NATIONAL TECHNICAL UNIVERSITY OF ATHENS
Parallel CFD & Optimization Unit
Laboratory of Thermal Turbomachines

Pseudo-Compressibility based implicit solver in OpenFOAM

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Incompressible flow solvers

- **Aim:** Solution of the incompressible Navier-Stokes equations
- **Problem:** No inherent coupling for the continuity and momentum equations
- **Popular solution:** The SIMPLE family methods. Loose coupling through a prediction-correction scheme. Inherently segregated algorithm. Slow convergence
- **OpenFOAM (standard) implementation:** Segregated solution of the momentum equations
- **Different approach:** Implicit solver. Simultaneous solution of the continuity and momentum equations. Faster convergence. More robust. Less memory efficient.
- **Motivation:** *a)* Faster primal and adjoint equations solver, *b)* Implicit treatment of the stiff ATC term in the OpenFOAM environment.

Incompressible Navier-Stokes equations

- **Equations/constraints**

$$R_i^{\upsilon} = \frac{\partial(\upsilon_i \upsilon_j)}{\partial x_j} - \frac{\partial}{\partial x_j}\left[(\nu + \nu_t)\left(\frac{\partial \upsilon_i}{\partial x_j} + \frac{\partial \upsilon_j}{\partial x_i}\right)\right] + \frac{\partial p}{\partial x_i} = 0$$

$$R^p = \frac{\partial \upsilon_j}{\partial x_j} = 0$$

Pseudo-compressibility approach

- **Equations/constraints reformulation**

$$R_i^{\upsilon} = \frac{\partial \upsilon_i}{\partial t} + \frac{\partial (\upsilon_i \upsilon_j)}{\partial x_j} - \frac{\partial}{\partial x_j}\left[(\nu + \nu_t)\left(\frac{\partial \upsilon_i}{\partial x_j} + \frac{\partial \upsilon_j}{\partial x_i} \right) \right] + \frac{\partial p}{\partial x_i} = 0$$

$$R^p = \frac{1}{\beta^2}\frac{\partial p}{\partial t} + \frac{\partial \upsilon_j}{\partial x_j} = 0$$

- **Purpose**

Elliptic system
Inco N-S

→ ***Pseudo-compressibility*** →

Hyperbolic system –
Viscous,inco N-S

- **Discretization**

Convective fluxes

$$F(q_L, q_R) = \frac{1}{2}\left[F(q_L) + F(q_R)\right] - \frac{1}{2}\left|A_{Roe}^{LR}\right|(q_R - q_L) \qquad q = [p \quad \upsilon_i]^T$$

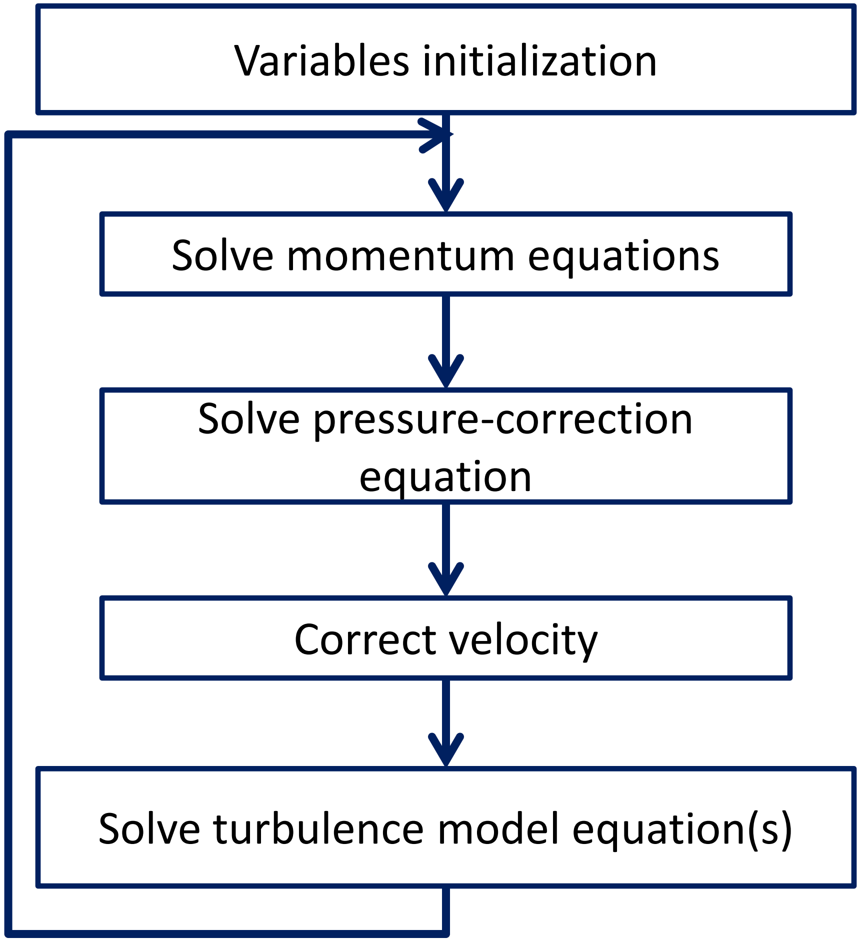
$$\left|A_{Roe}^{LR}\right| = R|\Lambda|R^{-1}, \quad \Lambda = diag[\phi \quad \phi \quad \phi + c \quad \phi - c], \quad \phi = u_k n_k$$

