Towards the Next Generation in CFD

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Overview

- Next-generation CFD capabilities
  - Reliably achieve required accuracy
  - Reasonable time
  - Automation
- Critical ingredients
  - Error estimation & adaptation
  - Higher-order discretization
  - Direct interface to CAD

CFD Today

- Integral part of aerospace design with wind tunnel & flight testing
- Has decreased amount of testing through improved screening
- Flows with complex geometry and physics can be approximated
- Viewed by many as a mature technology

Managing Risks with CFD Today

- Risks largely managed by standards of practice involving:
  - Grid topology and density
  - Turbulence models and parameters
  - Iterative methods and parameters
  - Corrections based on testing
- These standards are only reliable within scope
- Off-design conditions and/or novel design concepts require significant human intervention to attempt to manage risks

The next generation of CFD must provide simulations

- at engineering-required accuracy
- in a reasonable time
- in an automated manner

Objective of Error Estimation & Adaptation

- The goal of error estimation and adaptation is automated reliability
- When considering the relative costs of solution-based adaptive methods, human costs must be included
- For simpler problems, solution-based adaptive methods are unlikely to be competitive

Error Estimation & Adaptive Indicators

- Feature-based
- Interpolation error
- Residual-based
- Output-based

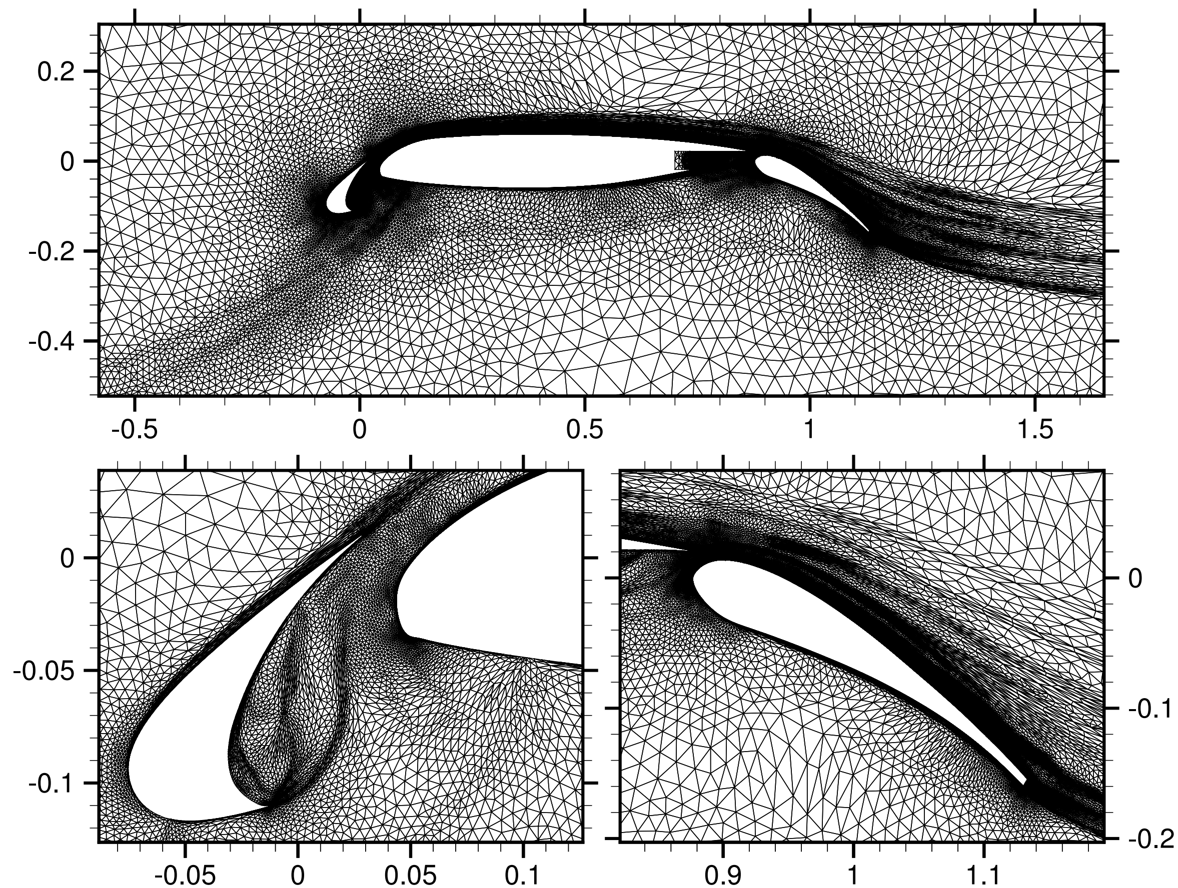
Output Error Estimation

- Several efforts have investigated estimating errors in engineering outputs:
  - FEM: Rannacher, Patera & Peraire, Suli & Giles, Larson & Barth
  - General discretizations: Giles & Pierce
- Key concept:

