Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
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# A Higher-Order Unstructured Finite Volume Solver for Three-Dimensional Compressible Flows

#### Shayan Hoshyari Supervisor: Dr. Carl Ollivier-Gooch

University of British Columbia

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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary

#### Computational Fluid Dynamics — Application



#### Optimal shape design of an Onera M6 wing (SU2)

Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	0000000	0

• Conventional methods are second-order accurate  $||u - u_h|| = O(h^2)$ 

Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	000000	00	000000	0000000	0

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- Higher-order methods can reduce computational costs



Inviscid flow around a sphere

Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	000000	00	000000	0000000	0

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- Unstructured finite volume methods

Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	0000000	0

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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	000000	00	000000	0000000	0

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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	00000000	0

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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	00000000	0

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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	0000000	0

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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	0000000	0

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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	0000000	0

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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	0000000	0

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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	0000000	0

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  - 3-D turbulent flow
- Long term goal at ANSLab:

3-D higher-order finite volume flow solver for all flow conditions

Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
○○●	0000000	00		00000000	O
Objective					

Introduction ○○●	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Objective					

 3-D finite volume formulation for Reynolds Averaged Navier-Stokes + Spalart-Allmaras turbulence model

Introduction ○○●	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Objective					

- 3-D finite volume formulation for Reynolds Averaged Navier-Stokes + Spalart-Allmaras turbulence model
- Implementing the mesh preprocessing steps in 3-D (mesh curving)

Introduction ○○●	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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- 3-D finite volume formulation for Reynolds Averaged Navier-Stokes + Spalart-Allmaras turbulence model
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- Solution of the discretized system of nonlinear equations

Introduction ○○●	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Objective					

- 3-D finite volume formulation for Reynolds Averaged Navier-Stokes + Spalart-Allmaras turbulence model
- Implementing the mesh preprocessing steps in 3-D (mesh curving)
- Solution of the discretized system of nonlinear equations
- Verification of performance and accuracy

Introduction 000	Discretization ••••••	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Finite V	olume Met	hod			

• Given a set of control volumes  $\mathcal{T}_h$ 



Introduction 000	Discretization ••••••	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Finite V	olume Met	hod			

- Given a set of control volumes  $\mathcal{T}_h$
- Find  $\mathbf{u}_h(\mathbf{x}; \mathbf{U}_h)$



Introduction 000	Discretization ●○○○○○○	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Finite V	olume Metl	hod			

- Given a set of control volumes  $\mathcal{T}_h$
- Find  $\mathbf{u}_h(\mathbf{x}; \mathbf{U}_h)$
- $\mathbf{U}_h \equiv \text{DOF}$  vector  $\equiv$  control volume average values



Introduction 000	Discretization ••••••	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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- Find  $\mathbf{u}_h(\mathbf{x}; \mathbf{U}_h)$
- $\mathbf{U}_h \equiv \text{DOF}$  vector  $\equiv$  control volume average values
- Equations must be in the conservative form:  $\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (F(\mathbf{u}) - Q(\mathbf{u}, \nabla \mathbf{u})) = \mathbf{S}(\mathbf{u}, \nabla \mathbf{u})$



Introduction 000	Discretization ••••••	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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#### Finite Volume Method

Using the divergence theorem

$$\begin{aligned} \frac{d\mathbf{U}_{h,\tau}}{dt} + \frac{1}{\Omega_{\tau}} \int_{\partial \tau} \left( \mathcal{F}(\mathbf{u}_{h}^{+},\mathbf{u}_{h}^{-}) - Q(\mathbf{u}_{h}^{+},\nabla\mathbf{u}_{h}^{+},\mathbf{u}_{h}^{-},\nabla\mathbf{u}_{h}^{-}) \right) dS \\ - \frac{1}{\Omega_{\tau}} \int_{\tau} \mathbf{S}(\mathbf{u}_{h},\nabla\mathbf{u}_{h}) d\Omega = 0 \end{aligned}$$



Introduction 000	Discretization ••••••	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Finite Vol	lume Metho	od			

Discretized system of equations

$$\frac{d\mathbf{U}_h}{dt} + \mathbf{R}(\mathbf{U}_h) = 0$$



Introduction 000	Discretization ••••••	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Finite Vo	olume Met	hod			

Discretized system of equations

$$\frac{d\mathbf{U}_h}{dt} + \mathbf{R}(\mathbf{U}_h) = 0$$

#### Building blocks

- *K*-exact reconstruction: Defining  $\mathbf{u}_h$  in terms of  $\mathbf{U}_h$
- Numerical fluxes  $\mathcal{F}$  and Q

Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	000000	00	000000	0000000	0

# RANS + Negative S-A Equations

$$\mathbf{u} = \begin{bmatrix} \rho \\ \rho \mathbf{v} \\ E \\ \rho \tilde{\mathbf{v}} \end{bmatrix} \quad \mathbf{F} = \begin{bmatrix} \rho \mathbf{v}^T \\ \rho \mathbf{v} \mathbf{v}^T + P \mathbf{I} \\ (E+P) \mathbf{v}^T \\ \tilde{\mathbf{v}} \rho \mathbf{v}^T \end{bmatrix} \quad \mathbf{Q} = \begin{bmatrix} 0 \\ (E+P)\tau \mathbf{v} + \frac{R\gamma}{\gamma-1} \left(\frac{\mu}{Pr} + \frac{\mu_T}{Pr_T}\right) \nabla T \\ -\frac{1}{\sigma} (\mu + \mu_T) \nabla \tilde{\mathbf{v}} \end{bmatrix}$$
$$\mathbf{S} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ Diff + \rho (Prod - Dest + Trip) \end{bmatrix}$$

EulerLaminar Navier-StokesRANS + S-A

Introduction 000	Discretization 000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O

#### *K*-exact reconstruction

#### Average values $\mathbf{U}_h \longrightarrow \text{piecewise continuous } \mathbf{u}_h(\mathbf{x})$



Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	0000000	0

# *K*-exact reconstruction — Continued

For every control volume  $\tau$ :

$$u_h(\mathbf{x};\mathbf{U}_h)|_{x\in\tau} = u_{h,\tau}(\mathbf{x};\mathbf{U}_h) = \sum_{i=1}^{N_{\text{rec}}} a_{\tau}^i(\mathbf{U}_h)\phi_{\tau}^i(\mathbf{x}),$$

where

$$\begin{cases} \phi_{\tau}^{i}(\mathbf{x}) | i = 1 \dots N_{\text{rec}} \end{cases} = \\ \begin{cases} \frac{1}{a! b! c!} (x_{1} - x_{\tau 1})^{a} (x_{2} - x_{\tau 2})^{b} (x_{3} - x_{\tau 3})^{c} | a + b + c \le k \end{cases}.$$

Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	0000000	0

#### *K*-exact reconstruction — Continued

- Select a specific set of each control volume's neighbors as its reconstruction stencil *Stencil*(τ)
- $|Stencil(\tau)| \ge MinNeigh(k) \approx 1.5N_{rec}(k)$





Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00	000000	0000000	0

#### *K*-exact reconstruction — Continued

- Predict the average values of  $Stencil(\tau)$  members closely
- Satisfy conservation of the mean

$$\begin{array}{ll} \underset{a_{\tau}^{1}...a_{\tau}^{N_{\text{rec}}}}{\text{minimize}} & \sum_{\sigma \in Stencil(\tau)} \left( \frac{1}{\Omega_{\sigma}} \int_{\sigma} u_{h,\tau}(\mathbf{x}) d\Omega - U_{h,\sigma} \right)^{2} \\ \text{subject to} & \frac{1}{\Omega_{\tau}} \int_{\tau} u_{h}(\mathbf{x}) d\Omega = U_{h,\tau} \end{array}$$

Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	000000	00	000000	0000000	0

# Numerical Flux Functions

Inviscid flux — Roe's flux function

 $\mathcal{F}(\mathbf{u}_h^+, \mathbf{u}_h^-)$  = approximate flux in

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial F(\mathbf{u})\mathbf{n}}{\partial s} = 0$$

Viscous flux — averaging with damping  

$$Q(\mathbf{u}_{h}^{+}, \nabla \mathbf{u}_{h}^{+}, \mathbf{u}_{h}^{-}, \nabla \mathbf{u}_{h}^{-}) = Q(\mathbf{u}_{h}^{*}, \nabla \mathbf{u}_{h}^{*})\mathbf{n}$$
  
where  $\mathbf{u}_{h}^{*} = \frac{1}{2} (\mathbf{u}_{h}^{+} + \mathbf{u}_{h}^{-})$   
and  $\nabla \mathbf{u}_{h}^{*} = \frac{1}{2} (\nabla \mathbf{u}_{h}^{+} + \nabla \mathbf{u}_{h}^{-}) + \eta (\frac{\mathbf{u}_{h}^{+} - \mathbf{u}_{h}^{-}}{\|\mathbf{x}_{\tau^{+}} - \mathbf{x}_{\tau^{-}}\|_{2}})\mathbf{n}$ 

Introduction 000	Discretization 0000000	Mesh Curving ●0	Solution Scheme	3-D Results	Summary O
Mesh Cu	rving				

• Mesh boundary must match the actual geometry



Introduction 000	Discretization 0000000	Mesh Curving ●○	Solution Scheme	3-D Results	Summary O
Mesh Cur	ving				

- Mesh boundary must match the actual geometry
- No mesh tangling



Introduction 000	Discretization 0000000	Mesh Curving ●○	Solution Scheme	3-D Results	Summary O
Mesh Cu	irving				

- Mesh boundary must match the actual geometry
- No mesh tangling
- FEM elasticity solver for displacing internal mesh faces (LibMesh)



Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	⊙●		00000000	O

# Mesh Curving – Continued




Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Solution	Scheme –	– PTC			

• Seeking the steady state solution of:

$$\frac{d\mathbf{U}_h}{dt} + \mathbf{R}(\mathbf{U}_h) = 0$$

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Solution	Scheme -	– PTC			

• Seeking the steady state solution of:

$$\frac{d\mathbf{U}_h}{dt} + \mathbf{R}(\mathbf{U}_h) = 0$$

• Pseudo transient continuation:

$$\left(\frac{\mathbf{V}}{\Delta t} + \frac{\partial \mathbf{R}}{\partial \mathbf{U}_h}\right) \delta \mathbf{U}_h = -\mathbf{R}(\mathbf{U}_h)$$

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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• A linear system must be solved:

$$A\mathbf{x} = \mathbf{b}$$

Introduction 000	Discretization 0000000	Mesh Curving	Solution Scheme	3-D Results	Summary O
Solution S	Scheme —	GMRES			

• Generalized minimal residual method (GMRES)

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Solution S	Scheme — (	GMRES			

- Generalized minimal residual method (GMRES)
  - Finds  $\mathbf{x}^{(k)} \in \text{Span}\{\mathbf{b}, \mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, \cdots, \mathbf{A}^{k-1}\mathbf{b}\}$

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
Solution	Scheme –	- GMRES			

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    That minimizes ||Ax<sup>(k)</sup> − b||<sub>2</sub>

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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  - That minimizes  $\|\mathbf{A}\mathbf{x}^{(k)} \mathbf{b}\|_2$
- Preconditioning APy = b, x = Py

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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$$A^* \approx \tilde{L}\tilde{U}$$



Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O
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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
000	0000000	00		00000000	O
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$$A^* \approx \tilde{L}\tilde{U}$$
  
•  $P = (\tilde{L}\tilde{U})^{-1}$  (to find  $\mathbf{v} = P\mathbf{z}$ , solve  $(\tilde{L}\tilde{U})\mathbf{v} = \mathbf{z}$ )

Introduction 000	Discretization 0000000	Mesh Curving	Solution Scheme	3-D Results	Summary O
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Reordering





Reordered A

Introduction 000	Discretization 0000000	Mesh Curv 00	ing	Solution Scheme	3-D Results	Summary O
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• HO-ILUp (Jalali and Ollivier-Gooch, 2017)

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•  $A \simeq (\tilde{L}\tilde{U})$  (fill level  $p \ge 3$ )

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O

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• 
$$A \simeq (\tilde{L}\tilde{U})$$
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Memory consuming

Introduction 000	0000000	00	OO●○○○	3-D Results 00000000	0 Summary
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- HO-ILUp (Jalali and Ollivier-Gooch, 2017)
  - $A \simeq (\tilde{L}\tilde{U})$  (fill level  $p \ge 3$ )
  - Memory consuming
- LO-ILUp: (Nejat and Ollivier-Gooch, 2008; Wong and Zingg, 2008)

Introduction 000	0000000	00	oo●○○○	3-D Results 00000000	0 Summary
~ 1 .	~ .				

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Introduction 000	Discretization 0000000	Mesh Curving	Solution Scheme	3-D Results 00000000	Summary O
~ .	~ .				

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$$A^* \simeq (\tilde{L}\tilde{U})$$

•  $A^*$  is k = 0 LHS matrix

Introduction 000	Discretization 0000000	Mesh Curving	Solution Scheme	3-D Results 00000000	Summary O
~ .	~ .				

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Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O

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Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O

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  - Imitates  $P(.) = (A^*)^{-1}(.)$
  - Solve  $(A^*) \{ \mathbf{P}(.) \} = (.)$  using ILU preconditioned GMRES

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O

- HO-ILUp (Jalali and Ollivier-Gooch, 2017)
  - $A \simeq (\tilde{L}\tilde{U})$  (fill level  $p \ge 3$ )
  - Memory consuming
- LO-ILUp: (Nejat and Ollivier-Gooch, 2008; Wong and Zingg, 2008)
  - $\bullet \ A^* \simeq (\tilde{L}\tilde{U})$
  - $A^*$  is k = 0 LHS matrix
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Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O

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  - RCM (minimizes fill of  $A^*$ )

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O

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- ILU reordering
  - RCM (minimizes fill of  $A^*$ )
  - QMD (minimizes fill of  $\tilde{L}\tilde{U}$ )

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary O

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- ILU reordering
  - RCM (minimizes fill of *A*\*)
  - QMD (minimizes fill of  $\tilde{L}\tilde{U}$ )
  - Lines of strong coupling between unknowns (this thesis)

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Introduction 000	Discretization 0000000	Mesh Cur 00	ving So	olution Scheme	3-D Results	Summa O

Solution Scheme — Lines of Strong Unknown Coupling



Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
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#### Solution Scheme — Results

- k = 3
- 2-D turbulent flow over NACA 0012
- $Re = 6 \times 10^6$ , Ma = 0.15,  $\alpha = 10^\circ$
- Mixed mesh with  $N_{CV} = 100$ K and  $N_{CV} = 25$ K

