THE UNIVERSITY of TENNESSEE at CHATTANOOGA

SIMCENTER
NATIONAL CENTER for COMPUTATIONAL ENGINEERING

A Perspective on High-Order Accurate Solvers for Field Equations

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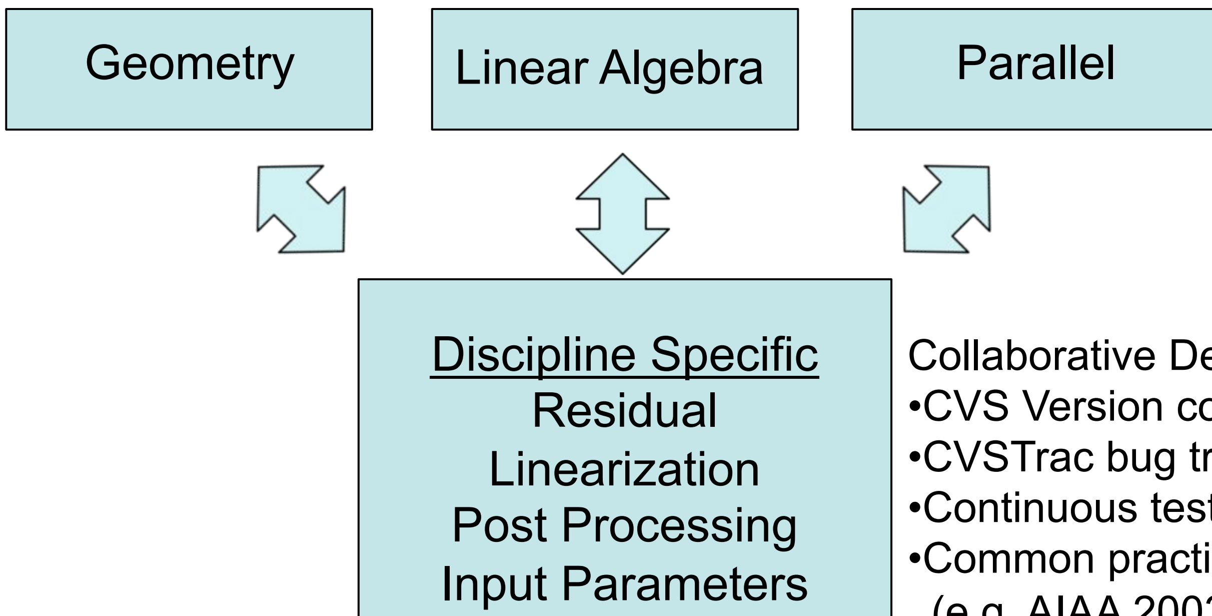
Program Description

- Development of a simulation framework easily adaptable for multidisciplinary applications
- High-order finite elements
- Share common modules between disciplines
  - Mesh-related routines
  - Parallel routines
  - Linear algebra
- Requires primarily residual and left-hand side for discipline
- Integration with CAPRI for CAD-based surface representation
- Adaptive (both h- and p-adaptation under development)
- Managed code base

New Simulation Framework

- Most computational simulation programs have similar structure and common components can be isolated into a single framework (code reuse)
- Discipline-specific applications (e.g. E&M + fluids) require new code in the form of residual routine and linearization (often just residual)
- Existing programs refactored to provide workable framework



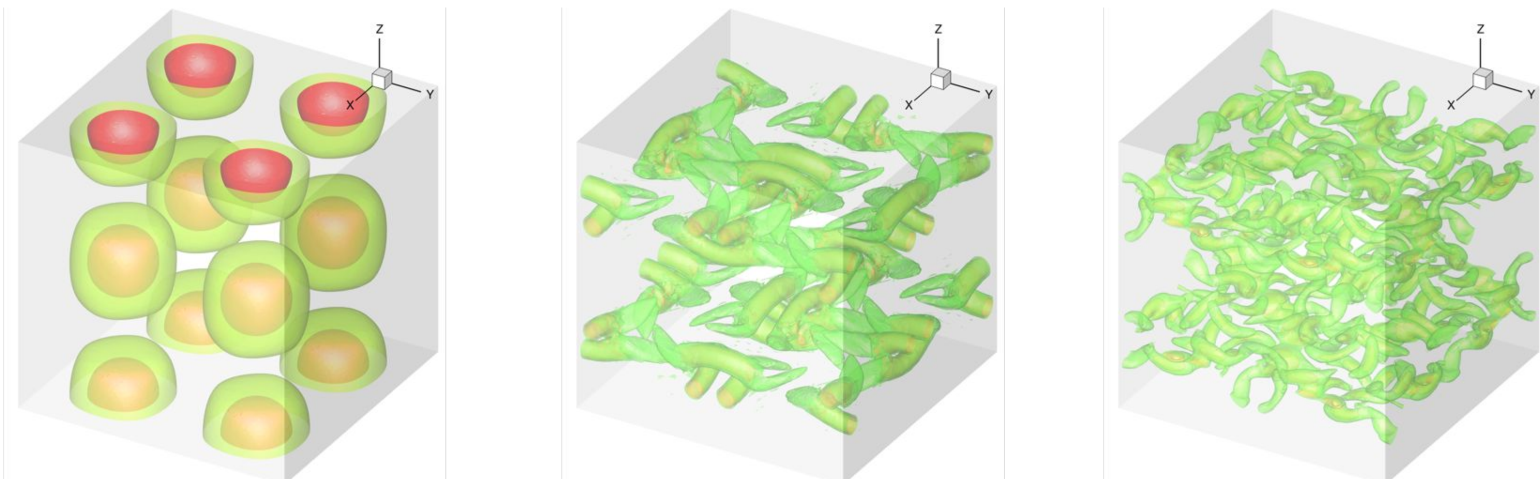
Collaborative Development (PG)
•CVS Version control
•CVSTrac bug tracking
•Continuous testing (future)
•Common practices
(e.g. AIAA 2003-3978)

Engineering Disciplines

- Fluid dynamics
- Electromagnetics
- Structural Analysis
- Lithium-Ion Batteries
- Hydrogen Reforming (under development)

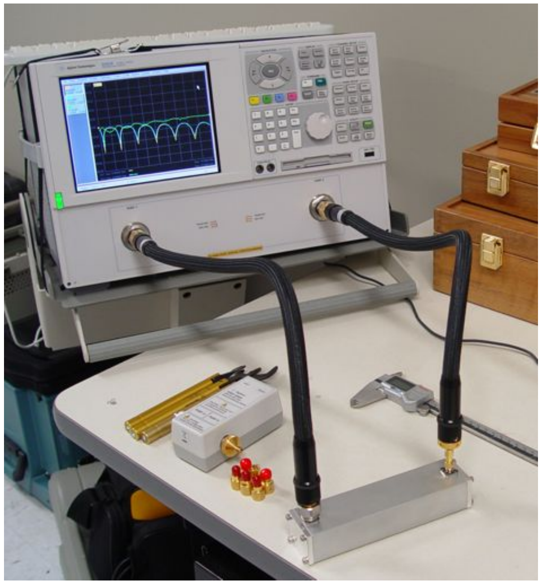
Fluid Dynamics

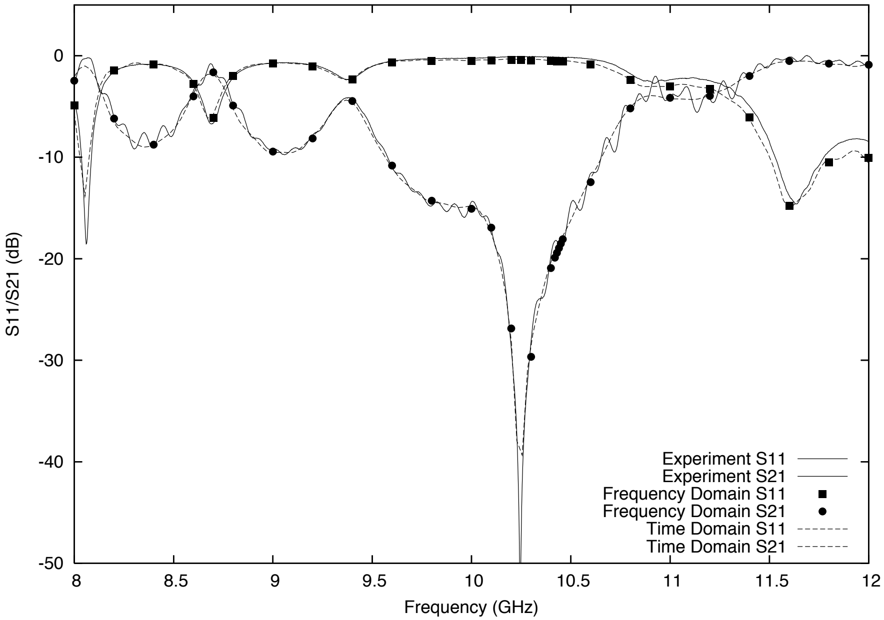
- Implicit time stepping
- Full Navier Stokes with Spalart-Allmaras turbulence model
- Petrov-Galerkin and discontinuous-Galerkin discretization



Electromagnetics

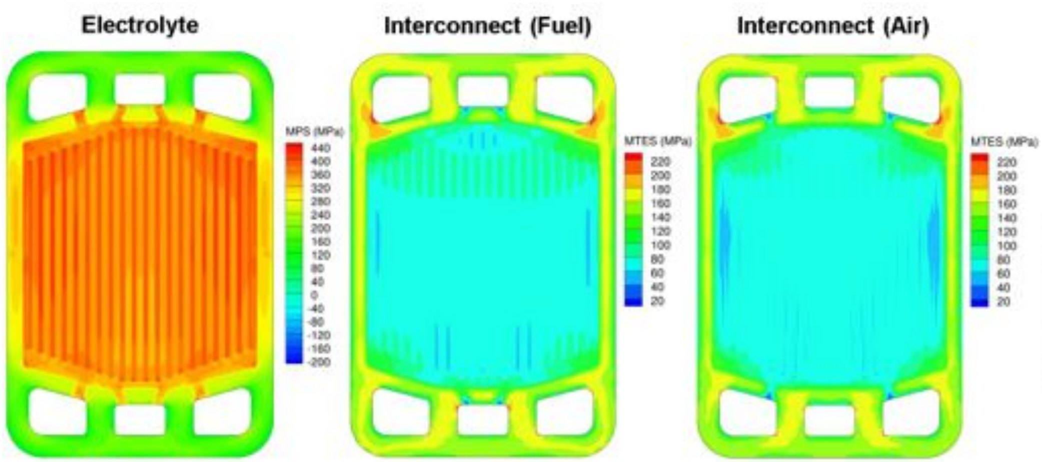
- Frequency domain and time-domain (implicit time stepping)
- Petrov-Galerkin and discontinuous-Galerkin discretization
- Frequency-dependent material properties

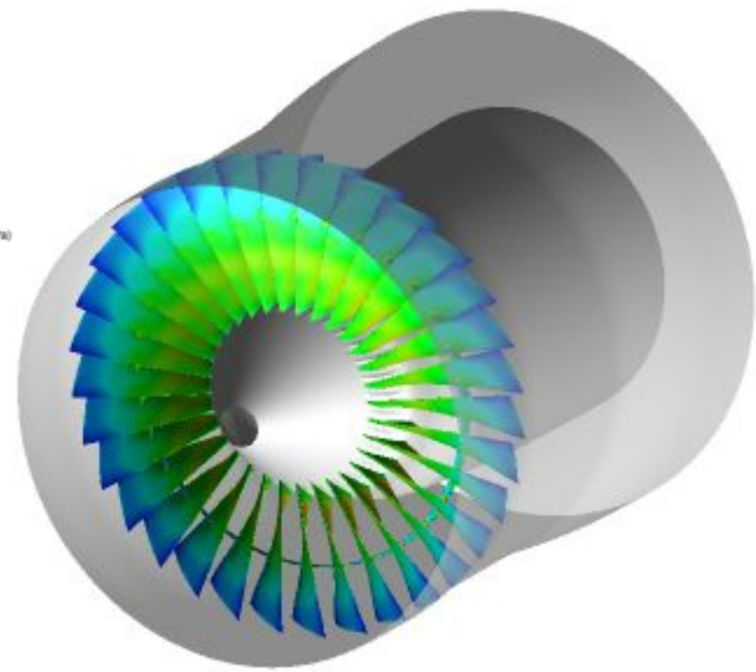




Structural Analysis

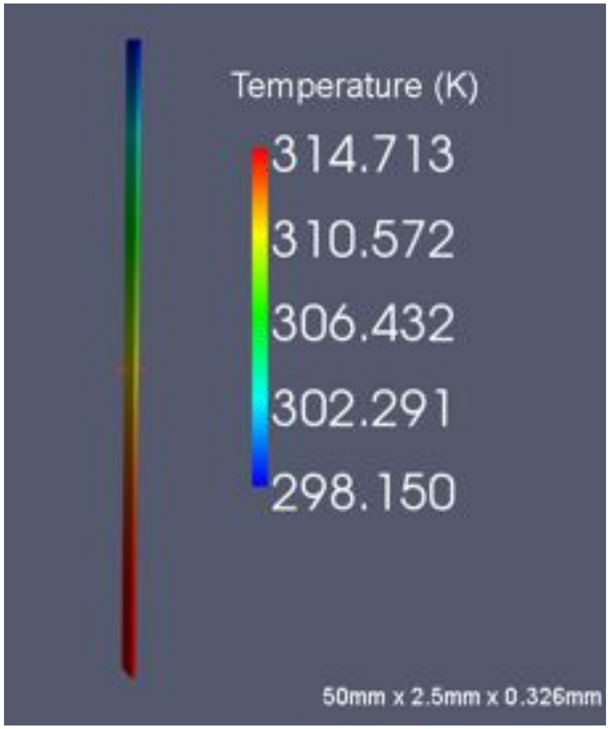
- Displacement-based structural dynamics
- Galerkin finite element
- Geometric and/or material nonlinearity
- Mechanical and thermal stresses

