Stanford Workshop on Error Estimation, Uncertainty, and Reliability

Aug. 20-22, 2005

A-Posteriori Error Estimation for Godunov Finite Volume Methods

Tim Barth

Exploration Technology Directorate

NASA Ames Research Center

Moffett Field, California 94035-1000 USA

barth@nas.nasa.gov

Additional Information

`http://science.nas.nasa.gov/~barth/stanford_workshop/*`

- These slides:

  `fv_error_estimation.pdf`

- Related lecture notes (Chapter 3):

  `lecture_notes.pdf`

Objectives

- Construct the (exact) non-perturbative error representation formula for *user specified* functionals for the class of high order Godunov finite volume methods including
  - MUSCL (van Leer)
  - TVD (Harten)
  - UNO (Harten-Osher-Engquist-Chakravarthy)
  - ENO (Harten-Engquist-Osher)

Objectives

- Construct the (exact) non-perturbative error representation formula for *user specified* functionals for the class of high order Godunov finite volume methods including
  - MUSCL (van Leer)
  - TVD (Harten)
  - UNO (Harten-Osher-Engquist-Chakravarthy)
  - ENO (Harten-Engquist-Osher)
- Devise computable error estimates

Objectives

- Construct the (exact) non-perturbative error representation formula for *user specified* functionals for the class of high order Godunov finite volume methods including
  - MUSCL (van Leer)
  - TVD (Harten)
  - UNO (Harten-Osher-Engquist-Chakravarthy)
  - ENO (Harten-Engquist-Osher)
- Devise computable error estimates
- Demonstrate sharpness of the estimates

Objectives

- Construct the (exact) non-perturbative error representation formula for *user specified* functionals for the class of high order Godunov finite volume methods including
  - MUSCL (van Leer)
  - TVD (Harten)
  - UNO (Harten-Osher-Engquist-Chakravarthy)
  - ENO (Harten-Engquist-Osher)
- Devise computable error estimates
- Demonstrate sharpness of the estimates
- Use the estimates in an adaptive meshing procedure

Higher Order Godunov FV Method

Higher order Godunov formulation in operator composition form

$$u_0^{n+1} = \Pi_0 \cdot E(\tau) \cdot R_q^0(\cdot) u_0^n$$

- R_q^0, q-th order reconstruction operator
- $E(\tau)$, evolution in the small
- Π_0, cell averaging operator

$$u_{0,K} = \Pi_0 u|_K = \frac{1}{\text{meas}(K)} \int_K u \, da$$

Additional requirements

- $R_q^0(x)\Pi_0 u = u(x) + O(h^{q+1})$ whenever u is smooth
- $\Pi_0|_K R(x) u_0 = u_0|_K, \ \forall K \in \mathcal{T}$ yielding a diagonal mass matrix

The Basic Idea

Observations:

1. Godunov finite volume (FV) methods and the discontinuous Galerkin (DG) methods both utilize discrete broken space, $\mathcal{V}_q^{\mathrm{B}}$, approximation

The Basic Idea

Observations:

1. Godunov finite volume (FV) methods and the discontinuous Galerkin (DG) methods both utilize discrete broken space, $\mathcal{V}_q^{\mathrm{B}}$, approximation

2. Godunov FV methods can be written abstractly as a Petrov-Galerkin variant of the Discontinuous Galerkin (DG) method: Find $u \in \mathcal{V}_0^{\mathrm{B}}$ such that

$$B_{\mathrm{DG}}(R_q^0 u, v) = F(v), \quad \forall v \in \mathcal{V}_0^{\mathrm{B}}, \quad R_q^0 : \mathcal{V}_0^{\mathrm{B}} \mapsto \mathcal{V}_q^{\mathrm{B}}$$

The Basic Idea

Observations:

1. Godunov finite volume (FV) methods and the discontinuous Galerkin (DG) methods both utilize discrete broken space, $\mathcal{V}_q^{\mathrm{B}}$, approximation

2. Godunov FV methods can be written abstractly as a Petrov-Galerkin variant of the Discontinuous Galerkin (DG) method: Find $u \in \mathcal{V}_0^{\mathrm{B}}$ such that

$$B_{\mathrm{DG}}(R_q^0 u, v) = F(v), \quad \forall v \in \mathcal{V}_0^{\mathrm{B}}, \quad R_q^0 : \mathcal{V}_0^{\mathrm{B}} \mapsto \mathcal{V}_q^{\mathrm{B}}$$

Consequence:

- Any *a posteriori* error estimation theory for $B_{\mathrm{DG}}(\cdot,\cdot)$ that assumes general (unequal) broken trial and test spaces applies directly to Godunov FV methods

Error Representation of Functionals

Objective: Estimate the error

$$J(u) - J(u_h)$$

where $J(\cdot)$ is a given functional.

Related Preceding Work (partial listing):

- Eriksson, Estep, Hansbo, Johnson
- Becker and Rannacher
- Süli and Houston
- Oden and Prudhomme
- Giles and Pierce
- Barth and Larson

Coping with Nonlinearity

Mean-value linearized forms:

$$\begin{aligned} B(u,v) &= B(R_q^0 u_0, v) + \overline{B}(u - R_q^0 u_0, v) \quad \forall\, v \in \mathcal{V}^{\mathrm{B}} \\ M(u) &= M(R_q^0 u_0) + \overline{M}(u - R_q^0 u_0), \end{aligned}$$

Coping with Nonlinearity

Mean-value linearized forms:

$$\begin{aligned} B(u,v) &= B(R_q^0 u_0, v) + \overline{B}(u - R_q^0 u_0, v) \quad \forall\ v \in \mathcal{V}^{\mathrm{B}} \\ M(u) &= M(R_q^0 u_0) + \overline{M}(u - R_q^0 u_0), \end{aligned}$$

Example: $B(u,v) = (L(u), v)$ with $L(u)$ differentiable

$$\begin{aligned} L(u_B) - L(u_A) &= \int_{u_A}^{u_B} dL = \int_{u_A}^{u_B} \frac{dL}{du} du \\ &= \int_0^1 \frac{dL}{du}(\tilde{u}(\theta))\, d\theta \cdot (u_B - u_A) = \overline{L}_{,u} \cdot (u_B - u_A) \end{aligned}$$

with $\tilde{u}(\theta) \equiv u_A + (u_B - u_A)\ \theta$.

$$\begin{aligned} B(u,v) &= B(R_q^0 u_0, v) + (\overline{L}_{,u} \cdot (u - R_p^0 u_0), v) \\ &= B(R_q^0 u_0, v) + \overline{B}(u - R_q^0 u_0, v) \quad \forall v \in \mathcal{V}^{\mathrm{B}} \end{aligned}$$

Coping with Nonlinearity

Mean-value linearized forms:

$$\begin{aligned} B(u,v) &= B(R_q^0 u_0, v) + \overline{B}(u - R_q^0 u_0, v) \quad \forall\ v \in \mathcal{V}^{\mathrm{B}} \\ M(u) &= M(R_q^0 u_0) + \overline{M}(u - R_q^0 u_0), \end{aligned}$$