Case	Preconditioning	Reordering	Used in
name	method	algorithm	higher-order FV
А	HO-ILU3	QMD	(Jalali and Ollivier-Gooch, 2017)
В	LO-ILU0	RCM	(Nejat and Ollivier-Gooch, 2008)
С	LO-ILU0	lines	This thesis
D	GMRES-LO-ILU0	RCM	This thesis
Е	GMRES-LO-ILU0	lines	This thesis

Introduction 000	Discretization 0000000	Mesh Curving	Solution Scheme	3-D Results	Summary O
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#### Solution Scheme — Results

#### Comparison of residual histories



Introduction D	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
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## Inviscid Flow Around Sphere

- Ma = 0.38
- $N_{\rm CV} = 64$ K, 322K, 1M



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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary

Inviscid Flow Around Sphere — Entropy Norm

Subsonic flow  $\longrightarrow ||S - S_{\infty}||_2 = 0$ 



Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary
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# Turbulent Flow Over a Flat Plate

- $Re = 5 \times 10^6$
- Ma = 0.2
- Nested meshes:  $60 \times 34 \times 7$ ,  $120 \times 68 \times 14$ , and  $240 \times 136 \times 28$



Adiabatic wall. Symmetry Inflow/outflow
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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summa

#### Turbulent Flow Over a Flat Plate — Verification

Distribution of the turbulence working variable on the plane  $x_3 = 0.5$ 



Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summ
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### Turbulent Flow Over a Flat Plate — Verification

Eddy viscosity on the line  $(x_1 = 0.97) \land (x_3 = 0.5)$ 



Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summar
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### Turbulent Flow Over an Extruded NACA 0012

- Extrusion length = 1 in  $x_3$  direction
- $Re = 6 \times 10^6$ , Ma = 0.15,  $\alpha = 10^\circ$ ,  $\psi = 0$
- Hex mesh with  $N_{\rm CV} = 100$ K and mixed mesh with  $N_{\rm CV} = 176$ K



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Introduction	Discretization	Mesh Curving	Solution Scheme	3-D Results	Summary

### Extruded NACA 0012 — Convergence

- Norm of the residual vector per PTC iteration
- Order ramping
- Convergence only slightly affected by mesh type or *k*



 Introduction
 Discretization
 Mesh Curving
 Solution Scheme
 3-D Results
 Summary

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 0000000
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### Extruded NACA 0012 — Verification



Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary •
Summary	,				

• Derived the *k*-exact finite volume formulation of the RANS + negative S-A equations in 3-D.

Introduction 000	Discretization 0000000	Mesh Curving	Solution Scheme	3-D Results	Summary •
Summary	7				

- Derived the *k*-exact finite volume formulation of the RANS + negative S-A equations in 3-D.
- Developed a 3-D linear elasticity solver to prevent mesh tangling.

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary •
Summary	7				

- Derived the *k*-exact finite volume formulation of the RANS + negative S-A equations in 3-D.
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- Designed an efficient solution scheme.

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary •
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  - Lines of strong coupling between unknowns.

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary •
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  - Inner GMRES iterations based on the k = 0 scheme.

Introduction 000	Discretization 0000000	Mesh Curving 00	Solution Scheme	3-D Results	Summary •
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- Developed a 3-D linear elasticity solver to prevent mesh tangling.
- Designed an efficient solution scheme.
  - Lines of strong coupling between unknowns.
  - Inner GMRES iterations based on the k = 0 scheme.
- Verified the developed solver for benchmark problems.

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References

Backup Slides

### FV vs DG



Inviscid flow around a circle (Bassi and Rebay, 1997)

# Common Goal

- Given a PDE  $\mathcal{L}\mathbf{u}(\mathbf{x}) = 0$
- Find a discrete solution **u**<sub>*h*</sub>(**x**; **U**<sub>*h*</sub>)
- Such that the discretization error  $\mathbf{e}_h = \mathbf{u}_h \mathbf{u}$
- Has an asymptotic behavior  $\|\mathbf{e}_h\| = O(h^p)$

The method is said to be *p*th-order accurate.

Traditional methods are second-order accurate.

# Higher-Order Methods — Advantages

#### **Reduction of computational costs.**

- When modeling errors are dominant:
  - Limited level of reduction in discretization error is of interest.
  - *hp*-adaptive methods.
- When numerical errors are dominant:
  - E.g., complicated full-body aircraft geometries.
  - E.g., advanced turbulence modeling schemes.
  - More accurate solution are valuable ( 1% better accuracy in finding drag ).
  - Accurate solutions can be obtained on coarser meshes.
- Unstructured finite volume methods
  - Complex geometries
  - Fewer number of degrees of freedom.
  - Easier integration into commercial solvers.