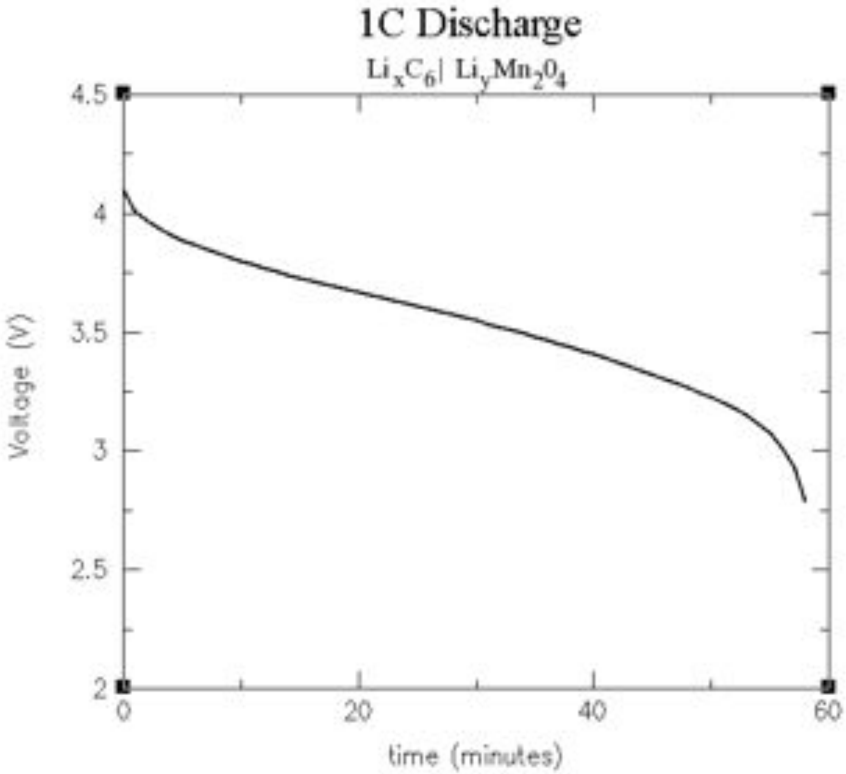




Lithium-Ion Batteries

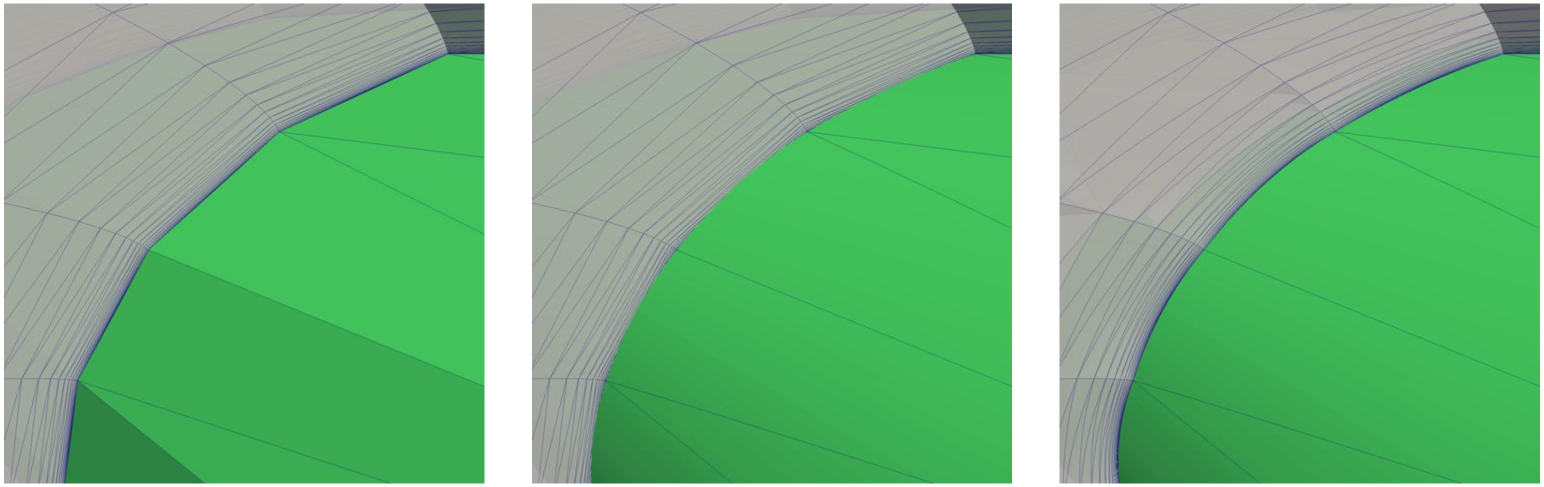
- High-order Galerkin discretization
- Current collectors, electrodes, and separator all modeled





CAPRI Interface for CAD Geometry

- CAD – Watertight geometry definition is required
- Linear mesh – Initial mesh generated using CAD definition
- CAPRI – Higher-order points inserted into linear mesh and projected onto CAD definition via CAPRI interface
- Linear Elasticity – Surface displacements provided by CAPRI are propagated into interior



Petrov-Galerkin

$$\iiint_{\Omega_k} w_i \frac{\partial Q}{\partial t} \partial\Omega_k - \iiint_{\Omega_k} \nabla w_i \cdot \left(F\left(Q\right) - F_v\left(Q\right)\right) \partial\Omega_k +$$

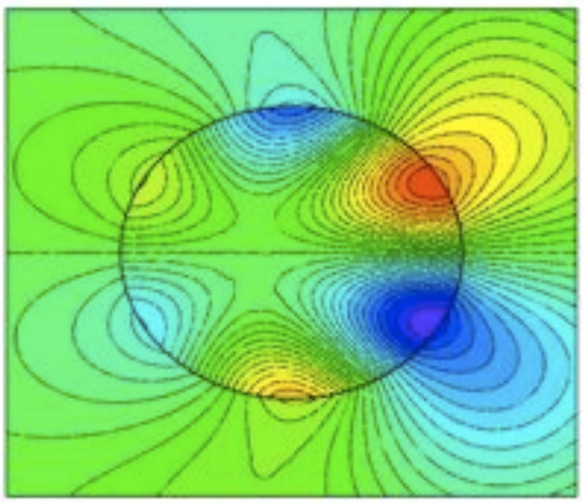
$$\iiint_{\Omega_k} \left\{ \left(\frac{\partial w_i}{\partial x}\left[A\right] + \frac{\partial w_i}{\partial y}\left[B\right] + \frac{\partial w_i}{\partial z}\left[C\right] \right) \left[\tau\right] \left(\frac{\partial Q}{\partial t} + \nabla \cdot \left(F\left(Q\right) - F_v\left(Q\right)\right) \right) \right\} \partial\Omega_k +$$

$$\iint_{\Gamma_k} w_k \left(F\left(Q\right) - F_v\left(Q\right)\right) \cdot \hat{n}\, \partial\Gamma_k = 0$$

- Not widely used for compressible flow: Approximately ten times fewer papers in AIAA conferences compared with discontinuous Galerkin
- Surface integral typically not evaluated because of continuity assumptions between elements. However, assumption not required (e.g. multiple materials in electromagnetics)

Evaluation of Surface Integral

- Typically ignored due to assumed continuity across elements
- Not a required assumption, such as multiple materials or port boundary conditions in electromagnetic applications
  - Create duplicate mesh points along interface
  - Resolve jumps in field parameters using Riemann solver
  - May also be used to easily create discontinuous-Galerkin



Stabilization Matrix

- Eigenvalue-based stabilization is "baseline"

$$\left[\tau\right]^{-1} = \sum_i \left(\left| \frac{\partial N_i}{\partial x}\left[\boldsymbol{A}\right] + \frac{\partial N_i}{\partial y}\left[\boldsymbol{B}\right] + \frac{\partial N_i}{\partial z}\left[\boldsymbol{C}\right] \right| + \frac{\partial N_i}{\partial x_j}\left[\boldsymbol{K}\right]_{jk} \frac{\partial N_i}{\partial x_k} \right)$$

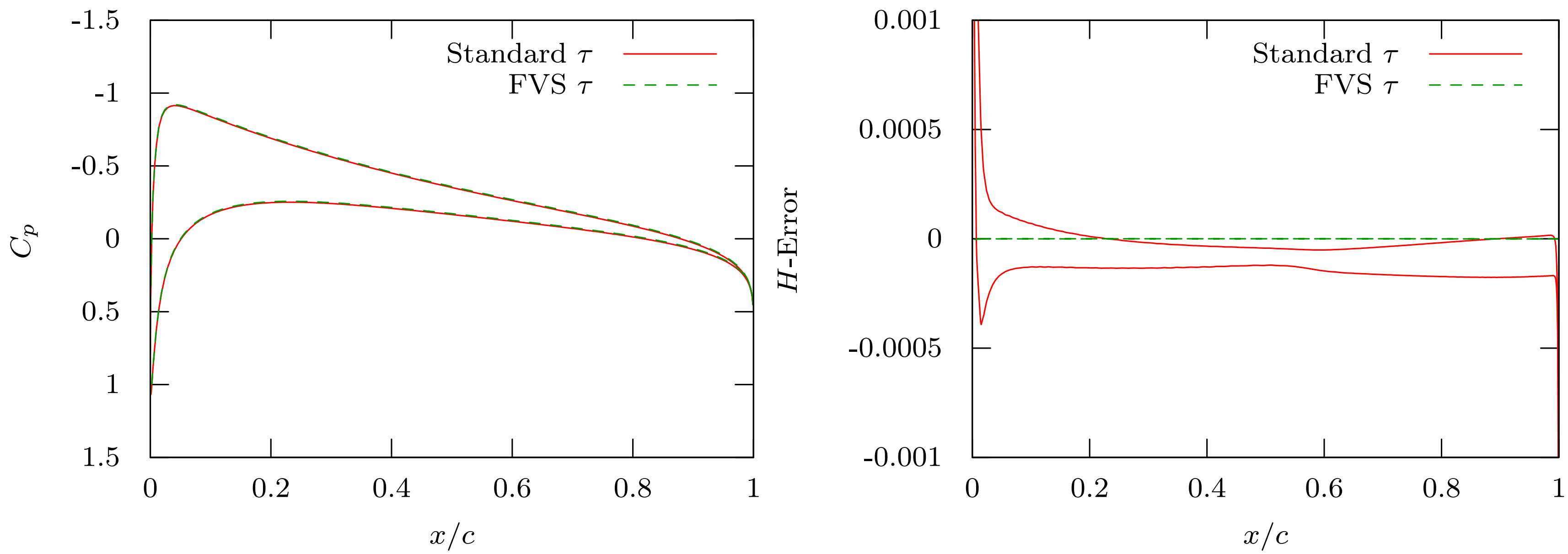
- Inviscid contribution may be defined using concepts from flux-vector splitting $\left|\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{Q}}\right| = \frac{\partial \boldsymbol{F}^+}{\partial \boldsymbol{Q}} - \frac{\partial \boldsymbol{F}^-}{\partial \boldsymbol{Q}}$

- $\frac{\partial \boldsymbol{F}^+}{\partial \boldsymbol{Q}}$ positive eigenvalues: $\frac{\partial \boldsymbol{F}^-}{\partial \boldsymbol{Q}}$ negative eigenvalues

$$\left[\tau\right]^{-1} = \sum_i \left(\frac{\partial}{\partial \boldsymbol{Q}} \left(\left(\boldsymbol{F}^+ - \boldsymbol{F}^- \right) \cdot \left\{ \frac{\partial N_i}{\partial \chi} \right\} \right) + \frac{\partial N_i}{\partial x_j}\left[\boldsymbol{K}\right]_{jk} \frac{\partial N_i}{\partial x_k} \right)$$

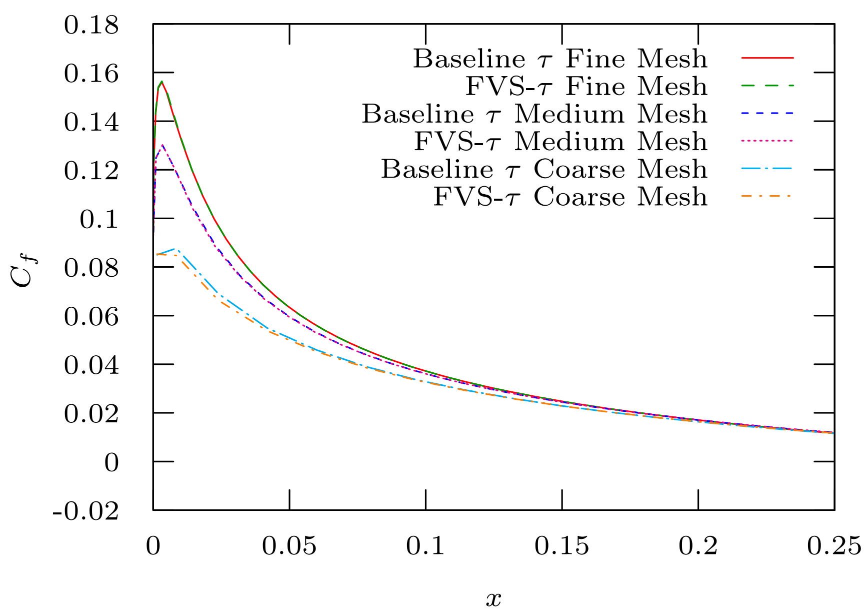
Stabilization Matrix Based on FVS

- Any flux-vector splitting formulation can be used
- Using van Leer FVS can maintain constant total enthalpy