Example: $B(u,v) = (L(u), v)$ with $L(u)$ differentiable

$$\begin{aligned} L(u_B) - L(u_A) &= \int_{u_A}^{u_B} dL = \int_{u_A}^{u_B} \frac{dL}{du} du \\ &= \int_0^1 \frac{dL}{du}(\tilde{u}(\theta))\, d\theta \cdot (u_B - u_A) = \overline{L}_{,u} \cdot (u_B - u_A) \end{aligned}$$

with $\tilde{u}(\theta) \equiv u_A + (u_B - u_A)\ \theta.$

$$\begin{aligned} B(u,v) &= B(R_q^0 u_0, v) + (\overline{L}_{,u} \cdot (u - R_p^0 u_0), v) \\ &= B(R_q^0 u_0, v) + \overline{B}(u - R_q^0 u_0, v) \quad \forall v \in \mathcal{V}^{\mathrm{B}} \end{aligned}$$

Orthogonality relationship: $\overline{B}(u - R_q^0 u_0, v) = 0 \quad \forall\ v \in \mathcal{V}_0^{\mathrm{B}}$

Error Representation: Godunov FV Case

Primal Godunov FV Problem: Find $u_0 \in \mathcal{V}_0^{\mathrm{B}}$ such that

$$B_{\mathrm{DG}}(R_q^0 u_0, v) = F_{\mathrm{DG}}(v) \quad \forall\, v \in \mathcal{V}_0^{\mathrm{B}}.$$

Linearized dual problem: Find $\Phi \in \mathcal{V}^{\mathrm{B}}$ such that

$$\overline{B}_{\mathrm{DG}}(v, \Phi) = \overline{M}(v) \quad \forall\, v \in \mathcal{V}^{\mathrm{B}}.$$

Error representation formula: ($B_{\mathrm{DG}}(\cdot,\cdot)$ and nonlinear $M(\cdot)$)

$$\begin{aligned}
M(u) - M(R_q^0 u_0) &= \overline{M}(u - R_q^0 u_0) && \text{(mean-value } M\text{)}\\
&= \overline{B}_{\mathrm{DG}}(u - R_q^0 u_0, \Phi) && \text{(dual problem)}\\
&= \overline{B}_{\mathrm{DG}}(u - R_q^0 u_0, \Phi - \pi_0 \Phi) && \text{(orthogonality)}\\
&= B_{\mathrm{DG}}(u, \Phi - \pi_0 \Phi) - B_{\mathrm{DG}}(R_q^0 u_0, \Phi - \pi_0 \Phi) && \text{(mean-value } B\text{)}\\
&= F_{\mathrm{DG}}(\Phi - \pi_0 \Phi) - B_{\mathrm{DG}}(R_q^0 u_0, \Phi - \pi_0 \Phi), && \text{(variational problem)}
\end{aligned}$$

Final error representation formula

$$M(u) - M(R_q^0 u_0) = F_{\mathrm{DG}}(\Phi - \pi_0 \Phi) - B_{\mathrm{DG}}(R_q^0 u_0, \Phi - \pi_0 \Phi)$$

Abstract A-Posteriori Estimate

We wish to study the sharpness of the following sequence of direct estimates

$$
\begin{aligned}
\left|M(u) - M(R_q^0 u_0)\right| &= \left|B_{\mathrm{DG}}(R_q^0 u_0, \Phi - \pi_0 \Phi) - F_{\mathrm{DG}}(\Phi - \pi_0 \Phi)\right| && \text{(basic representation)} \\
&= \Big|\sum_K \big(B_K(R_q^0 u_0, \Phi - \pi_0 \Phi) - F_K(\Phi - \pi_0 \Phi)\big)\Big| && \text{(element assembly)} \\
&\le \sum_K \left|\big(B_K(R_q^0 u_0, \Phi - \pi_0 \Phi) - F_K(\Phi - \pi_0 \Phi)\big)\right| && \text{(triangle inequality)} \\
&\le \sum_K R_K(R_q^0 u_0) \cdot W_K(\Phi - \pi_0 \Phi) && \text{(Cauchy-Schwarz)}
\end{aligned}
$$

$B_K(\cdot,\cdot)$ and $F_K(\cdot)$ are restrictions of $B_{\mathrm{DG}}(\cdot,\cdot)$ and $F_{\mathrm{DG}}(\cdot)$ to the element K

Adaptive Meshing

Define for each element K

$$\eta_K = B_K(R_q^0 u_0, \Phi - \pi_0\Phi) - F_K(\Phi - \pi_0\Phi)$$

$B_K(\cdot,\cdot)$ and $F_K(\cdot)$ are restrictions of $B_{\mathrm{DG}}(\cdot,\cdot)$ and $F_{\mathrm{DG}}(\cdot)$ to the element K

Adaptation Indictor:

$$\left|M(u) - M(R_q^0 u_0)\right| \leq \sum_K |\eta_K|$$

Stopping Criteria:

$$\left|M(u) - M(R_q^0 u_0)\right| = |\sum_K \eta_K|$$

Adaptive Meshing

1. Construct an intial mesh $\mathcal{T}_h$
2. Compute the numerical approximation to the primal problem on the current mesh $\mathcal{T}_h$
3. Compute a numerical approximation and postprocessing of the dual problem on the current mesh $\mathcal{T}_h$
4. Compute η_K for all elements in $\mathcal{T}_h$
5. If($|\sum_K \eta_K| < TOL$) STOP
6. Otherwise, refine and coarsen a user specified fraction of the total number of elements according to the size of $|\eta|_K$, generate a new mesh $\mathcal{T}_h$ and GOTO 2

Approximating $\Phi - \pi_0\Phi$

Some strategies for approximating $\Phi - \pi_0\Phi$

(1) Inherent two scale approximation: Compute the dual problem: Find $\Phi_0 \in \mathcal{V}_0^{\mathrm{B}}$ such that

$$B(v_0, R_q^0\Phi_0) = J(v_0), \quad \forall\, v_0 \in \mathcal{V}_0^{\mathrm{B}}$$

and approximate

$$\Phi - \pi_0\Phi \approx R_q^0\Phi_0 - \Phi_0$$

(2) Least-Squares patch recovery post-processing: (Zienkiewicz,Zhu,Aalto,Perala) Compute the dual problem: Find $\Phi_0 \in \mathcal{V}_0^{\mathrm{B}}$ such that

$$B(v_0, R_q^0\Phi_0) = J(v_0), \quad \forall\, v_0 \in \mathcal{V}_0^{\mathrm{B}}$$

and approximate using patch recovery technique $\overline{R}_{q+r}^q$ for $r > 0$

$$\Phi - \pi_0\Phi \approx \overline{R}_{q+r}^q R_q^0\Phi_0 - \Phi_0$$

Approximating $\Phi - \pi_0 \Phi$

(3) Higher order reconstruction: Compute the dual problem: Find $\Phi_0 \in \mathcal{V}_0^{\mathrm{B}}$ such that

$$B(v_0, R_q^0 \Phi_0) = J(v_0), \quad \forall\, v_0 \in \mathcal{V}_0^{\mathrm{B}}$$

and approximate using the reconstruction operator for $r > 0$

$$\Phi - \pi_0 \Phi \approx R_{q+r}^0 \Phi_0 - \Phi_0$$

(4) Global High Order Solves: Solve the dual problem global using a higher order method