### *K*-exact reconstruction — Continued

- Satisfy conservation of the mean.
- Predict the average values of  $Stencil(\tau)$  closely.

$$\begin{array}{ll} \underset{a_{\tau}^{1}...a_{\tau}^{N_{\text{rec}}}}{\text{minimize}} & \sum_{\sigma \in Stencil(\tau)} \left( \frac{1}{\Omega_{\sigma}} \int_{\sigma} u_{h,\tau}(\mathbf{x}) d\Omega - U_{h,\sigma} \right)^{2} \\ \text{subject to} & \frac{1}{\Omega_{\tau}} \int_{\tau} u_{h}(\mathbf{x}) d\Omega = U_{h,\tau} \end{array}$$

### *K*-exact reconstruction — Continued

- Satisfy conservation of the mean.
- Predict the average values of  $Stencil(\tau)$  closely.

$$I_{\tau\sigma}^{i} = \int_{\sigma} \phi_{\tau}^{i}(\mathbf{x}) d\Omega \qquad \sigma \in Stencil(\tau) \cup \{\tau\}$$

$$\frac{\begin{bmatrix} I_{\tau\tau}^{1} & \dots & I_{\tau\tau}^{N_{\text{rec}}} \\ I_{\tau\sigma_{1}}^{1} & \dots & I_{\tau\sigma_{1}}^{N_{\text{rec}}} \\ \vdots & \ddots & \vdots \\ I_{\tau\sigma_{\text{NS}(\tau)}}^{1} & \dots & I_{\tau\sigma_{\text{NS}(\tau)}}^{N_{\text{rec}}} \end{bmatrix} \begin{bmatrix} a_{\tau}^{1} \\ \vdots \\ a_{\tau}^{N_{\text{rec}}} \end{bmatrix} = \frac{\begin{bmatrix} U_{h,\tau} \\ U_{h,\sigma_{1}} \\ \vdots \\ U_{h,\sigma_{\text{NS}(\tau)}} \end{bmatrix}$$

### *K*-exact reconstruction — Continued

- Satisfy conservation of the mean.
- Predict the average values of  $Stencil(\tau)$  closely.

$$\begin{bmatrix} a_{\tau}^{1} \\ \vdots \\ a_{\tau}^{N_{\text{rec}}} \end{bmatrix} = \mathbf{A}_{\tau}^{\dagger} \begin{bmatrix} U_{h,\tau} \\ U_{h,\sigma_{1}} \\ \vdots \\ U_{h,\sigma_{\text{NS}(\tau)}} \end{bmatrix}$$

# **Reconstruction Optimization Problem**

- Ax = b subject to Bx = 0
- Change of variables x = By where the columns of *B* are the null space of *A*.
- Ax = 0 reduces to (AB = C)y = 0 which is always satisfied.
- Solve the unconstrained problem Cy = b, i.e.,  $y = C^{\dagger}b$ 
  - QR (Householder or Gram-schmidt):  $C = Q_1 R_1$ ,  $C^{\dagger} = R_1^{-1} Q^T$
  - SVD (most stable):  $C = U\Sigma V^T$ ,  $C^{\dagger} = W^T \Sigma^{-1} U$
  - Normal equations:  $C^{\dagger} = (CC^T)^{-1}C^T$
- Finally, x = By.

#### References

# Numerical Flux Functions

Inviscid Flux — Roe's Flux Function  

$$\mathcal{F}(\mathbf{u}_{h}^{+}, \mathbf{u}_{h}^{-}) = \text{approximate solution for } \boldsymbol{F}(s = 0)\mathbf{n} \text{ in}$$

$$\begin{cases} \frac{\partial \mathbf{u}}{\partial t} + \frac{\partial F(\mathbf{u})\mathbf{n}}{\partial s} = 0\\ \mathbf{u}(s < 0, t = 0) = u_{h}^{-}\\ \mathbf{u}(s > 0, t = 0) = u_{h}^{+} \end{cases}$$

Inviscid Flux — Averaging with Damping  $Q(\mathbf{u}_{h}^{+}, \nabla \mathbf{u}_{h}^{+}, \mathbf{u}_{h}^{-}, \nabla \mathbf{u}_{h}^{-}) = Q(\mathbf{u}_{h}^{*}, \nabla \mathbf{u}_{h}^{*})\mathbf{n},$ where  $\mathbf{u}_{h}^{*} = \frac{1}{2} \left( \mathbf{u}_{h}^{+} + \mathbf{u}_{h}^{-} \right),$ and  $\nabla \mathbf{u}_{h}^{*} = \frac{1}{2} \left( \nabla \mathbf{u}_{h}^{+} + \nabla \mathbf{u}_{h}^{-} \right) + \eta \left( \frac{\mathbf{u}_{h}^{+} - \mathbf{u}_{h}^{-}}{\|\mathbf{x}_{\tau^{+}} - \mathbf{x}_{\tau^{-}}\|_{2}} \right) \mathbf{n}$ 

# Parallel Scaling

#### Strong Scaling Test

- Solving the same problem with different number of processors
- Inviscid flow, sphere:  $N_{\rm CV} = 322$ K and k = 3
- Turbulent flow, flat plate:  $128 \times 68 \times 14$  mesh and k = 3