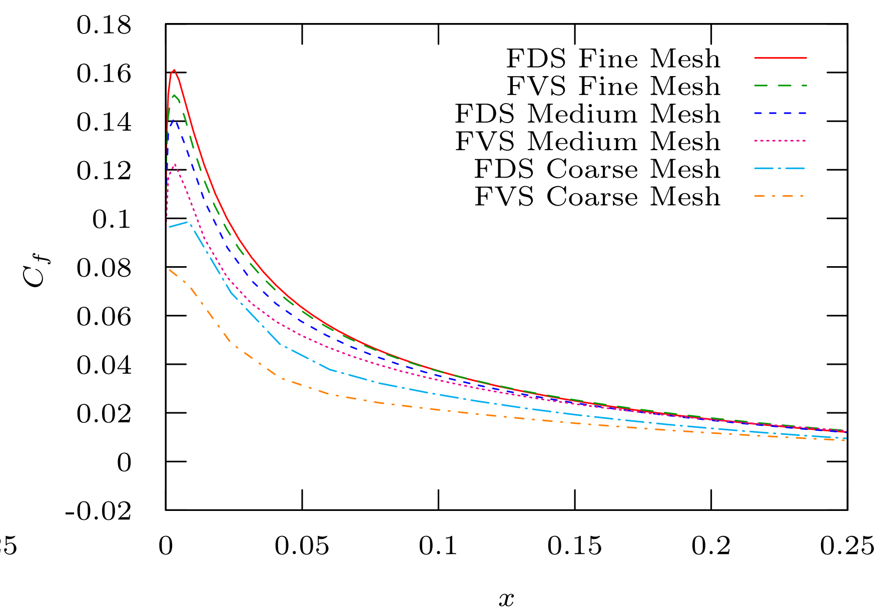


Stabilization Matrix Based on FVS

FVS-based stabilization not inferior to eigenvalue-based stabilization for viscous flows



Petrov Galerkin



Finite Volume

Stabilization Matrix

- Scaling necessary to maintain order property
- Varies as $O(h)$ for inviscid flows, $O(h^2)$ for viscous flow

$$a\frac{\partial u}{\partial x} - \frac{\partial}{\partial x}\left(\nu\frac{\partial u}{\partial x}\right) = a\frac{\partial u}{\partial x} - \frac{\partial}{\partial x}\left(f_v\right)$$

$$\tau^{-1} = \sum_i \left(\left|\frac{\partial N_i}{\partial x}a\right| + \frac{\partial N_i}{\partial x}\nu\frac{\partial N_i}{\partial x}\right)$$

$$\tau \propto \frac{L^2}{\left|aL\right| + \nu}$$

- Cotangent scaling based on Peclet number for systems in multiple dimensions found to be unreliable

Discontinuous Galerkin

$$\iiint_{\Omega_k} w_i \frac{\partial Q}{\partial t} \partial\Omega_k - \iiint_{\Omega_k} \nabla w_i \cdot \left(F\left(Q\right) - F_v\left(Q\right)\right) \partial\Omega_k +$$

$$\iint_{\Gamma_k} w_k \left(F\left(Q\right) - F_v\left(Q\right)\right) \cdot \hat{n}\, \partial\Gamma_k = 0$$

- Solution assumed discontinuous across element interfaces
- Surface integral evaluation using Riemann solver
- Viscous terms handled using symmetric interior penalty method

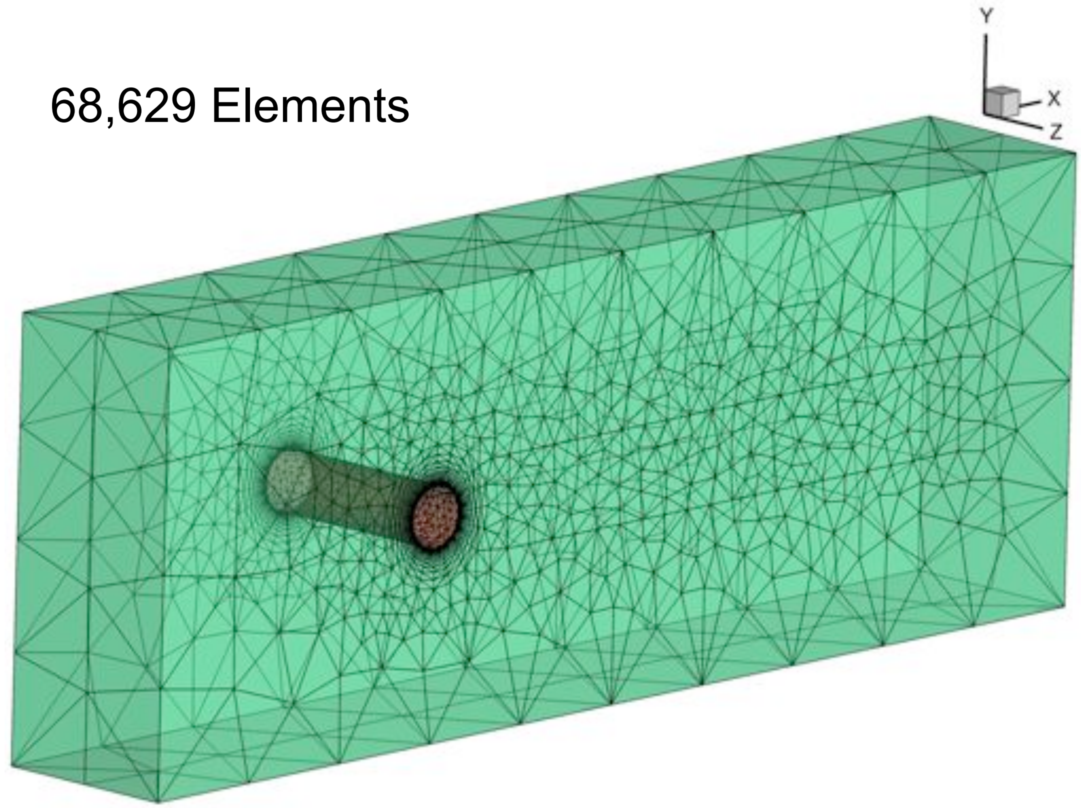
Example Applications

- Three-dimensional cylinder
- Multielement airfoil
- Onera M6
- Trap Wing
- Transonic airfoil

Three-Dimensional Cylinder

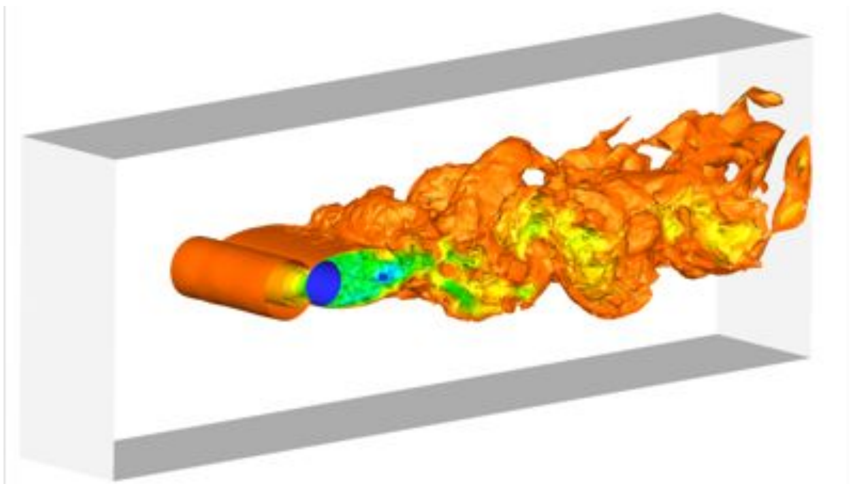
$$M_\infty = 0.2 \qquad \mathrm{Re} = 2580$$

