Debunking the Residuals Myth:

Using *residuals* to create accurate discretization schemes

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Instead of introduction

Why I did Residual-based schemes research ?

- (1996) Leading the CFD/CAE group (Centrifugal Compressors) at COMOTI Bucharest

- **Challenge:** to perform LES of turbulence inside high-PR CC

- Write a new CFD code (together with Aerospace Department at "Polytechnica" Institute Bucharest) for industrial LES

- Found a few papers about early Residual-Distribution schemes

- Learned more about these scheme at a VKI Advanced CFD course

- Went to Lund Institute to learn LES of turbulence and develop a (hopefully) best-in-class LES algorithm, for industry (Dec.1997)

A short early history of MU-RDS

Multidimensional Upwind Residual Distribution scheme :

- Fluctuation-Splitting (RDS) proposed in 1986 by professor Phil Roe

- Developed by professors and students at Michigan University (Roe), VKI (Deconinck), Bordeaux University (Abgrall), Polytechnica di Bari, Lund (Caraeni), Univ. of Leeds (Hubbard) etc.

- Compact matrix distribution schemes for *steady* Euler and Navier-Stokes equations (E.van der Weide, H. Paillere), 1996.

- Second order RD scheme for LES of turbulence using *a residual-property preserving*, dual time-step approach (Caraeni, 1999).

A short early history of MU-RDS (cont.)

Multidimensional Upwind Residual Distribution scheme:

- Second order space-time RD scheme for unsteady simulations (2000, VKI) (using space-time integration/residual-distribution to achieve accuracy)
- Third order RD scheme for *steady inviscid* flow simulations (2000, LTH) (node gradient-recovery for quadratic solution representation)
- Third order RD scheme for the *unsteady turbulent* flow simulations (2001, LTH). (node gradient-recovery and residual-property satisfying)
- Third order results with above gradient-recovery idea reported by Rad and Nishikawa (2002, MU).
- High-order (>3) RD scheme for scalar transport equations (2002, BU & MU). (sub-mesh reconstruction for high-order solution representation)

"Third-order non-oscillatory fluctuation schemes for steady scalar conservation laws" M. Hubbard, 2008.

What is a Residual–Distribution scheme ?

$$\nabla \cdot \mathcal{F}(u) = 0$$

1. $\forall K \in \Omega_h$ compute : $\phi^K = \int_K \nabla \cdot \mathcal{F}_h(u_h)$

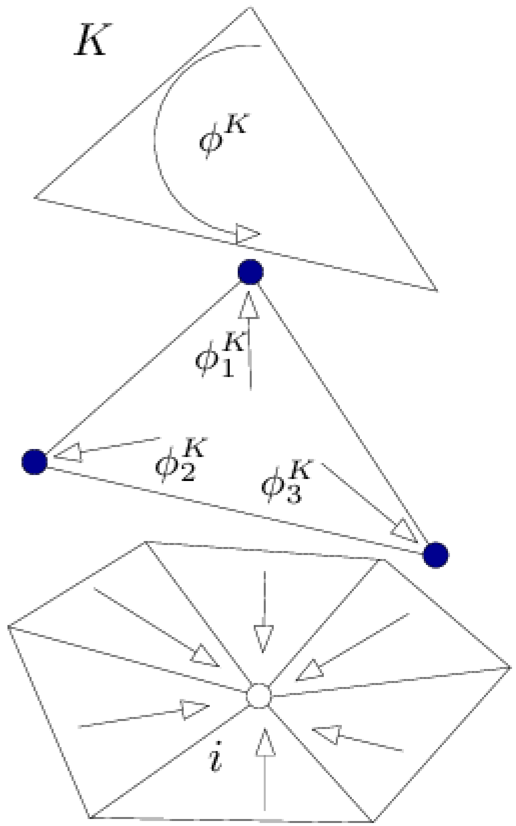
2. Distribution : $\phi^K = \sum_{i \in K} \phi_i^K$

   Distribution coeff.s : $\phi_i^K = \beta_i^K \phi^K$

3. Compute nodal values : solve algebraic system

$$\sum_{T|i \in T} \phi_i^K = 0, \quad \forall i \in \Omega_h \qquad (1)$$

$$|C_i| \frac{du_i}{dt} + \sum_{K|i \in K} \phi_i^K = 0$$



Ricchiuto, CEMRACS, 2012

A 3rd Order Residual-Distribution scheme for Navier-Stokes simulations

(Residual-property satisfying formulation)

(A Third Order Residual-Distribution Method for Steady/Unsteady Simulations: Formulation and Benchmarking, including LES, Caraeni, VKI, 2005)

High-order RD scheme
for Navier-Stokes equations

$$\begin{cases} \rho_{,t} + (\rho u_j)_{,j} = 0 \\ (\rho u_i)_{,t} + (\rho u_i u_j)_{,j} = -p_{,i} + \sigma_{ij,j} \\ (\rho e)_{,t} + (\rho u_j h)_{,j} = (u_i \sigma_{ij})_{,j} + (\lambda T_{,j})_{,j} \end{cases}$$

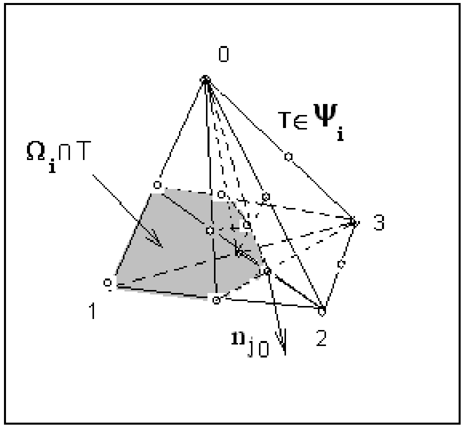
$$U = (\rho, \rho u_1, \rho u_2, \rho u_3, \rho e)^t$$

$$U_{,t} + F_{j,j}^{\;C} = F_{j,j}^{\;V}$$

Jameson dual-time algorithm

$$U_{,\tau} = -F_{j,j}^{\;c} + F_{j,j}^{\;v} - U_{,t}$$

$$\iiint_{\Omega} U_{,\tau}\, dv = \iiint_{\Omega} [(-F_j^{\;c} + F_j^{\;v})_{,j} - U_{,t}]\, dv$$



$$F_j^{\;C} = \begin{cases} \rho u_j \\ \rho u_1 u_j + p\delta_{1j} \\ \rho u_2 u_j + p\delta_{2j} \\ \rho u_3 u_j + p\delta_{3j} \\ \rho u_j h \end{cases}$$

$$F_j^{\;V} = \begin{cases} 0 \\ \sigma_{1j} \\ \sigma_{2j} \\ \sigma_{3j} \\ u_1\sigma_{1j} + u_2\sigma_{2j} + u_3\sigma_{3j} + \lambda T_{,j} \end{cases}$$

High-order RD scheme (cont.)
for Navier-Stokes equations

$$\Phi_T{}^c = \iiint_T F^c{}_{,j}.dv$$ ← Convection flux cell-residual

$$\Phi_T{}^v = \iiint_T F^v{}_{,j}.dv$$ ← Diffusion flux cell-residual

$$\Phi_T{}^{uns} = \iiint_T U_{,t}.dv$$ ← Unsteady term cell-residual

Update scheme for steady/unsteady simulations (Caraeni):

$$U_i^{n+1,k+1} = U_i^{n+1,k} - \frac{\delta\tau}{V_{\Omega_i}} \sum_{T,i\in T} B_i^T \left(\Phi_T{}^c - \Phi_T{}^v + \Phi_T{}^{uns}\right)^{n+1,k}$$

B_i^T ← Upwind matrix residual Distribution coefficient (bounded)

$$\sum_{i\in T} B_i^T = I$$

(conservativity)

High-order RD scheme (cont.)
for Navier-Stokes equations

Distribution schemes (for preconditioned system):

Low **D**iffusion **A** (**LDA**)

$$B_i^{T,LDA} = K_i^+ \left(\sum_j K_j^+\right)^{-1}$$

Lax-**W**endroff (**LW**)

$$B_i^{T,LW} = \left[\frac{1}{4} I + \eta \frac{1}{2} K_i \left(\sum_j \left| K_j \right|\right)^{-1}\right]$$

$$K_i = -\frac{1}{3} F_{j,U} n_{j,i} = \frac{1}{3} R_i \lambda_i R_i^{-1}$$

$$K_i^+ = \frac{1}{3} R_i \lambda_i^+ R_i^{-1}$$

$$K_i^- = \frac{1}{3} R_i \lambda_i^- R_i^{-1}$$

$$\Phi_T^c = \sum_1^4 K_i U_i$$

→ Computes the convective cell residual with second order accuracy (linear data)

High-order RD scheme (cont.)

How to construct a 3rd-order RDS (Ph.D. 2000, LTH):

1. Use (upwind or upwind-biased) uniformly bounded residual-distribution coefficients (linearity/accuracy preserving RD scheme), and apply to total cell-residual

2. Compute the total cell residual ***(convective + diffusive + unsteady terms)*** *with the required accuracy:*

- we used condition-1 + linear solution, second order accurate integration for 2^{nd} order RDS
- we need to use condition-1 + use quadratic reconstruction, 3^{rd} order accurate integration for 3^{rd} order RDS

The idea is to use the same accuracy-preserving RD scheme, as for second order schemes, but compute the total cell residual with 3^{rd} order accuracy.

