High-Order Spatial and Temporal Methods for Simulation and Sensitivity Analysis of High-Speed Flows

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Project Scope and Relevance

- Maturation of current algorithms
  - 20+ years of TLNS3D/CFL3D/Overflow/Laura/Unstructured FV

- Well known limitations
  - Grid convergence (DPW series for transonics)
  - Heating predictions for hypersonics
  - Stiffness for chemically reacting flows
  - Massive parallelism

Project Scope and Relevance

- Develop novel approaches for improving simulation capabilities for high-speed flows
  - Emerging consensus about higher-order methods
    - May be only way to get desired accuracy
      - Asymptotic arguments
    - Superior scalability
  - Sensitivity analysis and adjoint methods
    - Now seen as indispensible component of new emerging class of simulation tools
  - Other novel approaches: BGK methods

Definitions-Methodologies

- Higher order: Higher than 2^{nd} order
- In Space: Discontinuous Galerkin
- In Time:
  - Diagonally Implicit Runge-Kutta
  - Fully Implicit Runge-Kutta (for stiff problems ?)
  - Discontinuous Galerkin in Time (space-time)
- Sensitivity Analysis
  - Tangent and Adjoint Methods
  - Error estimation and adaptivity
- High Risk – Revolutionary Goals:
  - Still no competitive high-order method demonstrated for subsonic aerodynamics

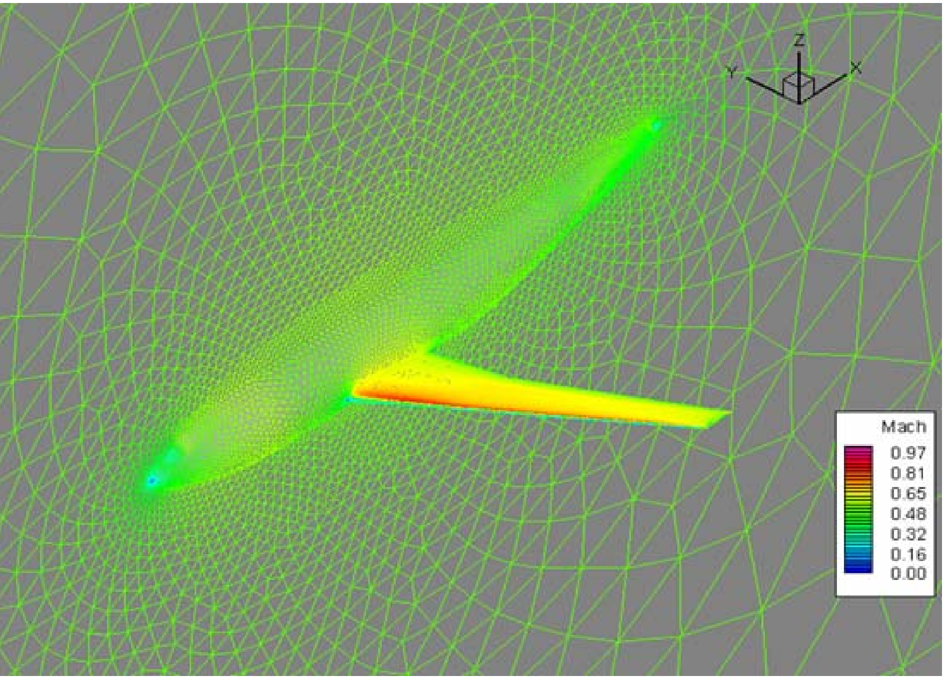
Overview

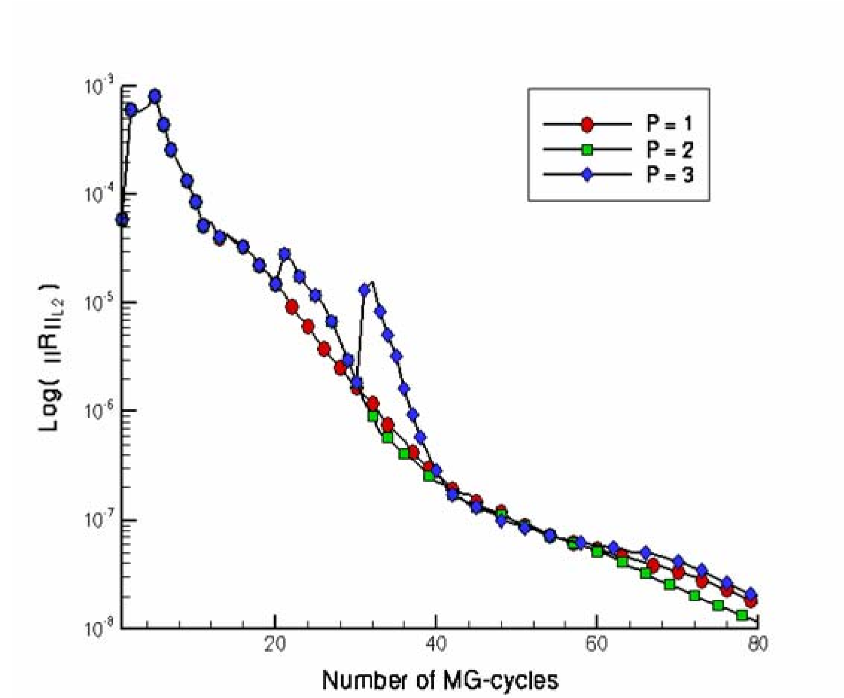
- Initial in-house DG Capability
    - h-p multgrid solver for steady-state (3D Euler)
    - h-p multigrid for unsteady problems
        - BDF and Diagonally Implicit RK Schemes

- Year 1 Achievements
    - Extension to Navier-Stokes equations
        - Implementation of diffusion terms using Interior Penalty (IP) Method
        - Implementation of BGK fluxes for finite volume unstructured code
    - Simulation of Strong Shock waves
        - Shock capturing using artificial viscous terms
        - Shock capturing using limiting and h-refinement
        - Shock fitting approaches
    - ALE (moving grid) formulation for DG
    - Adjoint sensitivity analysis for DG
        - Shape optimization
        - h-p adaptive refinement for functional outputs

- Plans for Out-Years

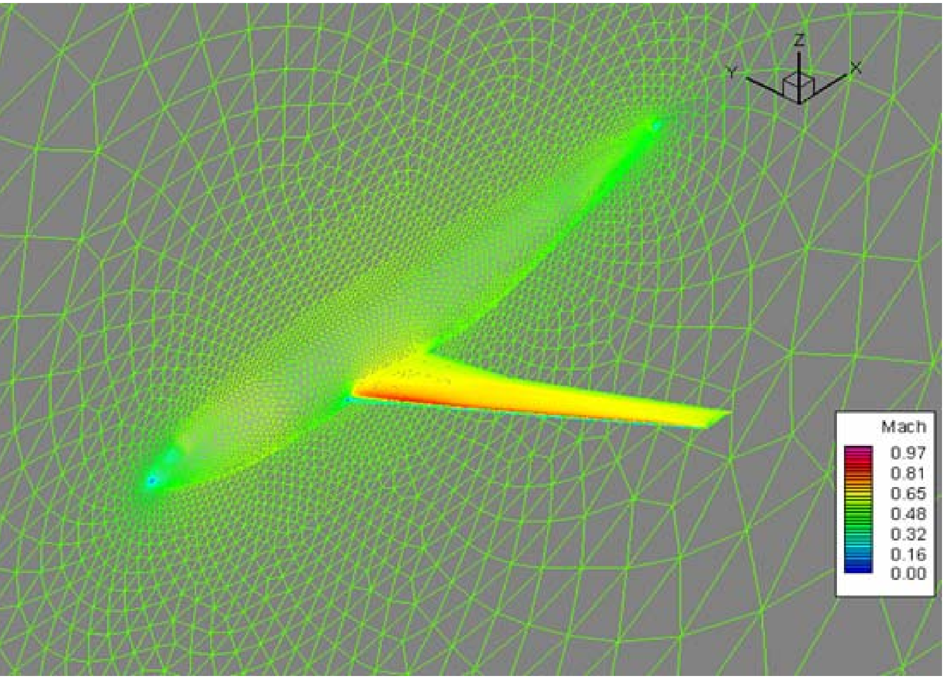
Initial 3D DG Solver (Euler)

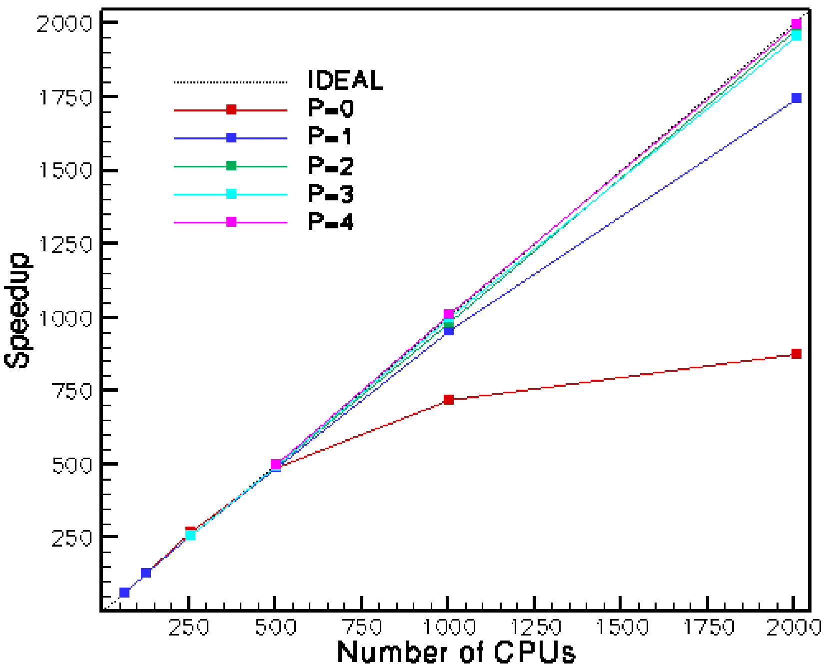




- Accuracy, convergence, scalability validated
- Subsonic inviscid flows only

Initial 3D DG Solver (Euler)





- Accuracy, convergence, scalability validated
- Subsonic inviscid flows only

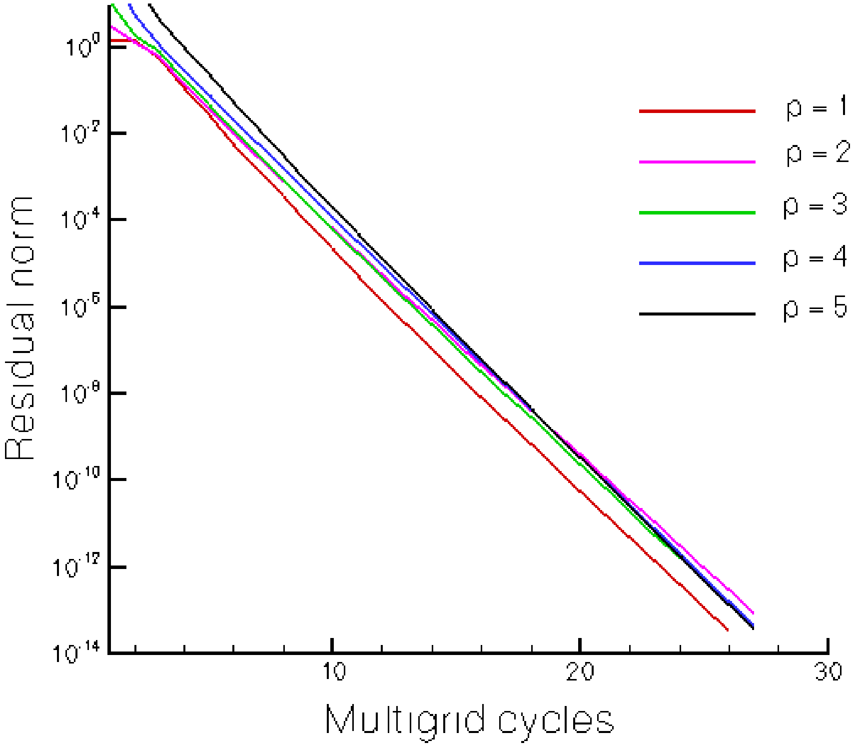
Extension to Viscous Flows

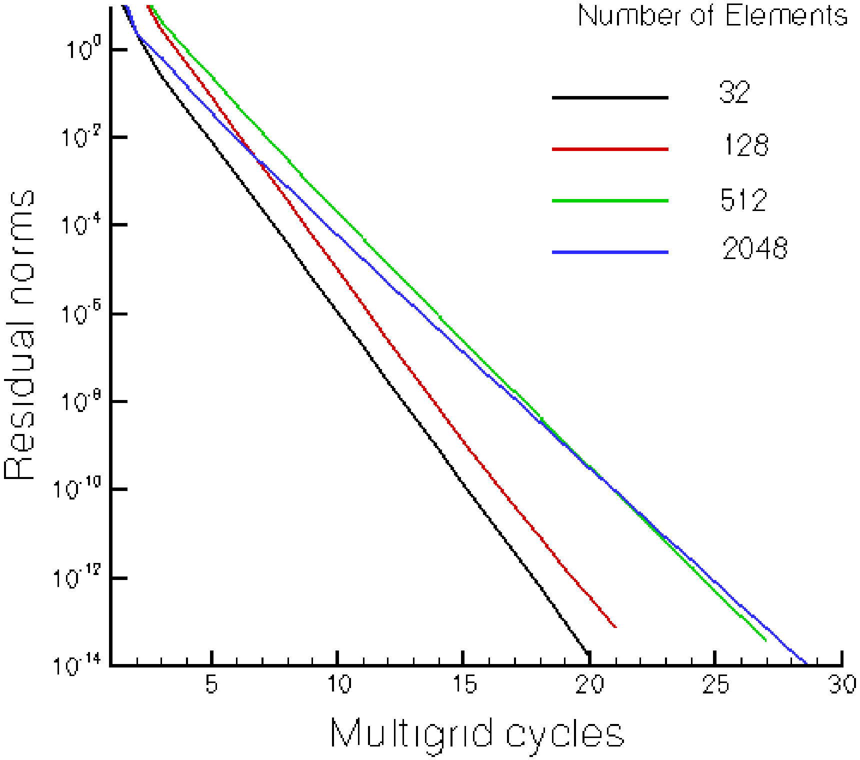
- DG methods developed initially for hyperbolic problems
  - Diffusion terms for DG non-trivial

- New Postdoc hire with experience in this area (March 2007)
  - Interior Penalty (IP) method
  - Explicit expression for penalty parameter derived (JCP)