68,629 Elements

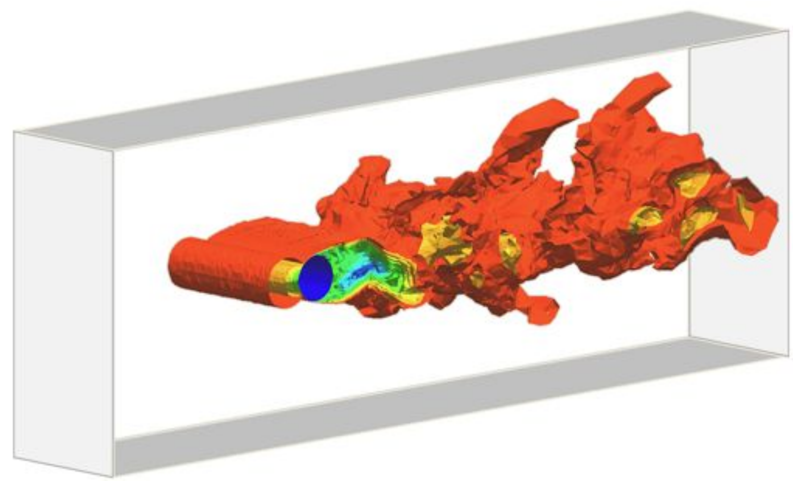


Three-Dimensional Cylinder

$$M_\infty = 0.2 \qquad \mathrm{Re} = 2580$$



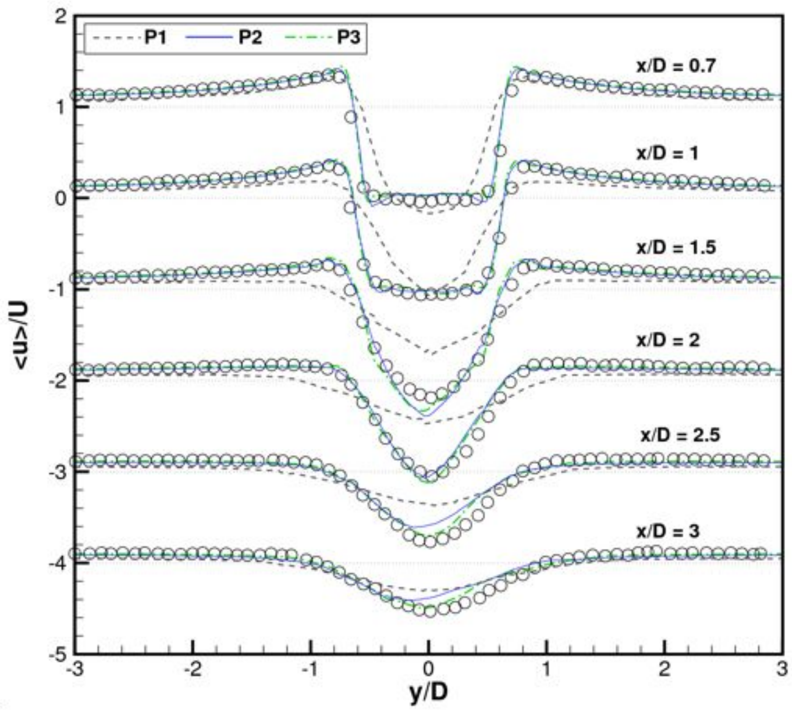
Discontinuous Galerkin P3



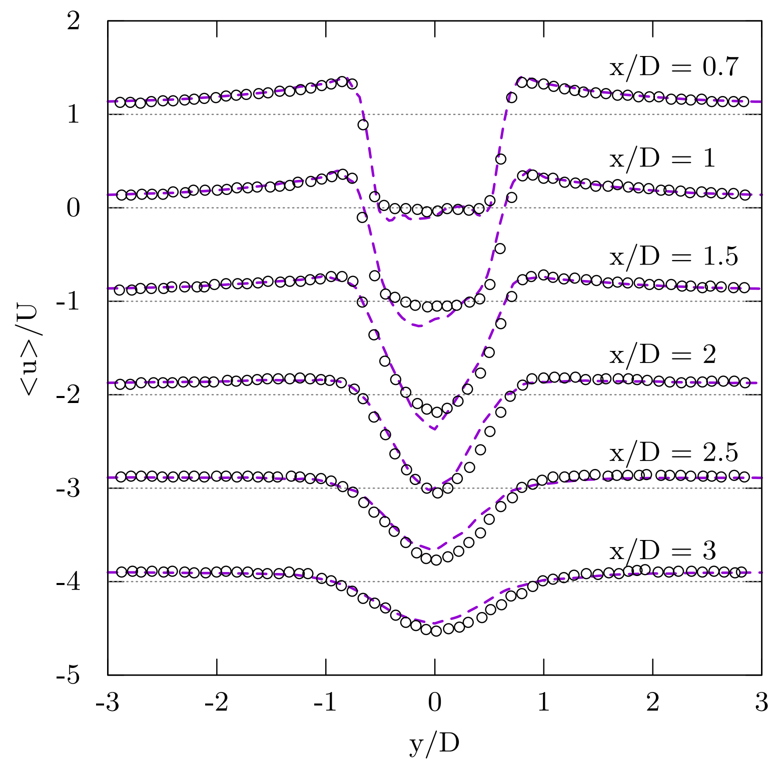
Petrov Galerkin P2

Three-Dimensional Cylinder Time-Averaged U-Velocity Component

$$M_\infty = 0.2 \quad \text{Re} = 2580$$



Discontinuous Galerkin

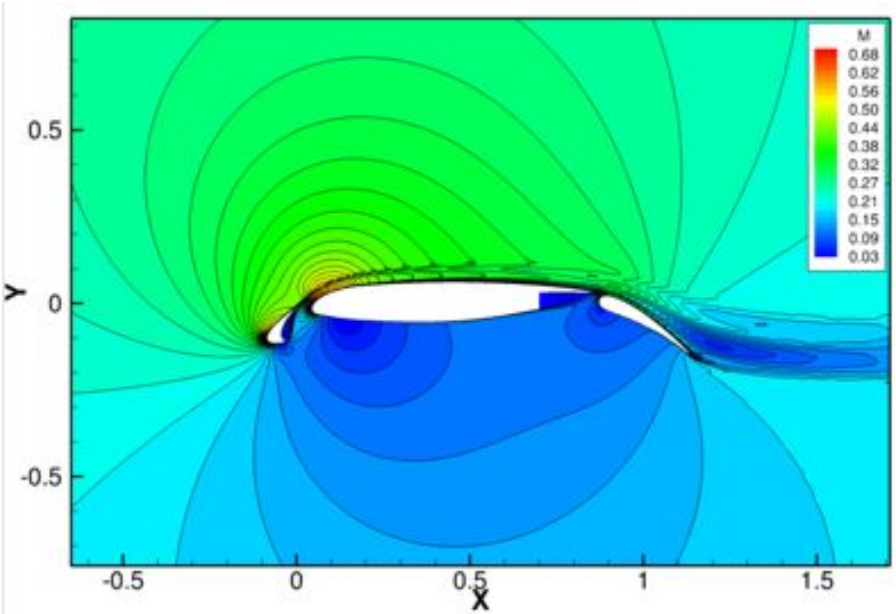


Petrov Galerkin

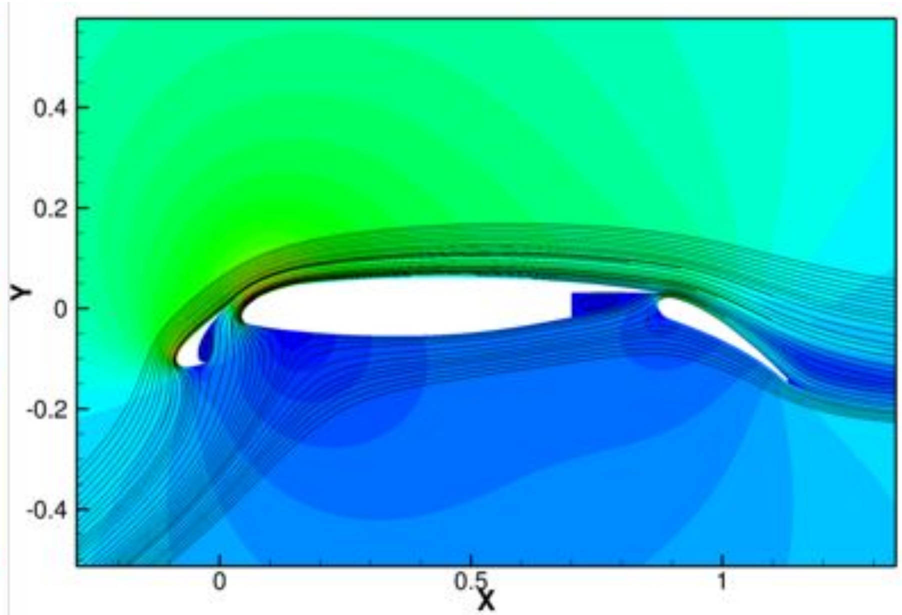
Multielement Airfoil

Douglas 30P-30N

$M_\infty = 0.2 \qquad \alpha = 16^o \qquad \mathrm{Re} = 9{,}000{,}000$



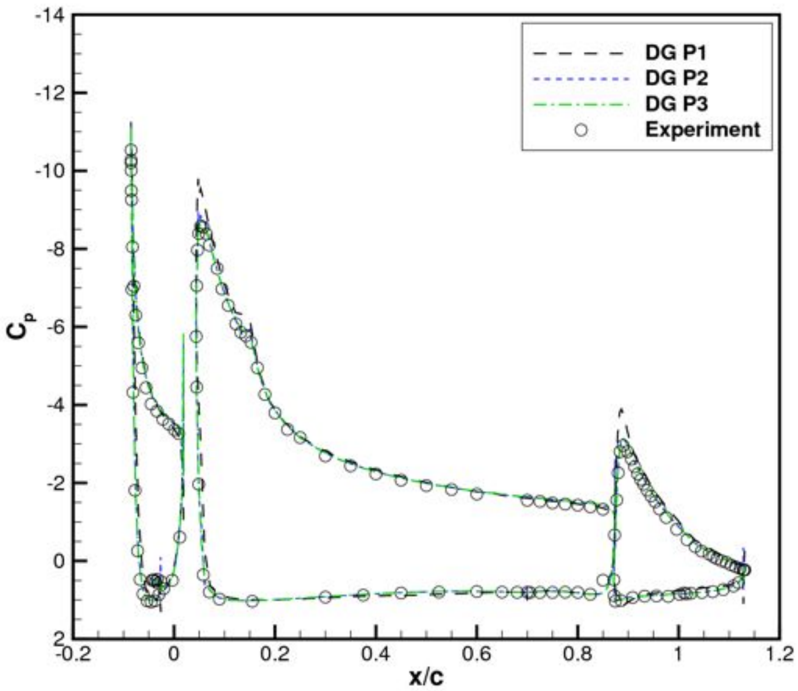
Mach Number Contours



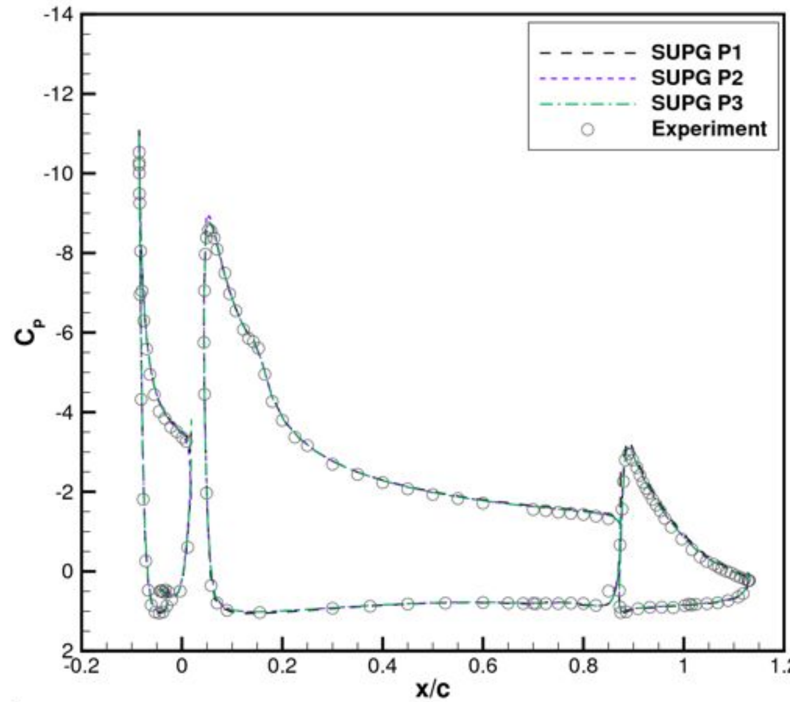
Streamlines

Multielement Airfoil

Pressure Distribution



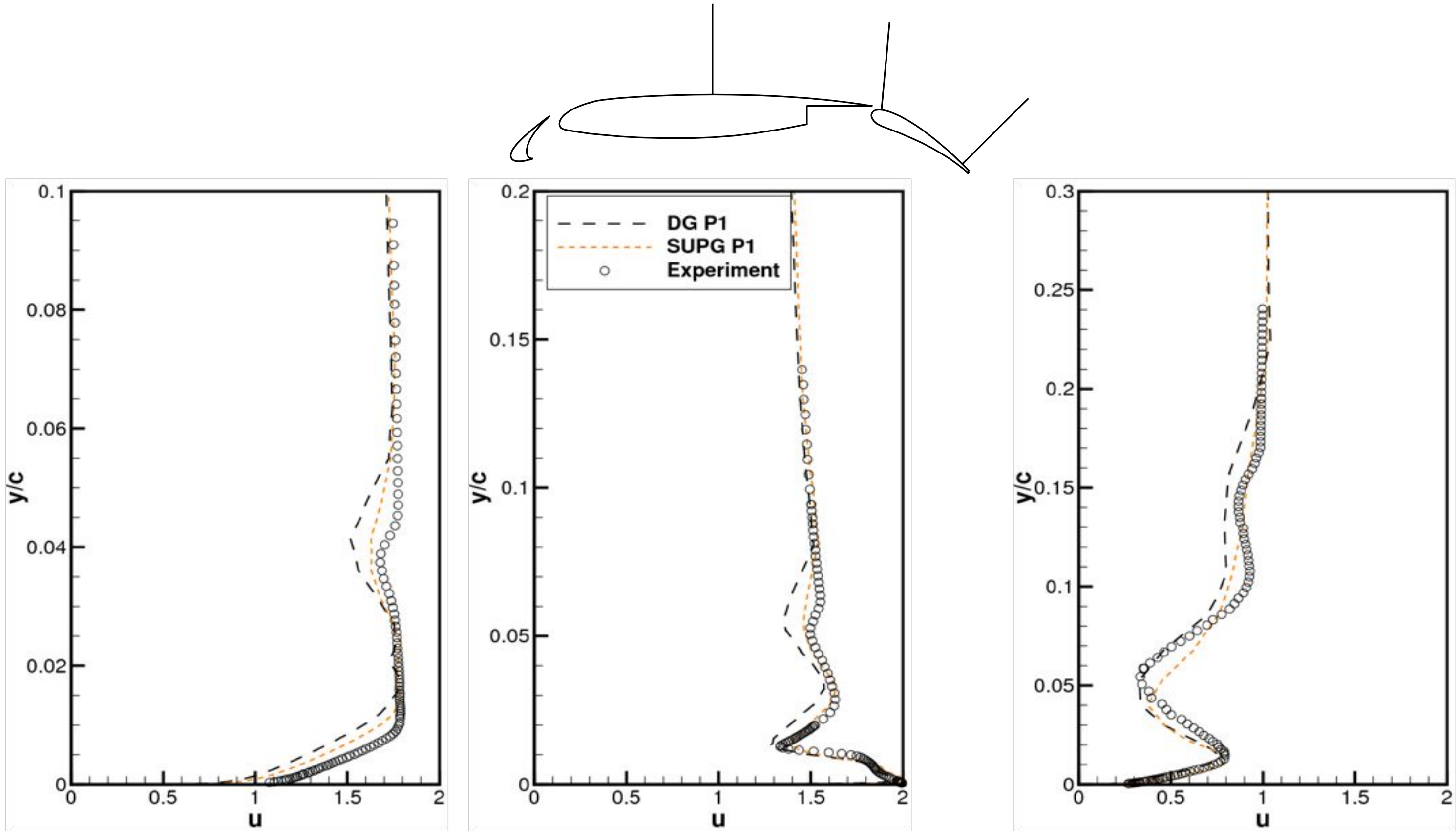
Discontinuous Galerkin



Petrov Galerkin

Multielement Airfoil

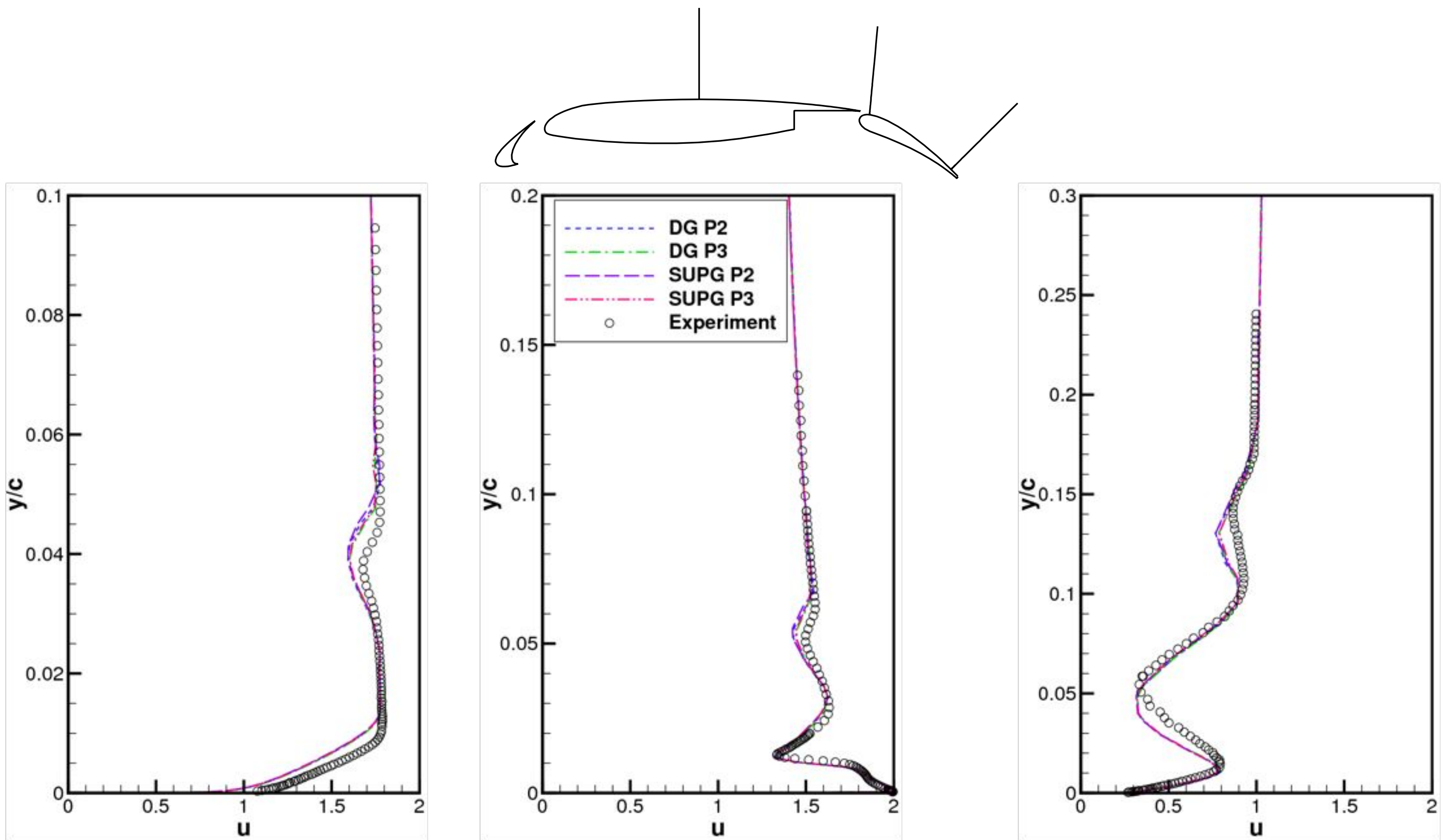
Velocity Profiles Linear Elements



x/c=0.45 (Main) x/c=0.8982 (Flap) x/c=1.1125 (Flap)