High-order RD scheme (cont.)

Convection residual discretization, 3rd order.

$$Z = \sqrt{\rho}(1, u_1, u_2, u_3, H)$$

Use parameter variable Z and assume a quadratic variation over the tetrahedral cell.

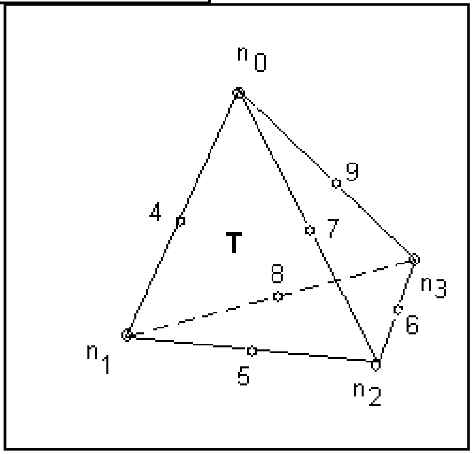
$Z_{,j}$ computed with 2nd order accuracy (multi-step algorithm)

Cell-residual in integral form:

$$\Phi_T{}^c = \iiint_T F_{,j}{}^c . dv = \iint_{\partial T} F^c . \overrightarrow{dS}$$

$$\overline{Z}^{(mid)} = \frac{\overline{Z}^{i_0} + \overline{Z}^{i_1}}{2} + \frac{(\overline{Z}_{,j}^{i_0} - \overline{Z}_{,j}^{i_1})}{8}(\vec{r}^{i_1} - \vec{r}^{i_0})$$

$$F^c = \begin{Bmatrix} Z_0 Z_j \\ Z_1 Z_j + p\delta_{1j} \\ Z_2 Z_j + p\delta_{2j} \\ Z_3 Z_j + p\delta_{3j} \\ Z_4 Z_j \end{Bmatrix}$$



$$p = \frac{\gamma - 1}{\gamma}(Z_0 Z_4 - \frac{Z_1^2 + Z_2^2 + Z_3^2}{2})$$

$$H = c_p T + \frac{u_i^2}{2}$$

High-order RD scheme (cont.)

Convection residual discretization, 3rd order.

$$\Phi_T{}^c = \iint_{\partial T} F^c . \overrightarrow{dS} = \sum_{i=1}^{4} \{ \iint_{face_i} (F_j{}^c \frac{n_{j,i}}{\left\| n_{j,i} \right\|} d\sigma)\}$$

$$\iint_{face_i} (F_j{}^c \bar{n}_{j,i}) d\sigma = \begin{cases} \bar{n}_{j,i} \iint_{face_i} (Z_0 Z_j) d\sigma \\ \bar{n}_{j,i} \iint_{face_i} (Z_1 Z_j + p\delta_{1j}) d\sigma \\ \bar{n}_{j,i} \iint_{face_i} (Z_2 Z_j + p\delta_{2j}) d\sigma \\ \bar{n}_{j,i} \iint_{face_i} (Z_3 Z_j + p\delta_{3j}) d\sigma \\ \bar{n}_{j,i} \iint_{face_i} (Z_4 Z_j) d\sigma \end{cases}$$

$$I_{Z_J Z_k}^{face_i} = \iint_{face_i} (Z_k Z_j) d\sigma$$

$$\iint_{face_i} (Z_k Z_j) d\sigma = \sum_{i_0, i_1 = 1}^{6} \{ Z_k^{i_0} Z_j^{i_1} \iint_{face_i} H^{(i_0)} H^{(i_1)} d\sigma \}$$

$$\iint_{face_i} H^{(j)} H^{(k)} d\sigma = A_{face_i} [I_{HH}]_{j,k}$$

$[I_{HH}]_{j,k}$ Pre-computed matrix

High-order RD scheme (cont.)

Diffusion residual discretization, 3rd order.

$$\Phi_T{}^v = \iiint_T F_{,j}{}^v dv = \oiint_{\partial T} F^v . \overrightarrow{ds}$$

Assuming a quadratic variation of the Z variables over the cell, the diffusive flux vector integral can be computed over the cell-face.

Use the values of the Z variable and its gradients,
defined in the nodes of the high-order FEM tetrahedral-cell.

$$\Phi_T{}^v = \oiint_{\partial T} F^v . \overrightarrow{ds} = \sum_{k=1}^{4} \overline{F}^v{}_{(face_k)} . \vec{n}_k$$

$$u_{i,\alpha} = \frac{[(\sqrt{\rho} u_i)_{,\alpha} - u_i(\sqrt{\rho})_{,\alpha}]}{\sqrt{\rho}}$$

High-order RD scheme (cont.)

Unsteady residual discretization , 3rd Order.

$$U_{,t} = \frac{3U^{n+1,k} - 4U^{n} + U^{n-1}}{2.\Delta t}$$

2^{nd} order discretization in time, and 3^{rd} order in space:

$$\Phi_T{}^{v} = \iiint_T U_{,t}.dv = \iiint_T \sum_{\alpha=0}^{9} Q^{(\alpha)} U_{,t}{}^{(\alpha)}.dv$$

$$\Phi_T{}^{v} = \sum_{\alpha=0}^{9} U_{,t}{}^{(\alpha)} \iiint_T Q^{(\alpha)}.dv$$

$$I_\alpha = \iiint_T Q^{(\alpha)}.dv;$$

$$I_\alpha = -0.05V_T; \alpha = 0,..,3$$

$$I_\alpha = +0.20V_T; \alpha = 4,..,9$$

High-order RD scheme (cont.)

Monotone shock capturing

1. Shock detection $\Psi = \Psi(\frac{h^2 \nabla^2 p}{p_{av}})$ or $\Psi = \Psi(\frac{|\nabla . V|^2}{|\nabla \times V|^2})$ or $\Psi = \frac{|\Phi^{\Omega}|}{\sum_{1}^{\#nodes} |\Phi_j^N|}$

2. Blending between the high-order scheme and a first order positive RD scheme (the N-scheme)

$$\Phi_i^T = (1-\psi).\Phi_i^{LDA} + \psi.\Phi_i^N$$
$$where: \psi = f(P, \rho, ..)$$

ψ = 0 for a smooth flow
= 1 (discontinuity detected)

Summary of this 3rd order RD algorithm

- Uses a Multi-D Upwind Residual-Distribution scheme

- Formulated for fully unstructured grids (tetrahedrons),

- Compact scheme, highly efficient parallel algorithm.

- Implicit time integration (dual time-stepping algorithm).

- 3rd - order accuracy in space (using FEM integration)

- 2nd - order time discretization (BDF2 scheme)

- Acceleration techniques: **preconditioning**, point-implicit relaxation, geometric multi-grid, etc.

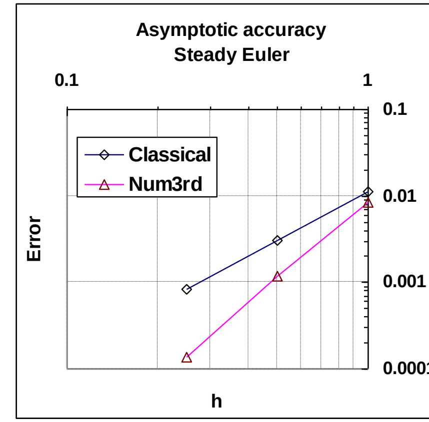
Results

- Steady inviscid flows
  a. Sine-bump channel flow inlet Mach 0.5.
- Steady viscous flows
  c. Laminar flat-plate boundary layer, Reynolds 2000.
- Unsteady inviscid flows
  b. Vortex transport by uniform flow Mach 0.04.
- Shock capturing
  d. Shock vortex interaction.
- Large Eddy Simulation
  e. LES of turbulent channel flow.

Steady Euler

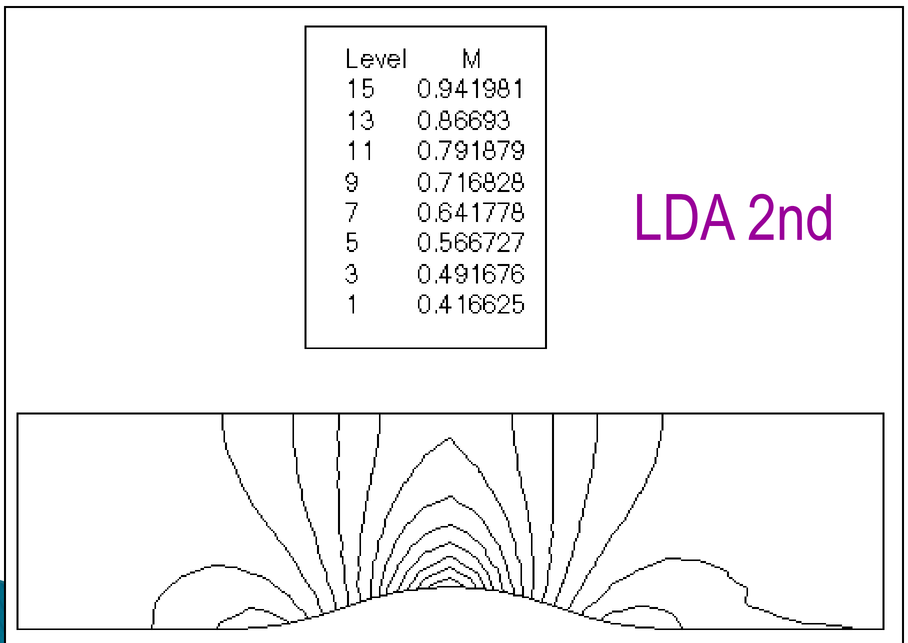
Inviscid sine bump channel flow:

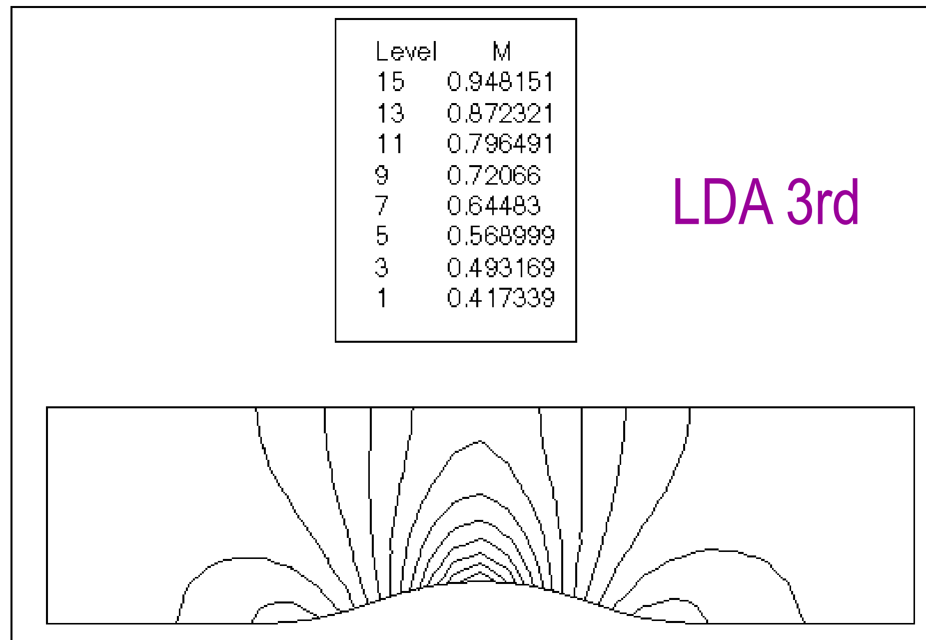
- Inlet Mach number 0.5



Maximum entropy production:

- 2nd order scheme E=2.3 e-4
- 3rd order scheme E=5.1 e-6
- Cell centered FVM(2ndO) E=4.2 e-4

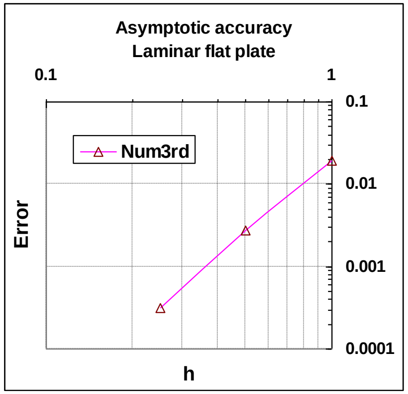


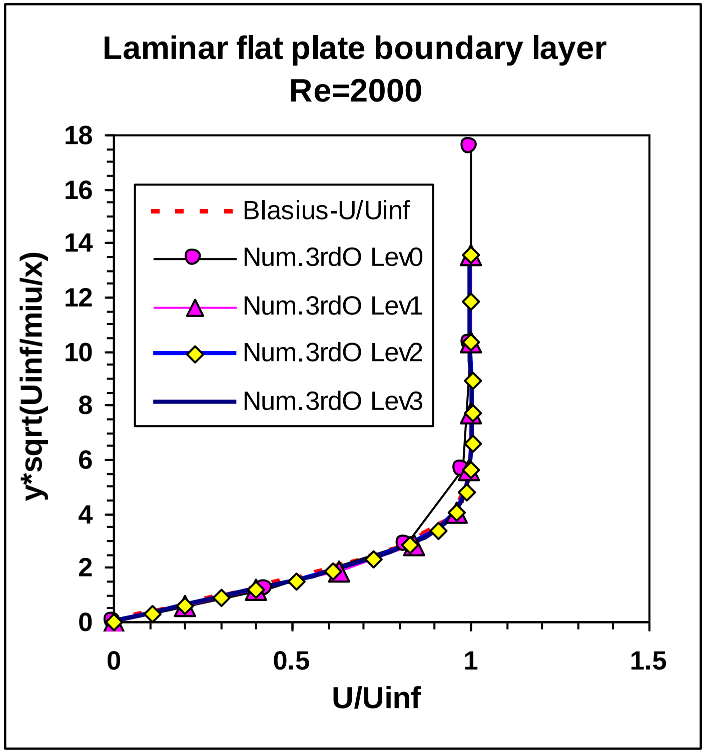


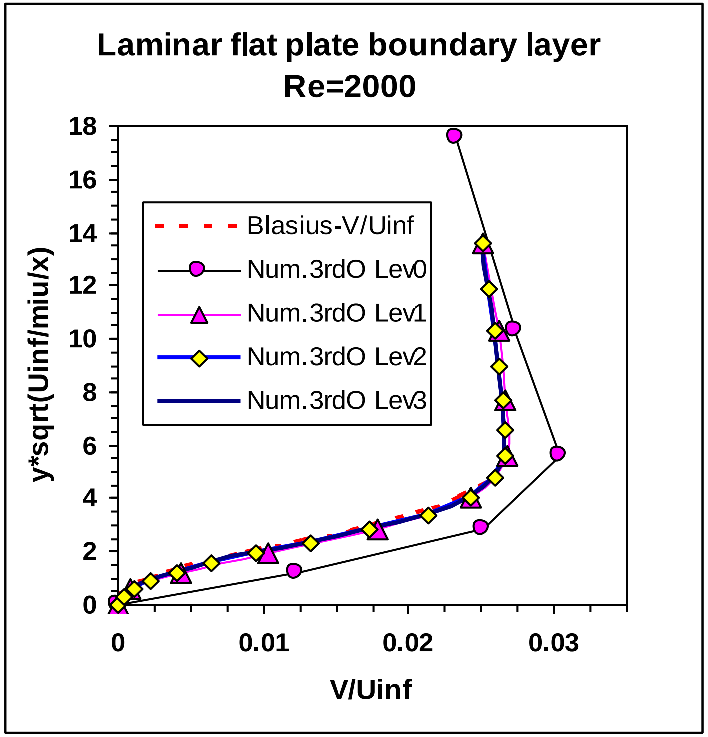
RDS Solution on 32x8 grid

Steady Navier-Stokes

Laminar viscous flow over a flat plate:
- Infinite Mach # 0.5, Re 2000
- Grid0 of 32x18 grid points



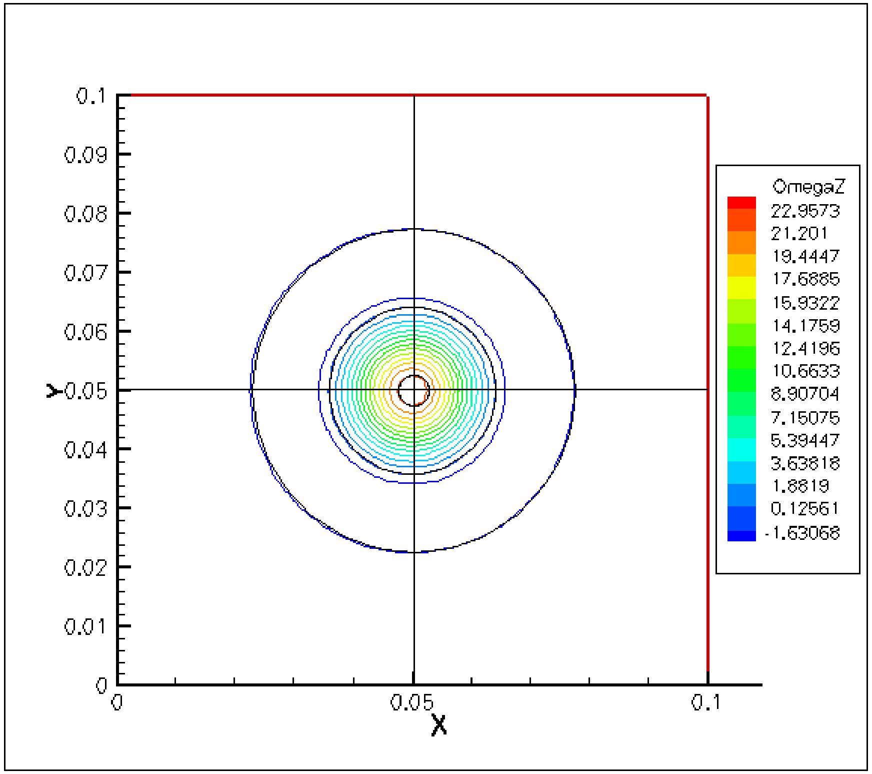




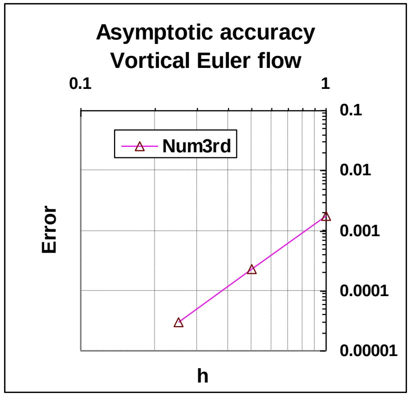
Unsteady Euler

Vortex transport by Inviscid flow.
- Uniform flow Mach = 0.04

Third order results, grid 64x64



Unsteady Euler (cont.)