- IP method derived and implemented for compressible Navier-Stokes formulation up to p=5
  - Studied symmetric and non-symmetric forms for IP
    - Non-symmetric: Accuracy order=p, lower penalty parameter/better convergence
    - Symmetric: Accuracy order=p+1, fast h-p multigrid convergence maintained using additional coarse (p=0) sweeps
  - h and p independent convergence observed for Poisson and Navier-Stokes problems

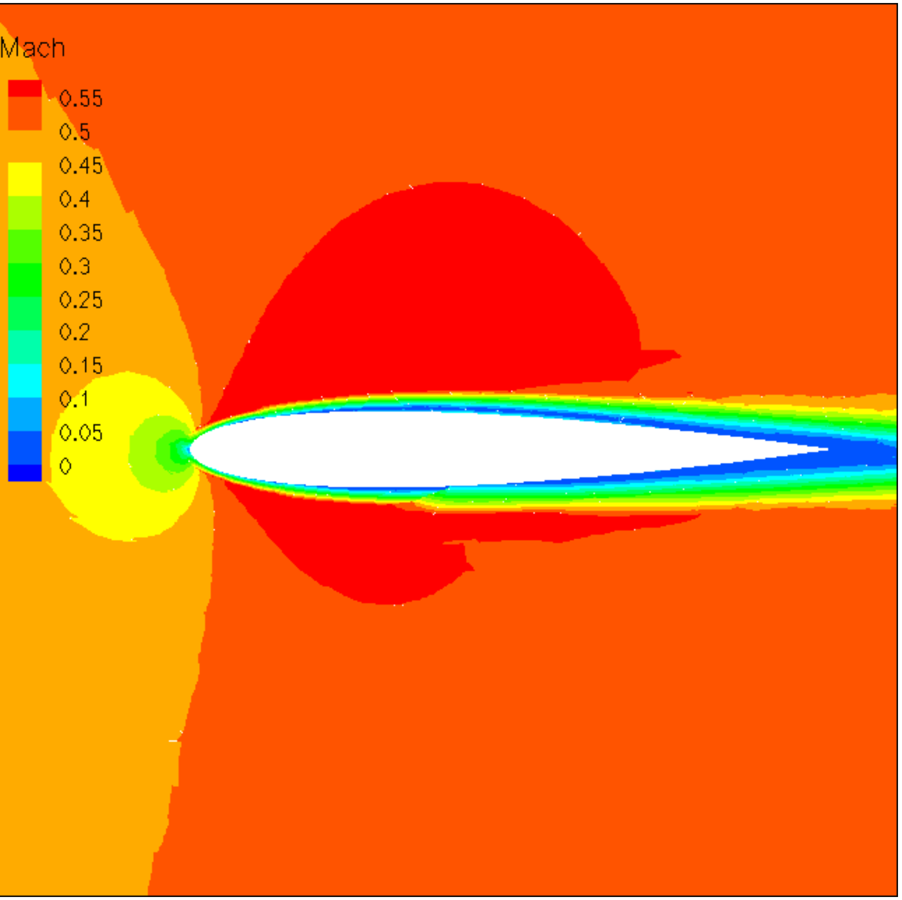
h-p Multigrid for Poisson Equation

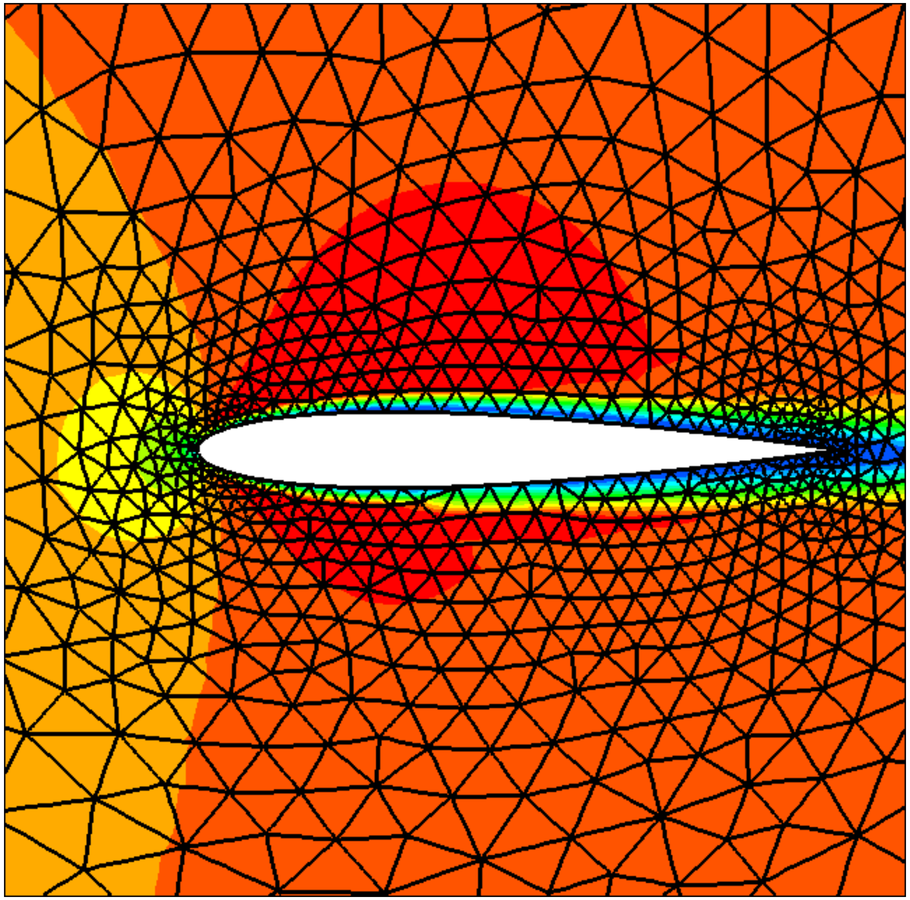




- h and p independent convergence rates

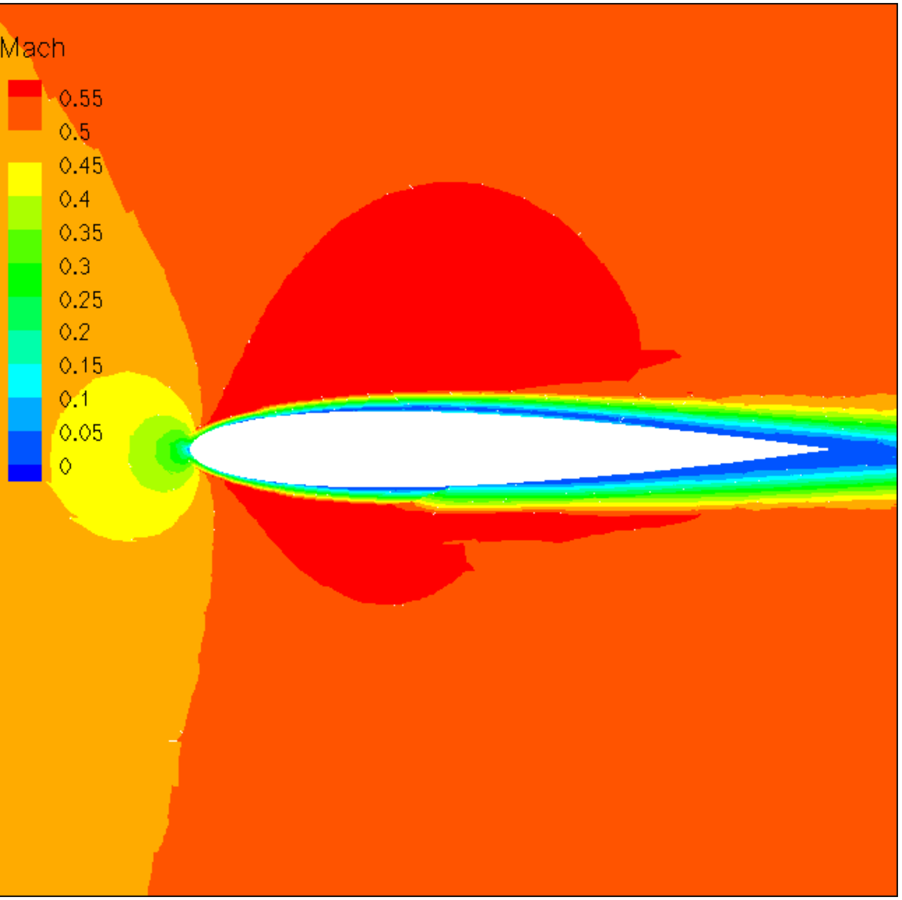
DG Navier-Stokes Solutions



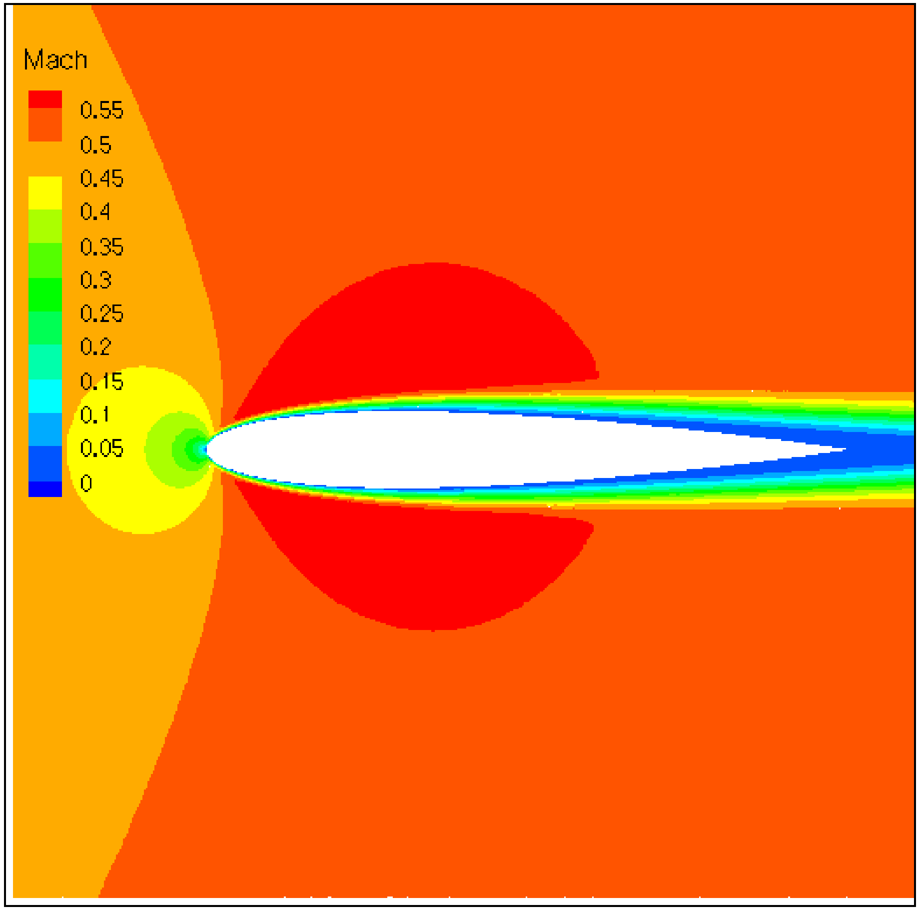


- Mach =0.5, Re =5000
- 2000 mesh elements
- Non-symmetric grid

DG Navier-Stokes Solutions



p=1: second-order accuracy



p=3: fourth-order accuracy

- h-p multigrid convergence maintained (50 – 80 cycles)
- Accuracy validated by comparison with high-resolution finite-volume results
  - Separation location ~ 81% chord (p=3)

Kinetic Based Flux Formulations (BGK)

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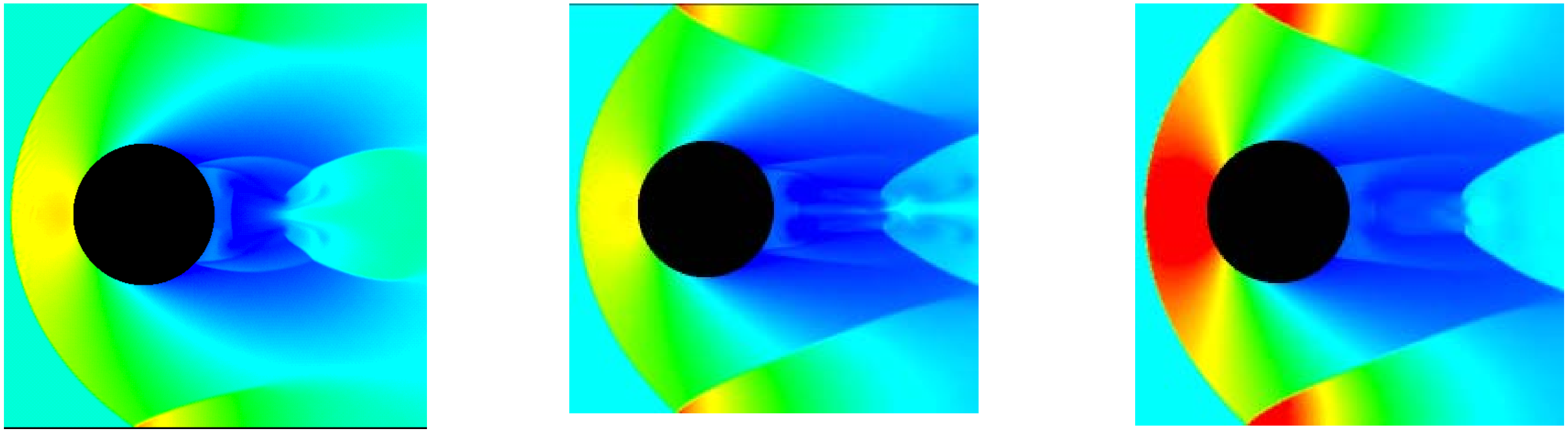
Princeton University

- Alternative for extension to Navier-Stokes:
  - It is not necessary to compute the rate of strain tensor in order to calculate viscous fluxes
- Automatic upwinding via the kinetic model.
- Satisfy Entropy Condition (H-Theorem) at the discrete level.
- Implemented in 2D Unstructured Finite-Volume code by Martinelli (Summer 2007)
- Extension to 2D DG code (Summer 2008)