### Nondimensionalization – Flow Variables

Reference values:

$$\begin{array}{ll} \rho^* \sim \rho_{\infty} & \mathbf{v}^* \sim c_{\infty} & T^* \sim \frac{c_{\infty}}{\gamma R} & P^* \sim \rho_{\infty} c_{\infty}^2 \\ t^* \sim \frac{L}{c_{\infty}} & \mu^* \sim \mu_{\infty} & \mu_T^* \sim \mu_{\infty} & \nu_T^* \sim \frac{\mu_{\infty}}{\rho_{\infty}} \\ \tilde{\nu}^* \sim \mu' & \boldsymbol{\tau} \sim \frac{\mu_{\infty} c_{\infty}}{L} & d \sim L \end{array}$$

Pressure and temperature:

$$c^* = \sqrt{\frac{\gamma P^*}{\rho^*}} \qquad \Rightarrow \qquad c = \sqrt{\frac{\gamma P}{\rho}}$$
$$P^* = \rho^* R T^* \qquad \Rightarrow \qquad P = \frac{\rho T}{\gamma}$$

$$E^* = \rho \frac{R(\gamma - 1)}{\gamma} T + \frac{1}{2} (\mathbf{v}^* \cdot \mathbf{v}^*) \Rightarrow P = (\gamma - 1) \left( E - \frac{1}{2} \rho (\mathbf{v} \cdot \mathbf{v}) \right)$$

Dimensionless numbers:

$$Ma = \frac{v_{\infty}}{c_{\infty}}$$
  $Re = \frac{\rho_{\infty}v_{\infty}L}{\mu_{\infty}}$   $Pr = \frac{c_{p}\mu}{k}$ 

### Nondimensionalization — Lift and Drag

Pressure Force ~ 
$$\rho_{\infty}c_{\infty}^2L^2$$
  
Viscous Force ~  $\mu_{\infty}c_{\infty}L^2$ 

$$C_D = \frac{D^*}{(1/2)\rho_{\infty}v_{\infty}^2 A} \implies C_D = \frac{D}{(1/2)Ma^2(A/L^2)}$$
$$C_{D\nu} = \frac{D^*}{(1/2)\rho_{\infty}v_{\infty}^2 A} \implies C_{D\nu} = \frac{D}{(1/2)MaRe(A/L^2)}$$
$$C_f = \frac{\mathbf{m}^T \boldsymbol{\tau}^* \mathbf{n}}{(1/2)\rho^* v_{\infty}^2 A} \implies C_f = \frac{\mathbf{m}^T \boldsymbol{\tau} \mathbf{n}}{(1/2)\rho MaRe(A/L^2)}$$

### Nondimensionalization — Sutherland's Law

$$\frac{\mu^{*}}{\mu_{ref}} = \left(\frac{T^{*}}{T_{ref}}\right)^{3/2} \frac{1 + (S^{*}/T_{ref})}{(T^{*}/T_{ref}) + (S^{*}/T_{ref})}$$
$$\mu = T \frac{\mu_{\infty}}{\mu_{ref}} \frac{(T_{ref}/T_{\infty}) + S}{T + S}$$

S = 110.4K  $T_{ref} = 273.15K$   $\mu_{ref} = 1.716 \times 10^{-5}$ 

### Nondimensionalization — Flux Matrices

$$\boldsymbol{F}^{*} = \begin{bmatrix} \rho^{*} \mathbf{v}^{*T} \\ \rho^{*} \mathbf{v}^{*} \mathbf{v}^{*T} + P^{*} \boldsymbol{I} \\ (E^{*} + P^{*}) \mathbf{v}^{*T} \\ \tilde{\boldsymbol{v}}^{*} \rho^{*} \mathbf{v}^{*T} \end{bmatrix} \quad \boldsymbol{Q}^{*} = \begin{bmatrix} 0 \\ \boldsymbol{\tau}^{*} \\ (E^{*} + P^{*}) \boldsymbol{\tau}^{*} \mathbf{v}^{*} + \frac{R_{Y}}{\gamma - 1} \left( \frac{\mu^{*}}{Pr} + \frac{\mu_{T}^{*}}{Pr_{T}} \right) \nabla T^{*} \\ -\frac{1}{\sigma} (\mu^{*} + \mu_{T}^{*}) \nabla \tilde{\boldsymbol{v}}^{*} \end{bmatrix}$$

$$\boldsymbol{F} = \begin{bmatrix} \rho \mathbf{v}^{T} \\ \rho \mathbf{v} \mathbf{v}^{T} + P \boldsymbol{I} \\ (E+P) \mathbf{v}^{T} \\ \tilde{\boldsymbol{v}} \rho \mathbf{v}^{T} \end{bmatrix} \quad \boldsymbol{Q} = \begin{bmatrix} 0 \\ \frac{Ma}{Re} \boldsymbol{\tau} \\ (E+P)\boldsymbol{\tau} \mathbf{v} + \frac{1}{\gamma-1} \left(\frac{\mu}{Pr} + \frac{\mu_{T}}{Pr_{T}}\right) \nabla T \\ -\frac{Ma}{Re\sigma} (\mu + \mu_{T}) \nabla \tilde{\boldsymbol{v}} \end{bmatrix}$$