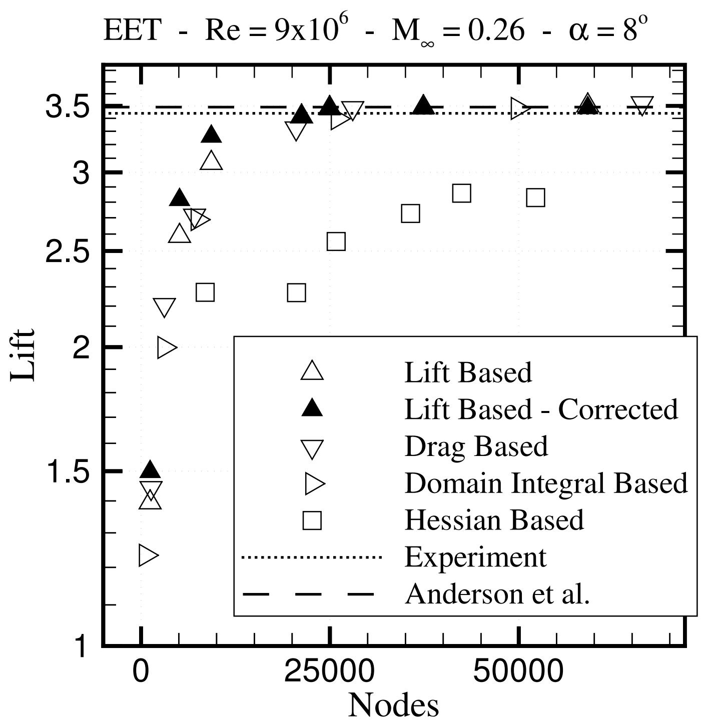
adjoint $\times$ solution residual $\Rightarrow$ output errors

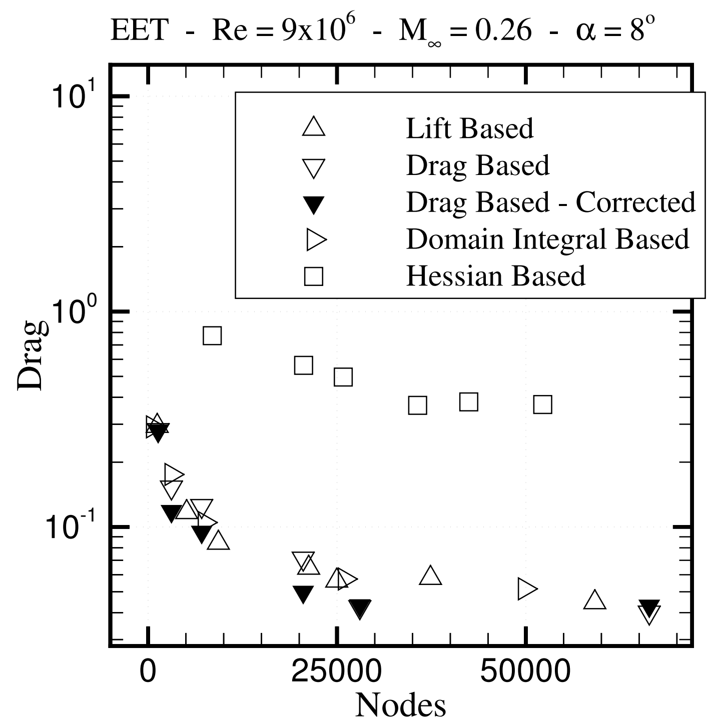
- Venditti & Darmofal have developed an adjoint-based, anisotropic approach and successfully applied it to a wide variety of aerodynamic flows

Output-based Adaptation: High-lift



Output-based Adaptation: High-lift





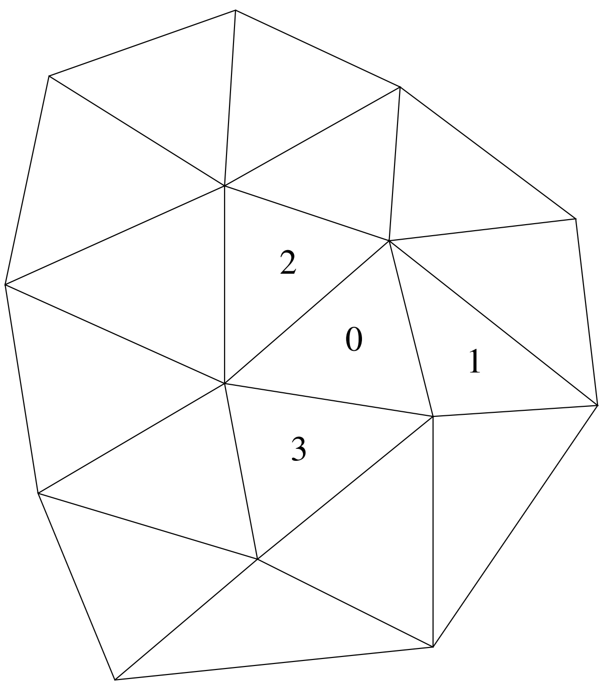
Adaptation: Challenges

- Time-dependent problems: Output-based = expensive
  - Requires backwards-in-time integration of adjoint
  - Must store primal iterates
- 'Steady'-state problems: Output-based methods can fail
  - Often, CFD simulations do not fully converge
  - Nonlinearity keeps residual bounded
  - Adjoint (linear) solutions will be unstable (Campobasso & Giles)
- Perhaps a middle ground exists: weighted residual-based indicators
- General challenge: 3-D anisotropic adaptation for complex geometries
- Modeling error poses another challenge

Motivation for higher order

- Higher-order methods are critical for simulation of unsteady flows with multiple scales, e.g.:
  - Applications of DNS, LES, or DES
  - Acoustics
- Even in aerodynamics, higher-order methods may offer benefits:
  - Existing 'industrial-strength' methods largely based on finite-volume with at best second order accuracy
  - Questions exist whether current discretizations are capable of achieving desired accuracy levels in practical time

First-order Accurate Finite Volume



In each triangle, assume $\mathbf{u}$ is constant.