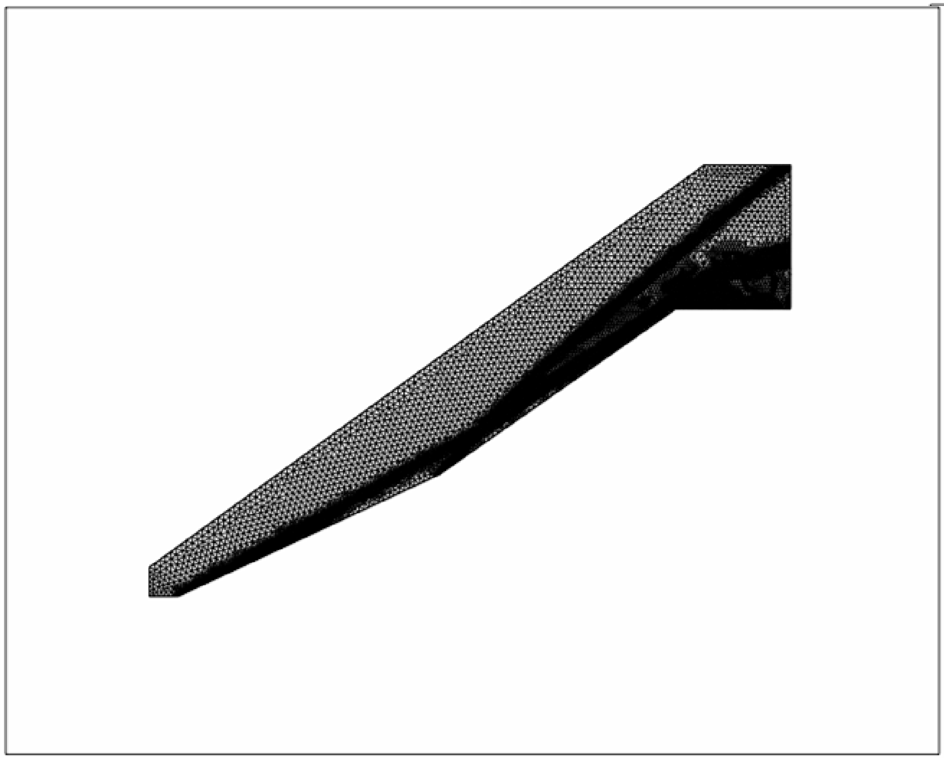
Mach 2 Flow (Ballistic Experiment)

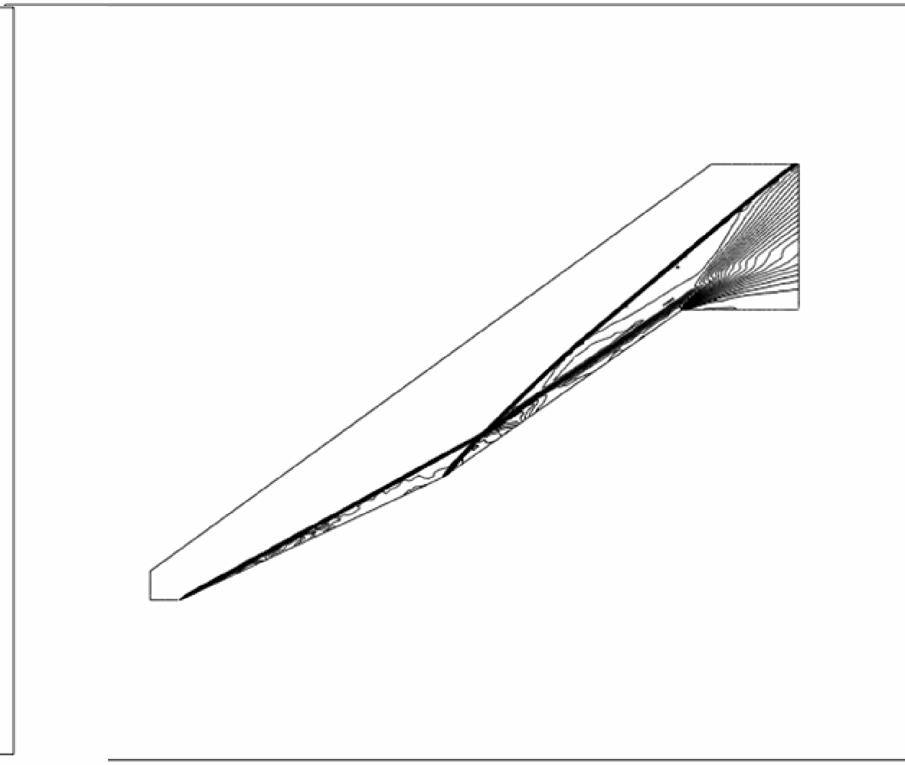


- The cylinder is impulsively started from rest
- Shocks are reflected at the walls

- Time Evolution of the the flow (left to right)
- All Shocks, expansion and contact are captured accurately using the Finite Volume BGK scheme on an adaptive triangular mesh
- The scheme is very robust

Mach 8 Flow
Axi-Symmetric Cone



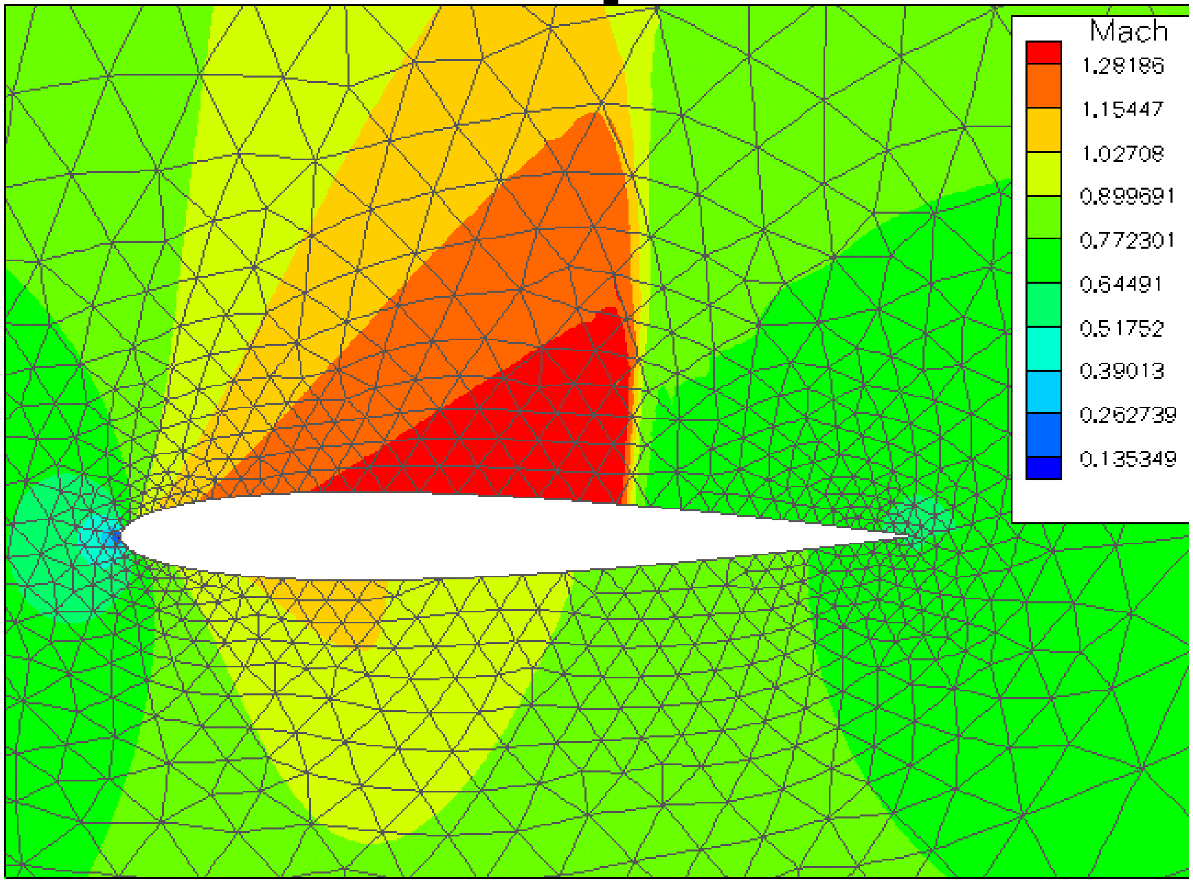


- Mesh (adapted) and computed iso-density contours on double edged cone (25 deg / 35 deg)
- Both Spatial and Temporal Slopes are included in the reconstruction of the flux
- Compares well with previous calculations and with experiments (qualitatively)

Treatment of Shock Waves

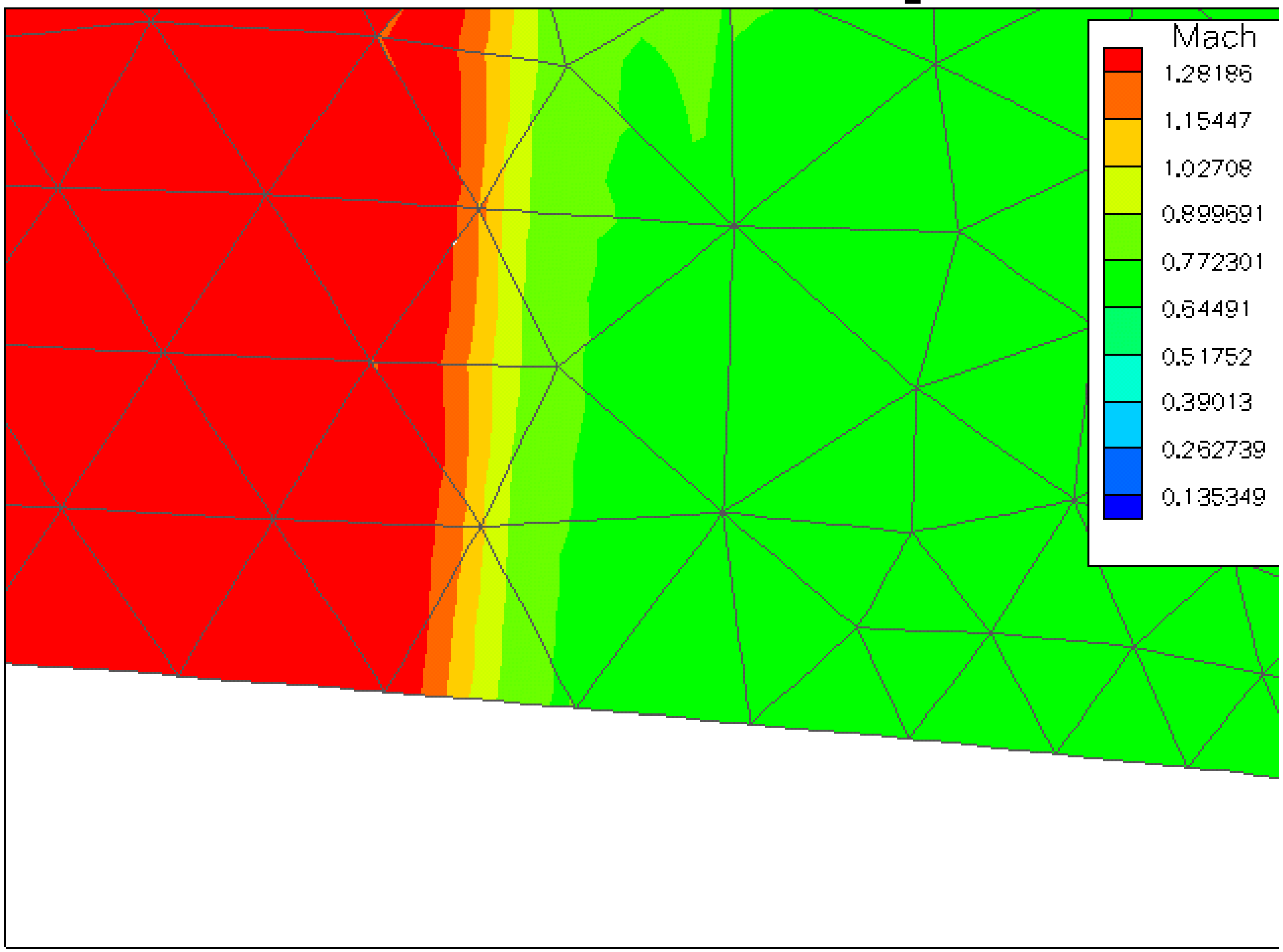
- High-order (DG) methods based on smooth solution behavior
- Shock wave simulation requires:
  - Smoothing out shock: Artificial viscosity
    - Use IP method discussed previously
  - Lowering order of DG discretization
    - Limiting, h-p adaptive
  - Shock fitting
    - Potential to relieve shock staircasing effect
    - Requires mesh optimization/movement

Shock Capturing with Artificial Dissipation



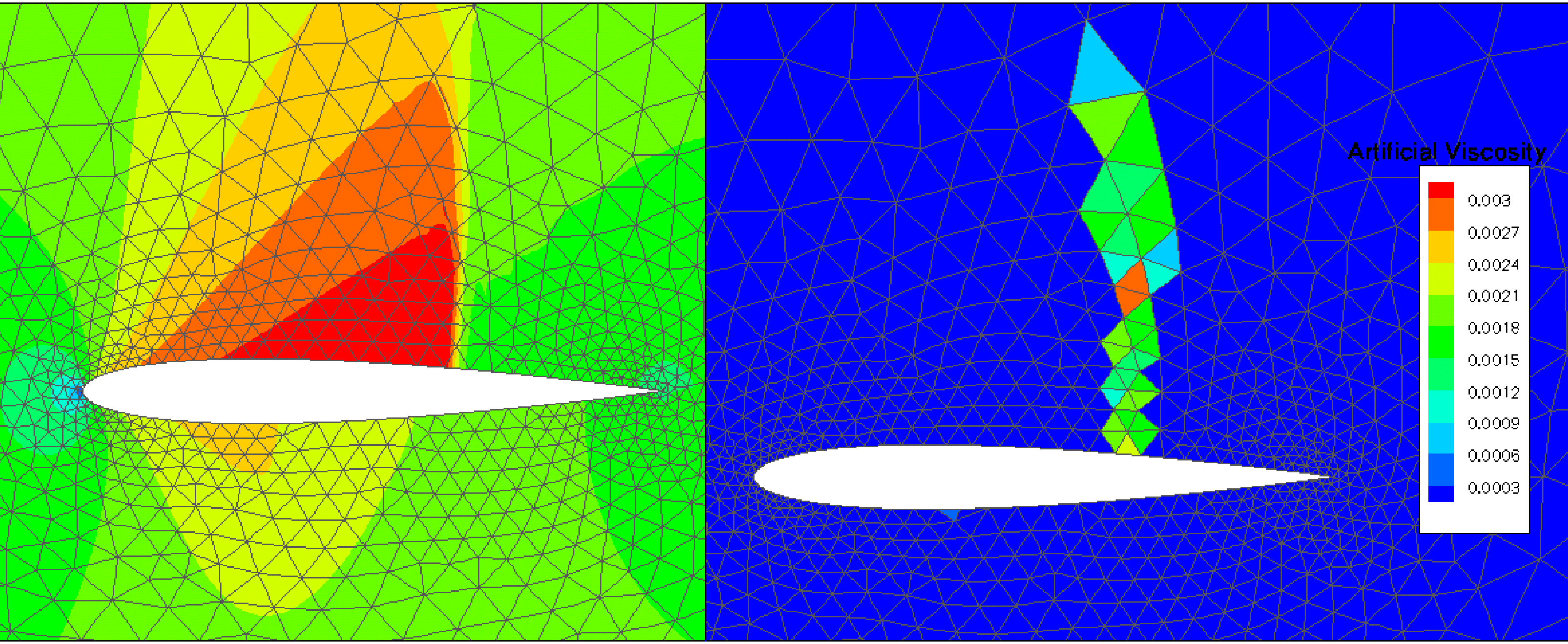
- Use IP method for artificial diffusion terms
  - Based on method of Persson & Peraire (2006)
- Transonic shock captured with p=4 (fifth order accuracy)