Multielement Airfoil

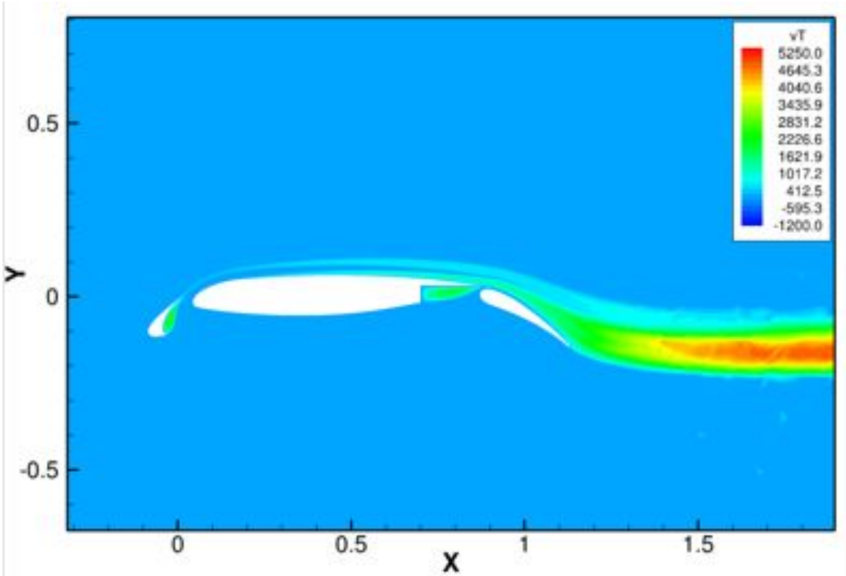
Velocity Profiles Quadratic and Cubic Elements

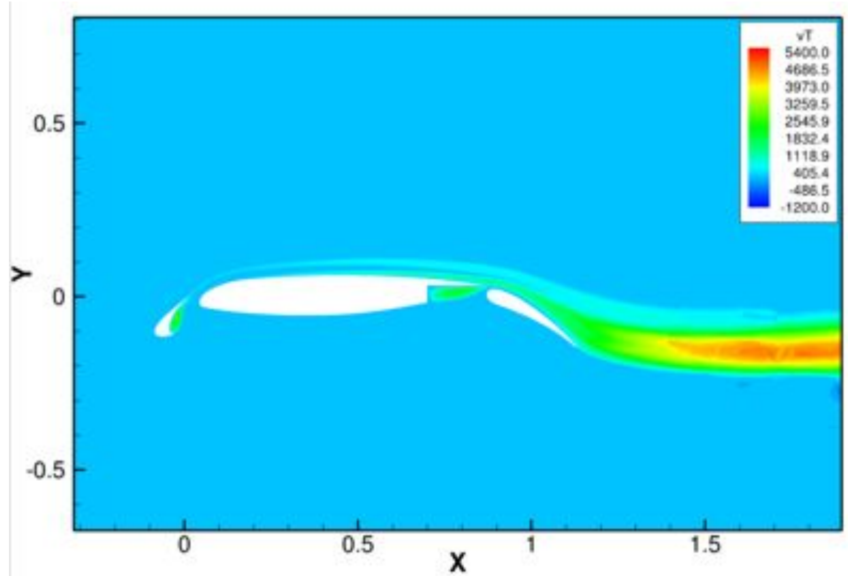


x/c=0.45 (Main) x/c=0.8982 (Flap) x/c=1.1125 (Flap)

Multielement Airfoil

Turbulence Working Variable Fourth Order DG and PG



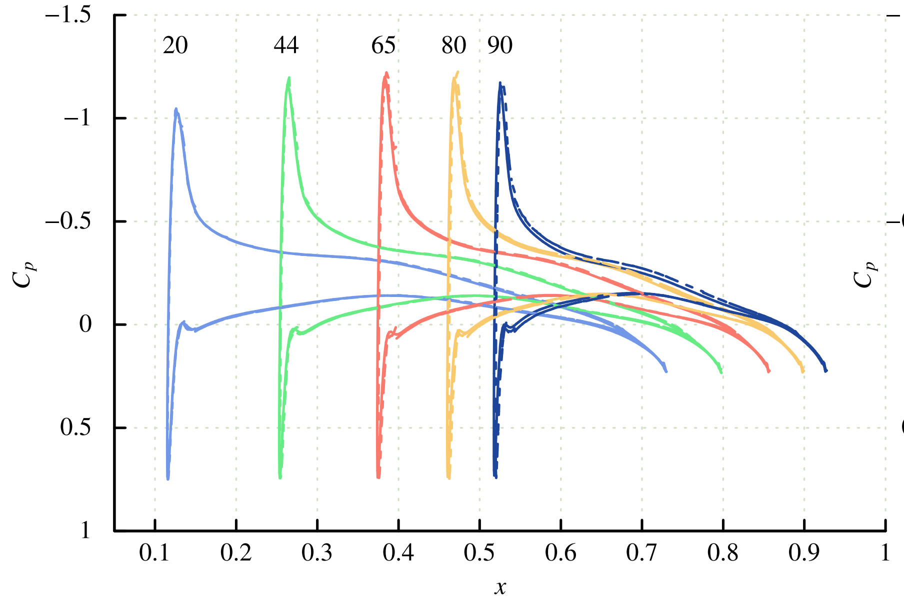


Discontinuous Galerkin

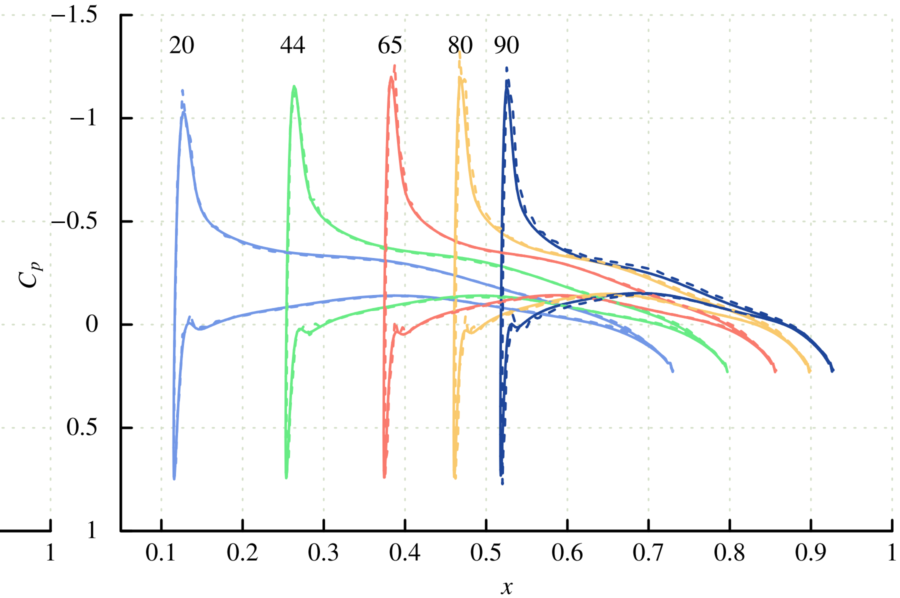
Petrov Galerkin

ONERA M6 Comparisons with CFL3D

$$M_\infty = 0.2 \qquad \alpha = 3.02^o \qquad \mathrm{Re} = 11,270,000$$



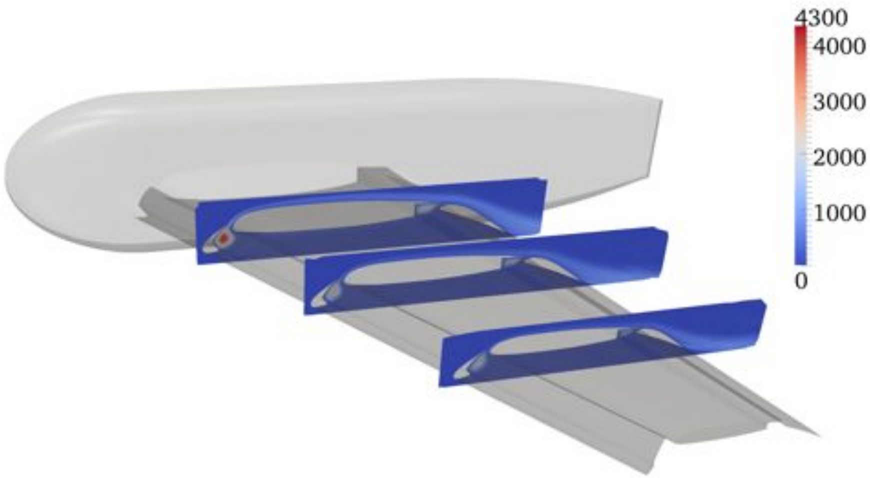
Discontinuous Galerkin P2



Petrov Galerkin P2

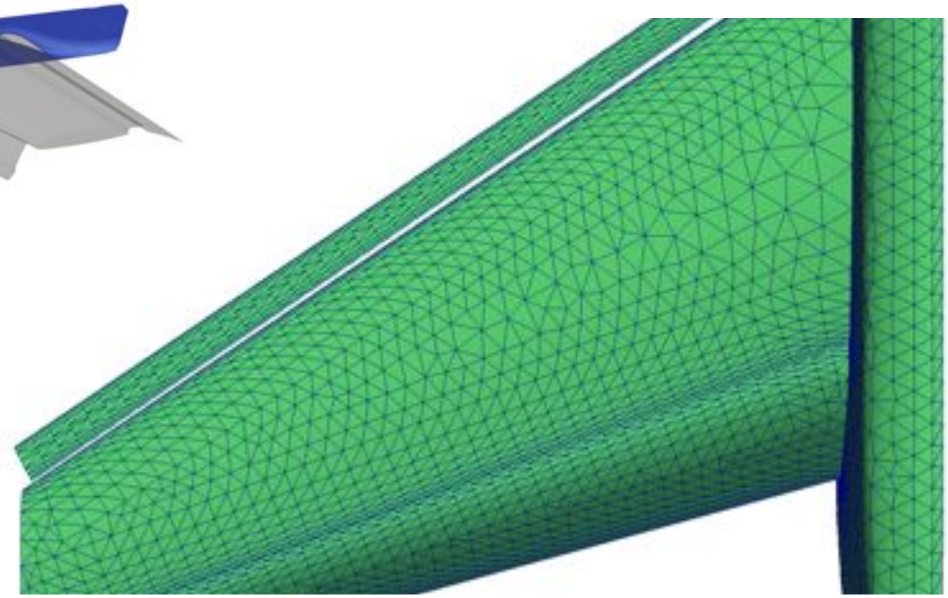
Trap Wing (Petrov-Galerkin Scheme)

$M_\infty = 0.2 \quad \alpha = 12.99^o \quad \mathrm{Re} = 4,300,000$



Turbulence Working Variable

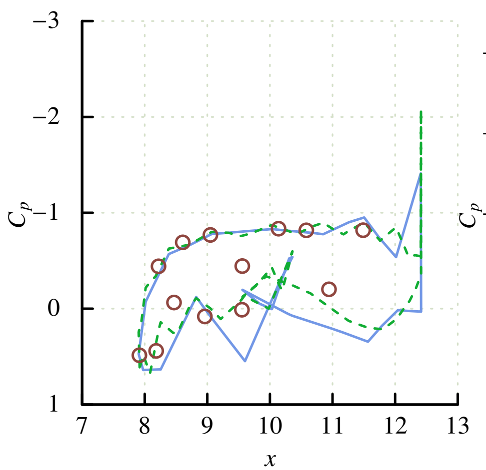
1,126,835 Elements
194,370 DOF P1
1,126,835 DOF P2