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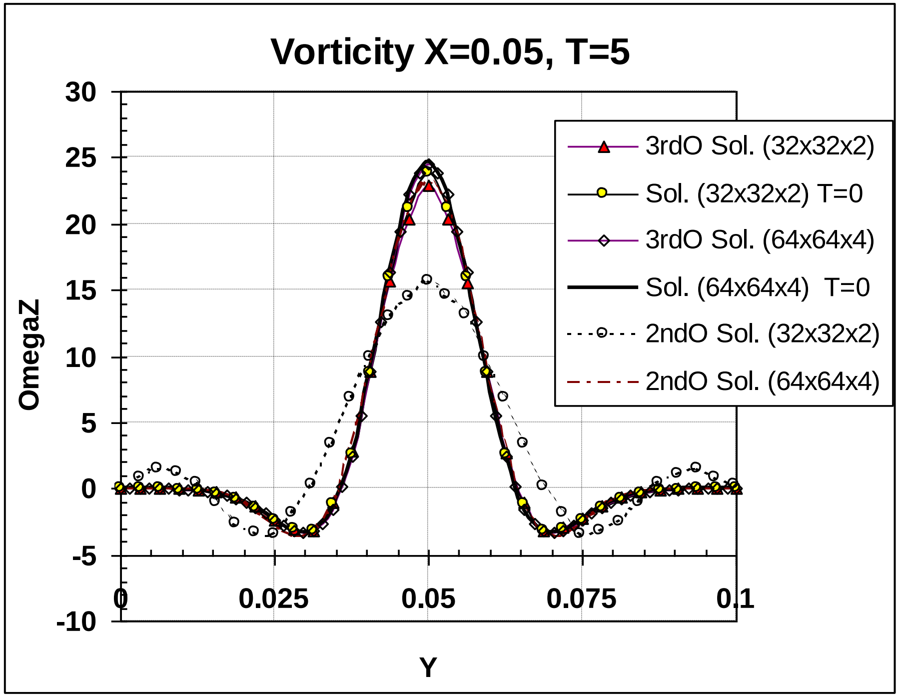

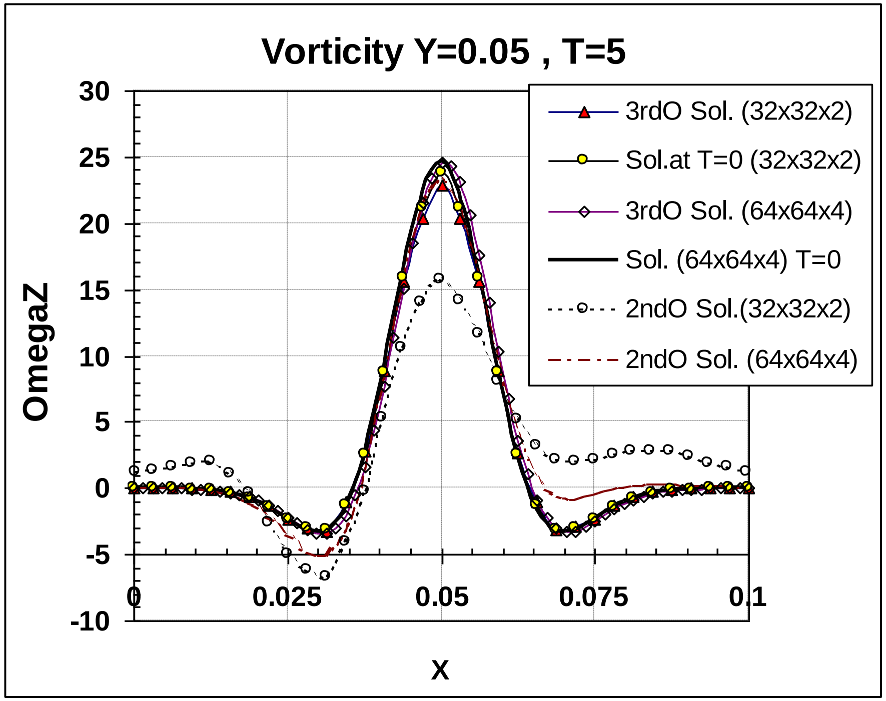

Unsteady Euler (cont.)

Vortex transport by Inviscid flow.
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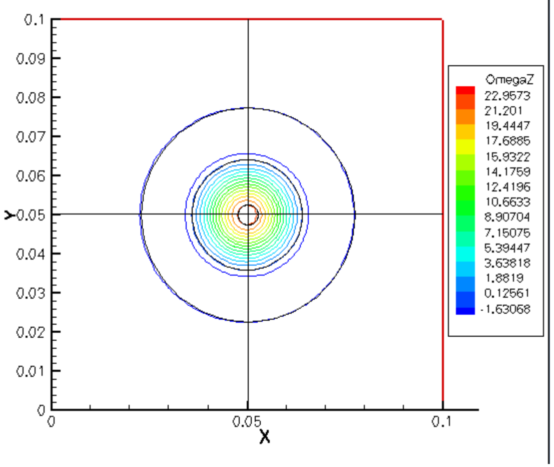
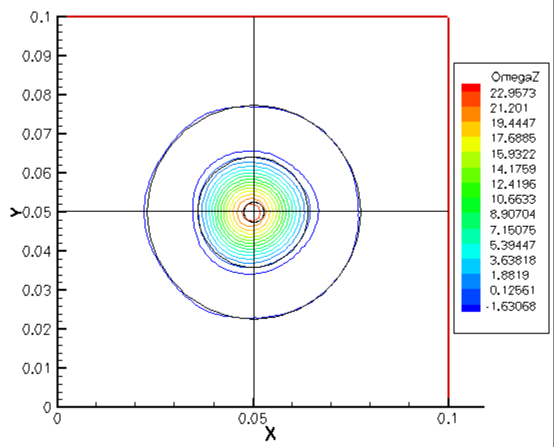
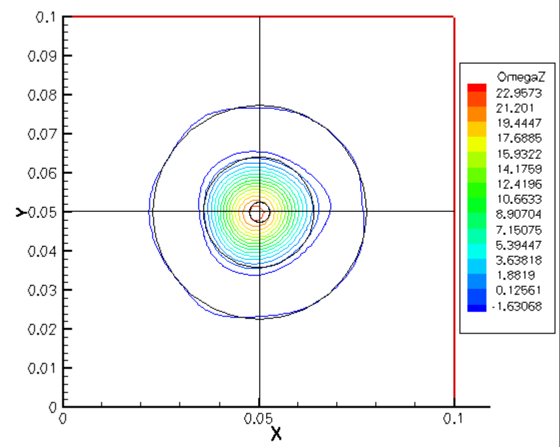


