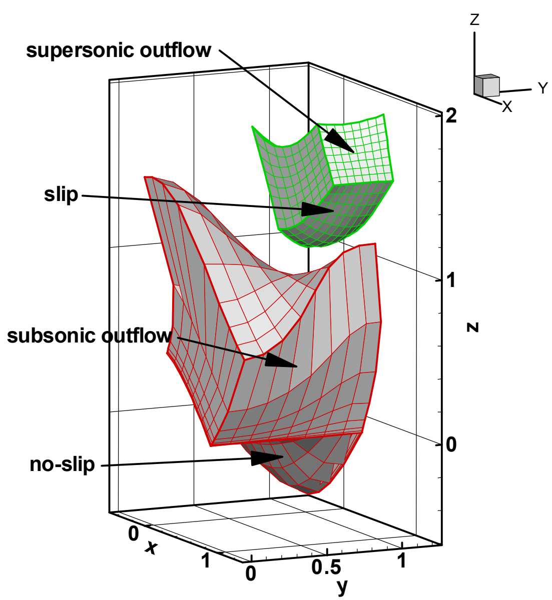
Meshes Used with Manufactured Solution

Original

$$F = \frac{1}{2}\cos(A_f x)\cos(B_f y) - z$$

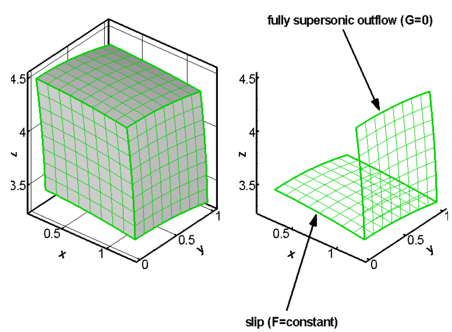
$$G = x - \frac{1}{2}\cos(A_g y)\sin(B_g y) - \frac{\pi}{4}$$

$$H = -y$$



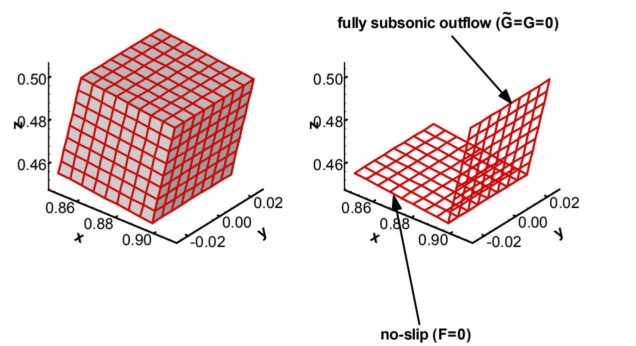
First Modification

Reduced the wave numbers by 4x (A_f, B_f, A_g and B_g)



Current

* Reduced computational domain by ~ 25x
* Created $\tilde{G}$ to handle $p \neq$ constant on outflow BC