# Solution Scheme — PTC

• Seeking the steady state solution of:

$$\frac{d\mathbf{U}_h}{dt} + \mathbf{R}(\mathbf{U}_h) = 0$$

Newton:

$$\frac{\partial \mathbf{R}}{\partial \mathbf{U}_h} \delta \mathbf{U}_h = -\mathbf{R}(\mathbf{U}_h), \quad \mathbf{U}_h \leftarrow \mathbf{U}_h + \delta \mathbf{U}_h$$

Backward Euler:

$$\frac{\mathbf{U}_{h}^{+} - \mathbf{U}_{h}}{\Delta t} + \mathbf{R}(\mathbf{U}_{h}) = 0$$

Pseudo transient continuation:

$$\left(\frac{\mathbf{V}}{\Delta t} + \frac{\partial \mathbf{R}}{\partial \mathbf{U}_h}\right) \delta \mathbf{U}_h = -\mathbf{R}(\mathbf{U}_h)$$

• A linear system must be solved:

 $A\mathbf{x} = \mathbf{b}$  (\*)

### Solution Scheme — Preconditioning

- GMRES can stall
- Right preconditioning APy = b, x = Py
- Incomplete LU factorization; fill level *p*

• 
$$A^* \approx \tilde{L}\tilde{U}$$
  
•  $P = (\tilde{L}\tilde{U})^{-1}$  (to find  $\mathbf{v} = P\mathbf{z}$ , solve  $(\tilde{L}\tilde{U})\mathbf{v} = \mathbf{z}$ )

• Reordering 
$$\sigma A \sigma^T P \mathbf{y} = \sigma \mathbf{b}$$



### Solution Scheme — Preconditioning

- GMRES can stall
- Right preconditioning APy = b, x = Py
- Incomplete LU factorization; fill level *p*

• 
$$A^* \approx \tilde{L}\tilde{U}$$
  
•  $P = (\tilde{L}\tilde{U})^{-1}$  (to find  $\mathbf{v} = P\mathbf{z}$ , solve  $(\tilde{L}\tilde{U})\mathbf{v} = \mathbf{z}$ )

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$$\sigma A \sigma^T P \mathbf{y} = \sigma \mathbf{b}$$



# Solution Scheme — Preconditioning

- GMRES can stall
- Right preconditioning APy = b, x = Py
- Incomplete LU factorization; fill level p

• 
$$A^* \approx \tilde{L}\tilde{U}$$
  
•  $P = (\tilde{L}\tilde{U})^{-1}$  ( to find  $\mathbf{v} = P\mathbf{z}$ , solve  $(\tilde{L}\tilde{U})\mathbf{v} = \mathbf{z}$  )

• Reordering 
$$\sigma A \sigma^T P \mathbf{y} = \sigma \mathbf{b}$$



# Solution Scheme — Lines of Strong Unknown Coupling

- Assign binary weights  $W_{\tau\sigma}$ .
- Advection-diffusion equation  $\nabla \cdot (\mathbf{v}u \mu_L \nabla u) = 0$ .

• 
$$W_{\tau\sigma} = \max\left(\frac{\partial R_{\sigma}}{\partial u_{\tau}}, \frac{\partial R_{\tau}}{\partial u_{\sigma}}\right)$$

- Greedy clustering algorithm
  - 1) Pick an unmarked control volume  $\tau$
  - 2) Pick the neighbour  $\sigma$  with the highest weight
  - 3 If  $\sigma$  is marked go to 1.
  - ④ Add  $\sigma$  to line and mark it.
  - $\mathbf{5} \ \tau = \sigma$ , go to 2.

### Solution Scheme — Comparison Details

Preconditioner	N-PTC	N-GMRES	Memory(GB)	LST(s)	TST(s)
		$N_{\rm CV} = 2$	25K		
A	37	956	1.4	416	635
В	44	10, 893	0.7	264	572
С	51	13,692	0.7	328	705
D	34	1,856	0.7	134	379
E	34	1, 787	0.7	118	361
		$N_{\rm CV} = 1$	00K		
A	39	4,640	5.9	3, 122	4,068
В	-	-	2.8	-	-
С	-	-	2.8	-	-
D	-	-	3.2	_	_
E	36	4, 396	3.2	1,308	2,348

### Poisson's Equation

- $\nabla^2 u = f$
- Manufactured solution
   u = sinh(sin(x<sub>1</sub>)) sinh(sin(x<sub>2</sub>)) sinh(sin(x<sub>3</sub>))
- Domain  $\Omega = \begin{bmatrix} 0 & 1 \end{bmatrix}^3$
- Dirichlet boundary conditions



Backup Slides

### Poisson's Equation — Accuracy Analysis



Error versus mesh length scale

Poor performance of k = 2 is expected (Ollivier-Gooch and Van Altena, 2002).

References

Backup Slides

# Poisson's Equation — Meshes

N = 10, 20, 40.