Apply conservation law on triangle:

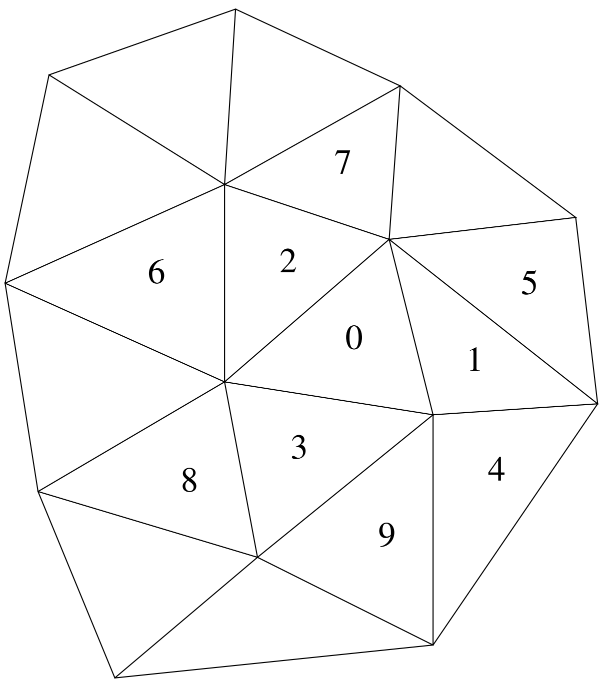
$$\frac{d\mathbf{u}_0}{dt}A_0 + \sum_{k=1}^{3}\int_{0k}\mathcal{H}_i(\mathbf{u}_0, \mathbf{u}_k, \hat{\mathbf{n}}_{0k})\, ds = 0$$

$\mathcal{H}_i(\mathbf{u}_L, \mathbf{u}_R, \hat{\mathbf{n}}_{LR})$ is flux function that determines inviscid flux in $\hat{\mathbf{n}}_{LR}$ direction from left and right states, $\mathbf{u}_L$ and $\mathbf{u}_R$.

Example flux functions: Godunov, Roe, Osher, Van Leer, Lax-Friedrichs, etc.

This discretization has a solution error which is $O(h)$ where h is mesh size.

Second-order Accurate Finite Volume



In each triangle, reconstruct a linear solution, $\tilde{\mathbf{u}}$, using neighboring averages:

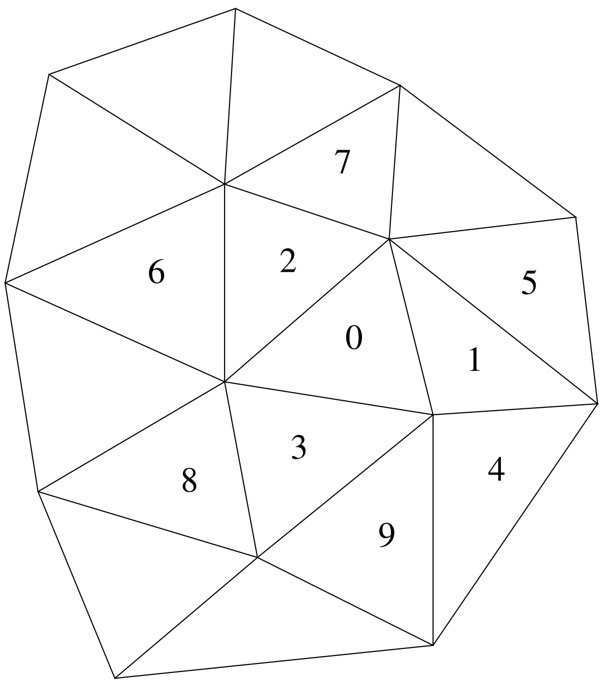
$$\tilde{\mathbf{u}}_0 \equiv \mathbf{u}_0 + (\mathbf{x} - \mathbf{x}_0) \cdot \nabla \mathbf{u}_0,$$
$$\nabla \mathbf{u}_0 \equiv \nabla \mathbf{u}_0 (\mathbf{u}_0, \mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3).$$

Apply conservation law on triangle:

$$\frac{d\mathbf{u}_0}{dt} A_0 + \sum_{k=1}^{3} \int_{0k} \mathcal{H}_i(\tilde{\mathbf{u}}_0, \tilde{\mathbf{u}}_k, \hat{\mathbf{n}}_{0k})\, ds = 0$$

On smooth meshes and flows, solution error is $O(h^2)$.

Pros/Cons of Higher-order Finite Volume



+ Increased accuracy on given mesh without additional degrees of freedom

– Difficulty in achieving higher-order on unstructured meshes and near boundaries

– Single stage, local iterative methods (e.g. Jacobi) are not stable for higher order (Godunov's theorem)

– Matrix fill-in increased resulting in high-memory requirements

Previous Work in DG

- Extensive work on DG for hyperbolic equations
  - Bassi and Rebay (1997)
  - Cockburn and Shu (1998, 2001)
  - Karniadakis et al. (1998, 1999)
- More recently work begun on elliptic equations
  - Bassi and Rebay (1997,1998)
  - Cockburn and Shu (1998, 2001)
  - Baumann and Oden (1997)
  - Brezzi et al. (1997)
- Only Bassi and Rebay have published RANS results (1997, 2003

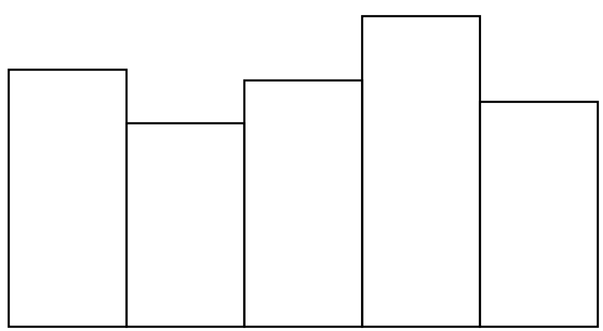
Discontinuous Polynomial Basis

- Triangulate domain Ω into non-overlapping elements $\kappa \in T_h$
- Define function space: Element-wise discontinuous polynomials of degree p

$$\mathcal{V}_h^p = \{\mathbf{v} \in L^2(\Omega) : \mathbf{v}|_\kappa \in P^p(\kappa) : \forall \kappa \in T_h\}$$