T= 0

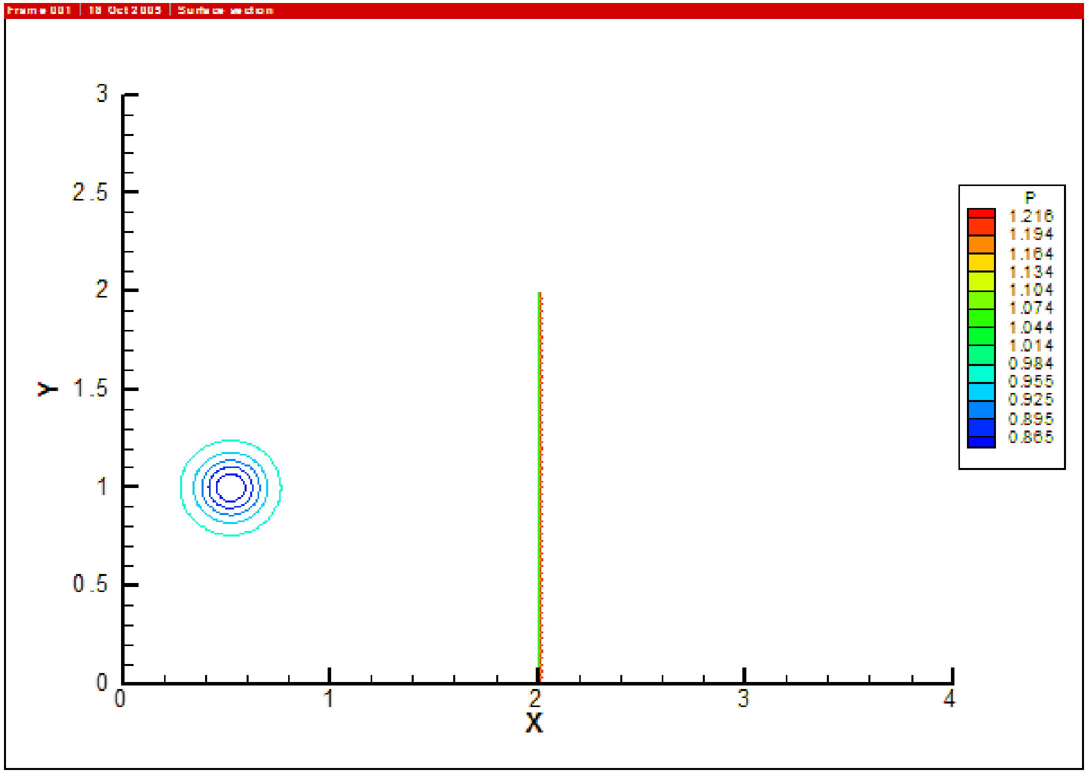


T = 12 periods



T = 24 periods

Shock vortex interaction



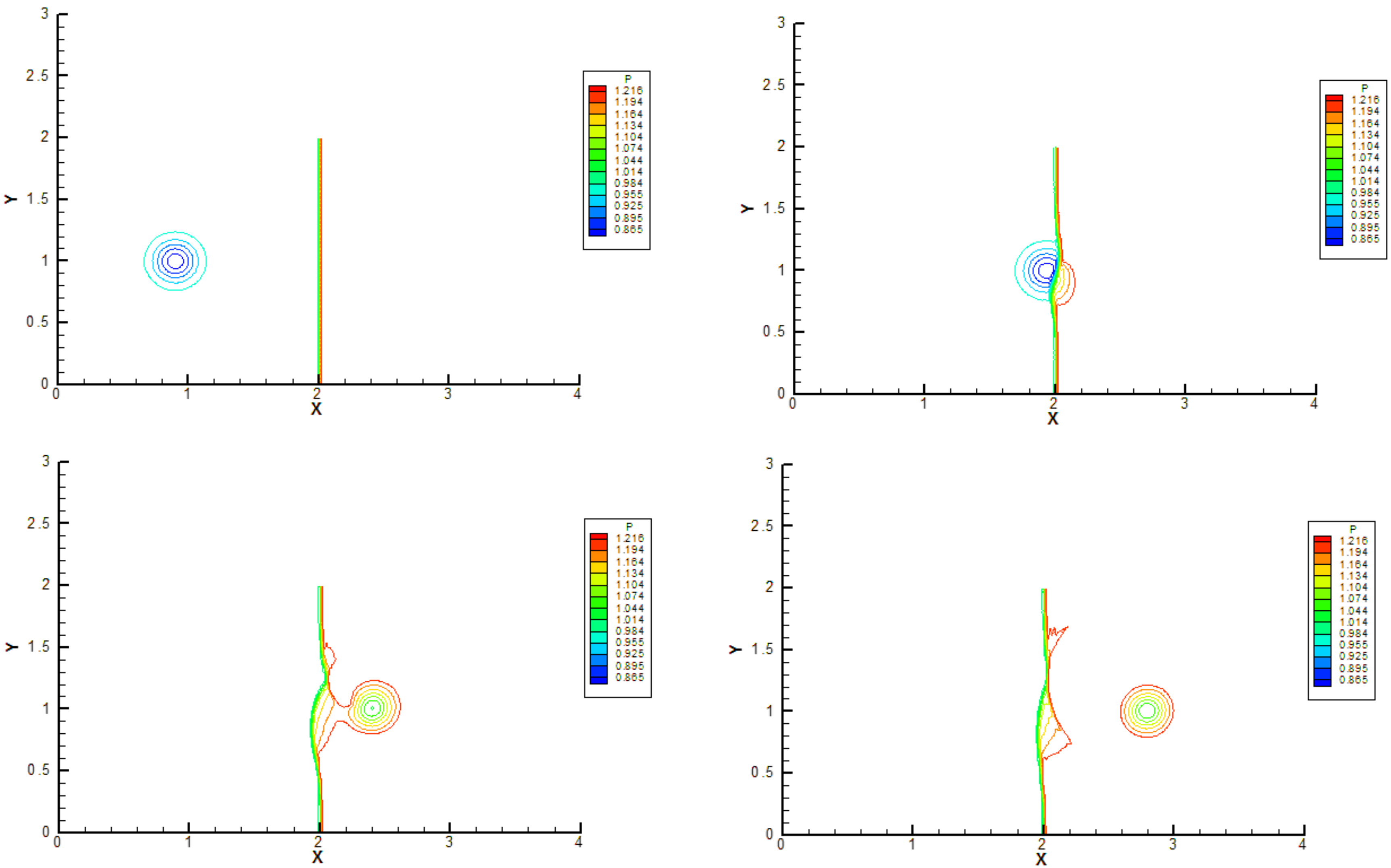
Shock-vortex interaction:

- Steady shock in mid channel

- Vortex moves from left to right

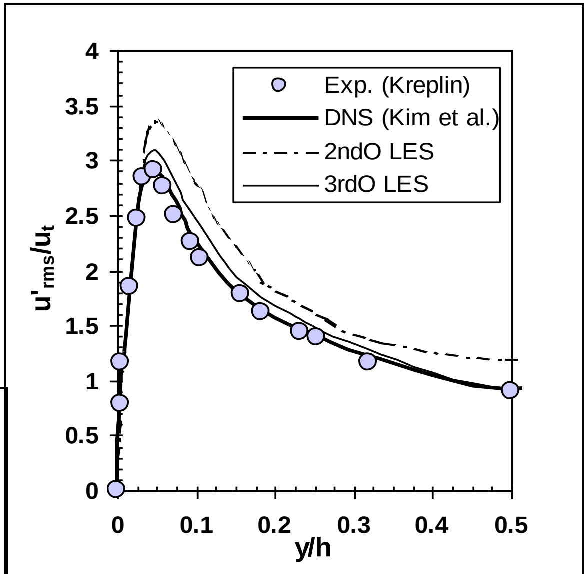
Note: vortex preserving strength, before and after crossing shock

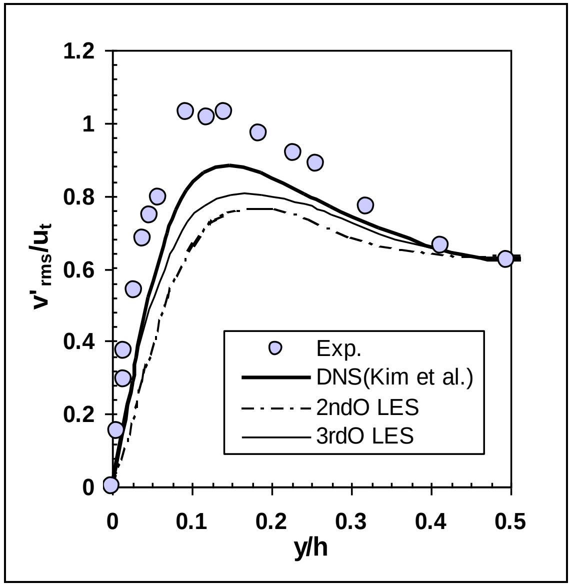
Shock vortex interaction

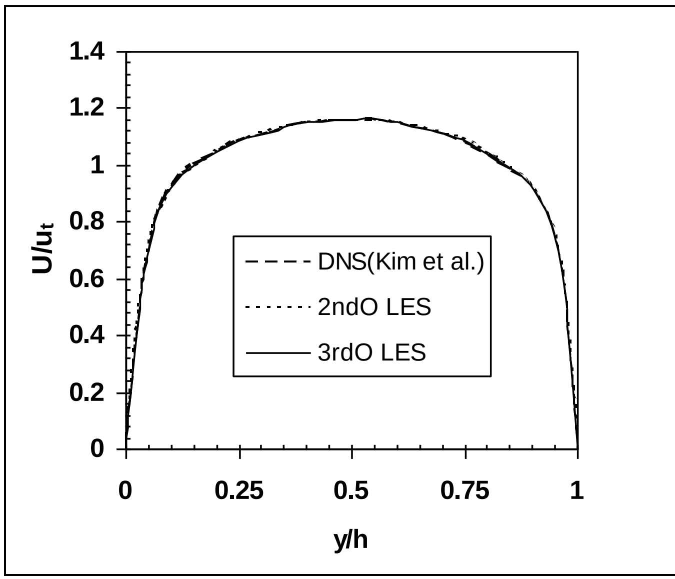


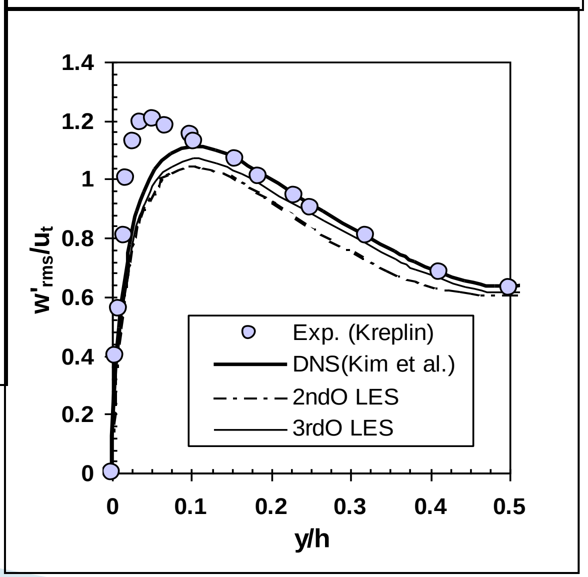
LES of turbulent channel flow

Turbulent channel flow:
- **Reynolds # = 5400**
- **Re_t= 344**









LES Smagorinsky	u_t/U_b	U_c/U_b
3rd O **MDU**	0.0640	1.164
2nd O **MDU**	0.0627	1.186
DNS (Kim et al.)	0.0643	1.162