Shock Capturing with Artificial Dissipation



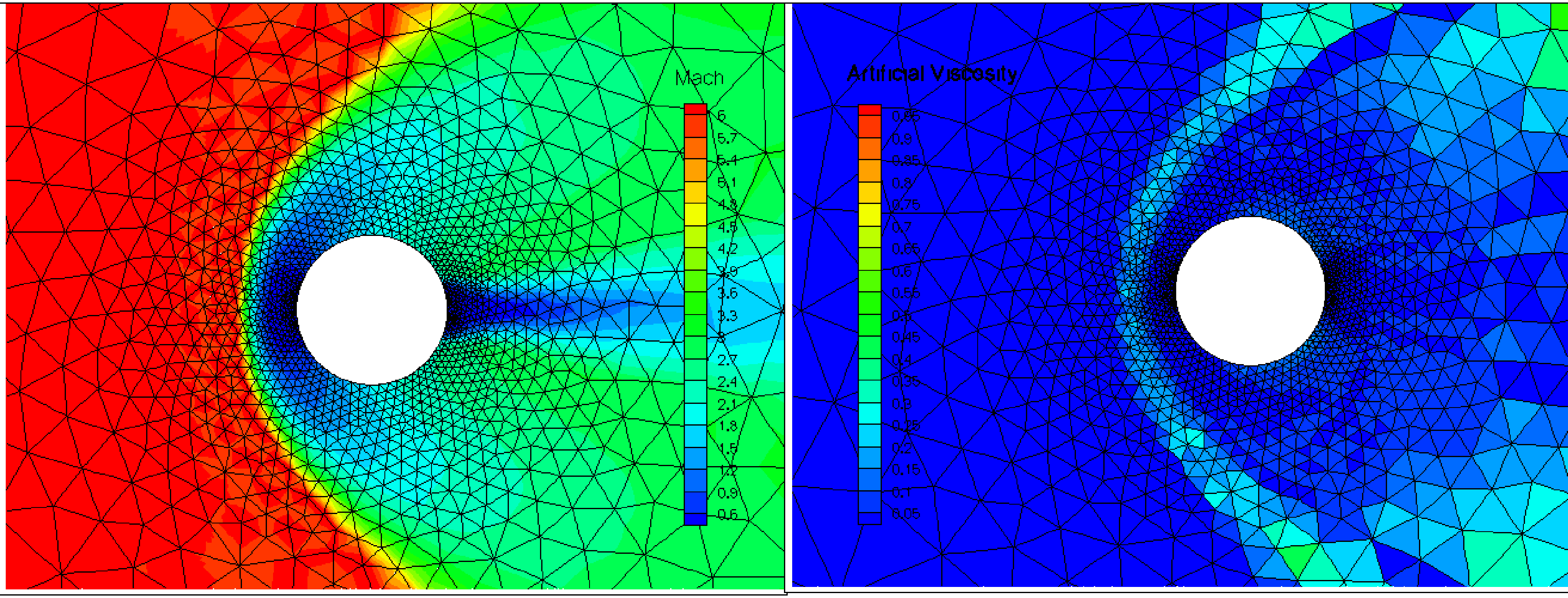
- Sub-cell shock capturing resolution (p=4)

Shock Capturing with Artificial Dissipation



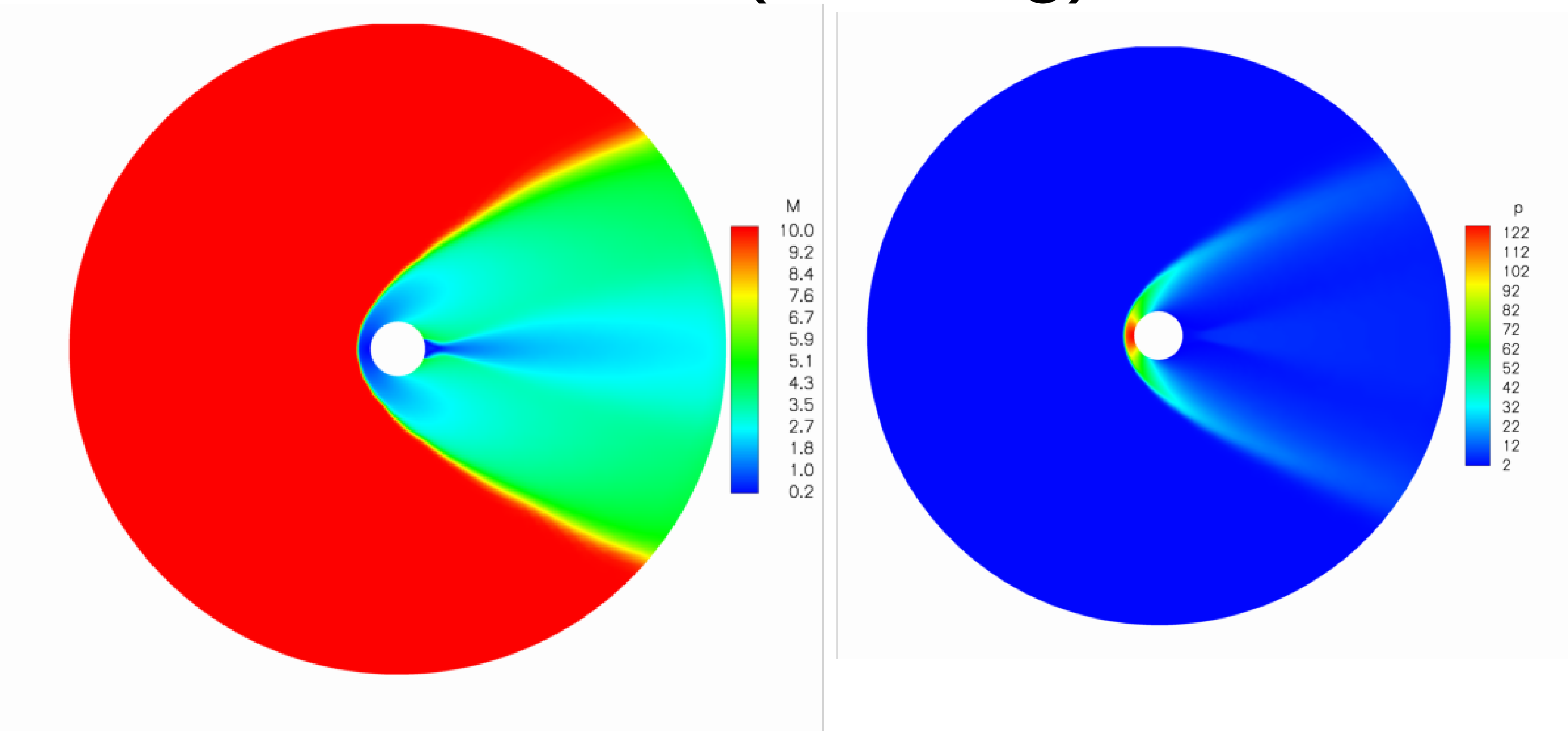
- Artificial Viscosity scales as ~ h/p
- An alternative to limiting or reducing accuracy in vicinity of non-smooth solutions
  - Raise p, or reduce h ?
- Robustness implications

Mach 6 Shock over Cylinder



- Applied to Mach 6 cylinder case
  - p=1 (second-order accuracy)

Alternative: Low-Order DG at Shock (Limiting)

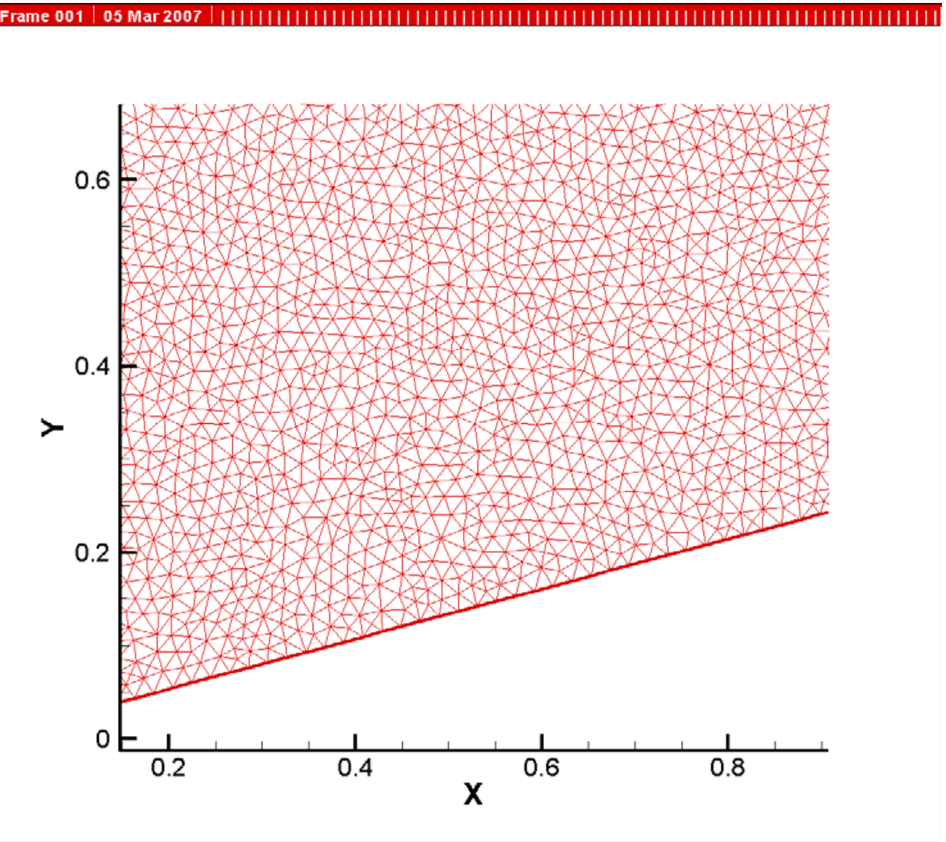


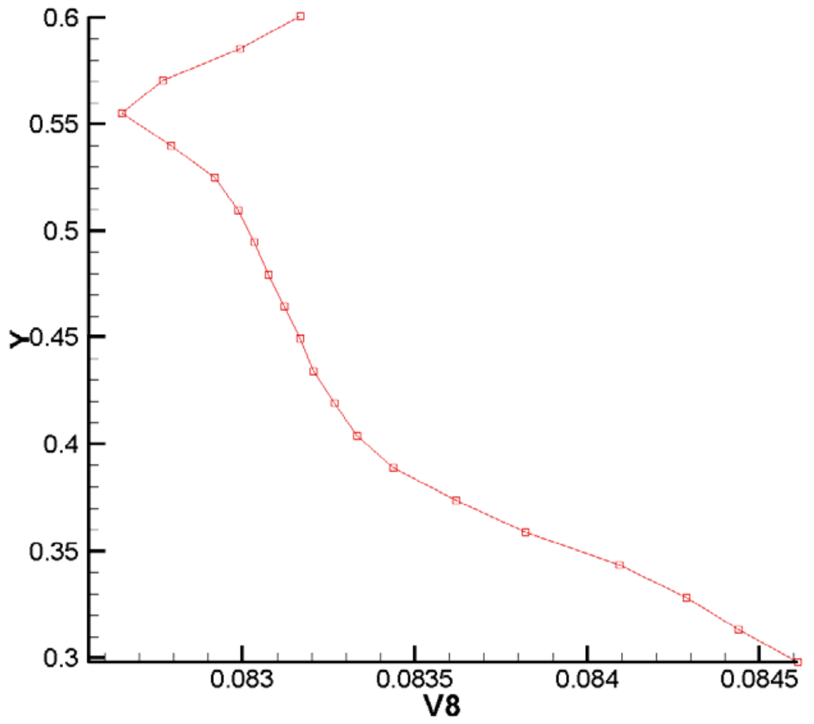
- Mach 10 shock over cylinder
  - p=0 in shock region
  - p=1,2 elsewhere (manually)

Shock Fitting / Mesh Optimization

- Shock capturing with unstructured mesh results in staircasing effect
  - Limited low order (p=0) approach
  - High-order artificial viscosity approach
- Resolution of this problem and its effect on accurate heating values may require mesh-alignment with shock