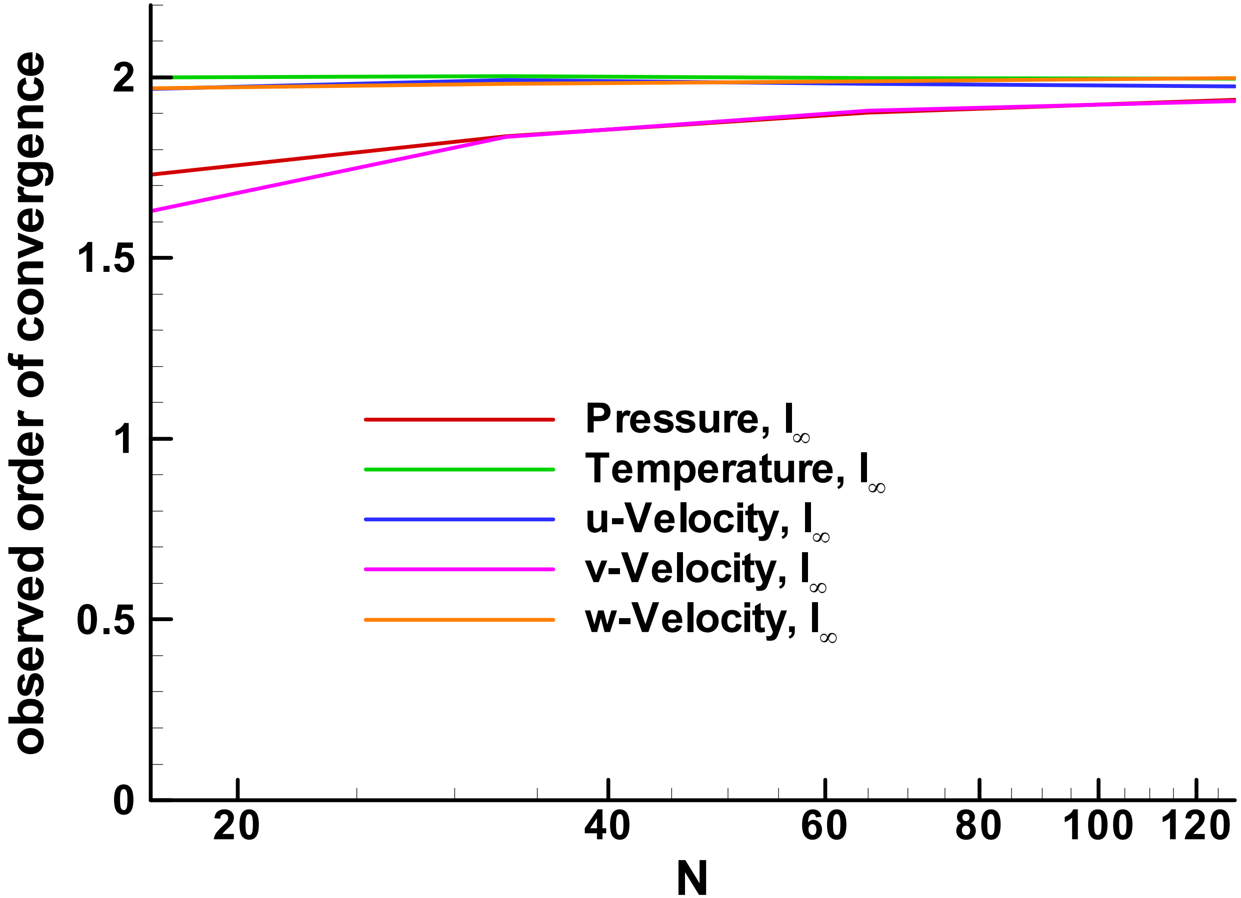


Coding Errors and Algorithmic Weaknesses

- Coding Errors
  - several parallel issues
  - indexing error for least squares gradient
  - CHAD gradient correction
  - several ‘kinks’ in fast-turnaround tests
  - other ‘bonus’ finds (bugs found while looking for others)
- Algorithmic Weaknesses
  - weak slip and outflow BC formulations
  - numerous gradient issues