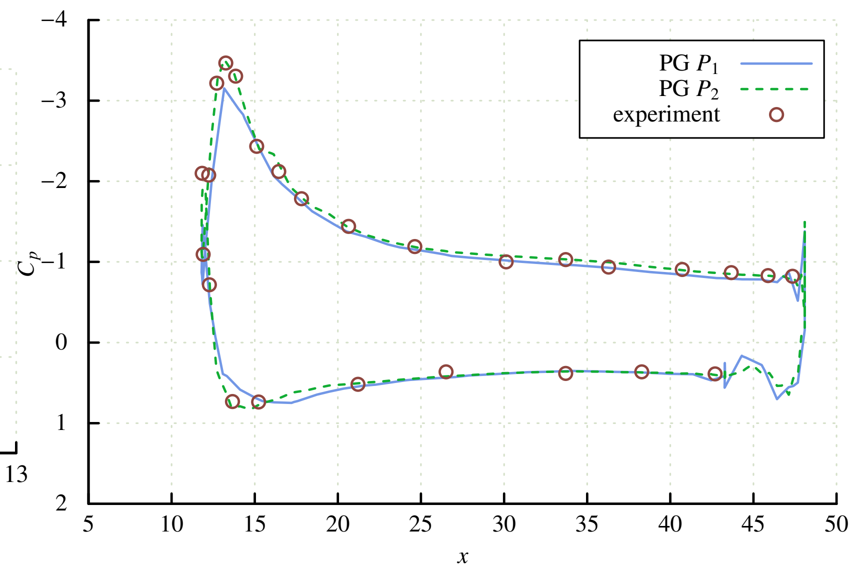
Trap Wing (Petrov Galerkin)

$M_\infty = 0.2 \quad \alpha = 12.99^o \quad \mathrm{Re} = 4,300,000$

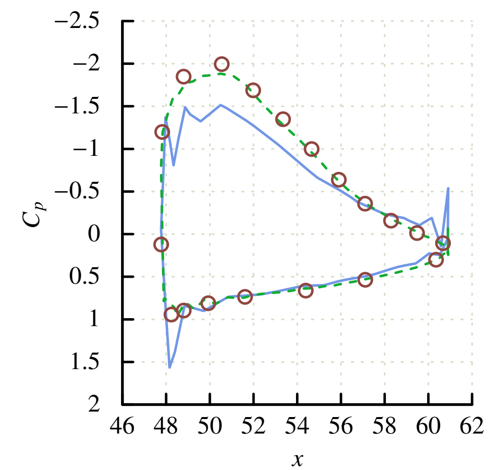
x/c=17%



Slat



Main Element

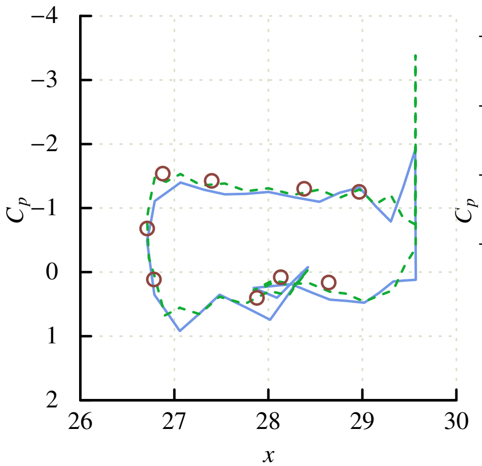


Flap

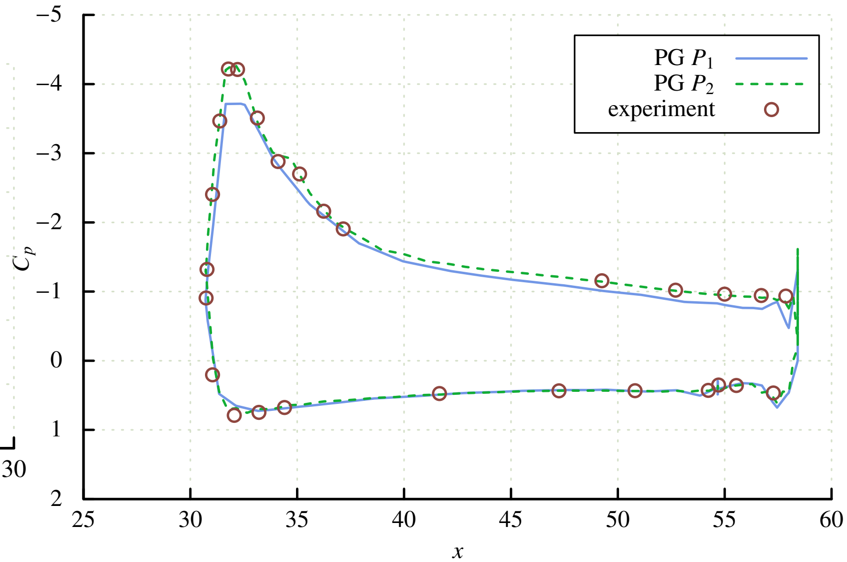
Trap Wing (Petrov Galerkin)

$M_\infty = 0.2 \quad \alpha = 12.99^o \quad \mathrm{Re} = 4,300,000$

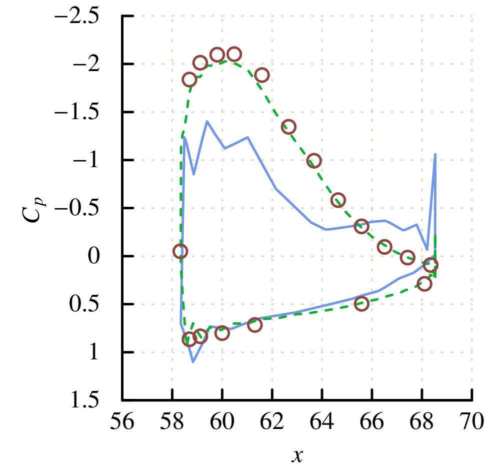
x/c=50%



Slat



Main Element

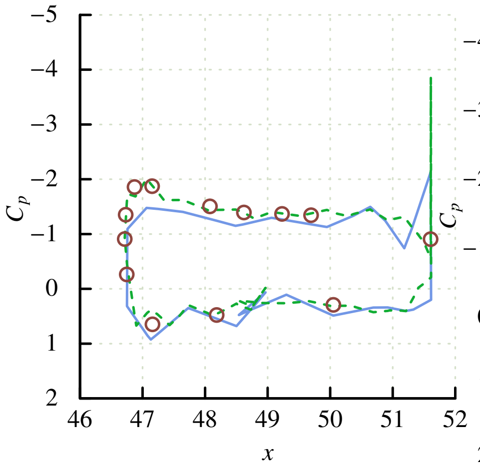


Flap

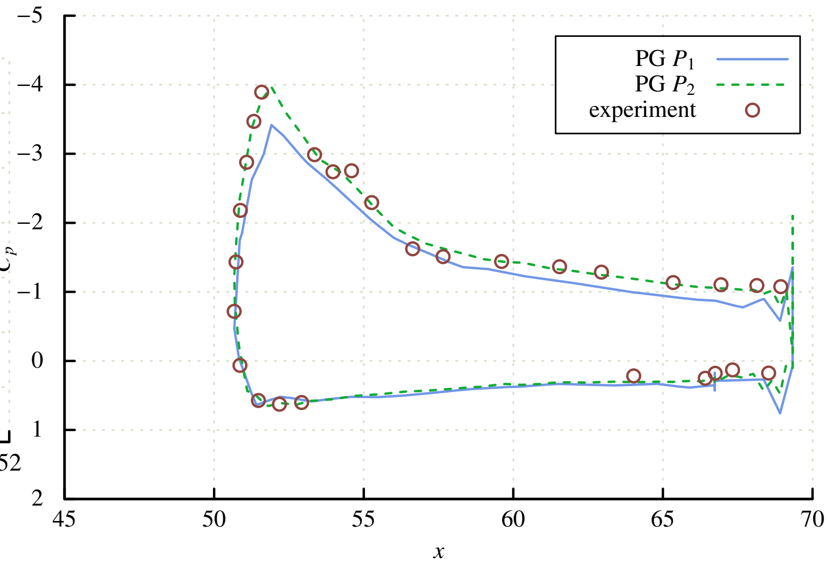
Trap Wing (Petrov Galerkin)