Multidimensional Residual-Distribution Solving for flow and "optimal" mesh

(Grids and solutions from Residual Minimization, Nishikawa, Rad, Roe, 2001)

Solving for flow and solution using RDS

Main ideas:

- Use multidimensional RDS to compute solution at vertices,

- There are 5-6 times less vertices than cells in the tetrahedral-cells mesh …

- Use the extra “conditions” (cell-residual must be driven to zero) to define mesh motion equations, using an LSQ approach,

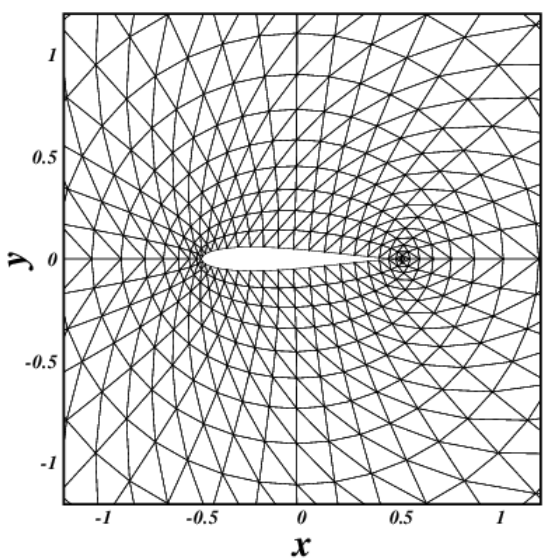
- Algorithm computes an improved solution on a “optimized” mesh, which minimizes the overall error in a specific norm.

(Nishikawa, 2001)

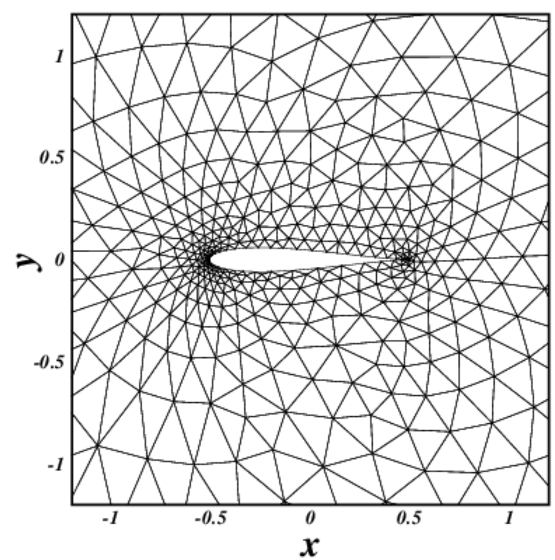
Solving for flow and solution using RDS

Flow over Joukowsky airfoil (known theoretical solution)

(Nishikawa, 2001)



Original mesh

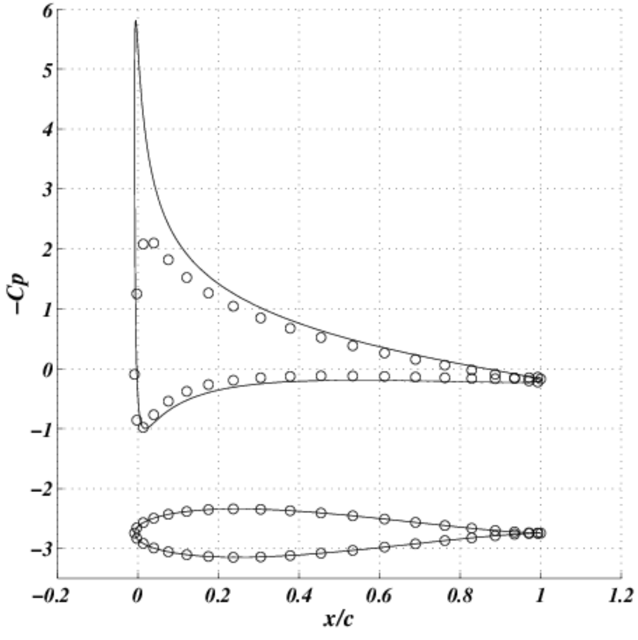


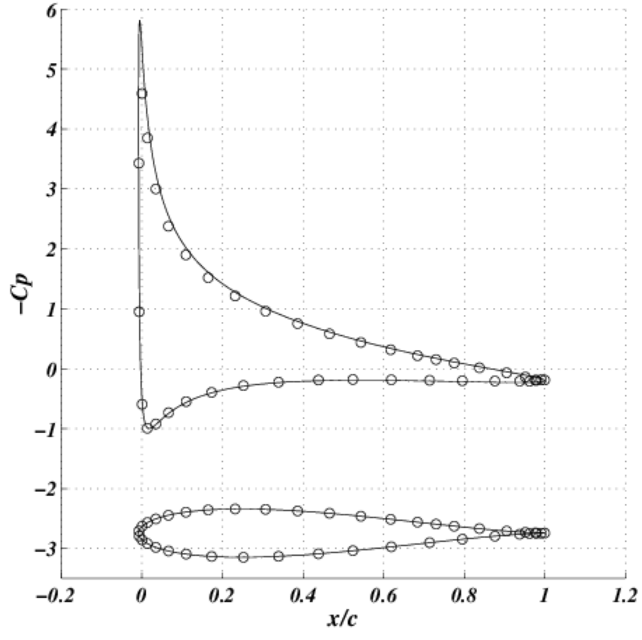
Adapted mesh

Solving for flow and solution using RDS

Flow over Joukowsky airfoil (known theoretical solution)

(Nishikawa, 2001)





Original mesh solution Cp, o

Adapted mesh Cp, o

Comparison with theoretical solution ----

Why using Multi-D Residual-Distribution schemes ?

- Resolves better real complex multidimensional physics (!)

- It is much more accurate that 2nd order Finite Volume method,

- It is capable of handling complex geometry (formulated tetrahedrons),

- Has a compact stencil algorithm, at every step (which leads to very efficient parallelization),

- It is relatively to easy to extend to high order accuracy (at least from 2nd to 3rd order), and 3rd order results are significantly more accurate,

- Can be used to **solve for flow and node location** - using the combined RDS/LSQ approach - for an optimal solution, on a given mesh topology.

Backup slides

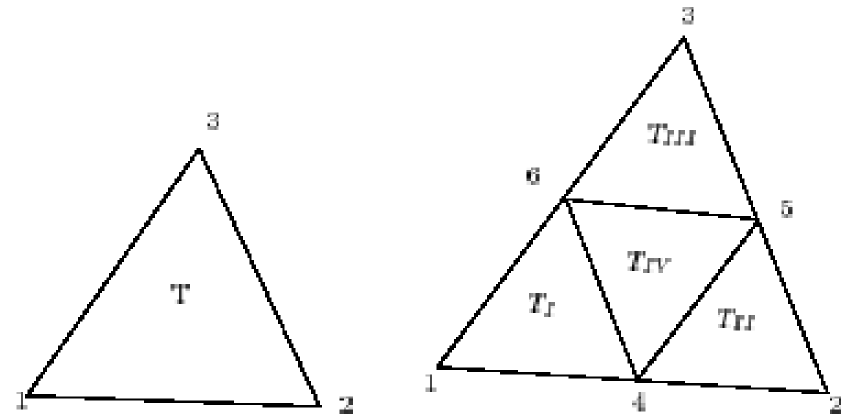
High-order Residual Distribution Scheme for Scalar Transport Equations on Triangular Meshes

From “*High-order fluctuations schemes on triangular meshes*”
R.Abgrall and Phil Roe, 2002

High-order RD scheme for scalar equations

$$u_\sigma^{n+1} = u_\sigma^n - \frac{\Delta t}{|C'_\sigma|} \sum_{T,\sigma\in T} \Psi_\sigma^T$$

$$\Psi_\sigma^T = \sum_{T'_T \subset T, \sigma \in T'_T} \Phi_\sigma^{T'_T}$$



$$\sum_{T'_T \subset T, \sigma \in T} \Phi_\sigma^{T'_T} = \int_T \text{div } f^h(u^h)dx.$$

$$\sum_{j=1}^{N} \beta_j = \sum_{j=1}^{N} \hat{\beta}_j = 1 \quad \text{Conservation}$$

$\beta_j \hat{\beta}_j \geq 0$ Monotonicity

$\hat{\beta}_j$ is bounded High-order accuracy

$$\beta_j = \frac{\phi_j^M}{\phi}, \qquad \hat{\beta}_j = \frac{\phi_j^H}{\phi^H}$$