(5) Local High Order Solves: Solve the dual problem on local patches using a higher order method

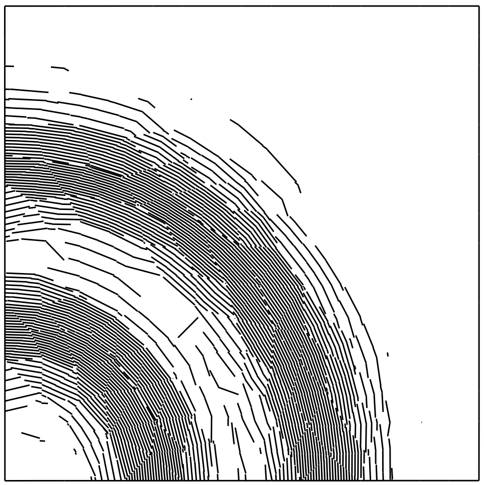
(6) ... ?

A Least Squares Reconstruction Operator

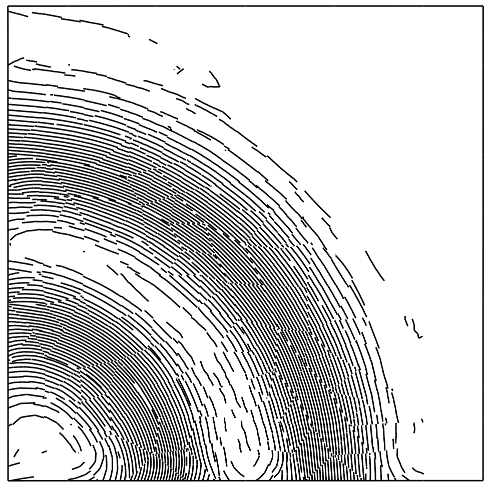
In the present calculations, a least square reconstruction operator R_q^0 has been implemented based on the following design principles:

1. **Exact Π_0 projection in element K.** The $\Pi_{0,K}$ projection of $R^0_{q,\mathcal{N}(K)} u_0$ is exact in element K,
$$\Pi_{0,K} R^0_{q,\mathcal{N}(K)} u_0 = u_{0,K} \quad \text{for each } u_0 \in \mathcal{V}_0^{\mathrm{B}}.$$
2. **Constrained least squares fitting on a patch $\mathcal{N}(K)$.** The L_2 deviation of the $\Pi_{0,K'}$ projection of $R^0_{q,\mathcal{N}(K)} u_0$ from given cell-averaged data in patch elements $K' \in \mathcal{N}(K)$ is minimized subject to constraints
$$\|u_0 - \Pi_0 R^0_{q,\mathcal{N}(K)}\, u_0\|_{\mathcal{N}(K)} = \min_{w \in \mathcal{Q}_q(\mathcal{N}(K))} \|u_0 - \Pi_0 w\|_{\mathcal{N}(K)},$$
for all $u_0 \in \mathcal{V}_0^{\mathrm{B}}$.

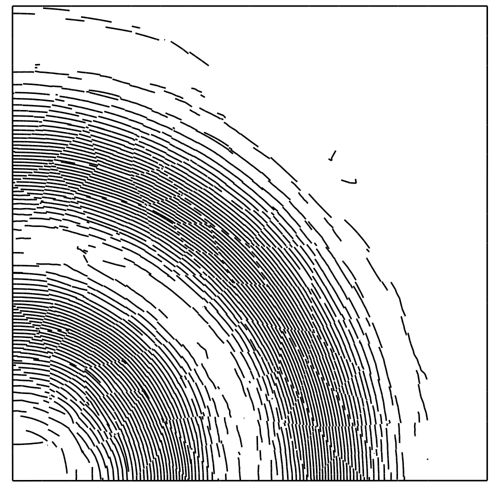
Least Squares Patch Postprocessing



Given $R_1^0 u_0$ data

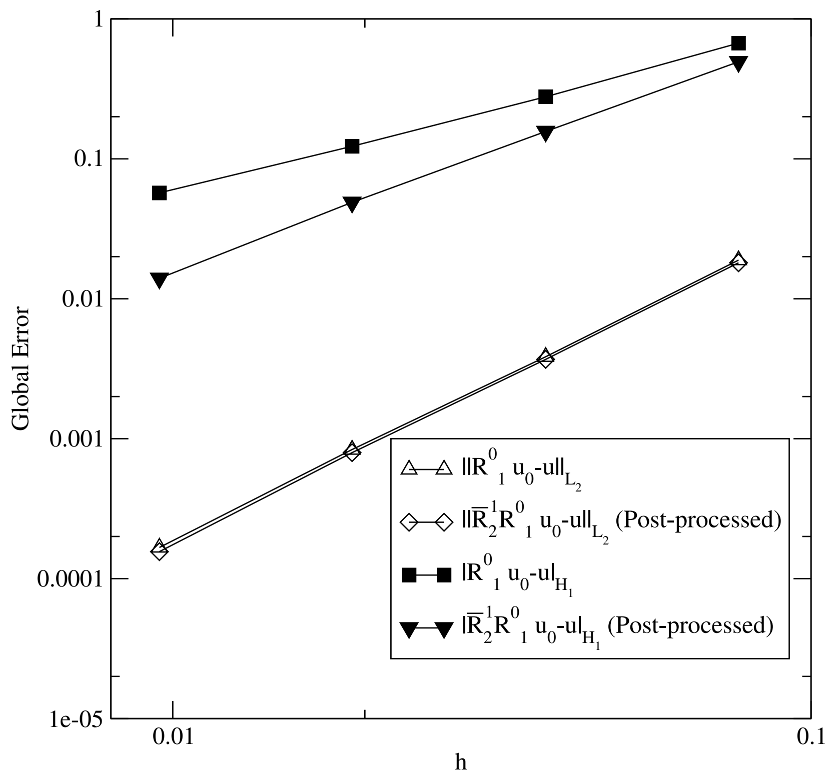


$\overline{R}_2^1 R_1^0 u_0$



$\overline{R}_2^1 R_1^0 u_0$ with $\lambda \cdot \nabla u = 0$ constraint on boundary only

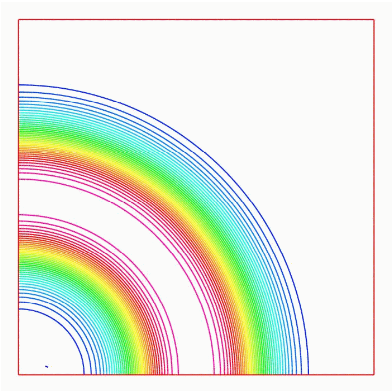
Least Squares Patch Postprocessing



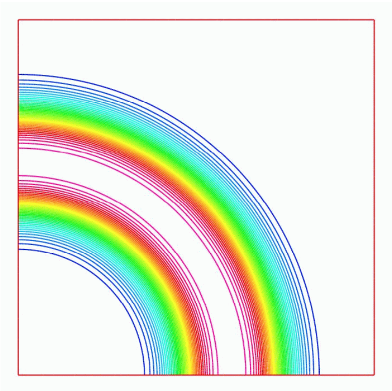
Global L_2 and H_1 semi-norm error.