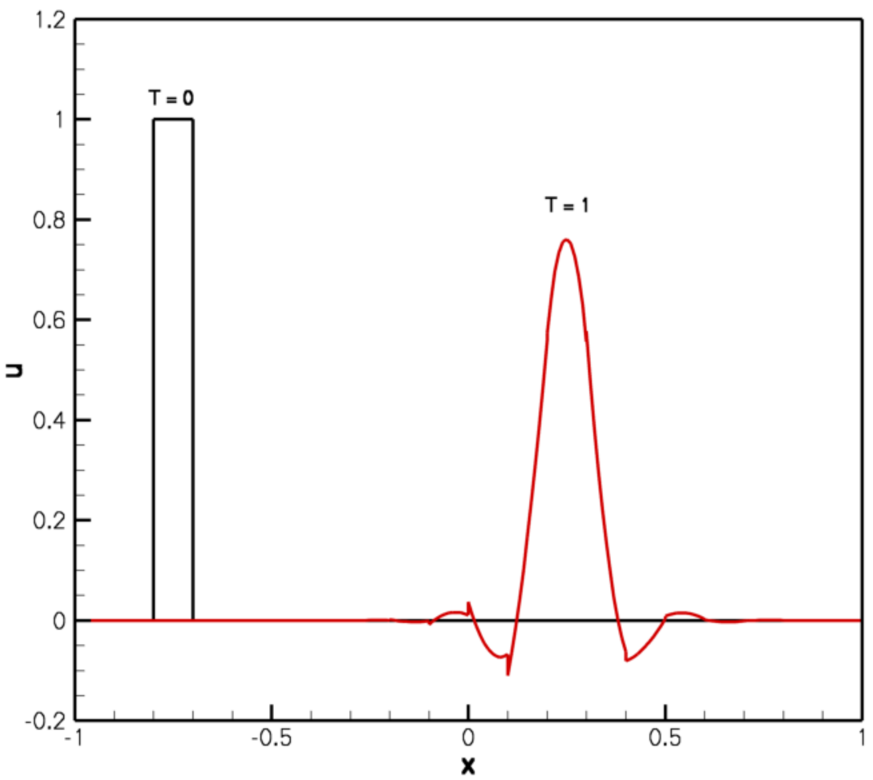
Adjoint-Based Shock Fitting

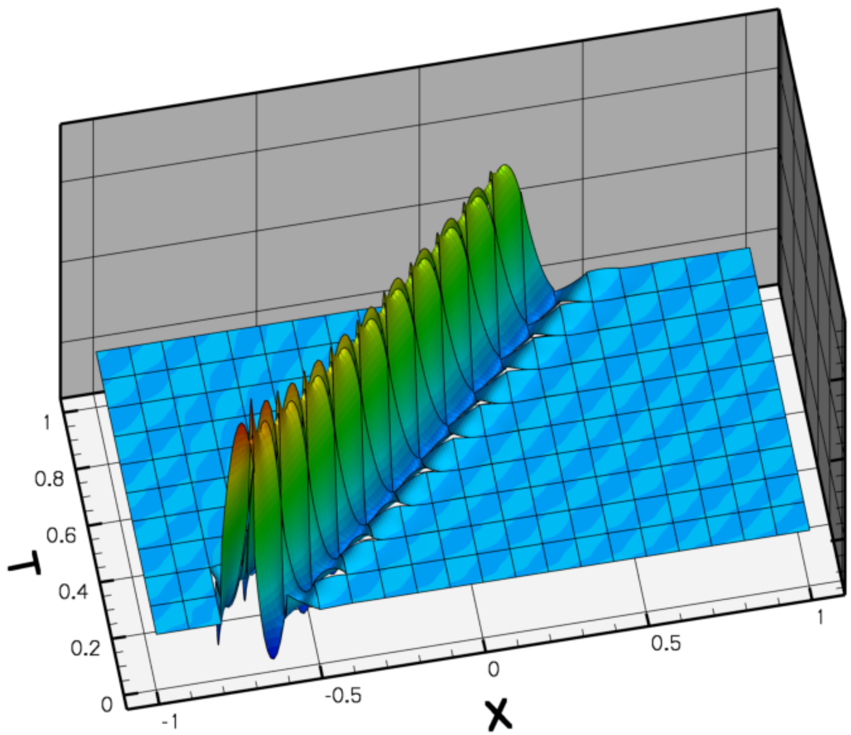




- Use adjoint to get sensitivity of grid points to entropy objective (heating)
- Mesh optimization results in shock fitting
- Perfect fit not always possible, but improvement always obtained
  - Based on knowledge of exact solution

Shock Fitting: High-Order Space Time Formulation

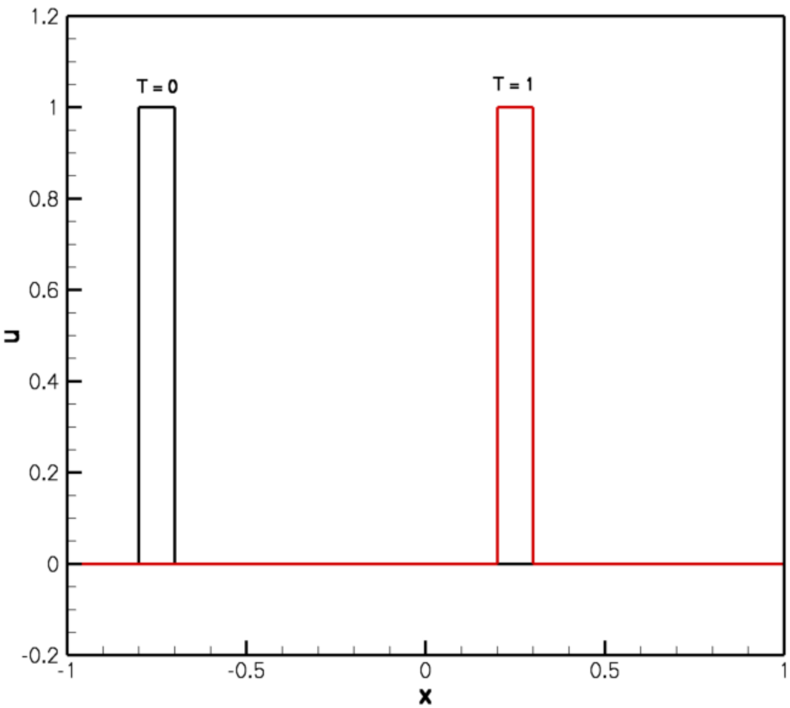


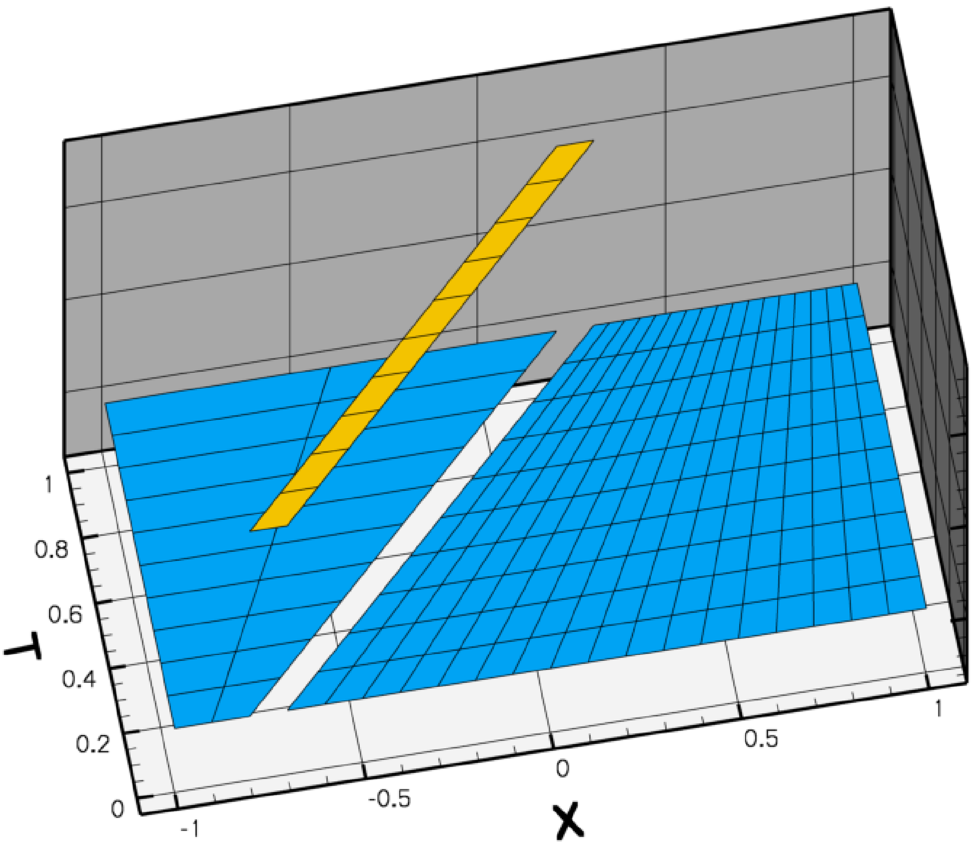


- Wave equation: Static Mesh
  - Produces oscillations

Yang and Mavriplis
AIAA 2008-0758

High-Order Shock Fitting





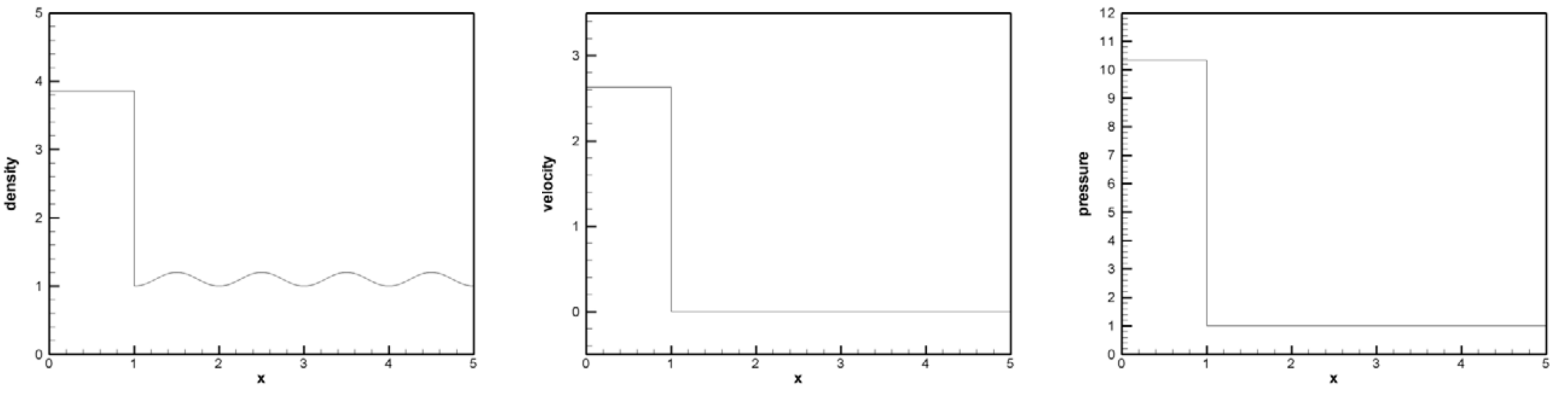
- Moving mesh: Fit moving shock in space-time
  - Discontinuity resolved exactly using high-order elements p=4

Shock Fitting: Euler Equations

- Shock Entropy Interaction
  - Initial condition:

$$\rho_1 = 3.857 \quad u_1 = 2.629 \quad p_1 = 10.333 \quad \text{if} \quad x < 1$$

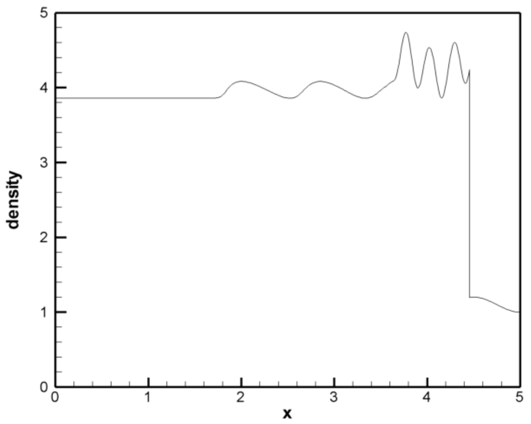
$$\rho_2 = 1 + 0.1(1 - \cos(2\pi x)) \quad u_2 = 0 \quad p_2 = 1 \quad \text{if} \quad x \geq 1$$

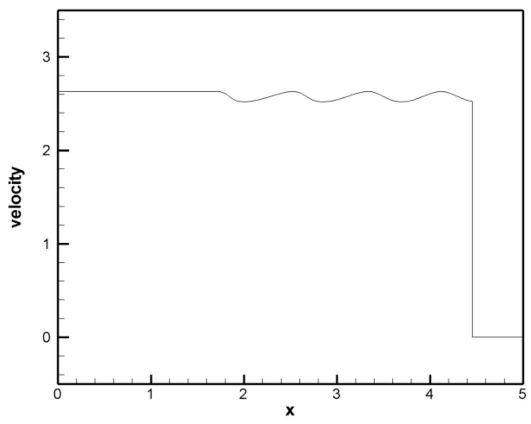


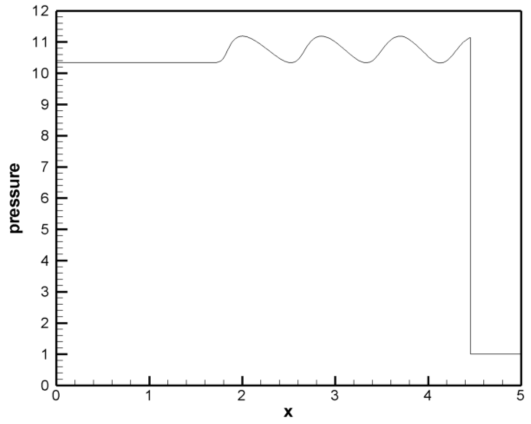
Shock Fitting: Euler Equations

- Shock Entropy Interaction, t = 1

Yang and Mavriplis AIAA 2008-0758







•Achieves design (high-order) accuracy (in 1D)
•Shock location computed using level set approach
•Most effective approach in 3D may involve combination of methodologies (to be investigated)

ALE Form for DG Methods

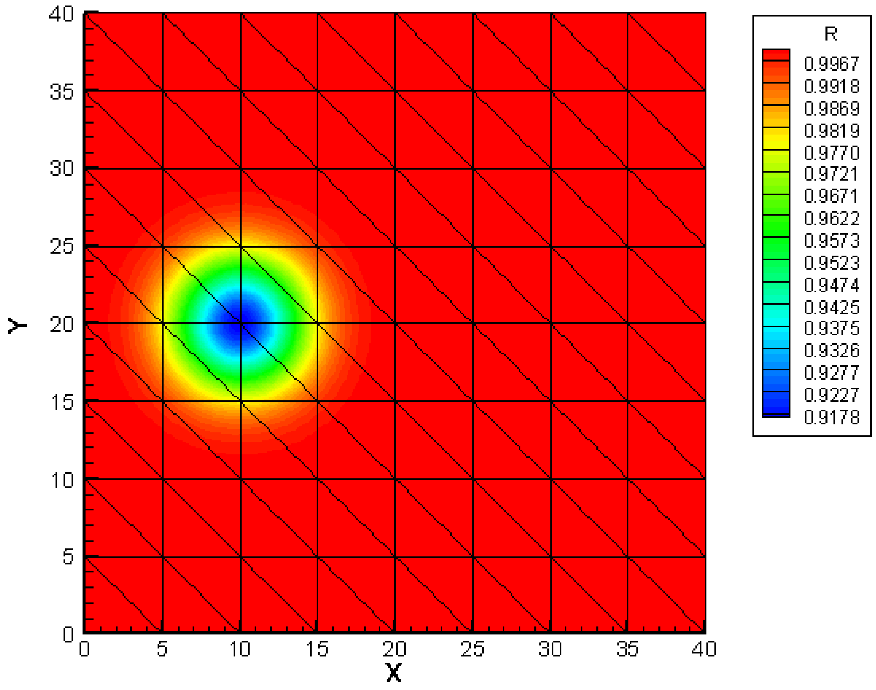
- Dynamic mesh problems important
  - Moving fitted shocks
  - Time-dependent ablation
  - Aeroelastics …
- Require discrete conservation for high-order DG methods with moving meshes: GCL
  - No current formulation available for general mesh motion
  - Derived and implemented new ALE/GCL formulation
    - Valid for any order p spatial discretization
    - Preserves temporal accuracy for BDF1, BDF2, IRK time discretizations
    - Valid for any type of mesh motion
      - Moving curved high-order elements