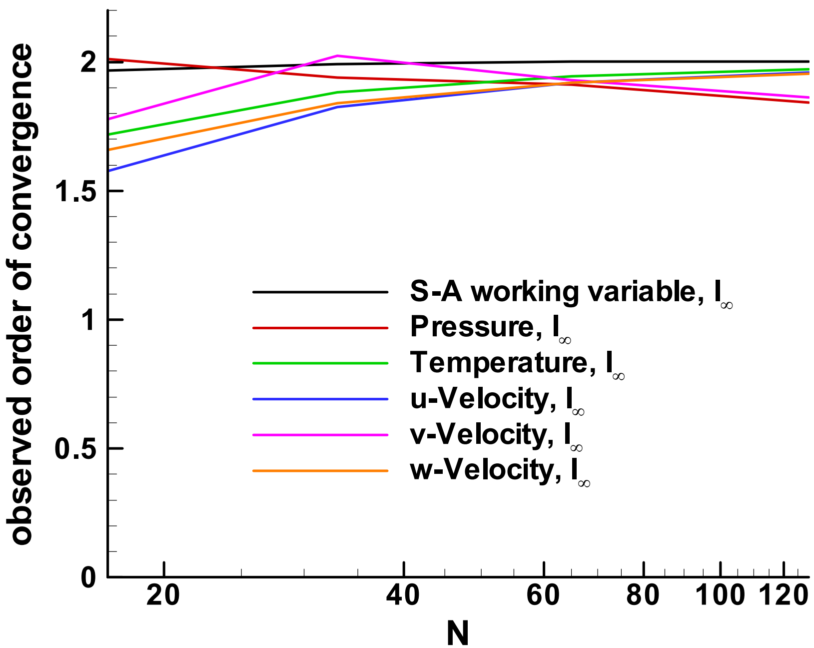
Euler Equations

Inverse Distance Weighted Least Squares

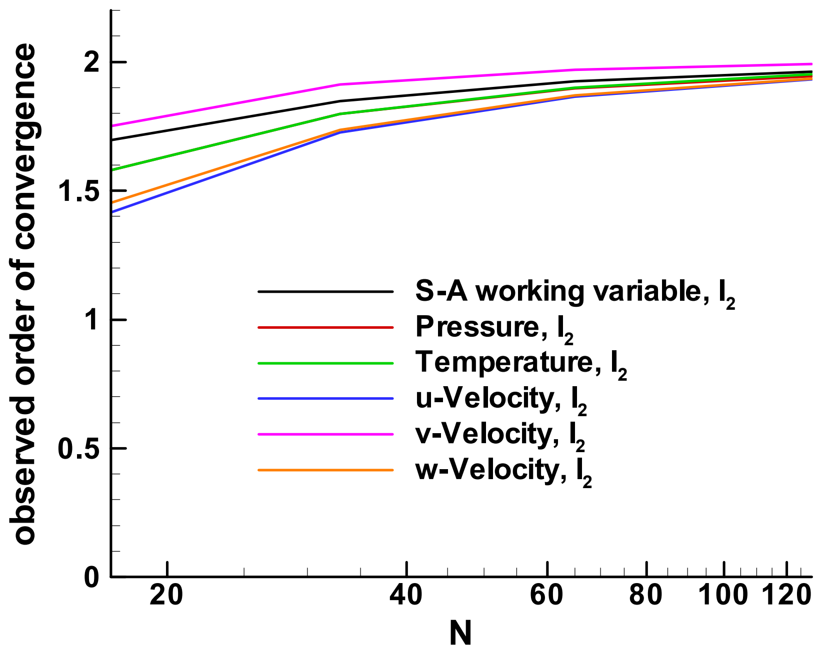


RANS w/ Spalart-Allmaras

l_∞ norms



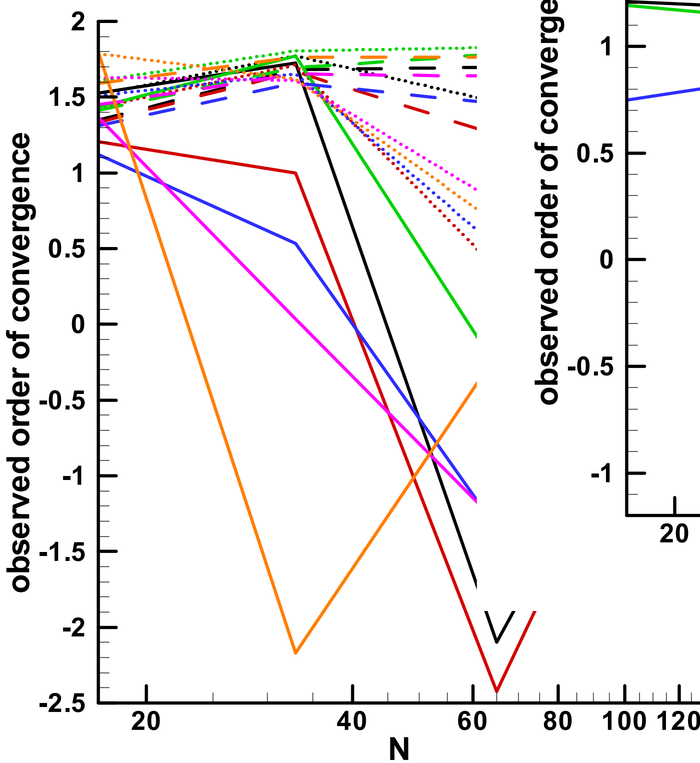
l_2 norms



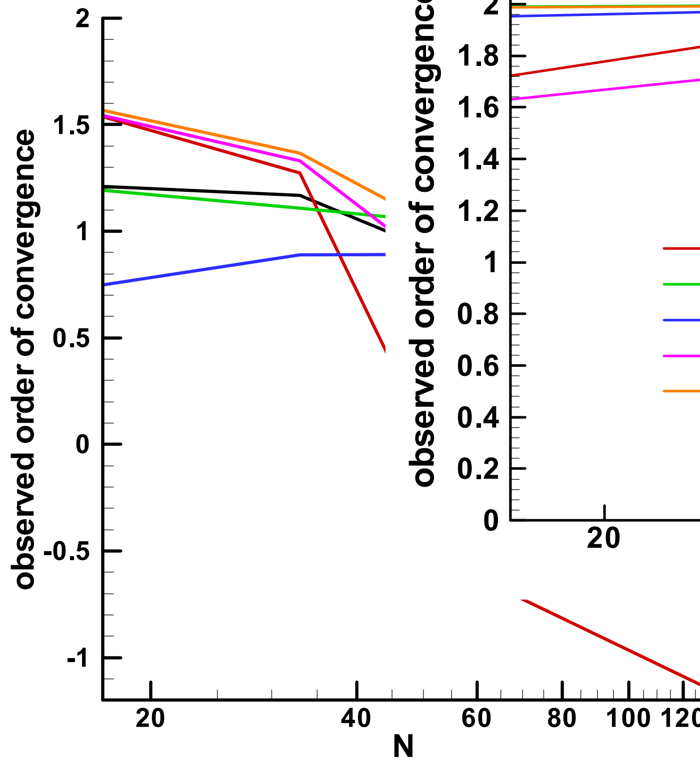
Sandia National Laboratories

Slip Condition

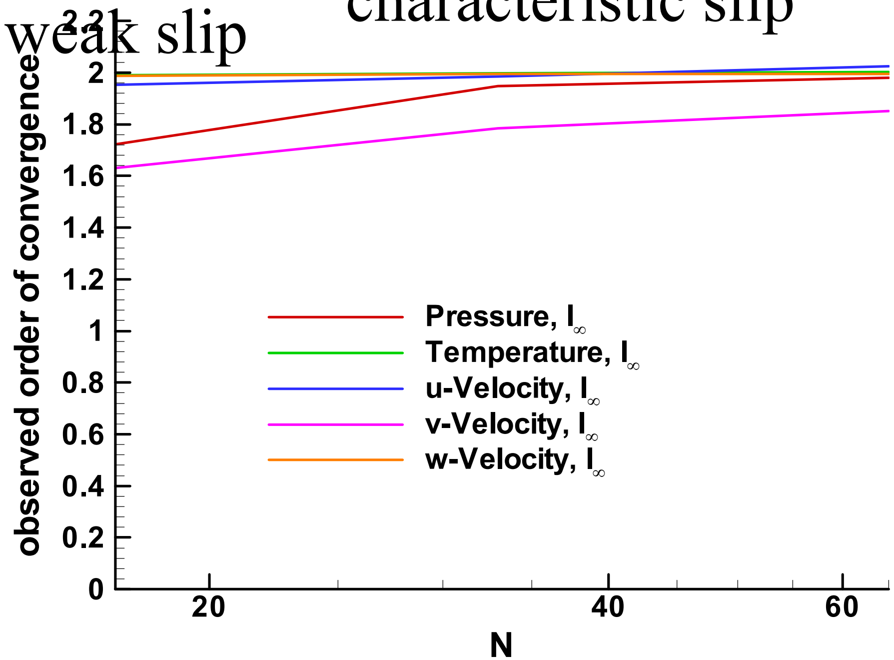
weak slip with parallel bug in surface normal



“correct” weak slip



characteristic slip



Sandia National Laboratories

Fast-Turnaround MMS

- Formal order verification is often viewed as a certification that takes place very late in the development cycle.
- Once the initial overhead of deriving and implementing manufactured solutions is done, new tests can be run very quickly.
- This fast-turnaround time allows order verification to be used early in the development cycle of new capabilities, especially when only one thing differs from a previous order verification exercise.