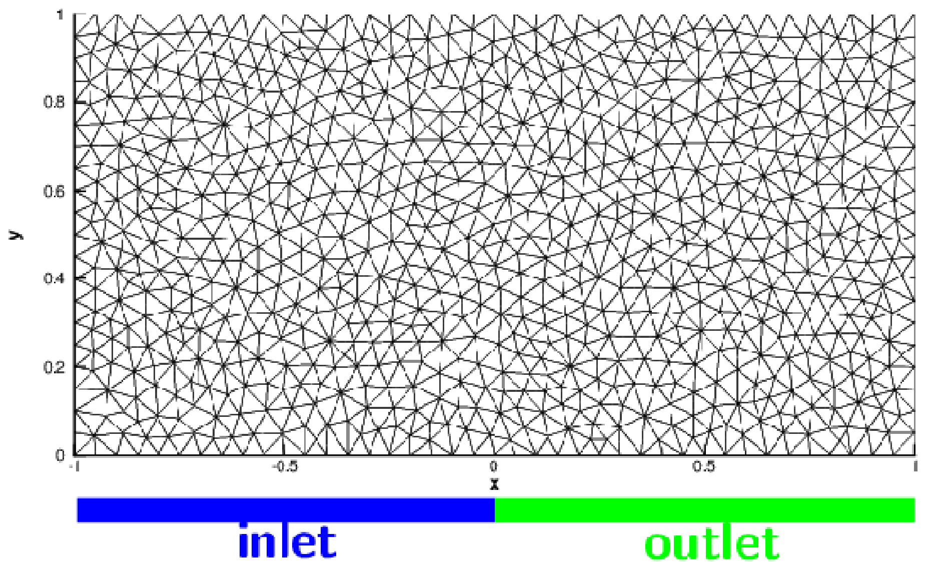
$$\hat{\beta}_j = \frac{\beta_j^+}{\sum_j \beta_j^+}$$

$$\Phi^H = 2\Phi^{IV} + \frac{2}{3}(\Phi^I + \Phi^{II} + \Phi^{III})$$

High-order RD scheme for scalar equations

Scalar example : $\vec{a} \cdot \nabla u = 0$ with $\vec{a} = (y, 1 - x)$ and bcs

$$u_{\text{in}} = \begin{cases} \cos(2\pi(x+0.5))^2 & \text{if} \quad x \in [-0.75, -0.25] \\ 0 & \text{otherwise} \end{cases}$$



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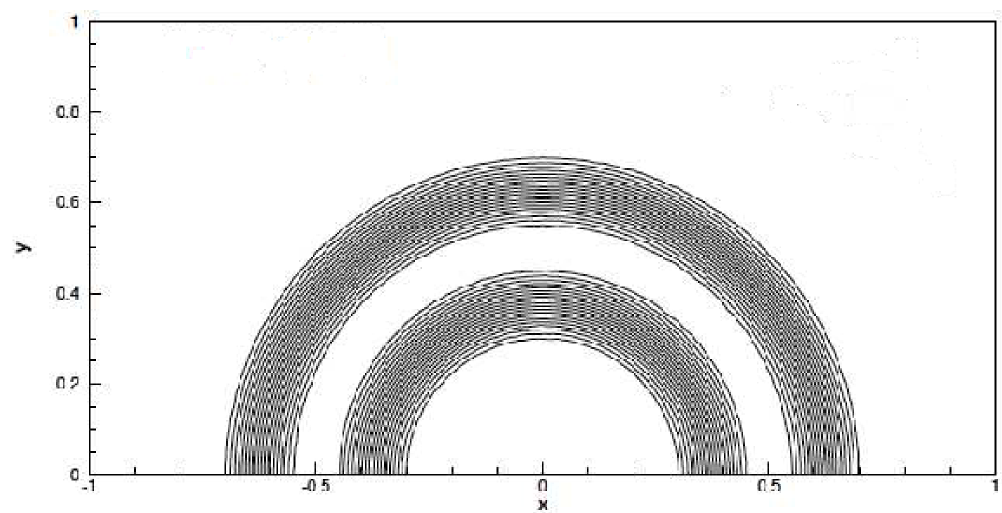
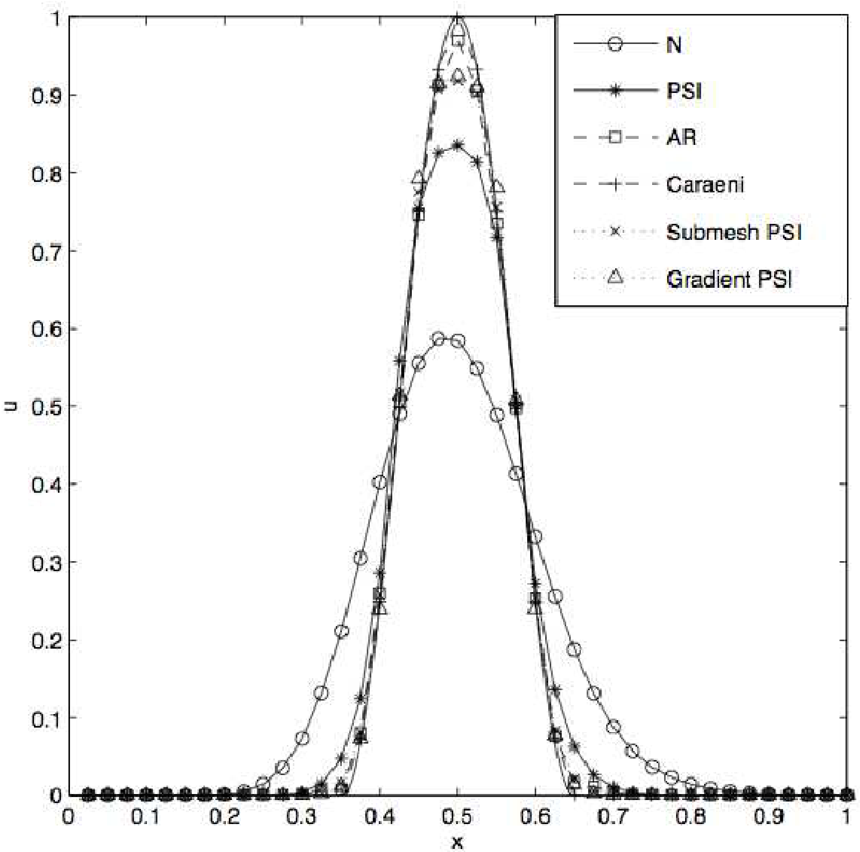
Scalar example : $\vec{a} \cdot \nabla u = 0$ with $\vec{a} = (y, 1 - x)$ and bcs

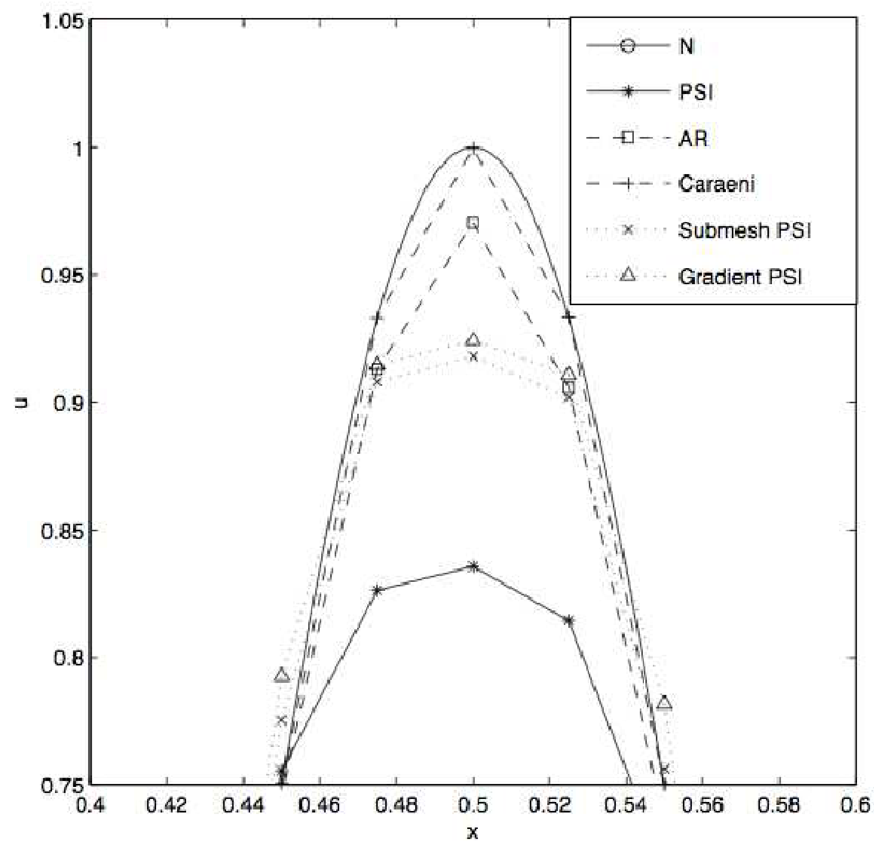
$$u_{\text{in}} = \begin{cases} \cos(2\pi(x + 0.5))^2 & \text{if} \quad x \in [-0.75, -0.25] \\ 0 & \text{otherwise} \end{cases}$$



High-order RD scheme for scalar equations

From (Hubbard, J. Computational Physics 2007)





Space-time Residual Distribution schemes for unsteady simulations

"*Status of Multidimensional Residual Distribution Schemes and Applications in Aeronautics*",
Deconinck et al. AIAA 2000-2328.