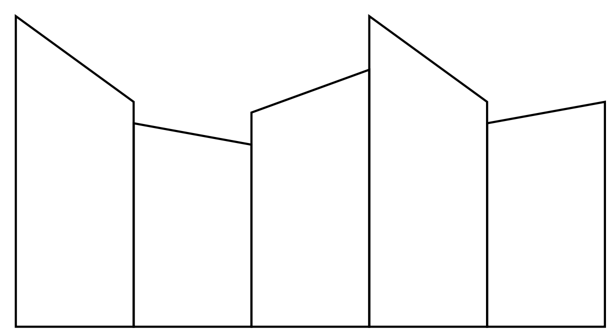
Example of One-Dimensional Bases

$p = 0$ basis



1 DOF/element

$p = 1$ basis



2 DOF/element

Relationship of DG to other methods

- For $p = 0$ discretization, DG is identical to first-order finite volume
- For $p > 0$, DG can be intrepreted as a moment method.
- Moment methods for hyperbolic problems were first suggested by Van Leer (1977) and then developed for the Euler equations by Allmaras (1987, 1989) and later Holt (1992).

Stability of Local Iterative Methods for DG

An elemental block Jacobi iterative method to solve this problem is,

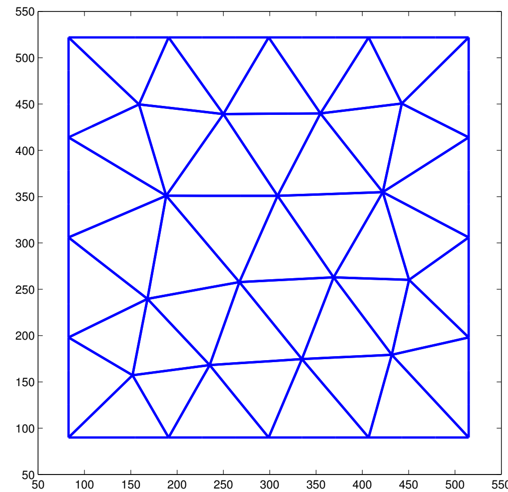
$$\mathbf{u}_j^{n+1} = \mathbf{u}_j^n - \omega \left(\partial \mathbf{R}_j / \partial \mathbf{u}_j\right)^{-1} \mathbf{R}_j(\mathbf{u}).$$

where $\partial \mathbf{R}_j / \partial \mathbf{u}_j$ is the diagonal block for the element j.

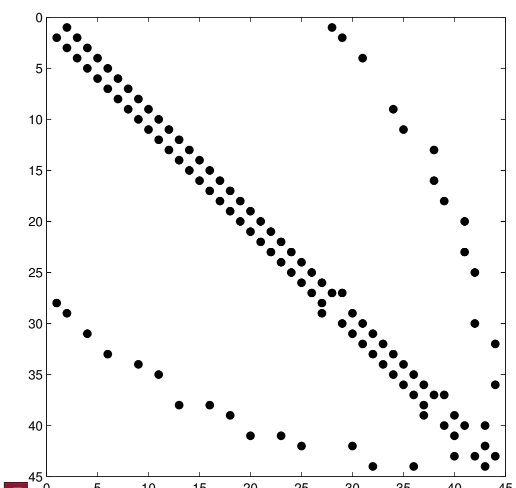
For 1-D hyperbolic systems, the eigenvalues of the higher-order modes are all collocated $\Rightarrow$ p-independent convergence.

For multiple dimensions, elemental block Jacobi is stable independent of p when $0 < \omega < 1$.

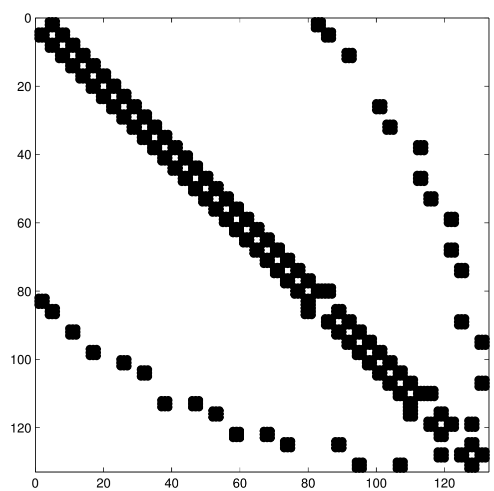
Matrix Fill for Higher-order DG



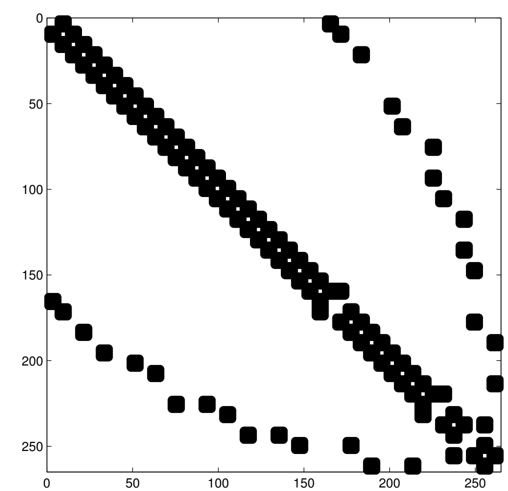
First-order ($p = 0$)



Second-order ($p = 1$)



Third-order ($p = 2$)



Iterative Solution of Higher-order DG (Fidkowski & Darmofal, 2004)

- Use a preconditioned iterative scheme to drive $\mathbf{R}(\mathbf{u}_h^n) \to 0$:

$$\mathbf{u}_h^{n+1} = \mathbf{u}_h^n - \mathbf{P}^{-1}\mathbf{R}(\mathbf{u}_h^n)$$

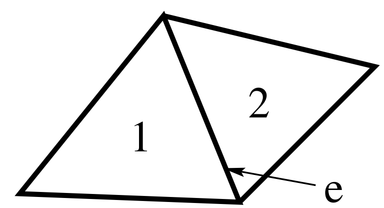
- Elemental line preconditioner: $\mathbf{P} = \mathbf{M}_{line}$
- Motivation: Transport of information in Navier-Stokes equations characterized by strong (anisotropic) coupling
  - Inviscid regions: Information follows characteristic directions set by convection
  - Boundary layers/wakes: Diffusion effects can be as strong if grid is well-resolved.
- Lines of elements from using an element-to-element coupling measure.