Numerical Calculations

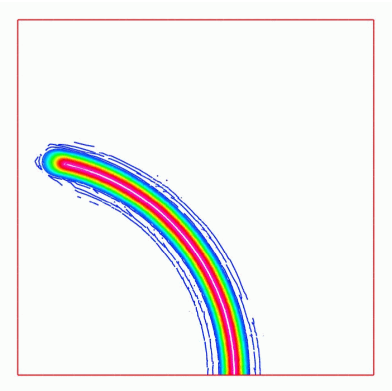
Advection Test Problem: $\mathrm{div}(\lambda u) = 0, \quad \lambda = (y, -x)$



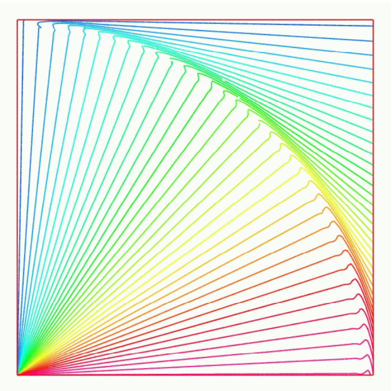
Primal Problem



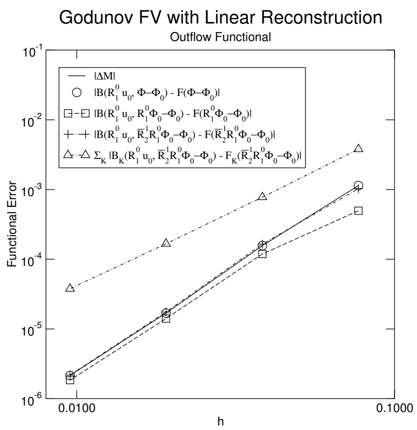
Dual Problem
(Outflow Functional)

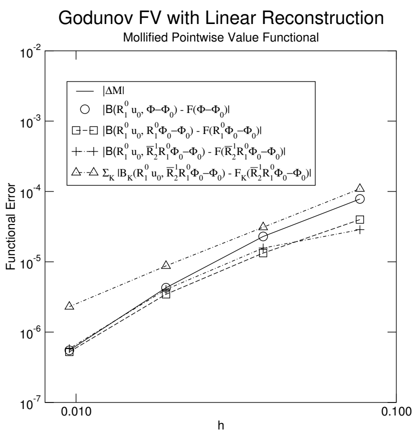


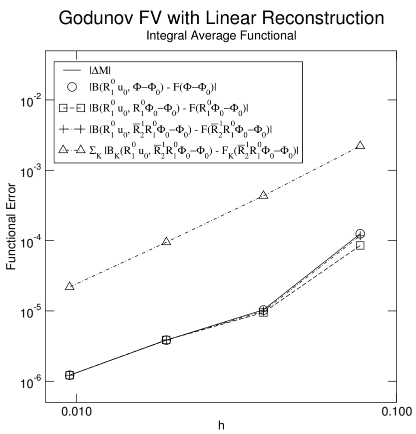
Dual Problem
(Mollified PW Value)



Dual Problem
(Integral Average)

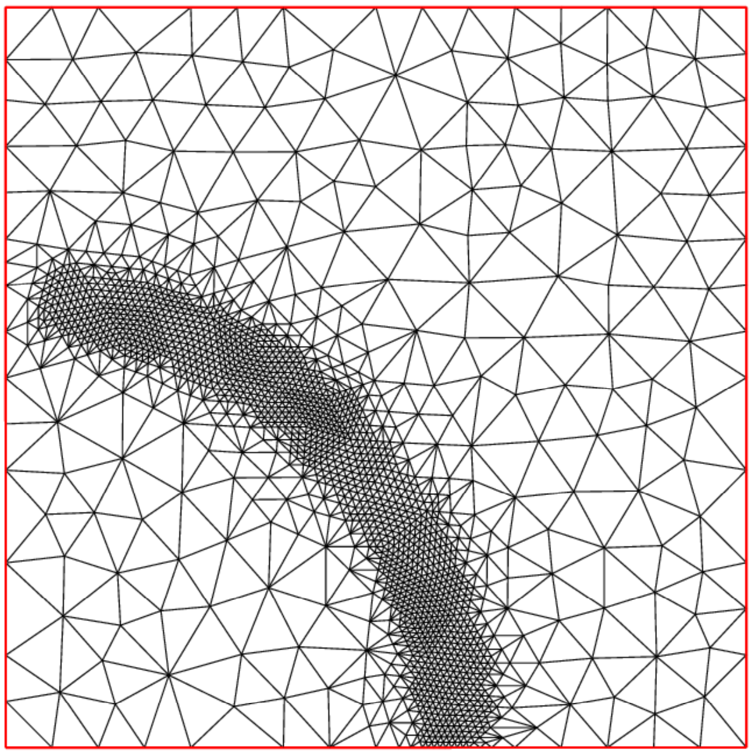






Numerical Calculations

Advection Test Problem: $\operatorname{div}(\lambda u) = 0, \quad \lambda = (y, -x)$. Mollified Pointwise Value Functional:

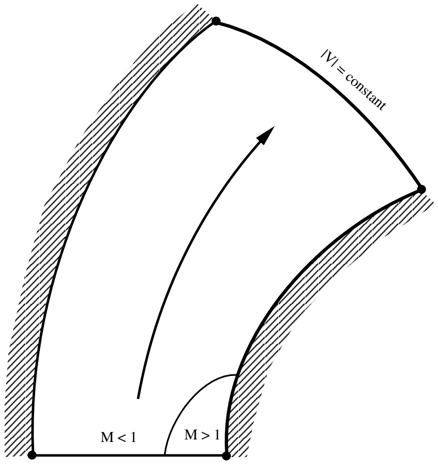


Adapt Levels	#cells	$\lvert\Delta M\rvert$
0	400	1.9E-3
1	602	9.4E-4
2	1232	1.7E-5
3	3418	5.8E-8

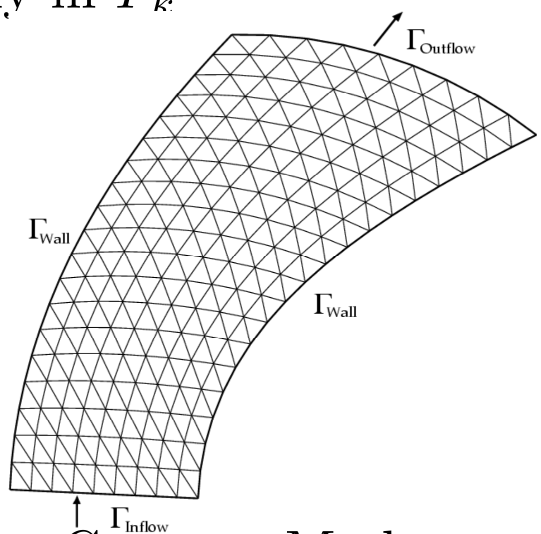
Numerical Calculations: Ringleb Flow

Ringleb Flow Test Problem

- Exact Solution of the 2-D Compressible Euler Equations
- Streamline pairs chosen to simulate turning duct geometry
- Solution is not represented exactly in P_k