$$M_\infty = 0.2 \quad \alpha = 12.99^o \quad \text{Re} = 4,300,000$$

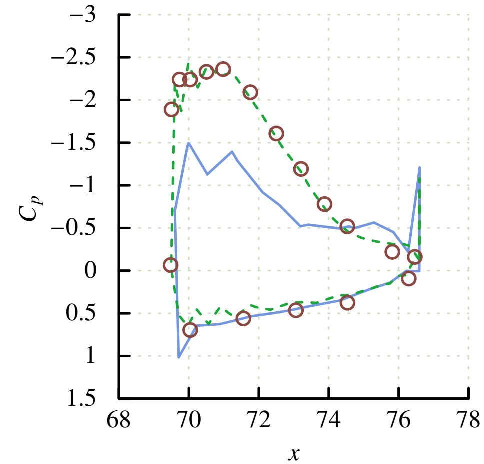
x/c=85%



Slat



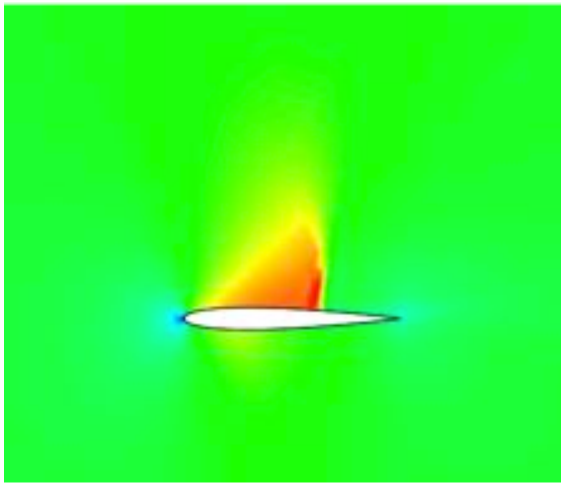
Main Element



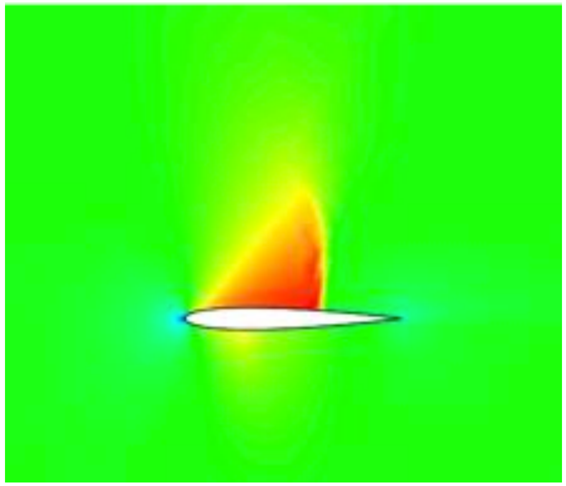
Flap

Transonic NACA 0012

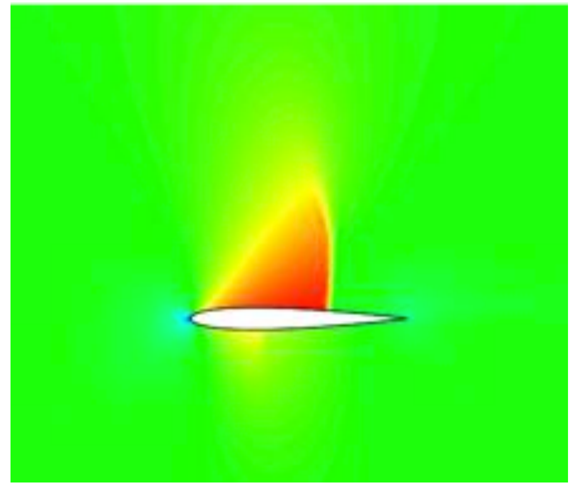
$M_\infty = 0.8 \qquad \alpha = 1.25^o$



Finite Volume



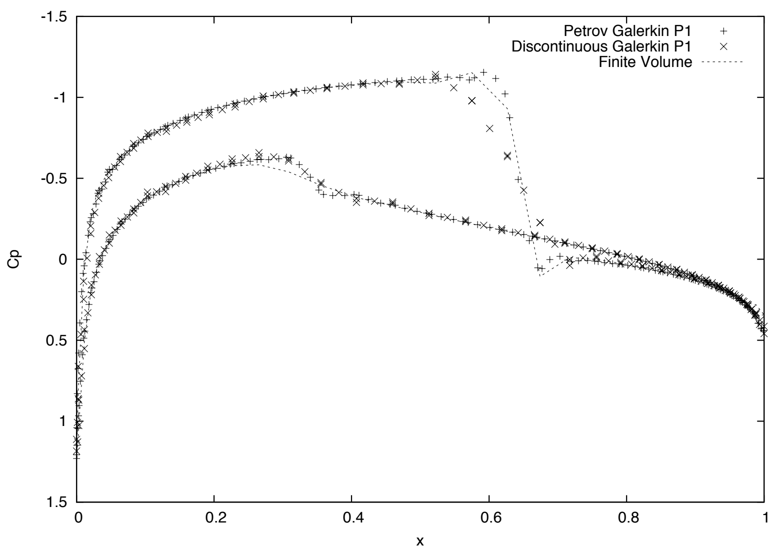
Petrov Galerkin P1



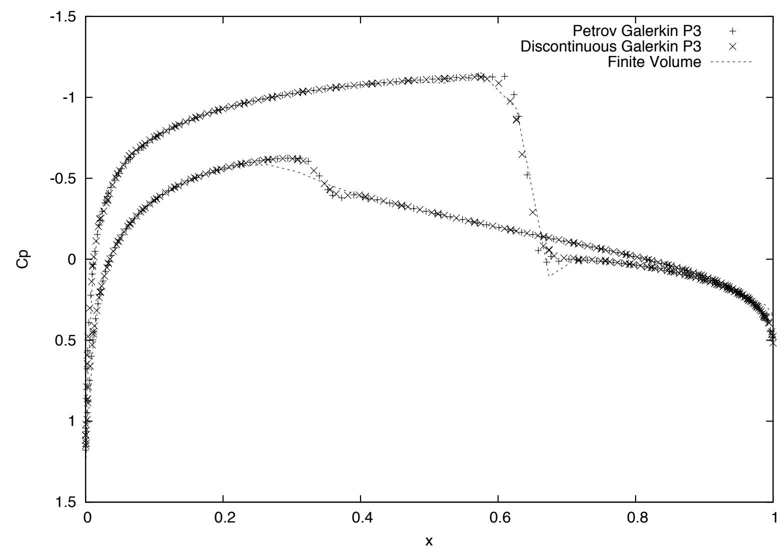
Petrov Galerkin P2

Transonic NACA 0012

$$M_\infty = 0.8 \qquad \alpha = 1.25^o$$



Linear Elements

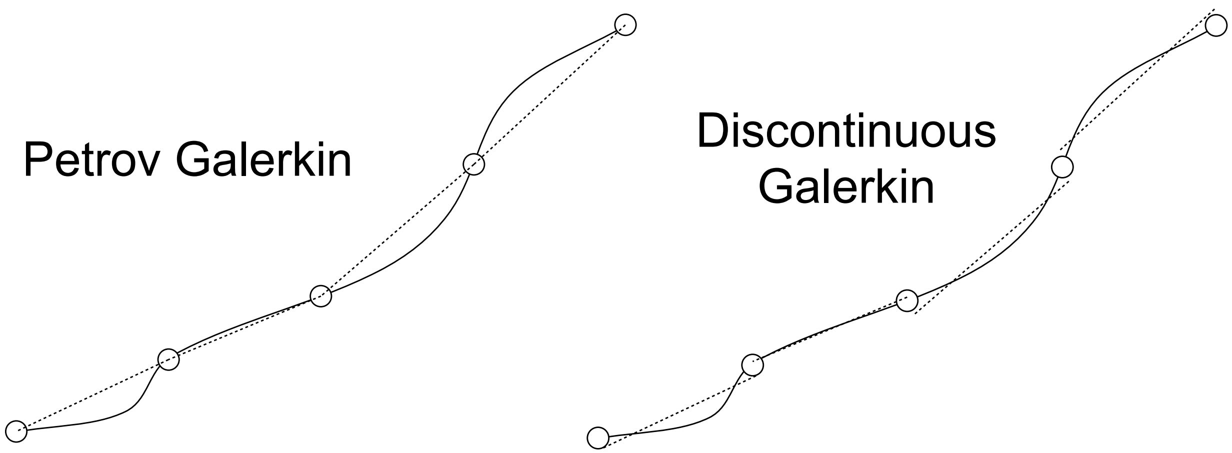


Cubic Elements

- Preliminary results adding switched viscous-like term
- Discontinuous Galerkin and Petrov-Galerkin terms not the same
- Don't make a general conclusion as to shock capturing!

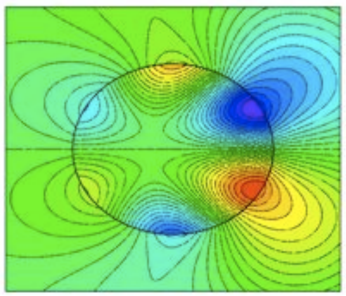
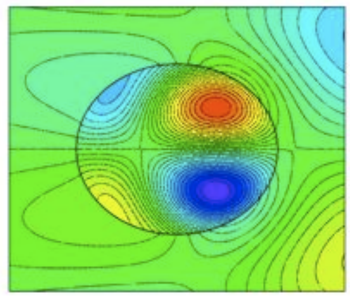
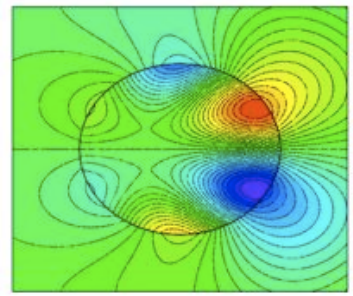
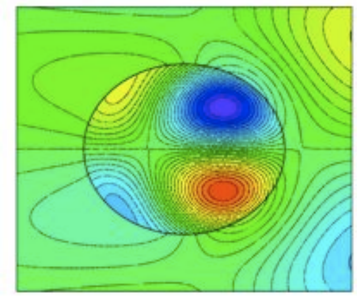
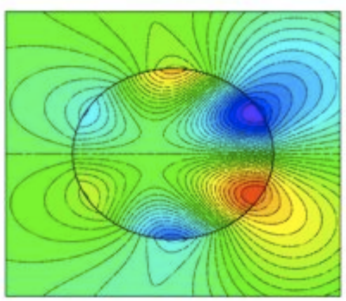
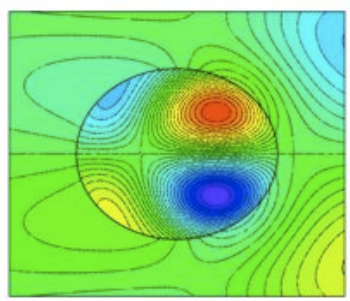
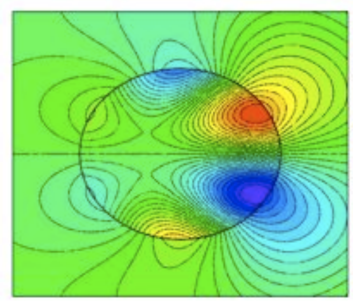
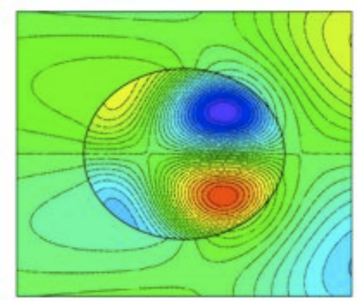
Which Scheme to Use?

- Intuition would indicate that there is an accuracy advantage on a given mesh for discontinuous Galerkin



- However, new degrees of freedom are created with discontinuities between elements
- Do the benefits outweigh the cost?

2D Time-Domain Scattering from Dielectric Cylinder

			
Exact T=0	Exact T=Pi/2	Exact T = Pi	Exact T = 3Pi/4
			
Petrov-Galerkin			

2D Time-Domain Scattering from Dielectric Cylinder (P1 Elements)

DOF	L1 Error	L1 Slope	L2 Error	L2 Slope
369	2.52E-01		2.37E-01	
1348	6.00E-02	2.22	5.60E-02	2.23
5153	1.49E-2	2.08	1.39E-02	2.07

Petrov Galerkin

DOF	L1 Error	L1 Slope	L2 Error	L2 Slope
1824	2.52E-01		1.42E-01	
7314	6.00E-02	2.22	3.35E-02	2.08
29,376	1.49E-2	2.08	8.30E-03	2.01

Discontinuous Galerkin

2D Time-Domain Scattering from Dielectric Cylinder (P2 Elements)

DOF	L1 Error	L1 Slope	L2 Error	L2 Slope
1345	1.03E-02		1.05E-02	
5133	1.23E-03	3.28	1.21E-03	3.34
20,097	1.50E-4	3.13	1.51E-04	3.10

Petrov Galerkin

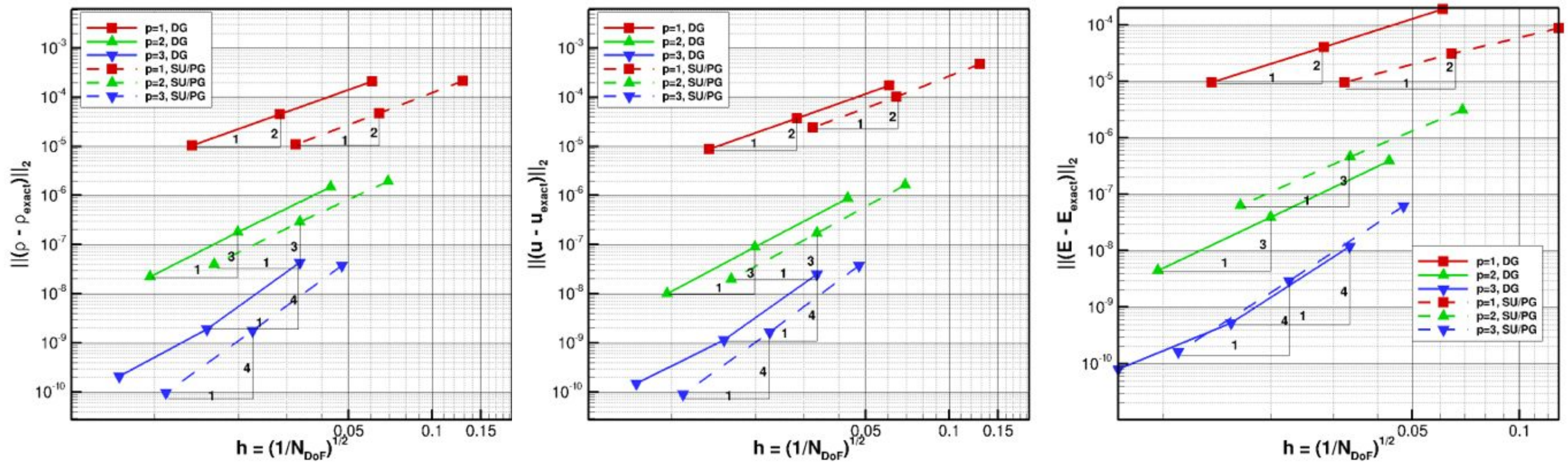
DOF	L1 Error	L1 Slope	L2 Error	L2 Slope
3648	1.00E-02		5.83E-03	
14,628	1.20E-03	3.06	6.69E-04	3.12
58,752	1.48E-4	3.01	8.42E-05	2.98

Discontinuous Galerkin

Which Scheme to Use?

Error in Manufactured Solution Per DOF

(Glasby et al. AIAA 2013-0692)

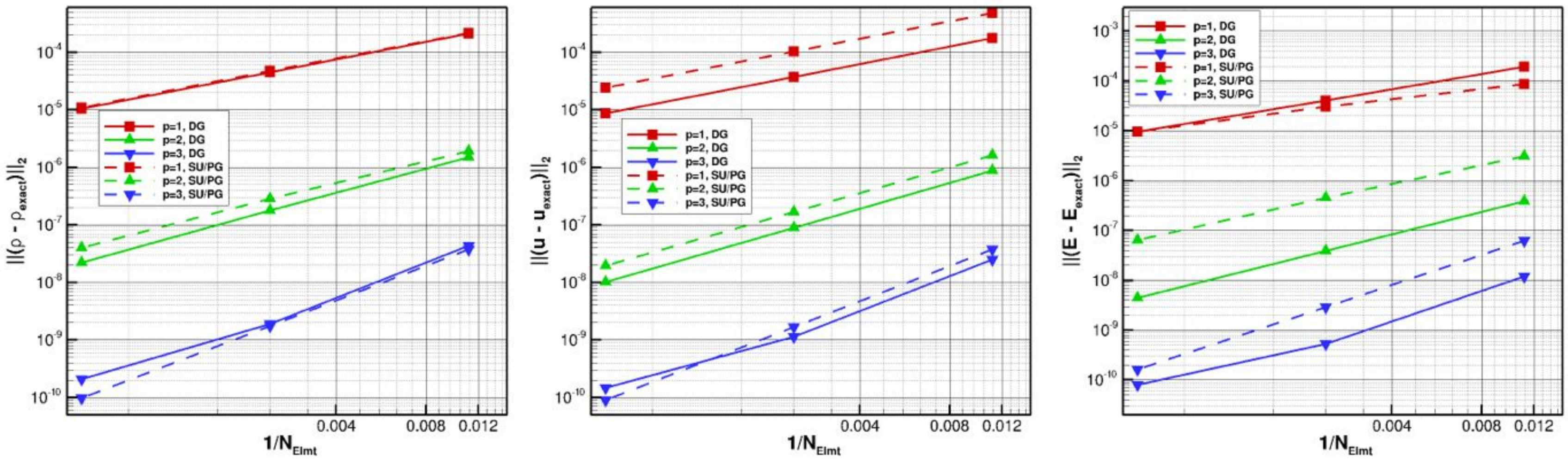


Petrov Galerkin exhibits lower error per degree of freedom

Which Scheme to Use?