ALE Form for DG Methods

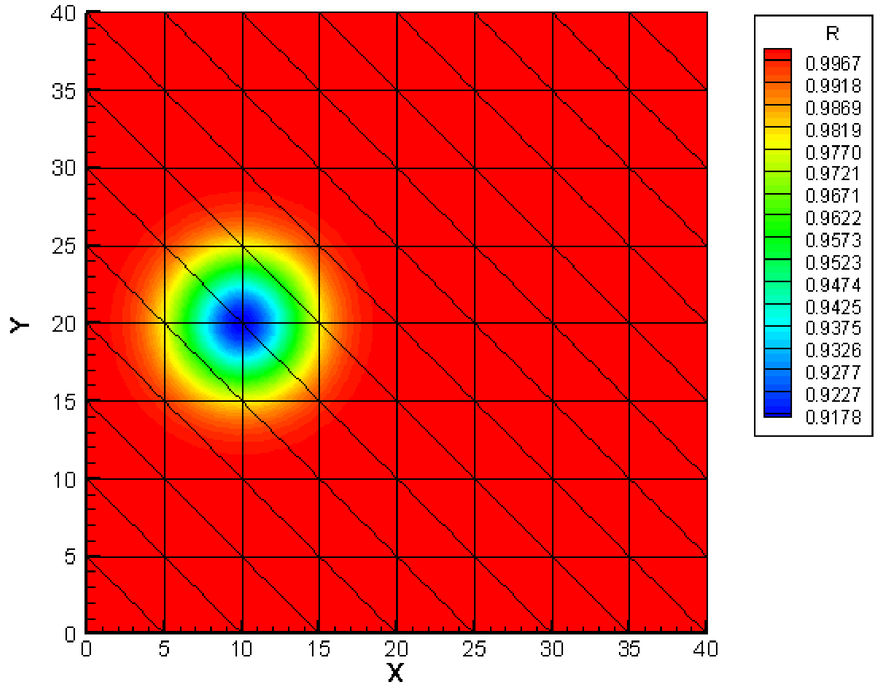
- Inspired from space-time formulation
  - Reduces to space-time formulation for BDF1
  - Easily extends to BDF2, BDF3, IRK
- ALE Formulation
  - extra grid speed terms multiplied by time dependent mesh metrics
- Principal requirement:
  - For each stage of BDF or IRK:
    - Grid speed terms at quadrature points computed to match exactly space time formulation (fully conservative - GCL)

Vortex Convection Test Case

- Prescribed mesh motion with curved elements
- Fully conservative: Uniform flow = exact discrete solution
- Static mesh design accuracy recovered for BDF1 (1st order) and BDF2 (2nd order)
  - AIAA paper 2008-0778
- Higher order implicit Runge-Kutta experiments underway

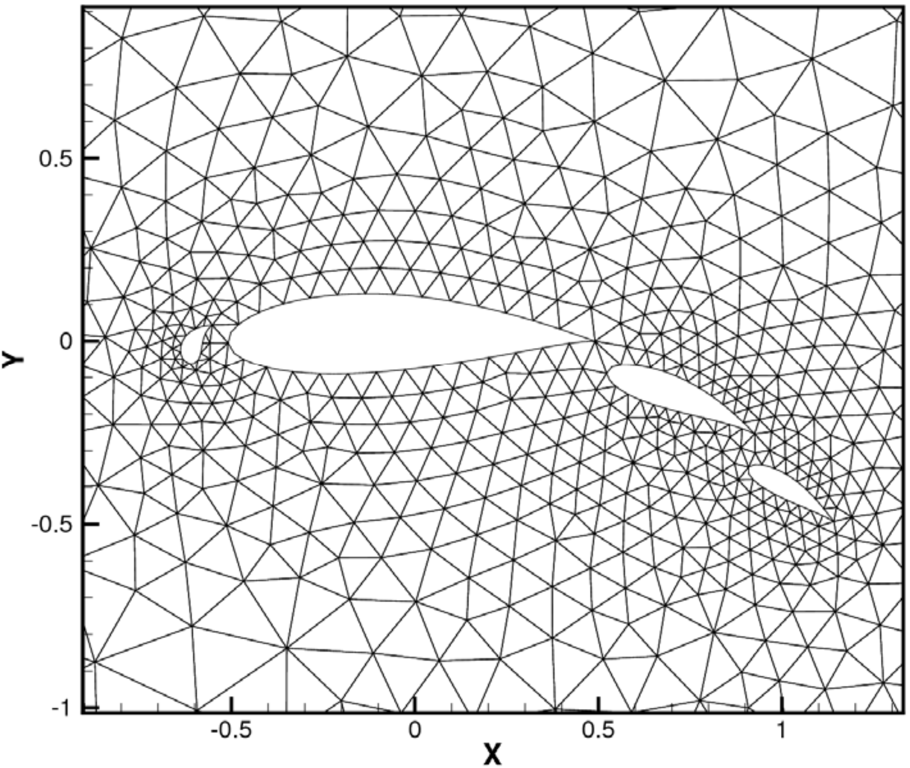


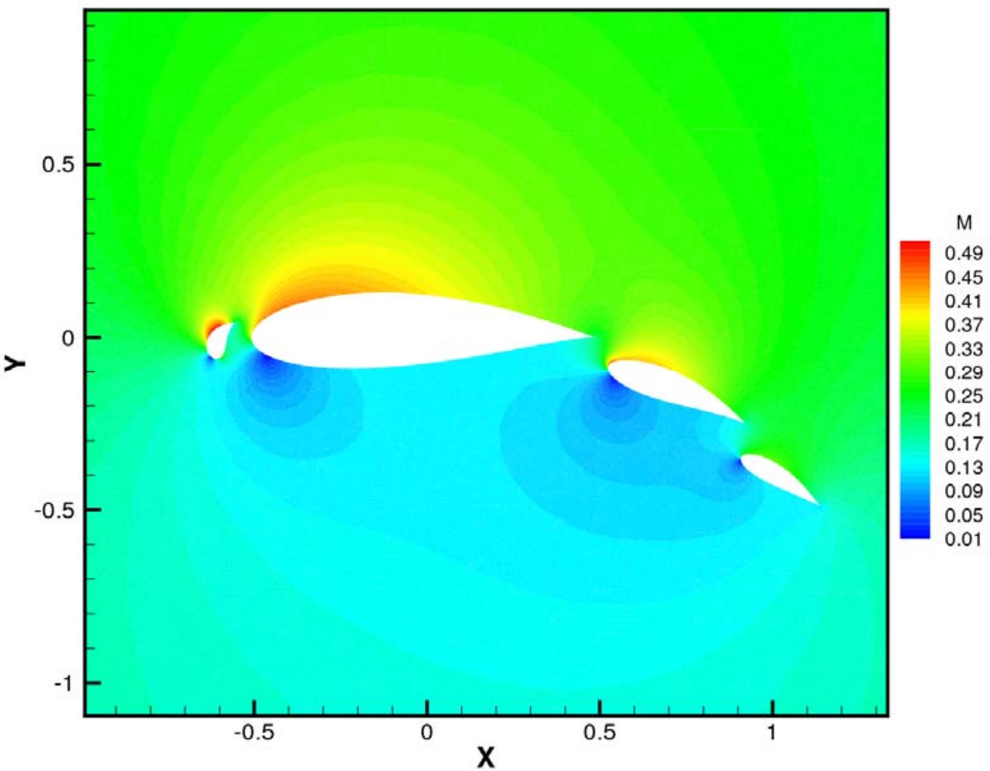
BDF 1



BDF 2

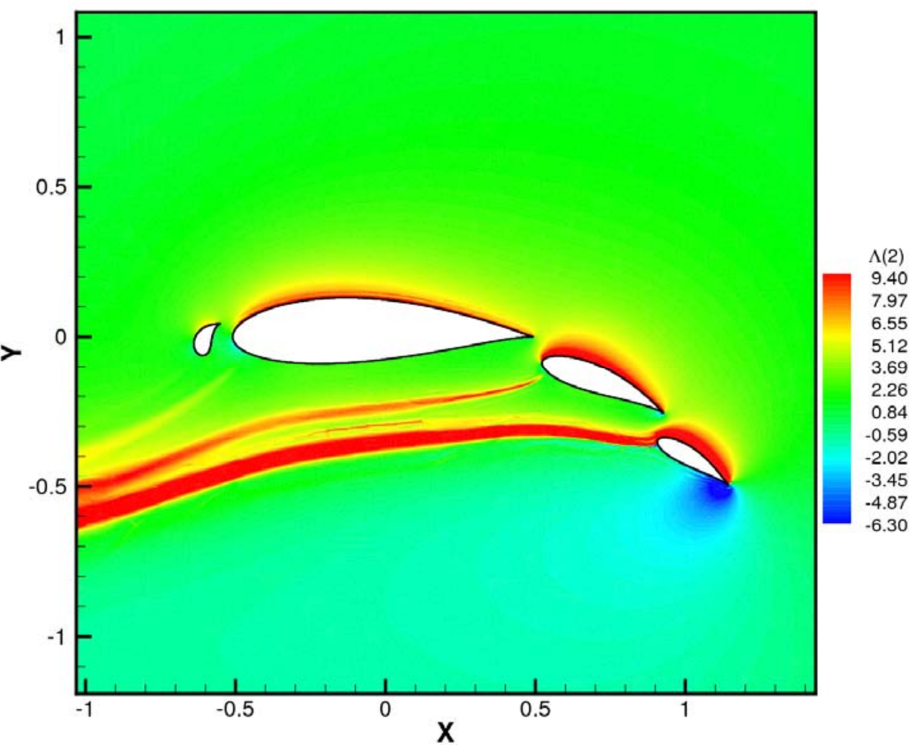
Adjoint-Based Adaptivity (h-p)

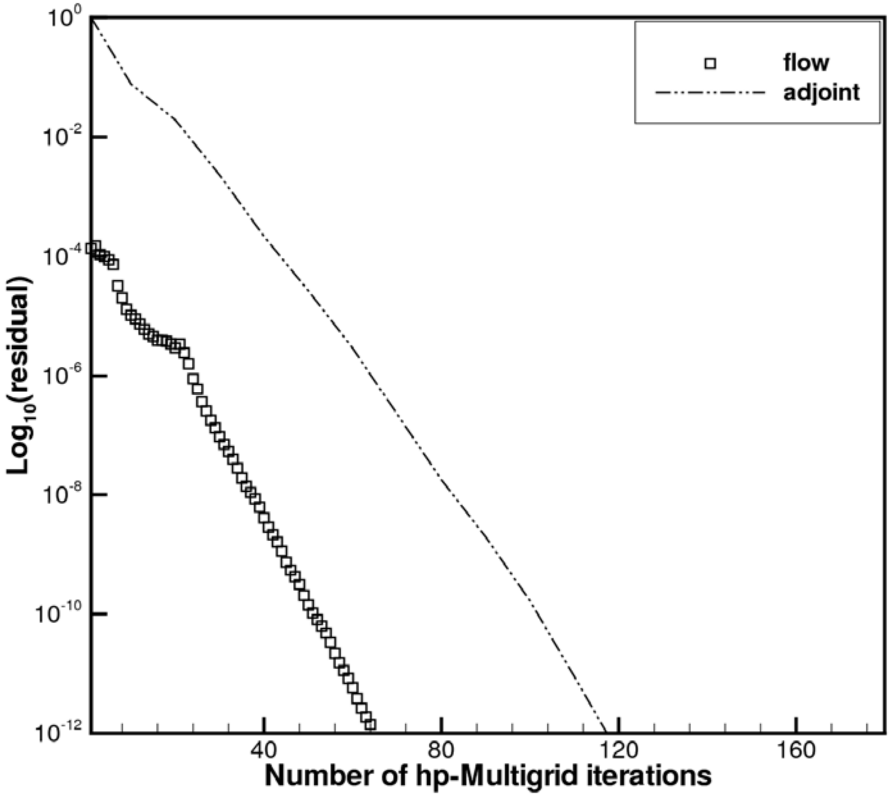




- Initial test case: Subsonic flow, complex geometry
- Smooth solution profiles
- Precursor to application to strong shocks