Schematic



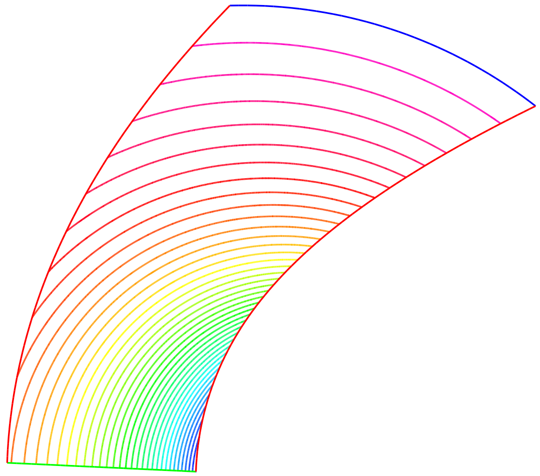
Coarsest Mesh

Numerical Calculations: Ringleb Flow

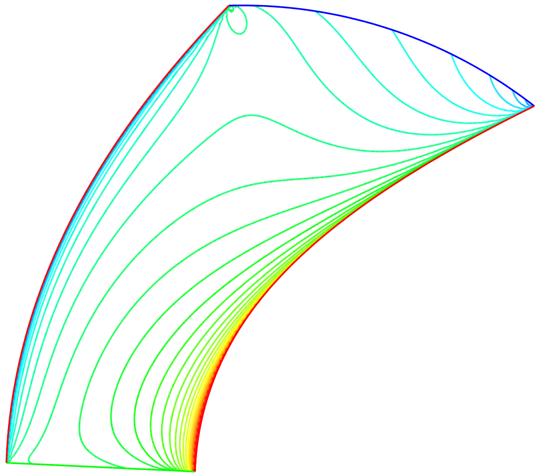
Force Component Functional in the direction $\boldsymbol{\psi}$

$$M_{\boldsymbol{\psi}}(u) = \text{Force}_{\boldsymbol{\psi}}(u) = \int_{\Gamma_{wall}} (\mathbf{n} \cdot \boldsymbol{\psi})\; Pressure(u)\; dx$$

Let $\boldsymbol{\psi}$ be a constant vertically directed vector. Compute the Ringleb flow primal and dual solutions computed using a FV discretization with linear reconstruction

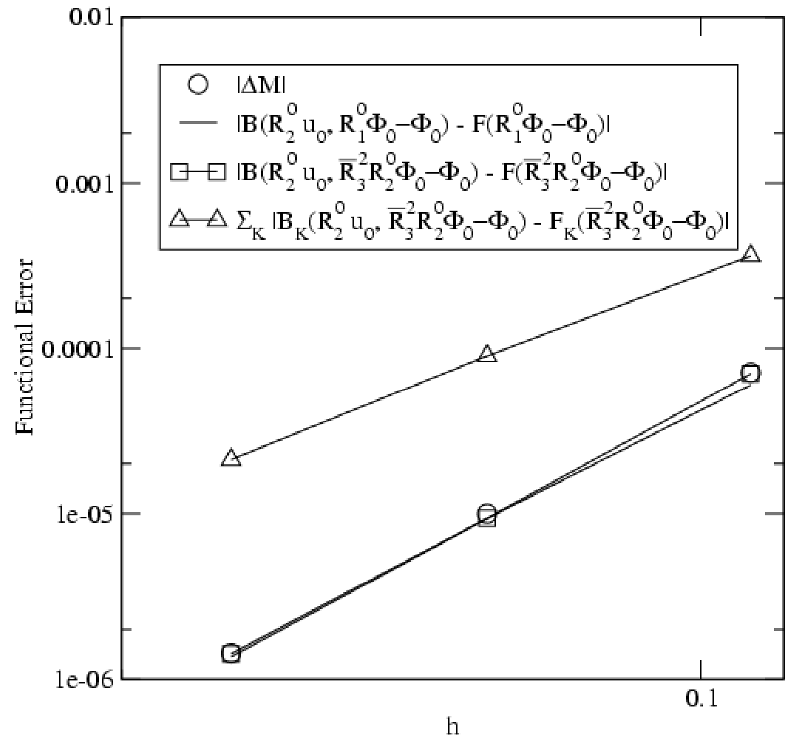


Iso-density contours of the primal solution.



Iso-density contours of the dual solution.