Sandia National Laboratories

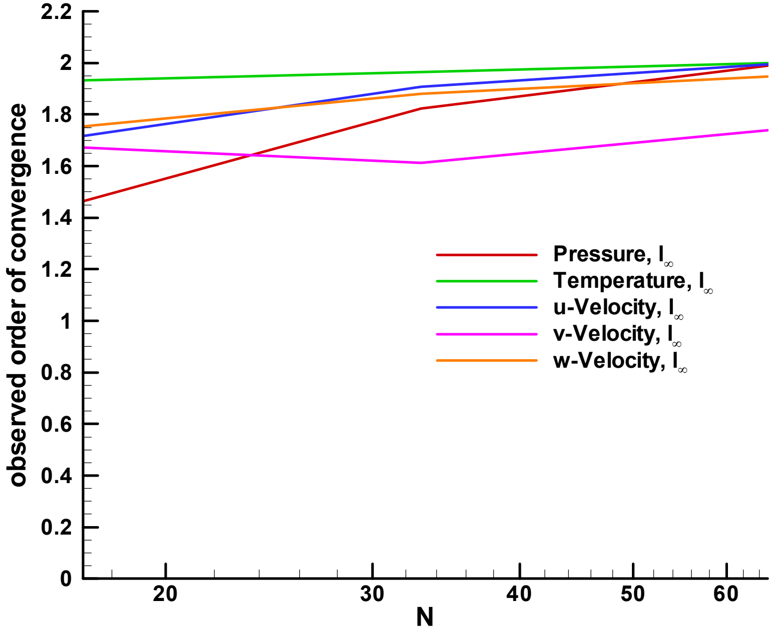
STVD Schemes

- Robustness issues were observed with MUSCL-based schemes in the edge-based discretization, suspected to be the result of limiter issues.
- These issues were improved with the introduction of a symmetric, total variation diminishing (STVD) scheme, since the limiter is “built-in”.
- Even better robustness was gained from the introduction of a collinear-edge-based STVD.
- 24 candidate formulations of these STVD schemes were tested in a week.
  – verification of correctness complimented other testing
  – head-to-head error comparison on manufactured solution