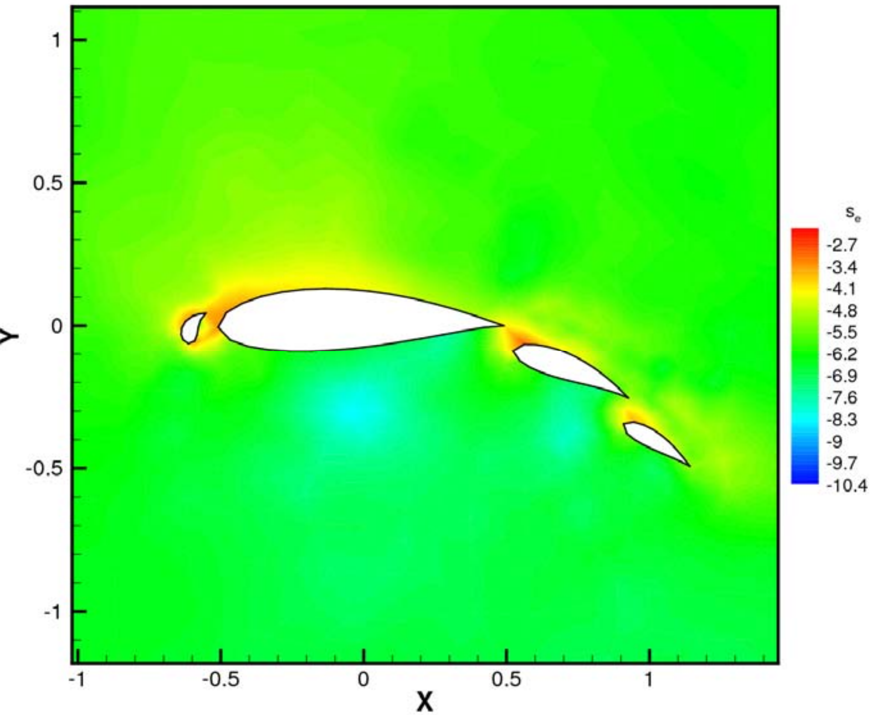
Discrete Adjoint



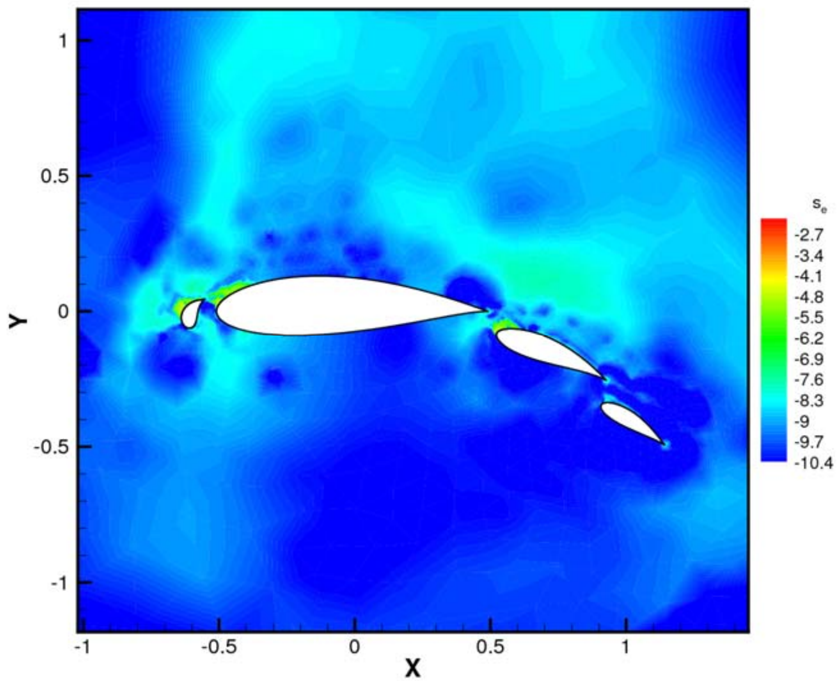


- Implemented in modular fashion
- Solved with h-p multigrid scheme
  - Achieves similar convergence rate as flow equations

Adjoint-Based Adaptivity (h-p)



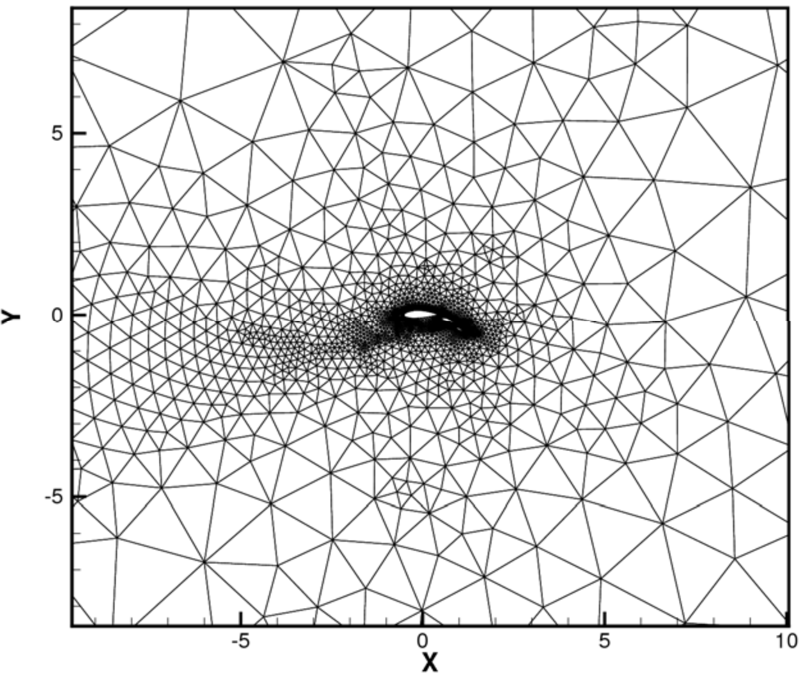
Initial error distribution for Lift

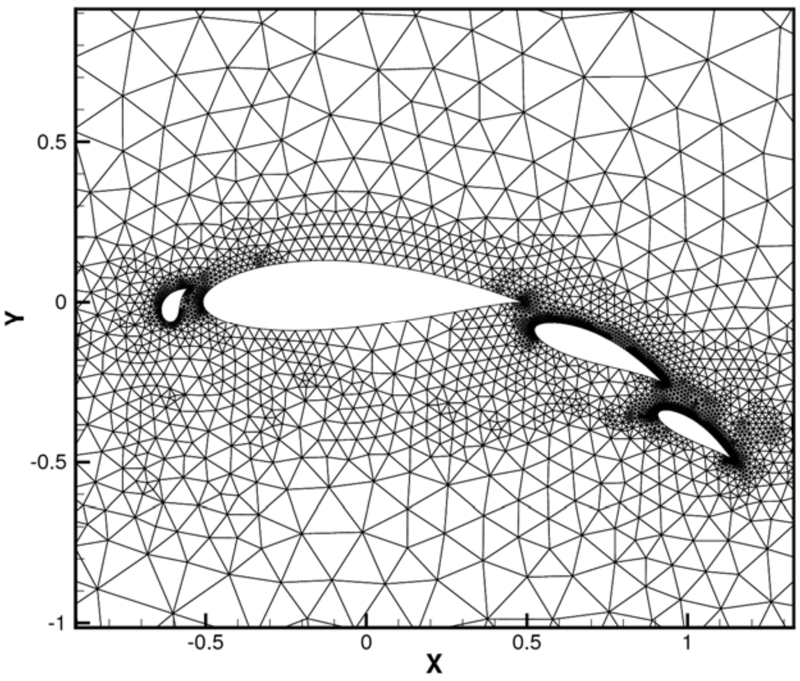


Error distribution after h-p adaptivity

- Inner product of adjoint solution with non-zero residual (on finer mesh) yields error estimate for output functional

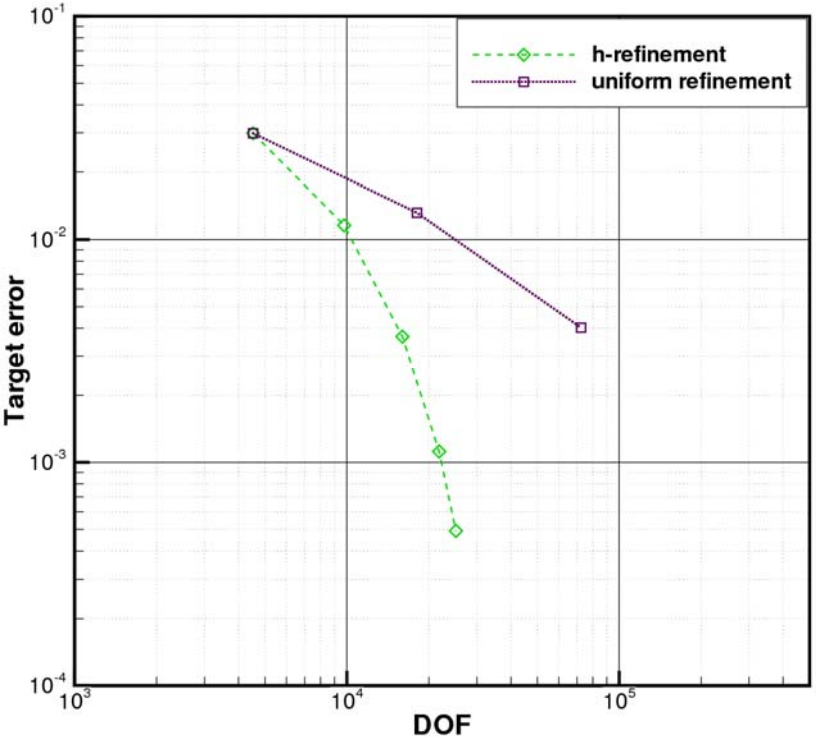
Adjoint-Based Adaptivity (h-alone)

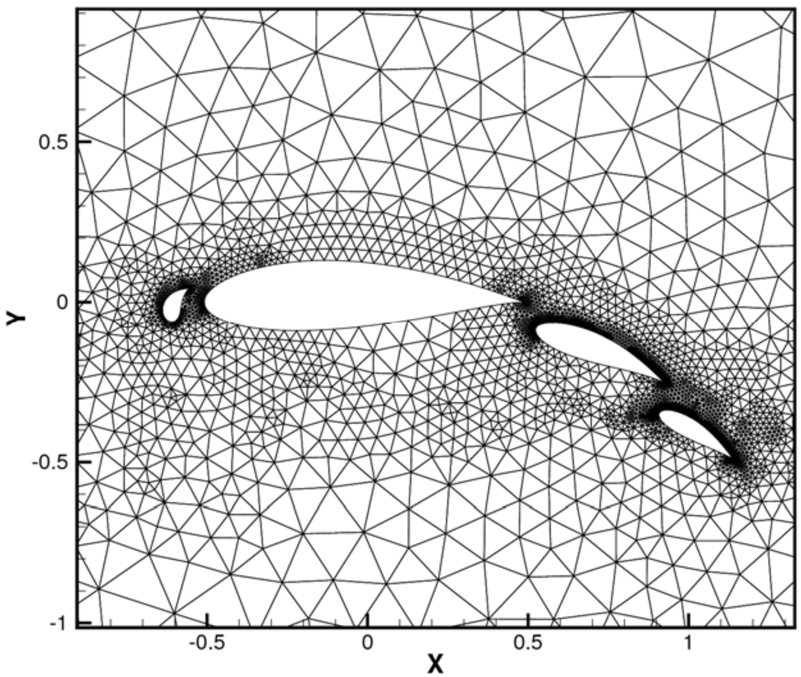




- h-adaptivity (mesh refinement) for drag

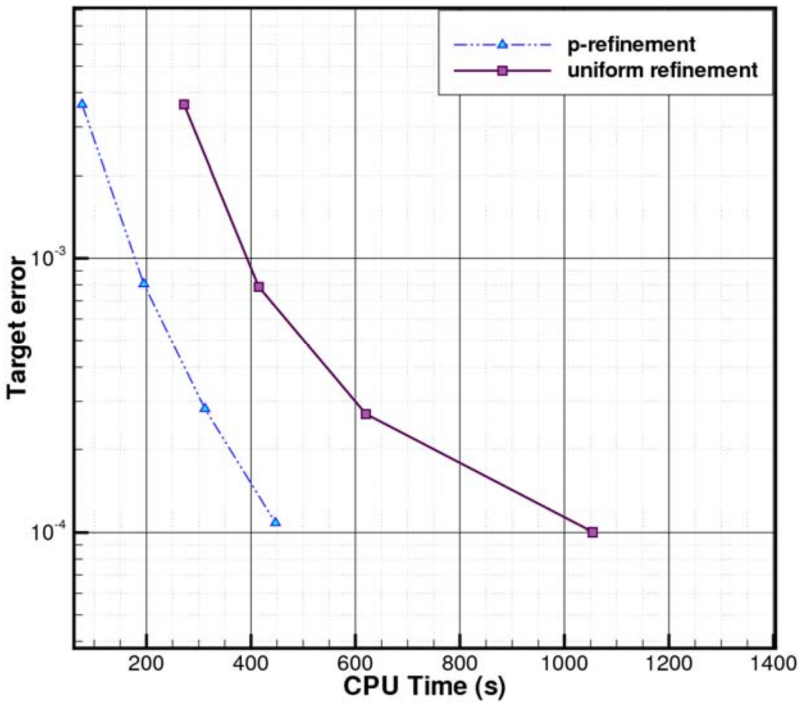
Adjoint-Based Adaptivity (h-p)

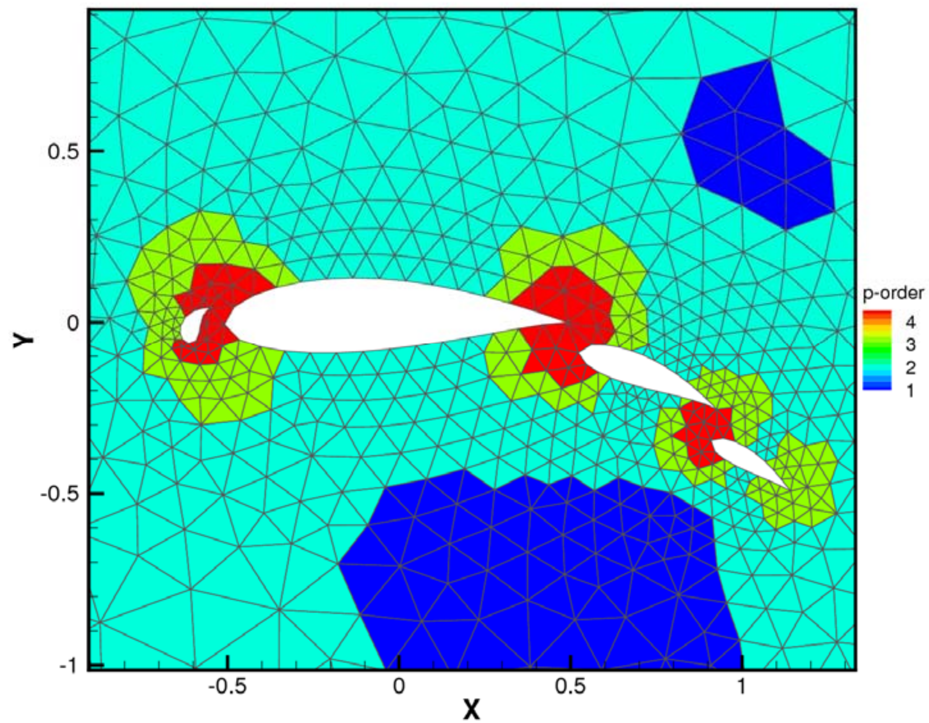




- Each adaptive level achieves same absolute error in objective (drag) as global mesh refinement
  - Best possible solution
  - Much lower cost