Numerical Calculations: Ringleb Flow



Ringleb flow vertical force functional. Piecewise Linear Reconstruction

Numerical Calculations: Ringleb Flow

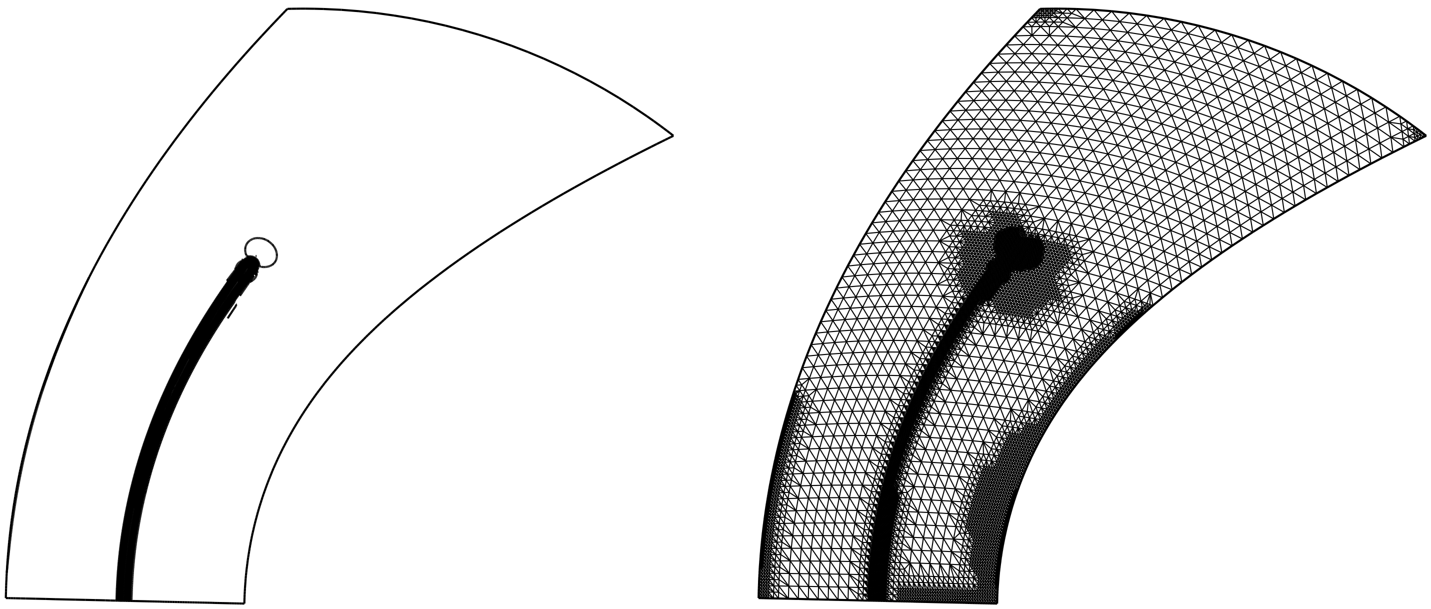
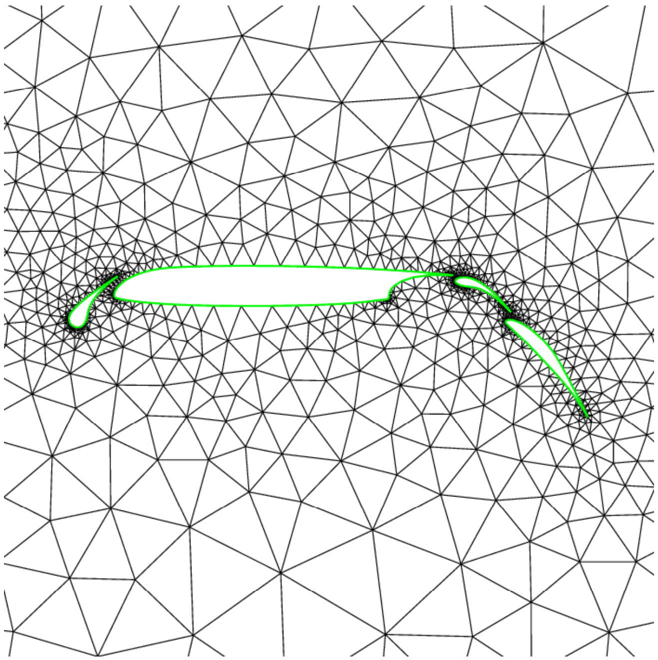


Figure 1: Ringleb channel geometry. Dual energy isocontours solution corresponding to mollified delta functional (left) and final adapted mesh (3 levels) (right).

Multi-element Airfoil Computation

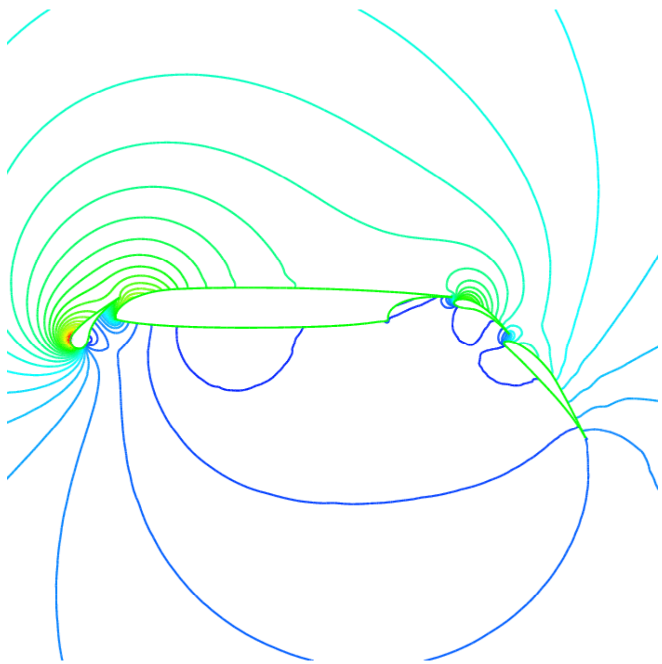
Test Problem: $M_\infty = 0.1, \alpha = 15.0^\circ$ flow over multiple component airfoil.

Domain Triangulation (2500 Vertices)



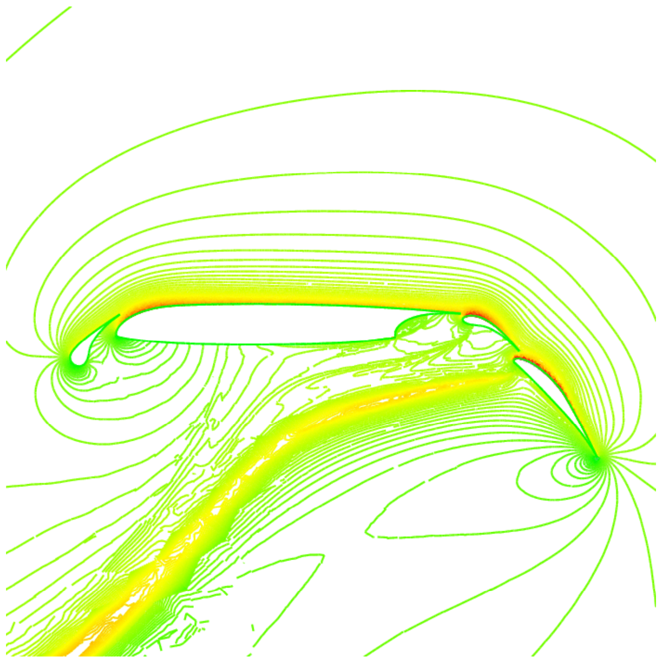
Multi-Element Airfoil Computation

Mach number contours of multielement airfoil Euler solution computed with linear reconstruction



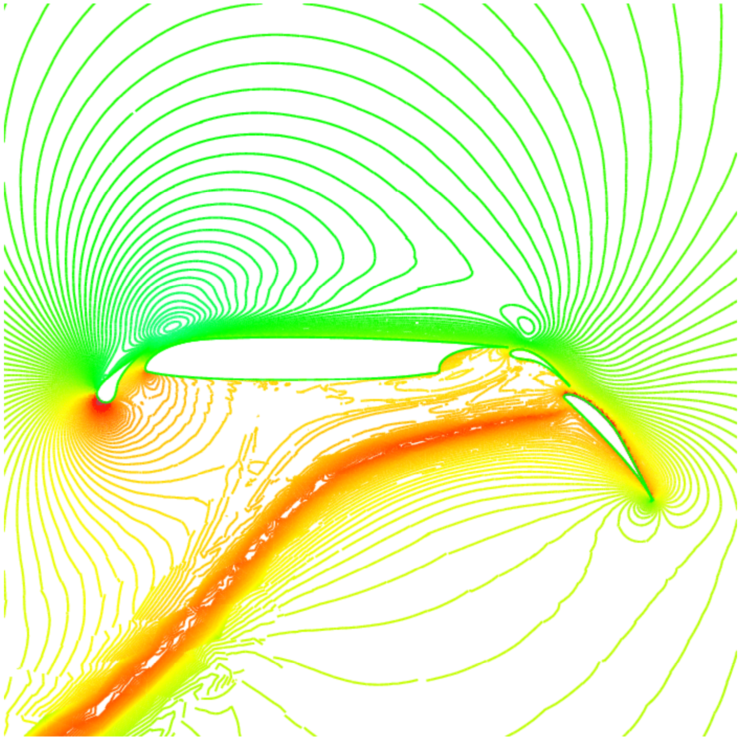
Lift Functional

Dual x-momentum solution, lift functional, $M_{\boldsymbol{\psi}}(u)$ with $\boldsymbol{\psi} \perp Velocity$