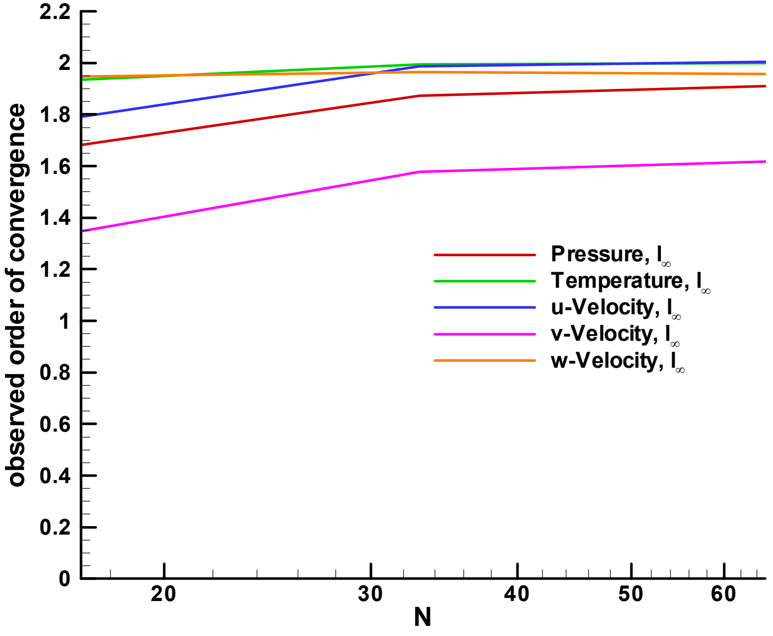
Sandia National Laboratories

Order of Accuracy for STVD Schemes

extrapolation-based



collinear-edge-based



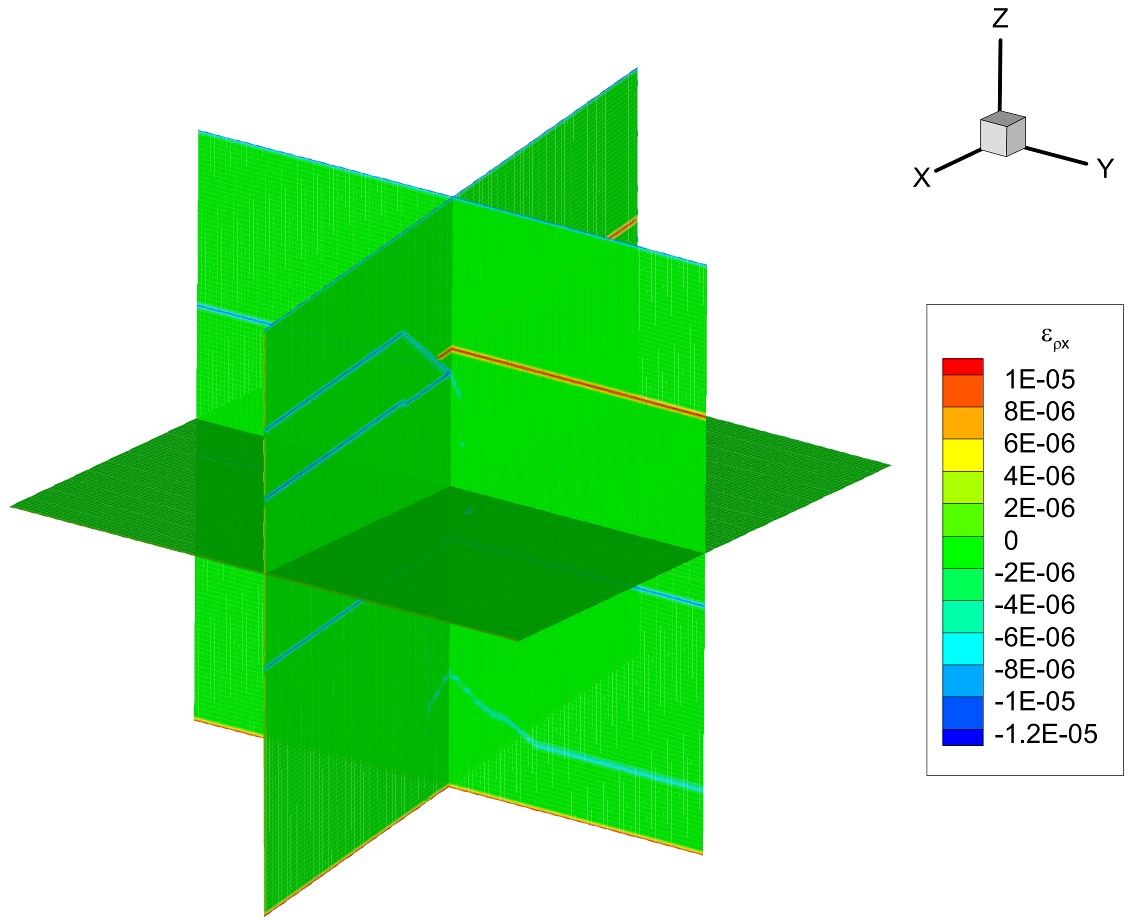
Sandia National Laboratories

Gradient Reconstruction Options in Premo

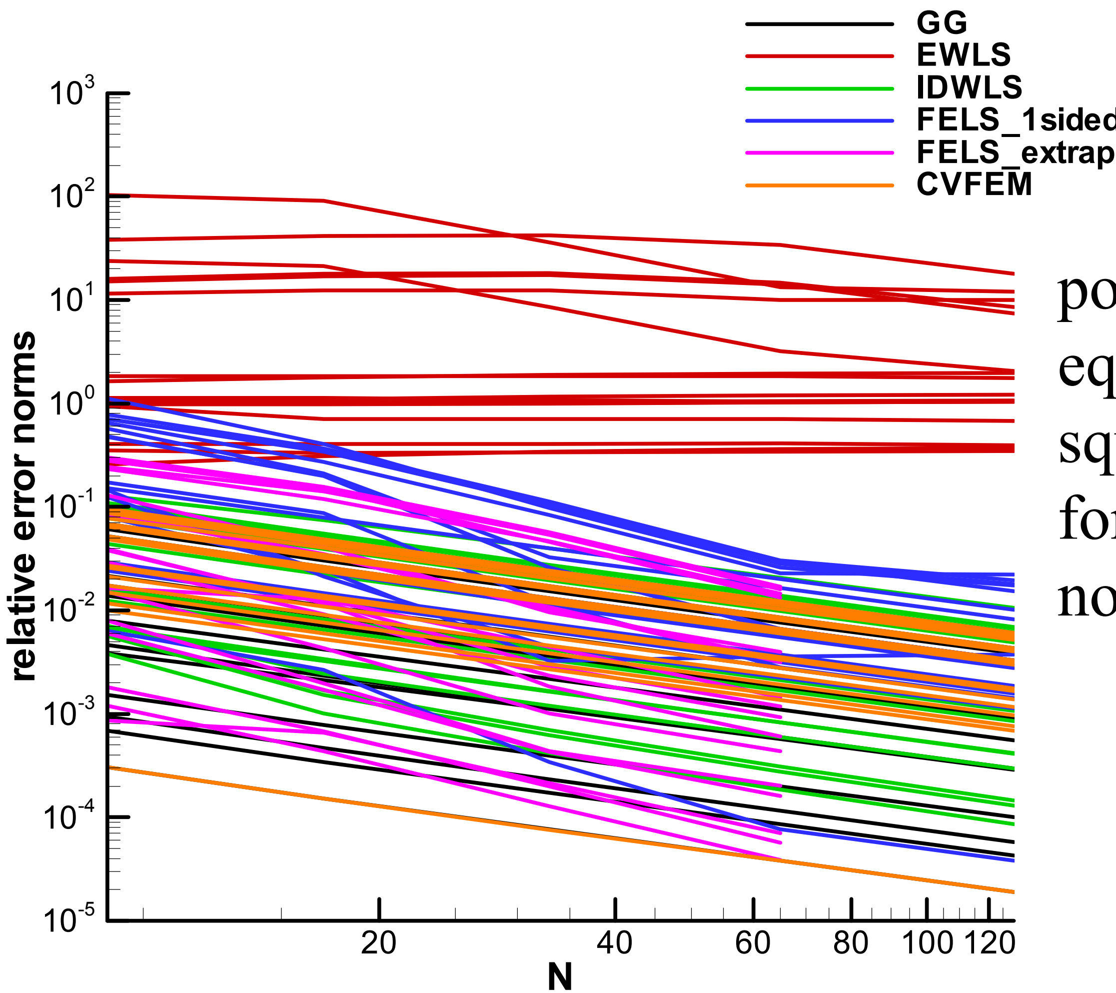
- Nodal gradients are used for
  - extrapolation of variables in MUSCL based schemes,
  - calculation of viscous fluxes, and
  - calculation of turbulence model source terms
- legacy options
  - Green-Gauss (GG) ← accuracy suffers for high mesh curvature/skewness
  - least squares (LS)
    - equally weighted ← accuracy suffers for high mesh aspect ratio
    - inverse-distance weighted ← robustness issues
- new options
  - control volume finite element (CVFEM)
    - three quadrature options
  - finite element least squares (FELS)
    - two options for boundary treatment

Sandia National Laboratories

Error Plot Representing Parallel Issue



Error Norms for High Aspect Ratio Mesh



poor accuracy of equally weighted least squares is a formulation weakness, not a coding mistake

Summary

- Formal order verification via the method of manufactured solutions has been instrumental in the development of Premo.
- Coding mistakes and formulation weaknesses have been detected and addressed.
- Order verification has been integrated into the development process so that new capabilities can be verified as soon as they are implemented.
- Order verification has become instrumental in advancing the state of the art in flux schemes and gradient reconstruction within Premo.

Selected References

- "A Manufactured Solution for Verifying CFD Boundary Conditions," AIAA Paper 2004–2629.
  - Parts II and III, AIAA 2005–0088, 2006–3722.
  - Upcoming AIAA Journal article.
- "Aspects of Reconstruction Schemes on Unstructured Mesh Flow Solvers," 9:45–10:10 on Wednesday in session MS63, Bristol 3 L.
- *Verification of Computer Codes in Computational Science and Engineering*, Knupp & Salari

Sandia National Laboratories