"*Construction of 2nd order monotone and stable residual distribution schemes: the unsteady case*",
Abgrall et al. VKI 2002

Space-time RD for unsteady simulations

$$u^h(x,t) = u^n(x)\frac{t_{n+1}-t}{\Delta t} + u^{n+1}(x)\frac{t-t_n}{\Delta t}$$

$\longrightarrow$

$$\Phi_{x.t} = \int_\Omega \int_{t_n}^{t_{n+1}} \left(\frac{\partial u^h}{\partial t} + A_i \frac{\partial u}{\partial x_i}\right) dx.dt$$

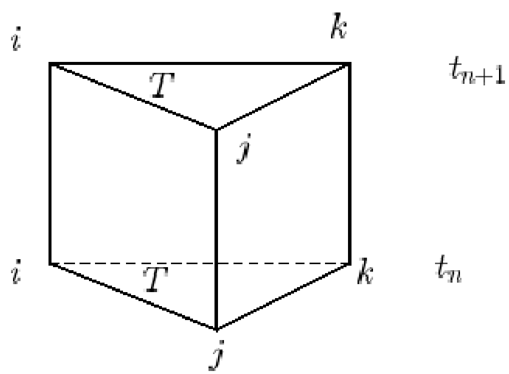
$$\Phi_{x,t} = \sum_{i\subset\Omega} \Phi_i^{\,t} + \Phi^s$$

$$\Phi_i^{\,t} = \frac{\Omega}{3}(u_i^{\,n+1} - u_i^{\,n})$$

$$\Phi^s = \frac{\Delta t}{2}\sum_{i\subset\Omega} K_i(u_i^{\,n+1} + u_i^{\,n})$$

$\Phi_{i,n}^{\;N} = 0$ “Upwind-in-time”

$$\Phi_{i,n+1}^{\;N} = \frac{V_\Omega}{3}(u_i^{\,n+1} - u_i^{\,n}) + \frac{\Delta t}{2}K_i^{\,+}(u_i^{\,n+1} - \overline{u}^{\,n+1}) + \frac{\Delta t}{2}K_i^{\,+}(u_i^{\,n} - \overline{u}^{\,n})$$



$$\overline{u}^{\,n+1} = \left(\sum_{i\subset\Omega} K_i^{\,-}\right)^{-1} \sum_i K_j^{\,-} u_j^{\,n+1}$$

$$\overline{u}^{\,n} = \left(\sum_{i\subset\Omega} K_i^{\,-}\right)^{-1} \sum_i K_j^{\,-} u_j^{\,n}$$

Space-time RD for unsteady simulations

LDA space-time scheme:

$$\Phi_{i,n}^{LDA} = 0$$

$$\Phi_{i,n+1}^{LDA} = (\beta_i + \frac{1}{6})\Phi_i^t + (\beta_i - \frac{1}{12})\sum_{j\neq i}\Phi_j^t + \beta_i\Phi^s$$

$$\beta_i = K_i^+ (\sum_j K_j^+)^{-1}$$

LDA+N space-time scheme:

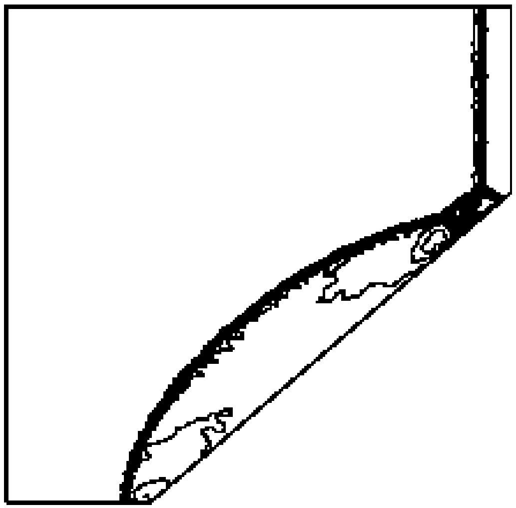
$$\Phi_{i,n}^{B} = 0$$

$$\Phi_{i,n+1}^{B} = l\Phi_{i,n+1}^{N} + (1-l)\Phi_{i,n+1}^{LDA}$$

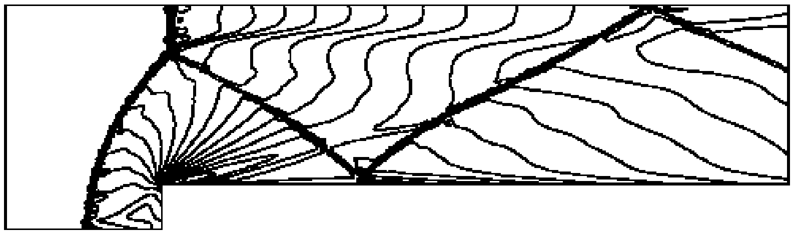
$$l = \frac{\left|\Phi_{x,t}\right|}{\sum_j \left|\Phi_{i,n+1}^{N}\right|}$$

"Status of Multidimensional Residual Distribution Schemes and Applications in Aeronautics" Deconinck et al. 2000

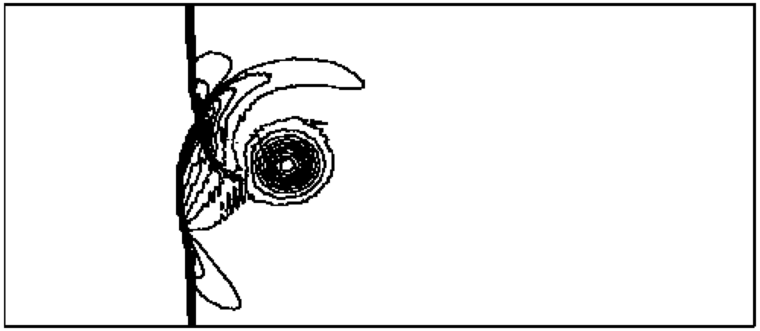
Space-time RD for unsteady simulations



Reflection of a planar
shock from a ramp (density plot)



Shock reflection on a forward facing
step (density plot)



Shock-vortex interaction

From “Construction of 2nd order monotone and stable residual distribution schemes: the unsteady case”, Abgrall et al. 2002

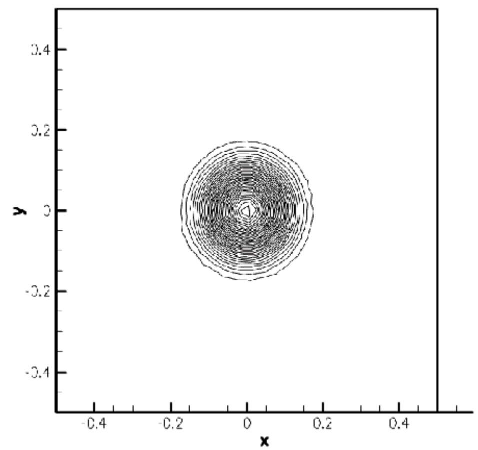
Space-time RD for unsteady simulations

Convection of vortex

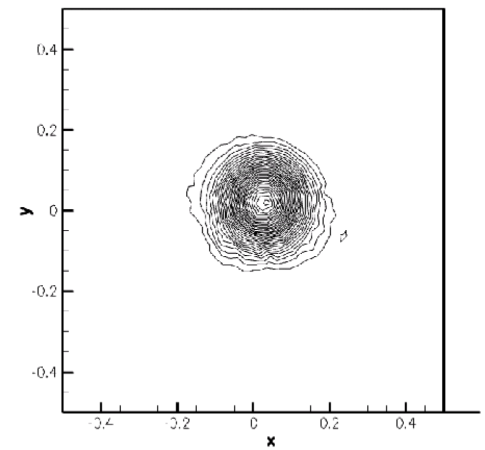
- Periodic BC's
- One revolution simulated
- 2nd and 3rd order ST-RDS compared

- Pressure contours displayed

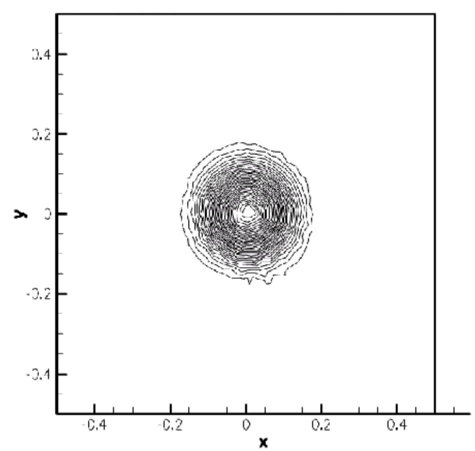
From (**Nadege Villedieu , VKI Ph.D., 2009**)



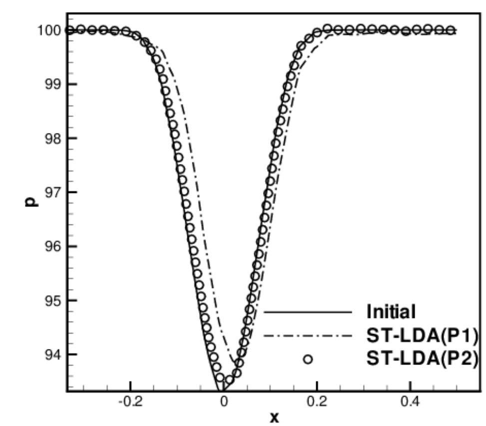
(a) $t = 0s$



(b) $t = \frac{1}{6}s$, ST-LDA(P^1)



(c) $t = \frac{1}{6}s$, ST-LDA(P^2)



(d) $t = \frac{1}{6}$, Slice at $y = 0$