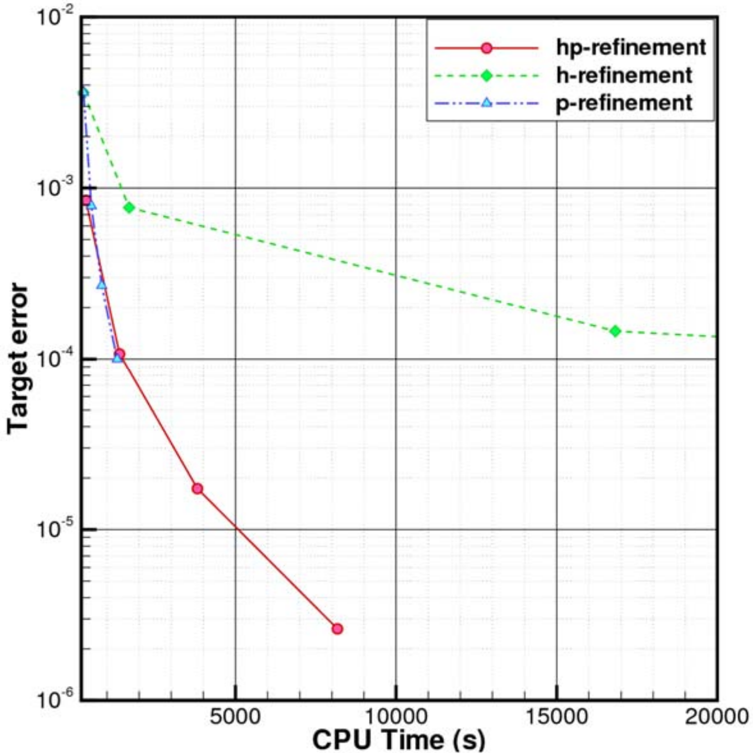
Adjoint-Based Adaptivity (p-alone)

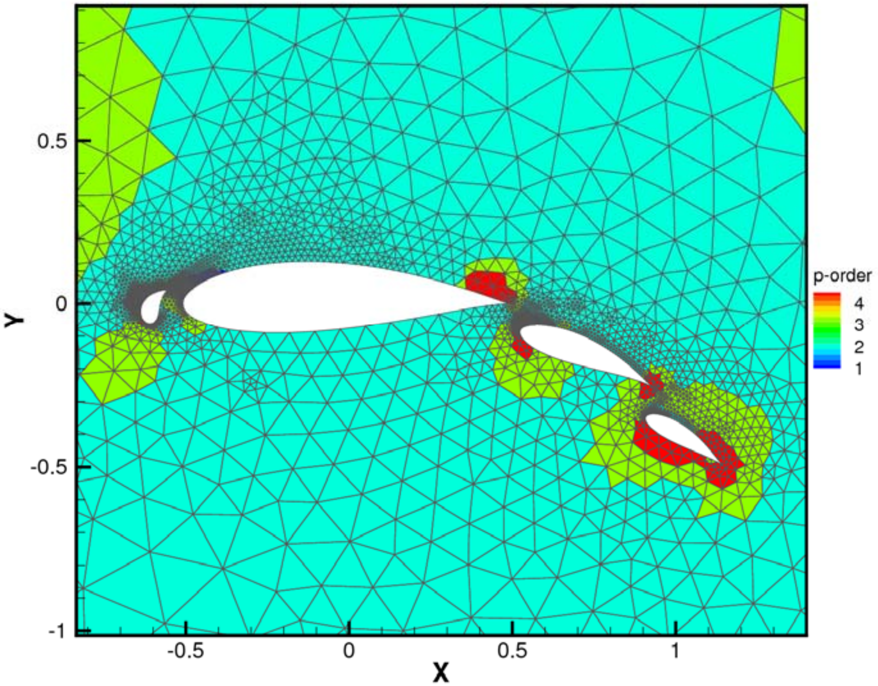




- p-refinement: raise p order locally, keep mesh fixed
  - Based on adjoint error estimate for drag
  - Achieves same error as global p enrichment at lower cost

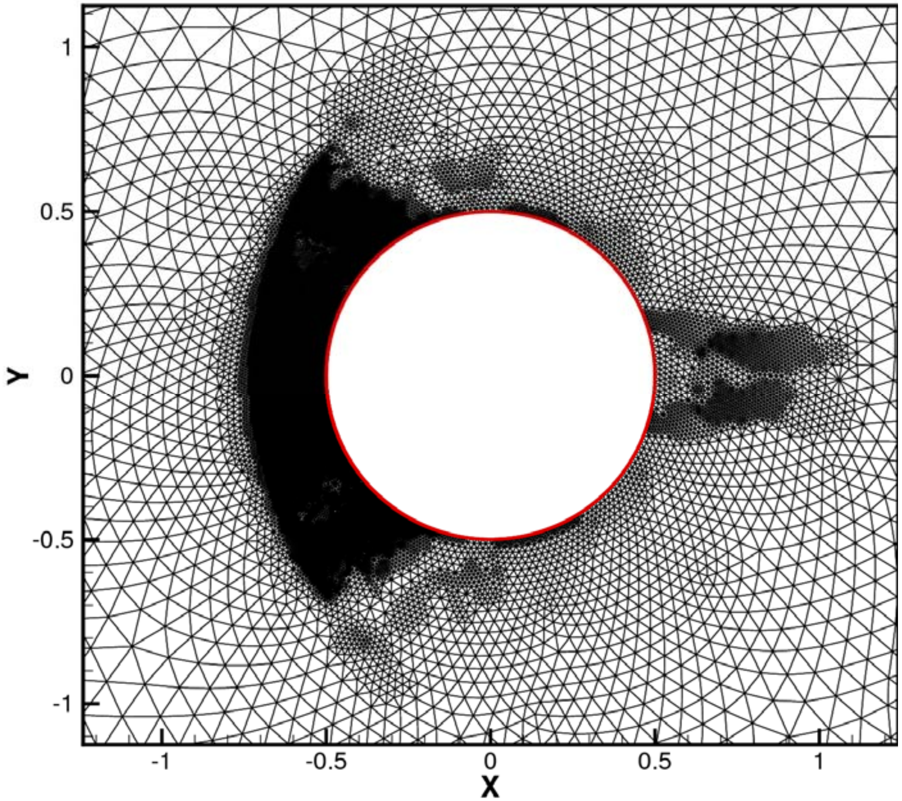
Adjoint-Based Adaptivity (h-p)

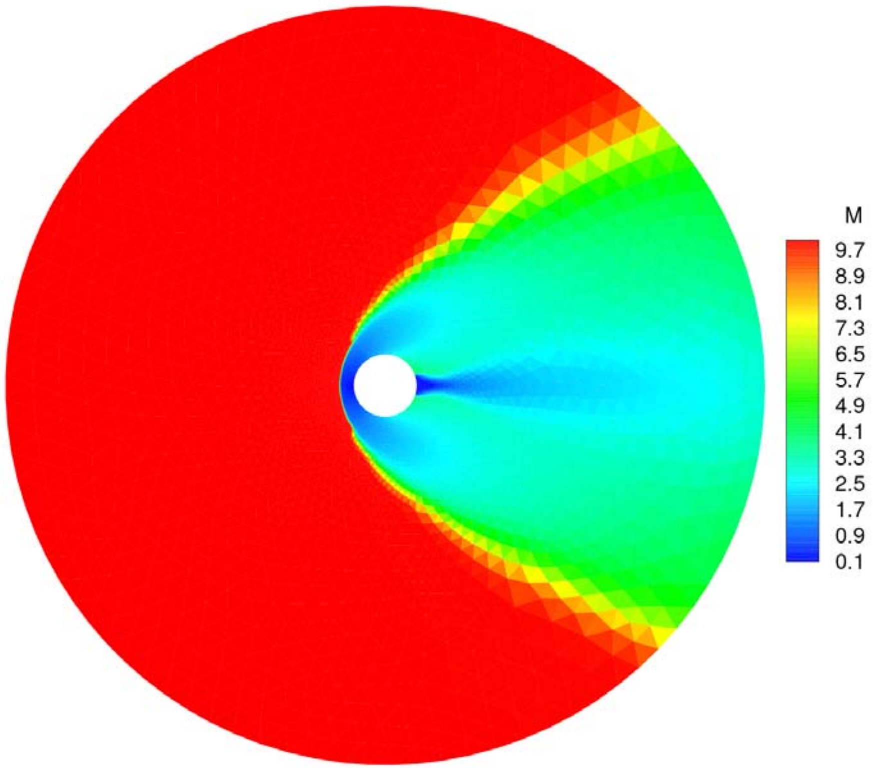




- Combined h-p refinement
  - Decision to refine h or p based on adjoint error estimate
  - Choice between h or p based on solution smoothness indicator
    - Decay of high order coefficients, edge jumps between elements
- Superior error reduction at lower cost
  - Theoretically exponential error reduction

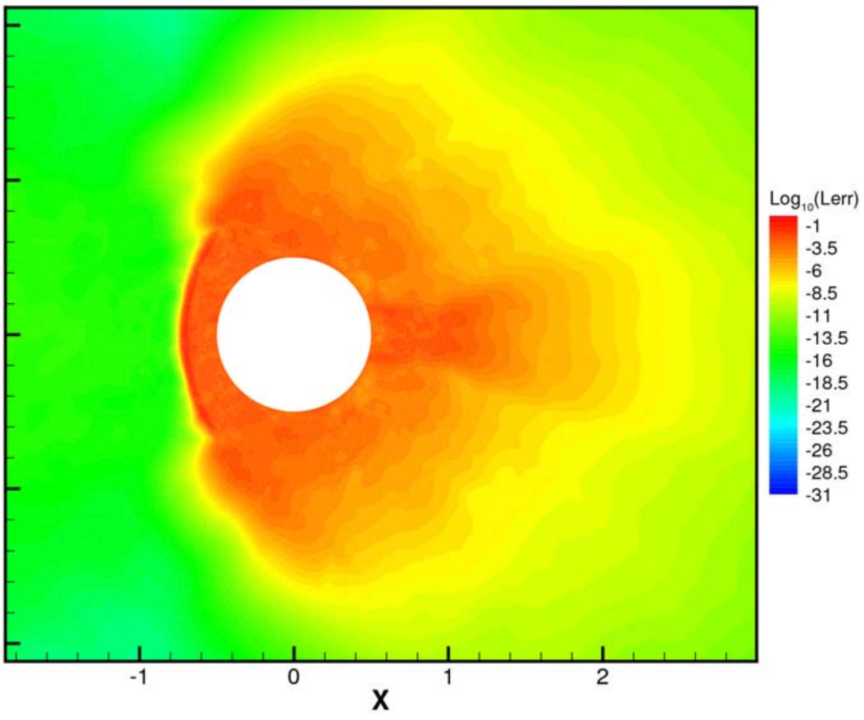
h-p Adaptivity for Shock Waves

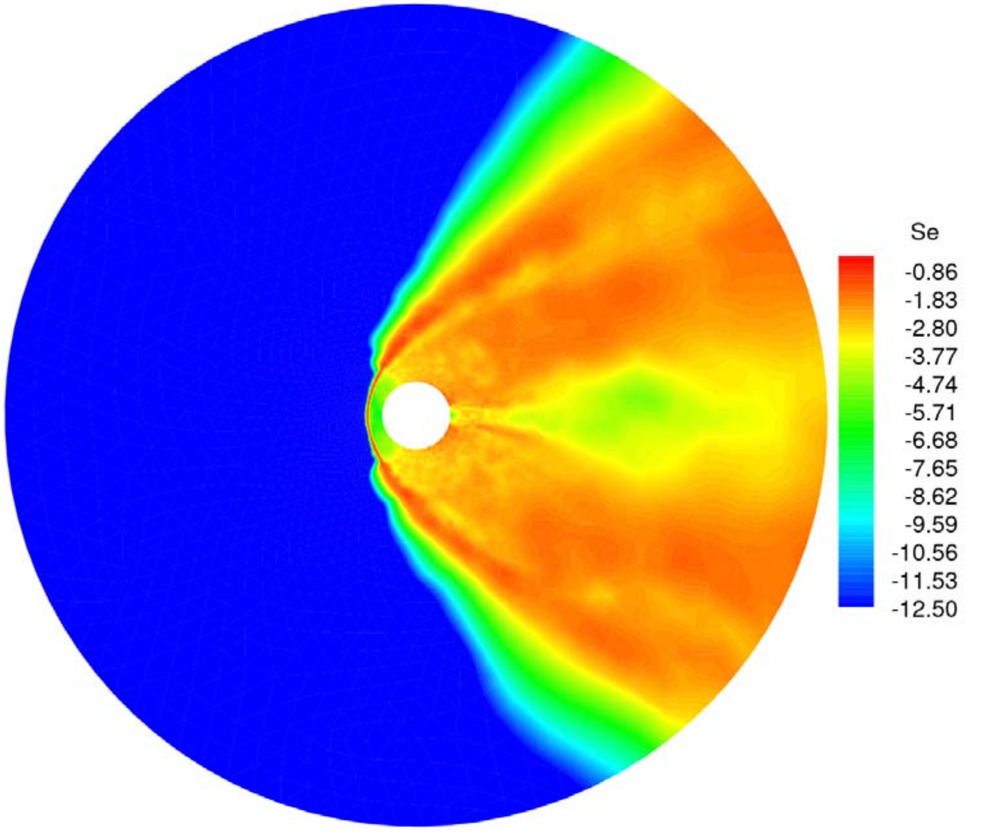




- h-refinement based on drag objective for Mach 10 shock wave (p=0 1st order accurate)

h-p Adaptivity for Shock Waves





Adjoint error for drag

Smoothness indicator

- Smoothness indicator identifies shock
- Can h-p adaptation be used in place of limiter ?
  - Or in conjunction with limiting (to be investigated)

Conclusions and Future Work

- Shock capturing
  - Artificial viscosity vs. limiting
  - Raise order p (fixed h) or lower p (limiting) and refine h
    - Investigate these tradeoffs
- Adjoint based h-p refinement for strong shocks with heating objectives
  - Incorporate mesh optimization techniques also
- BGK Fluxes to be incorporated into 2D DG code and tested up to p=5 (6^{th} order)

Conclusions and Future Work

- Various basic issues being resolved in simplified 2D setting
  - Shock capturing
  - Viscous fluxes
  - ALE formulation and GCL
  - Solvers and implicit time discretizations
- Extend into 3D DG parallel code
  - Diffusion terms
  - Shock capturing
  - h-p adaptivity (adjoint based)
- Real gas effects
  - 5 species, 2 temperature model for DG code
    - Solve using h-p muultigrid
    - Derive adjoint of real gas model
      - Use for h-p adaptivity
      - Investigate model parameter sensitivity with adjoint approach