Connectivity Criteria

- Measure of influence based on $p = 0$ discretization of scalar transport equation

$$\nabla \cdot (\rho \vec{u} \phi) - \nabla \cdot (\mu \nabla \phi) = 0$$

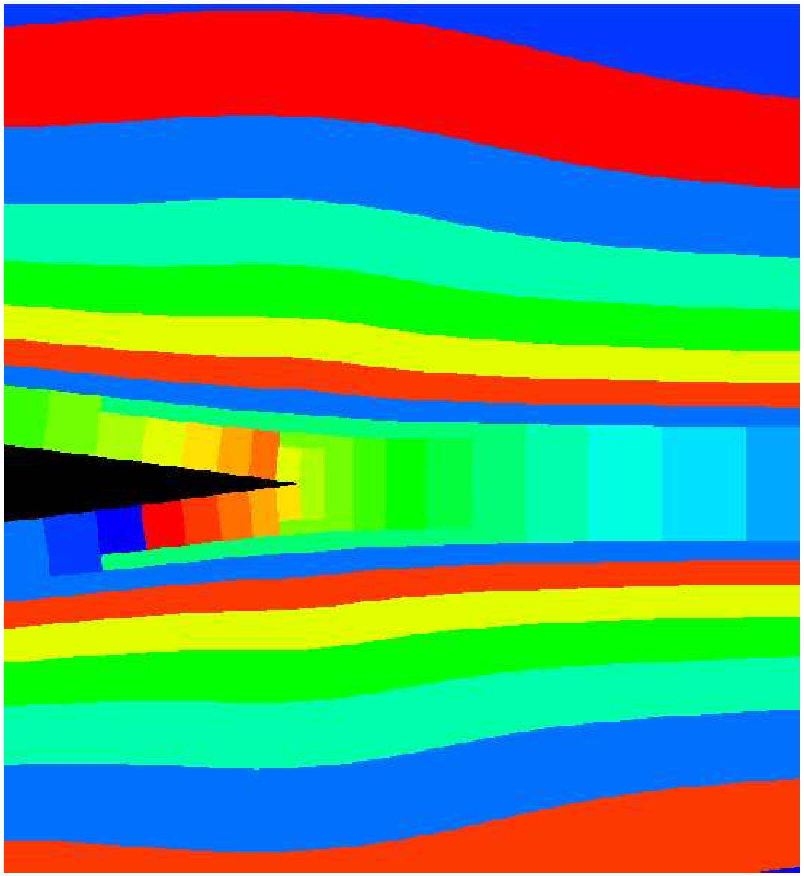
- $\rho \vec{u}$ and μ taken from current solution
- At each edge, compute off-diagonal components of Jacobian for adjoining elements

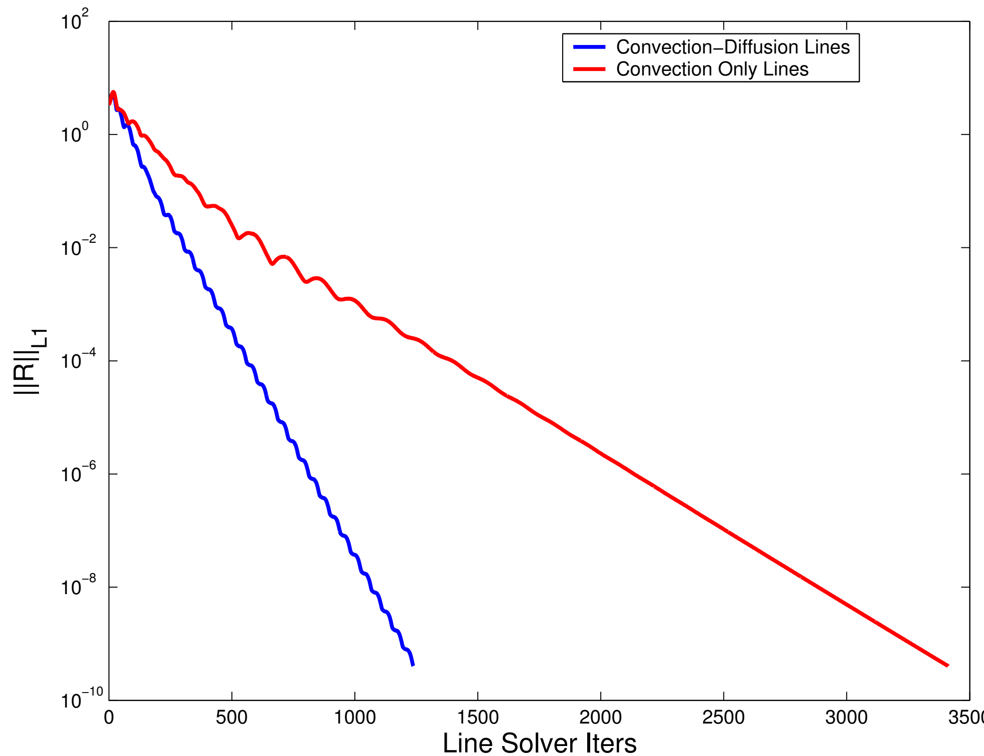


- Connectivity given by maximum absolute value

$$C_e = \max \left(\left| \frac{\partial R_1}{\partial \phi_2} \right|, \left| \frac{\partial R_2}{\partial \phi_1} \right| \right)$$