Drag Functional

Dual x-momentum solution, drag functional, $M_{\psi}(u)$ with $\boldsymbol{\psi} \parallel Velocity$



Multi-Element Airfoil

Error in lift functional assuming "exact" solution from DG(3) solution of 5500 cell mesh

#cells	ΔM	$error_{\text{est}}$	θ
1200	5.50E-4	4.52E-3	8.22
1950	4.45E-4	3.12E-3	7.01
3300	2.89E-4	1.42E-3	4.98
5500	9.76E-5	9.33E-4	9.56

$$error_{\text{est}} \equiv B(R_1^0 u_0, R_2^0 \Phi_0 - \Phi_0) - F(R_2^0 \Phi_0 - \Phi_0)$$

$$\theta \equiv \frac{error_{\text{est}}}{\Delta M}$$

Multi-Element Airfoil

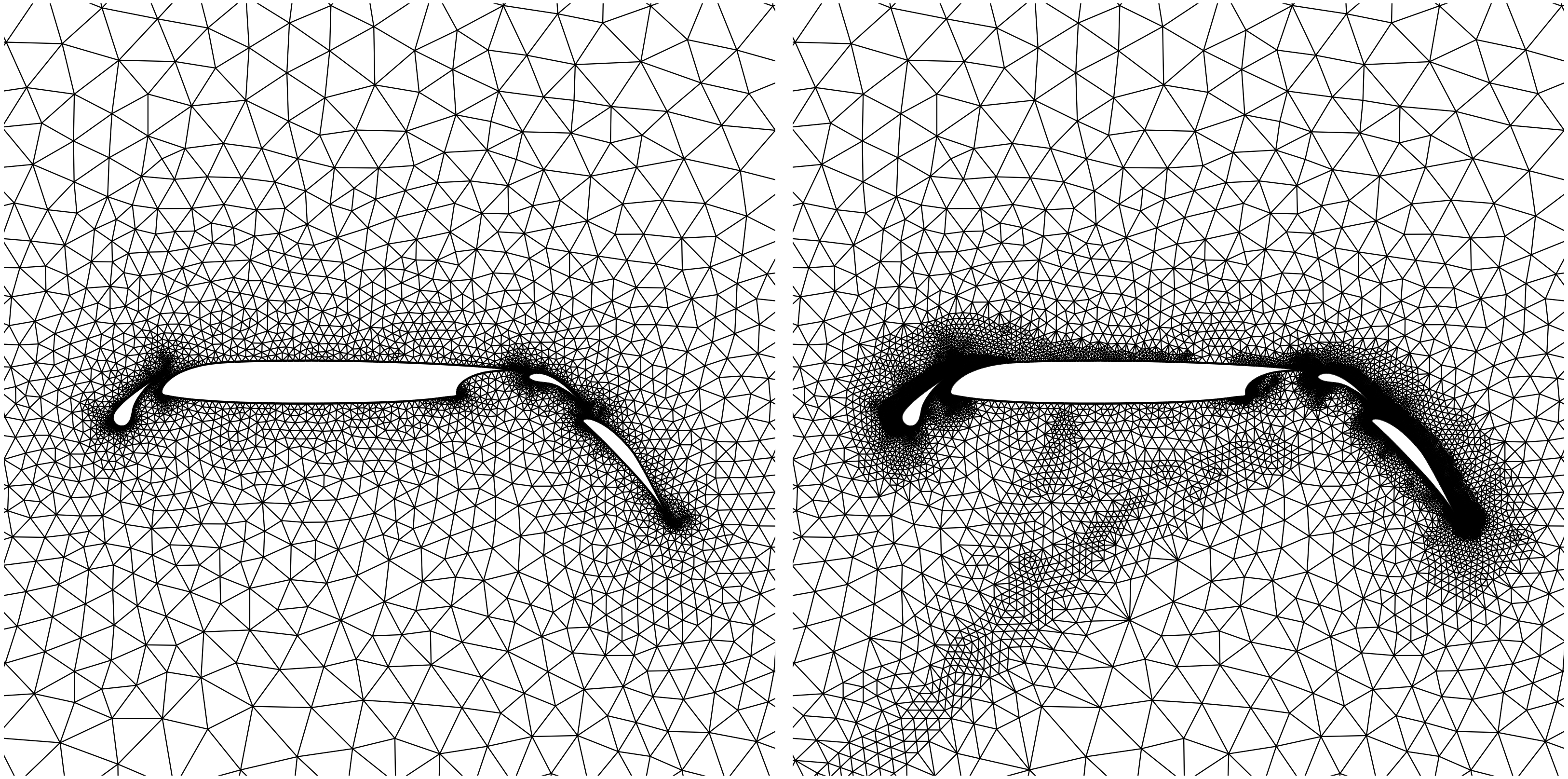


Figure 2: Multiple component airfoil meshes. Original mesh (left) and final adapted mesh with 50k triangles (right).