Error in Manufactured Solution Per Element

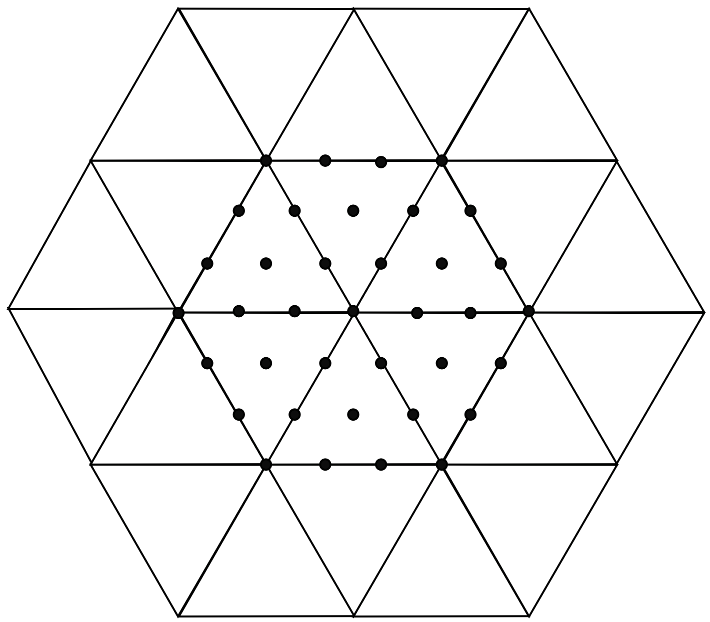
(Glasby et al. AIAA 2013-0692)



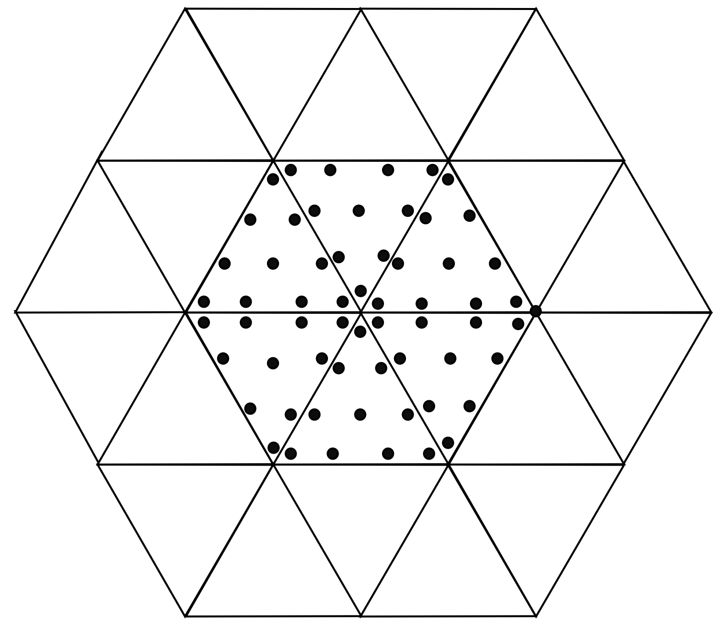
- Discontinuous Galerkin exhibits lower error per element
- Results are for low Reynolds number MMS but typical for Euler, Navier Stokes, and Electromagnetic application

Which Scheme to Use?

Estimating DOF and Number of Non Zero Entries in Matrix



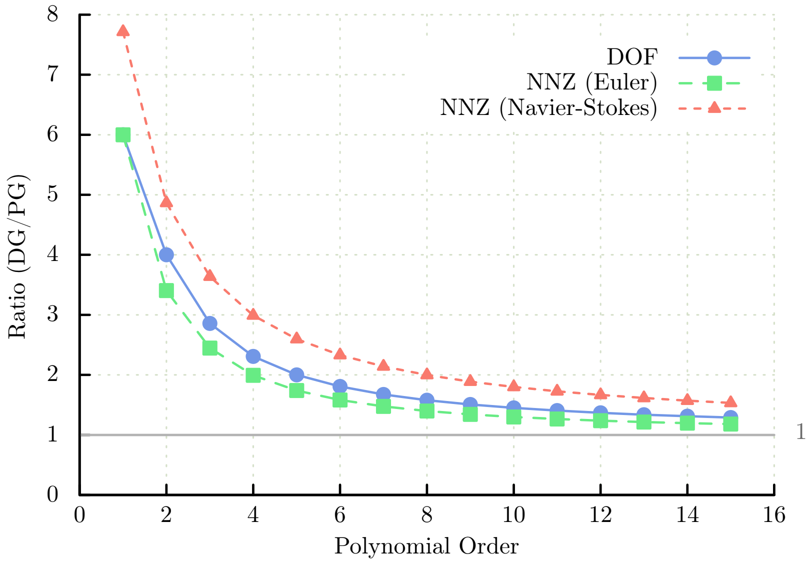
Petrov Galerkin



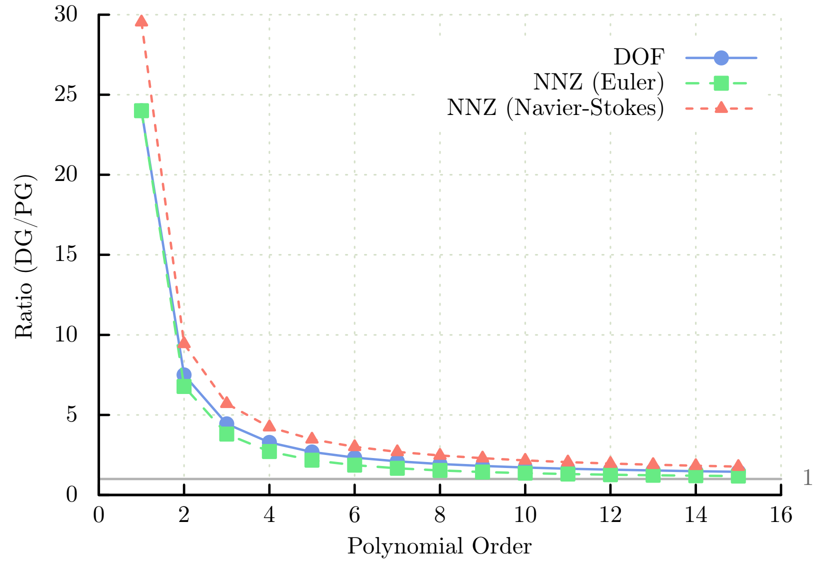
Discontinuous Galerkin

Which Scheme to Use?

Estimating Ratio of DOF and Number of Non Zero Entries in Matrix Between PG and DG



Two Dimensions
(Triangles)



Three Dimensions
(Tetrahedrons)

Which Scheme to Use?

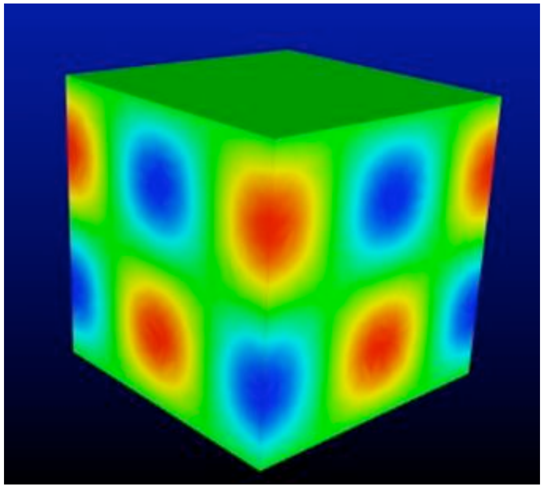
DOF and Number of Non Zero Entries in Matrix
Cubic Volume Subdivided into Elements

	Tetrahedron		Hexahedron		Prismatic	
	DOF	NNZ	DOF	NNZ	DOF	NNZ
P1	22.16	19.8	7.53	5.74	11.35	9.42
P2	7.19	6.20	2.92	2.14	4.02	3.15

- Discontinuous Galerkin compares more favorably for hexahedrons, worst case is for tetrahedrons
- Higher DOF and NNZ translates into more memory, more work per iteration, and generally more iterations (search directions for GMRES)
- At low-to-moderate orders, Petrov Galerkin appears to have advantages over discontinuous Galerkin
- Higher orders may favor discontinuous Galerkin

Which Scheme to Use?

Resonant Cavity: 1.85 GHz
Magnetic Field Intensity



- Advancing fixed number of time steps to compare efficiencies
- Independent of equation set

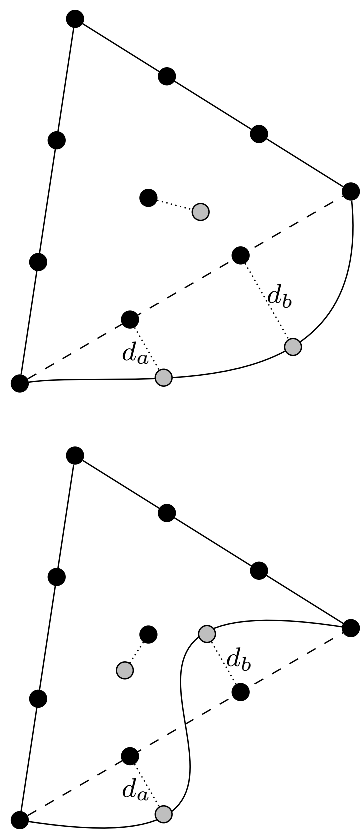
Ratio of time for fixed number of time steps		
	DOF Ratio	Actual Time Ratio
Linear	22.16	27
Quadratic	7.19	12

(DG required more search directions)

Which Scheme to Use?

- Many factors effect the accuracy of a given scheme so it is difficult, if not impossible, to make a broad conclusion
  - Boundary condition type / order / weak v. strong
  - Basis functions and quadrature rules
  - Solution and comparison variables
  - Flux function / stabilization matrix
- While number of stabilization matrices for PG is approximately the same as the number of flux evaluations for DG, stabilization matrix approximately twice as expensive
- Higher DOF translates to more search directions
- **Very high order is unclear but work advantages for PG at low-to-moderate orders are difficult for DG to overcome**

Curved Elements



- Isoparametric mapping requires more terms in (r,s) to obtain full polynomial representation in (x,y)
- Deficiency in higher-order terms
- Ciarlet's theory provides guidance as to how much an element can deviate from linear and still maintain order
- Edges for cubic elements must be order h**3 but geometry varies as h**2
- Verifiable with either discontinuous-Galerkin or Petrov-Galerkin method
- Also verifiable using downscaling

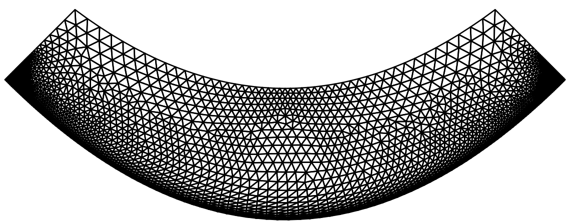
Curved Elements

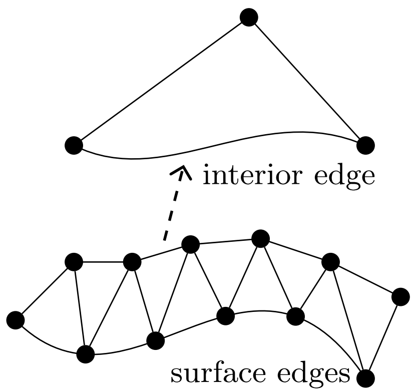
Order of Accuracy for Polynomial Curving of Elements
Using Downscaling

		Polynomial for Curving Edges		
	Mesh Reduction	Quartic (4)	Cubic (3)	Quad. (2)
P4	h**2	3	4	5
	h**3	4	5	5
	h**4	5	5	5
P3	h**2		3	4
	h**3		4	4
P2	h**2			3

Curved Elements

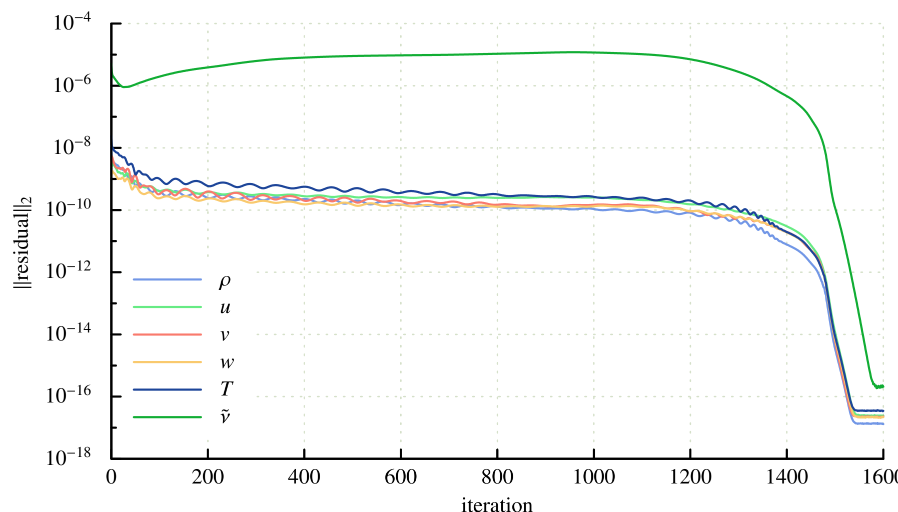
- Ciarlet's theorems assume element shape remains the same as the mesh is refined
- Uniform refinement changes shapes of elements. Experiments indicate that uniform refinement yields correct order property
- Mesh movement can, however, create problems
- For manufactured solution on parabolic domain, algebraic mesh movement failed to recover proper order while linear elasticity was successful





Ongoing Work

- Modifications to time-stepping scheme
  - Linear ramp of CFL number not robust or efficient
  - Switched Evolution Relaxation (SER) type schemes appear favorable



- Continue development of shock sensors
- DES / LES
- Tight integration between disciplines

Summary

- Developing framework for high-order finite element solutions to multidisciplinary problems
- Discontinuous-Galerkin and Petrov-Galerkin methods work well for inviscid, laminar, and turbulent flows
- Petrov-Galerkin method appears to be a much overlooked method for low-to-moderate orders of accuracy
- Curved elements need consideration but order property can be maintained as long as higher-order curves are not created during mesh movement