Example Lines and Performance



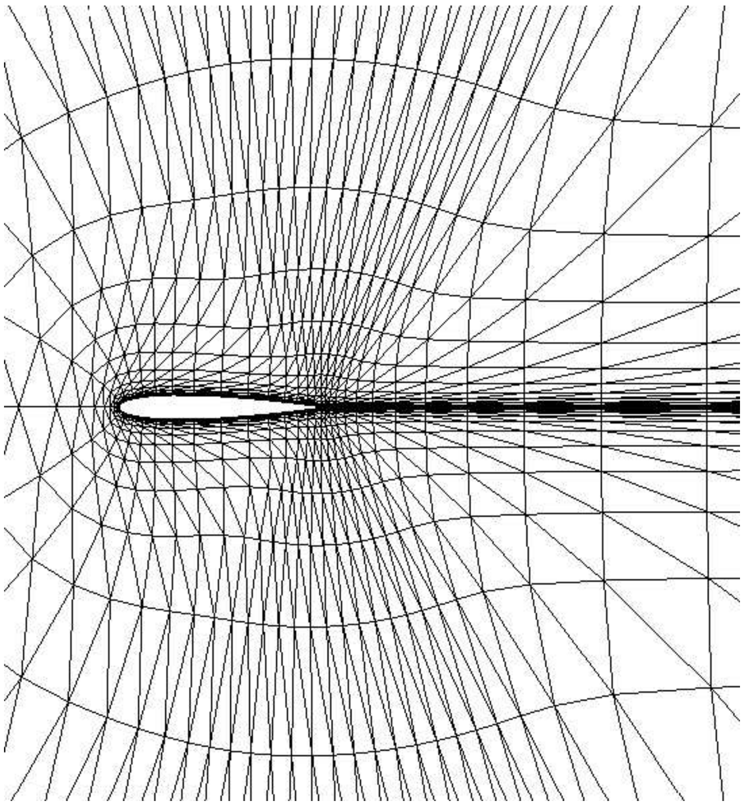


p-Multigrid: Motivation

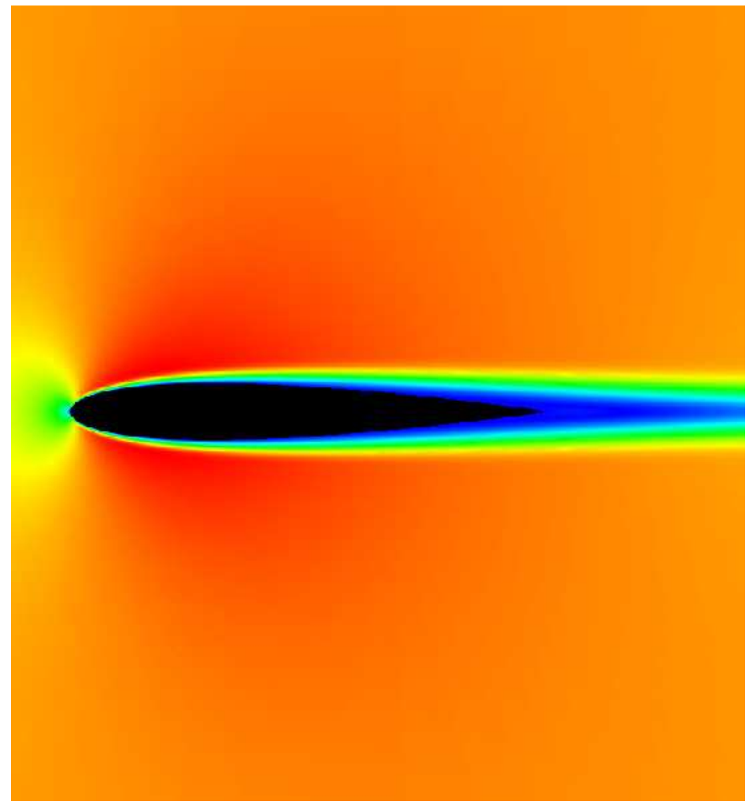
- Observation: Smoothers are inefficient at eliminating low frequency error modes on fine level
- h-Multigrid
  - Spatially coarse grid used to correct solution on fine grid
  - Grid coarsening is complex on unstructured meshes
- p-Multigrid (Ronquist & Patera, Helenbrook et al., Fidkowski & Darmofal)
  - Low order $(p-1)$ approximation used to correct high order (p) solution
  - Natural implementation in DG FEM discretization on unstructured meshes