Multi-Element Airfoil

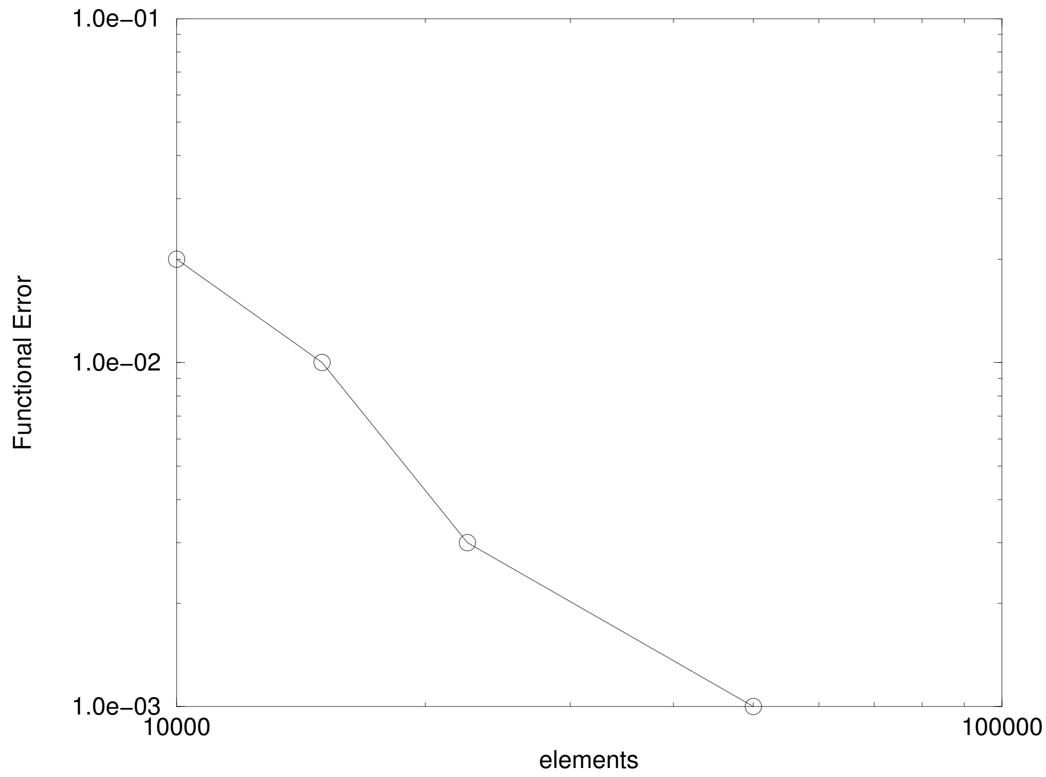


Figure 3: Multiple component airfoil problem. Functional error versus number of triangle elements during intermediate levels of refinement.

Transonic Airfoil

NACA0012 Airfoil, Mach = .85, $\alpha = 2.0^\circ$.

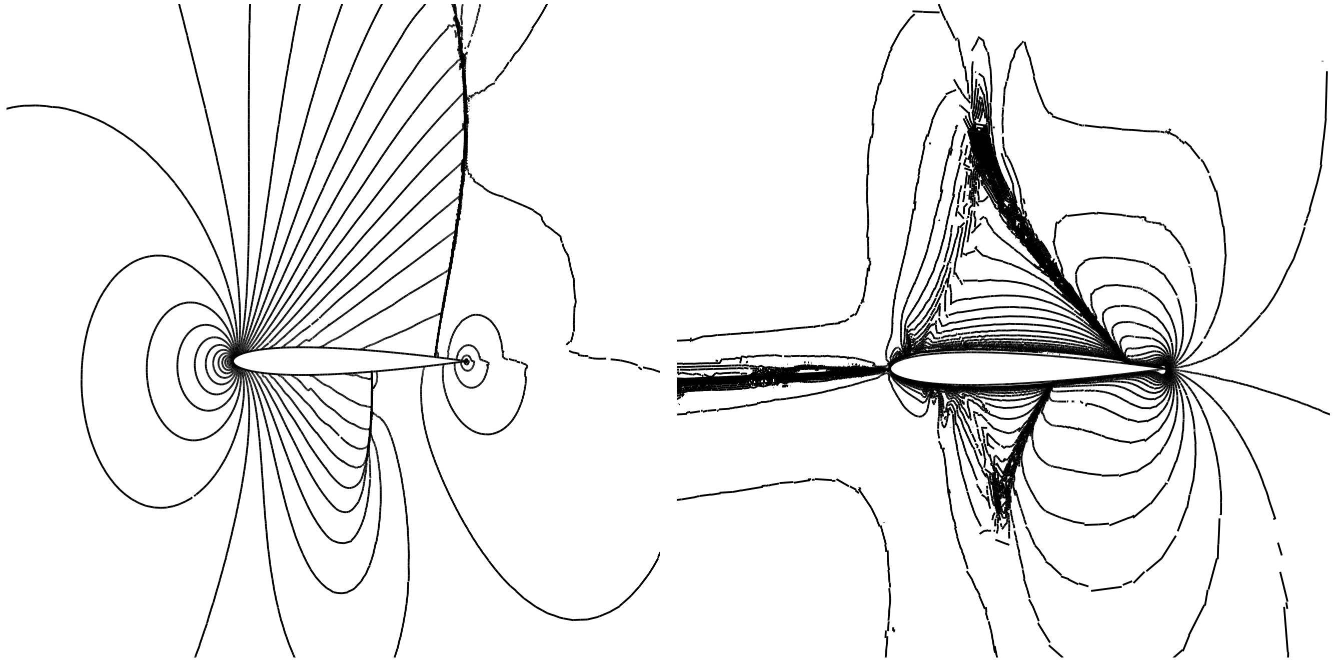


Figure 4: Isodensity contours of primal solution (left) and corresponding contours of the dual density solution (right) for the lift functional.

Transonic Airfoil

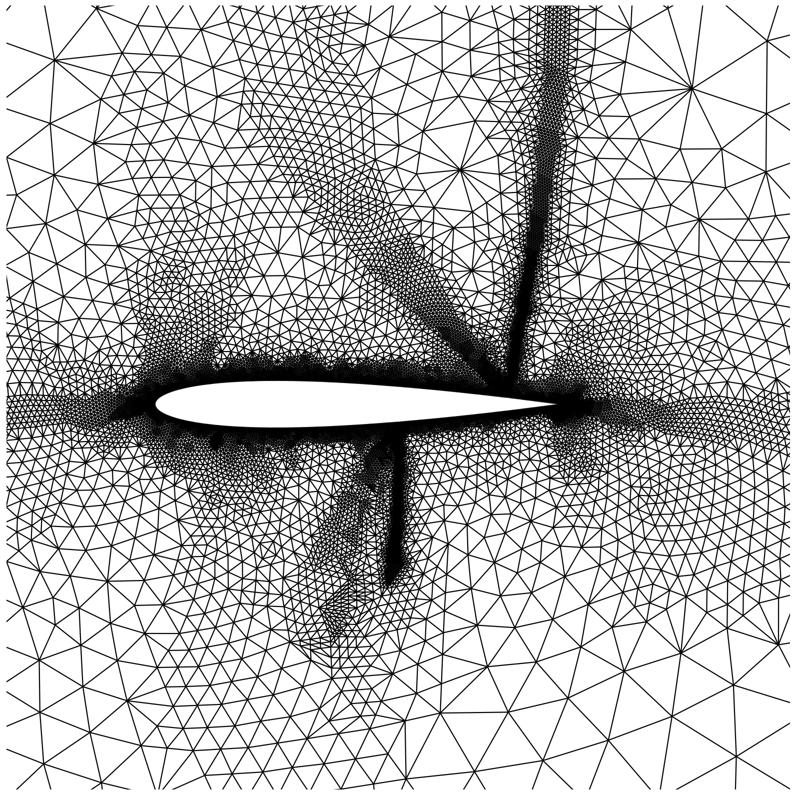


Figure 5: NACA airfoil, $M_\infty = .85, \alpha = 2.0°$. Final adapted mesh (3 levels refinement).

Concluding Summary and Remarks

- By exploiting the *a posteriori* error theory developed for the DG method, an *a posteriori* error estimation theory for the Godunov finite volume method has been developed
- The Petrov-Galerkin structure of the Godunov FV methods suggests a simple estimate of $\Phi - \pi_0 \Phi$ for the continuous dual problem

Open problems

- Analysis of discontinuous coefficients in the dual problem
- Mean-value linearization and non-differentiability
- Approximating $\Phi - \pi_0 \Phi$ and post-processing