References

Backup Slides

### Inviscid Flow Around Sphere — Mach Contours



Computed Mach contours on the  $x_3 = 0$  symmetry plane for the sphere problem
## Sphere — Convergence

- Norm of the residual vector per PTC iteration
- Free-stream state as initial conditions.



## Sphere — Performance

k	N-PTC	N-GMRES	Memory(GB)	LST(s)	TST(s)				
$N_{\rm CV} = 64 {\rm K}$									
1	15	182	2.94	24	107				
2	15	181	3.91	20	112				
3	15	255	6.00	31	320				
$N_{\rm CV} = 322 {\rm K}$									
1	16	207	13.24	134	579				
2	16	212	14.05	132	620				
3	16	300	28.39	271	1, 879				
$N_{\rm CV} = 1 { m M}$									
1	17	275	39.48	486	1, 969				
2	17	277	45.52	536	2,150				
3	17	385	85.78	793	5,904				

# Flat Plate — Convergence

- Norm of the residual vector per PTC iteration
- Solution of (*k* + 1)-exact scheme is initialized with that of *k*-exact.



### Flat Plate — Drag

Computed value and convergence order of the drag coefficient and the skin friction coefficient at the point  $\mathbf{x} = (0.97, 0, 0.5)$ 

	<i>CD</i>			$C_f$		
NASA TMR		0.00286			0.00271	
k Mesh	1	2	3	1	2	3
$60 \times 34 \times 7$	0.00396	0.00233	0.00233	0.00350	0.00228	0.00222
$120 \times 68 \times 14$	0.00301	0.00281	0.00285	0.00283	0.00268	0.00271
$240 \times 136 \times 28$	0.00287	0.00286	0.00286	0.00274	0.00273	0.00273
Convergence order	2.8	3.3	5.4	3	3	5.1

#### Flat Plate — Performance

k	N-PTC	N-GMRES	Memory(GB)	LST(s)	TST(s)	
	$60 \times 34 \times 7$ mesh					
1	26	844	0.42	31	55	
2	26	1,009	1.35	42	124	
3	26	1,071	2.10	57	202	
	$120 \times 68 \times 14$ mesh					
1	28	1,436	5.24	510	713	
2	29	1, 864	8.30	742	1, 489	
3	29	2,041	14.63	825	2, 124	
	$240 \times 136 \times 28$ mesh					
1	29	2, 492	38.77	6, 222	7, 884	
2	27	3, 305	60.70	12, 353	18, 137	
3	27	2,906	121.81	23, 141	35, 412	
	k 1 2 3 1 2 3 1 2 3	k         N-PTC           1         26           2         26           3         26           1         28           2         29           3         29           1         29           2         27           3         27	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{tabular}{ c c c c c c c } \hline k & N-PTC & N-GMRES & Memory(GB) \\ \hline & & 60 \times 34 \times 7 \text{ mesh} \\ \hline 1 & 26 & 844 & 0.42 \\ \hline 2 & 26 & 1,009 & 1.35 \\ \hline 3 & 26 & 1,071 & 2.10 \\ \hline & & 120 \times 68 \times 14 \text{ mesh} \\ \hline 1 & 28 & 1,436 & 5.24 \\ \hline 2 & 29 & 1,864 & 8.30 \\ \hline 3 & 29 & 2,041 & 14.63 \\ \hline & & 240 \times 136 \times 28 \text{ mesh} \\ \hline 1 & 29 & 2,492 & 38.77 \\ \hline 2 & 27 & 3,305 & 60.70 \\ \hline 3 & 27 & 2,906 & 121.81 \\ \hline \end{tabular}$	$\begin{tabular}{ c c c c c c c c c c c c c c c c c c c$	

# Extruded NACA 0012 — $\tilde{\nu}$

Distribution of the turbulence working variable for the extruded NACA 0012 problem on the  $x_3 = 0$  plane, k = 3.



(a) Hexahedral mesh



(b) Mixed prismatic-hexahedral mesh

# Extruded NACA 0012 — Drag

Computed value and convergence order of the drag coefficient and the skin friction coefficient at the point x = (0.97, 0, 0.5)

k	$C_{Dp}$	$C_{Dv}$	$C_L$					
NASA TMR								
_	0.00607	0.00621	1.0910					
Hex mesh								
1	0.01703	0.00582	1.0619					
2	0.01702	0.00497	1.0507					
3	0.00301	0.00472	1.0417					
Mixed mesh								
1	0.01129	0.00574	1.0735					
2	0.00365	0.00565	1.0776					
3	0.00550	0.00536	1.0869					

### Extruded NACA 0012 — Performance

k	N-PTC	N-GMRES	Memory(GB)	LST(s)	TST(s)				
Hex mesh, $N_{\rm CV} = 100 {\rm K}$									
1	33	1, 154	4.77	317	744				
2	31	1, 788	6.82	730	2,097				
3	31	2,415	12.23	1,057	3, 215				
Mixed mesh, $N_{\rm CV} = 176 {\rm K}$									
1	34	1, 132	8.70	458	1,164				
2	32	1, 769	10.87	800	2,427				
3	31	2, 185	26.47	1,311	4,666				