NACA 0012 Test Case

$M = 0.5$, $Re = 5000$, $\alpha = 0$
Grids are from Swanson at NASA Langley



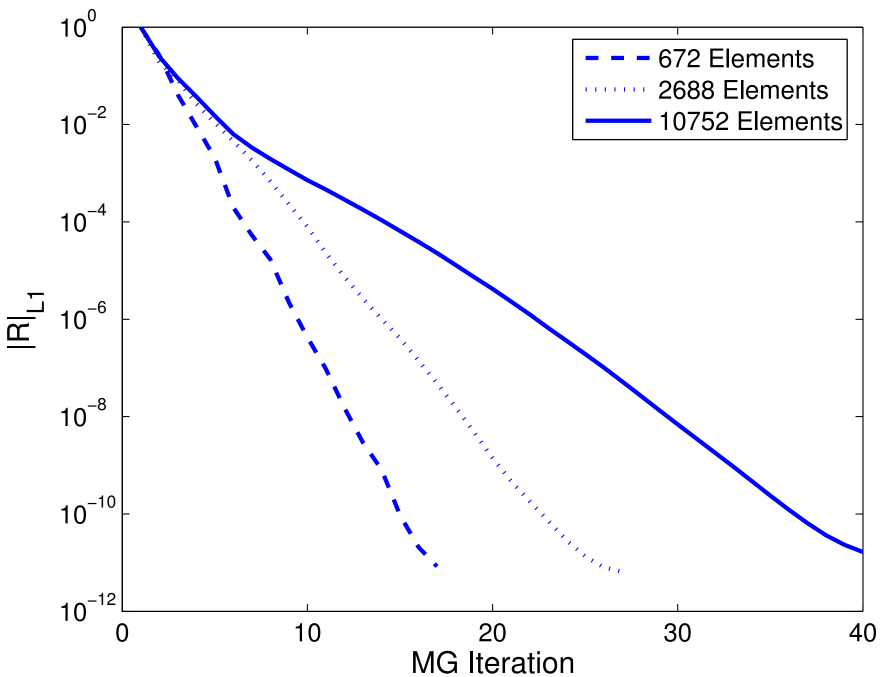
2112 element mesh



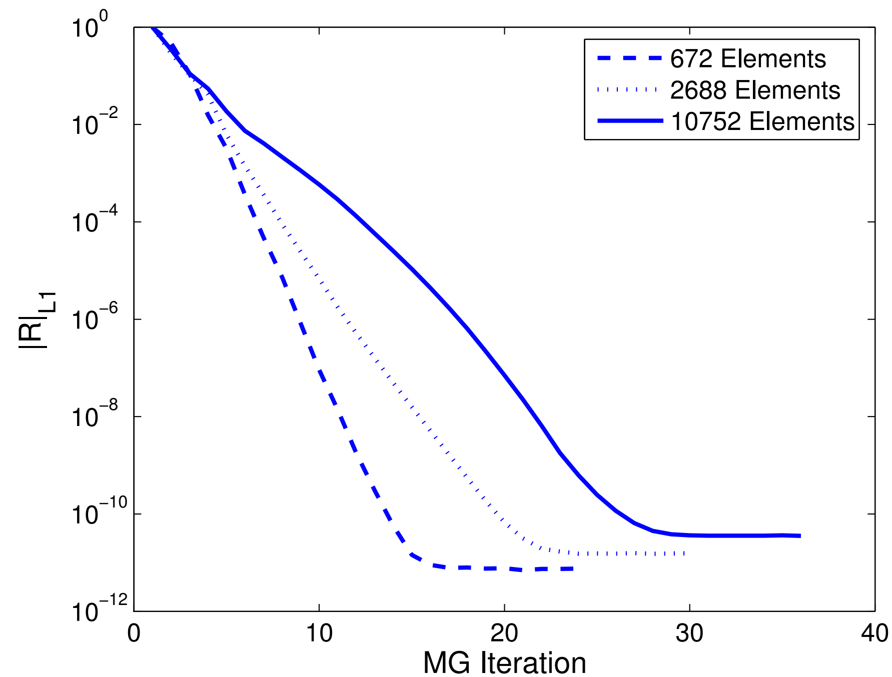
Mach contours

Iterative Behavior: p and h dependence

$p = 1$ convergence



$p = 3$ convergence

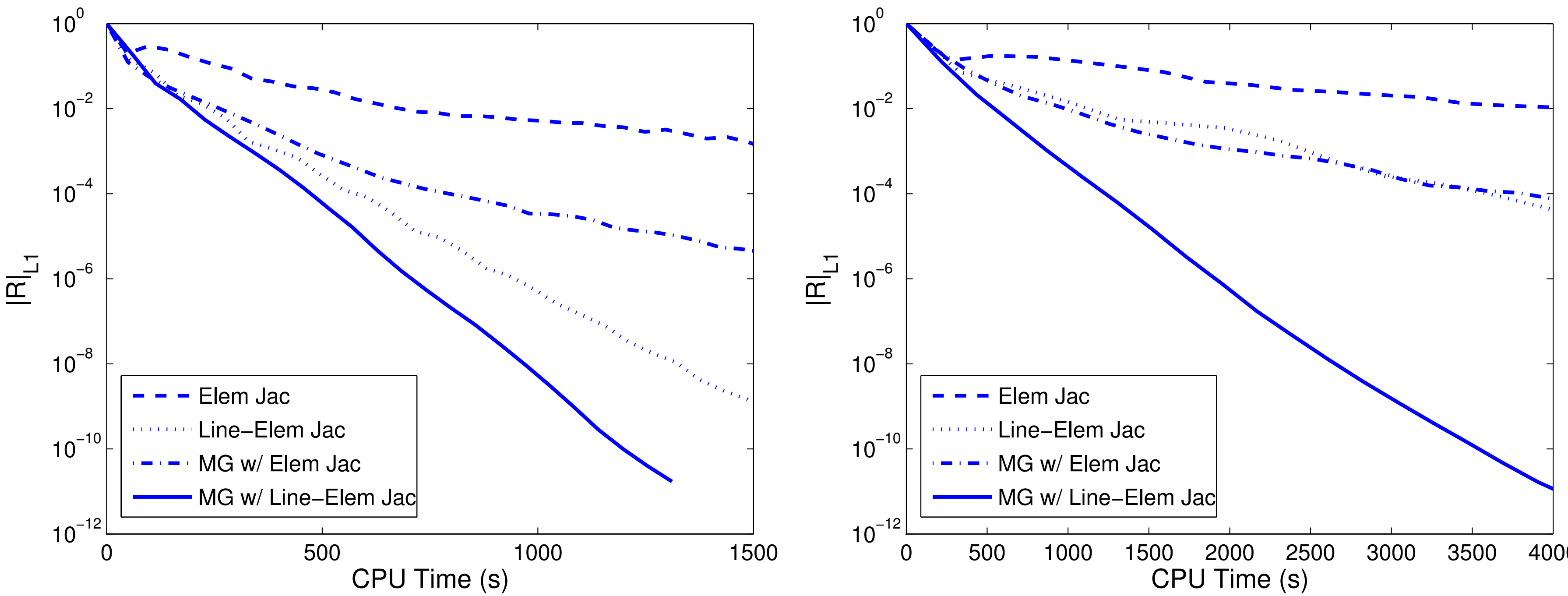


Iterative rate for p-multigrid with line smoothing:

- Nearly p-independent
- Some h-dependence

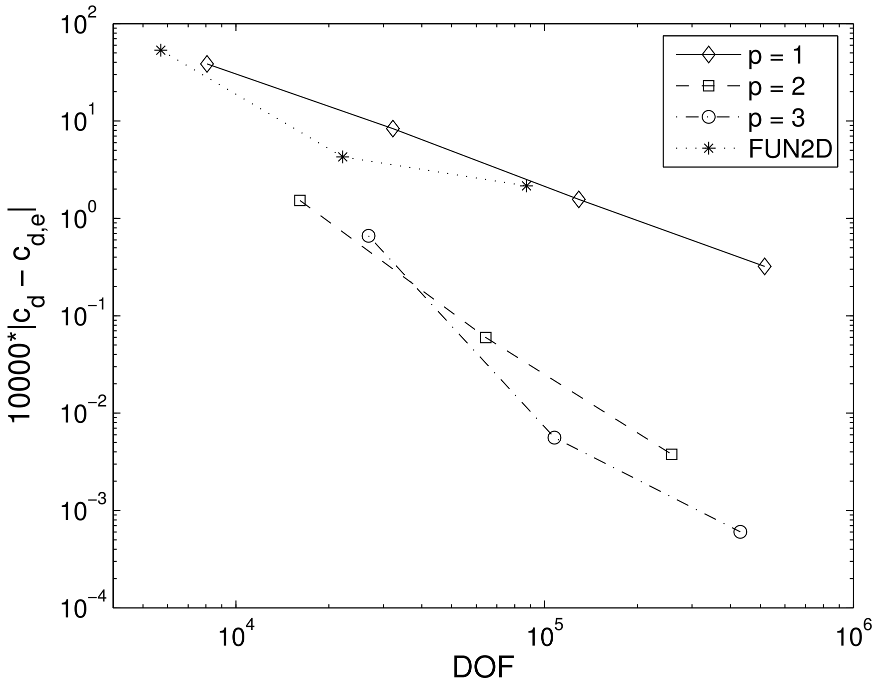
Comparison of Iterative Algorithms

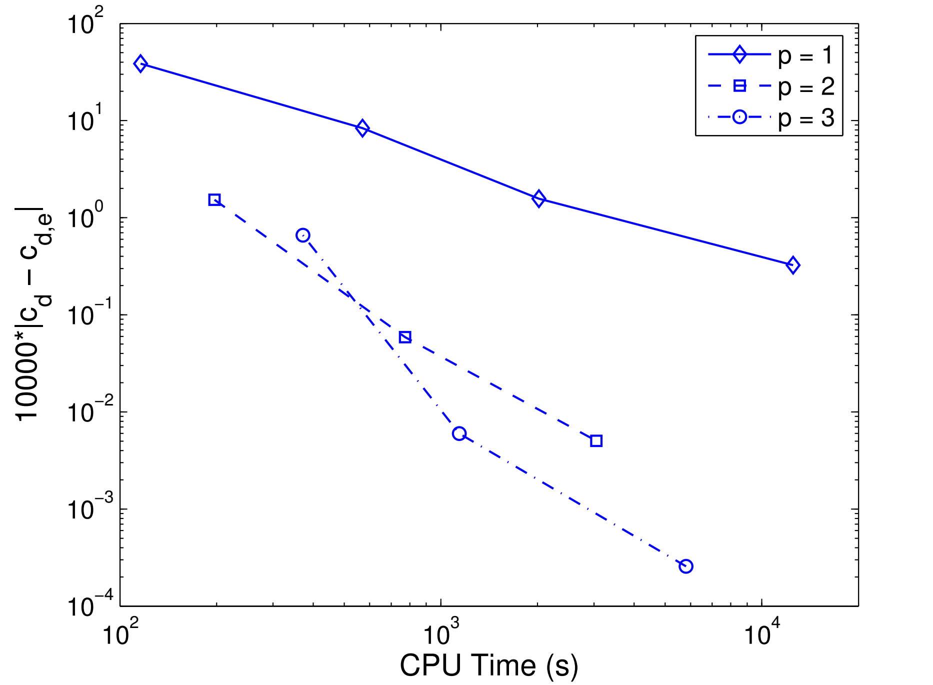
$p = 1$ convergence | $p = 3$ convergence



p-multigrid with line smoothing increasingly important with higher p

Drag Error Convergence





Note: FUN2D is an unstructured finite volume algorithm developed at NASA Langley by Anderson

Higher-order Methods: Challenges

- Turbulence modeling
- Shocks
- Higher-order geometry

Direct Interface to CAD

- Current interface commonly through static, one-way surfaces (IGES)
- CAD is the efficient manner to specify design intent
- CAD can provide a common geometry definition throughout design process and to multiple disciplines
- One approach to provide a CAD interface is CAPRI (Haimes)
- CAPRI provides triangulated surfaces which remain associated with underlying CAD model
- Several researchers have utilized CAPRI to provide direct CAD access (Alonso et al, Nemec et al, Zingg et al)
- *Cart3D* (Aftosmis & Berger) is an example of the potential of next-generation CFD

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