Local time stepping

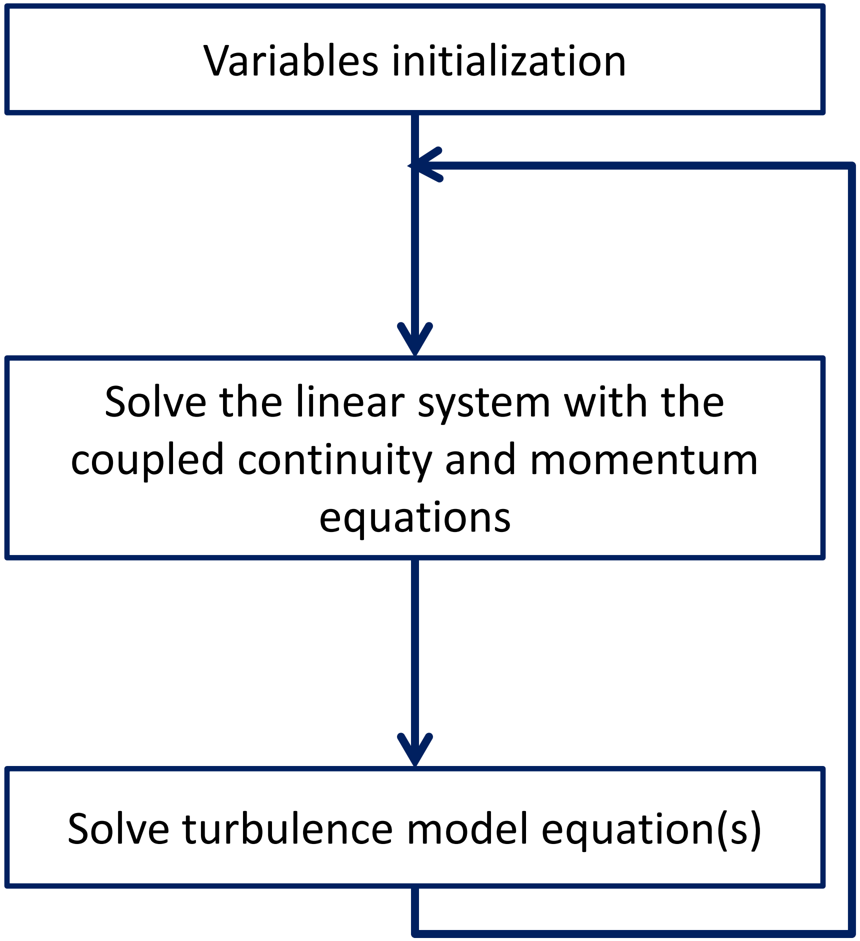
$$dt = CFL \frac{C_V}{\int (\upsilon_i + c) dS}$$

Solution algorithm outline

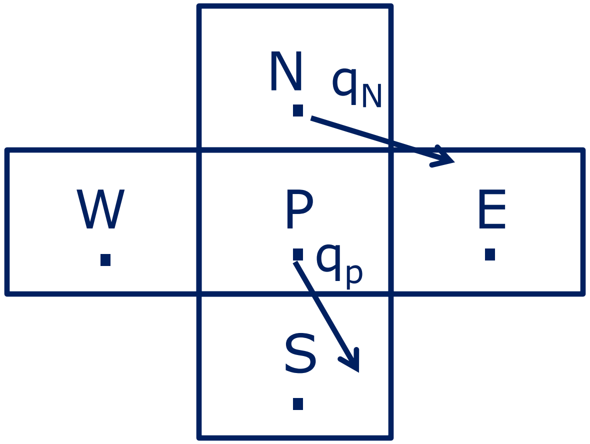
SIMPLE



Pseudo-Compressibility based solver



Incompressible flow implicit solver in OpenFOAM



Discretization for P

$$A_P \vec{q}_P + \sum_i C_{Pi} \vec{q}_i = \vec{b}_P$$

Diagonal contributions

$$A_P \vec{q}_P = \begin{bmatrix} \alpha_{pp} & \alpha_{px} & \alpha_{py} \\ \alpha_{xp} & \alpha_{xx} & 0 \\ \alpha_{yp} & 0 & \alpha_{yy} \end{bmatrix} \begin{bmatrix} p \\ \upsilon_x \\ \upsilon_y \end{bmatrix}$$

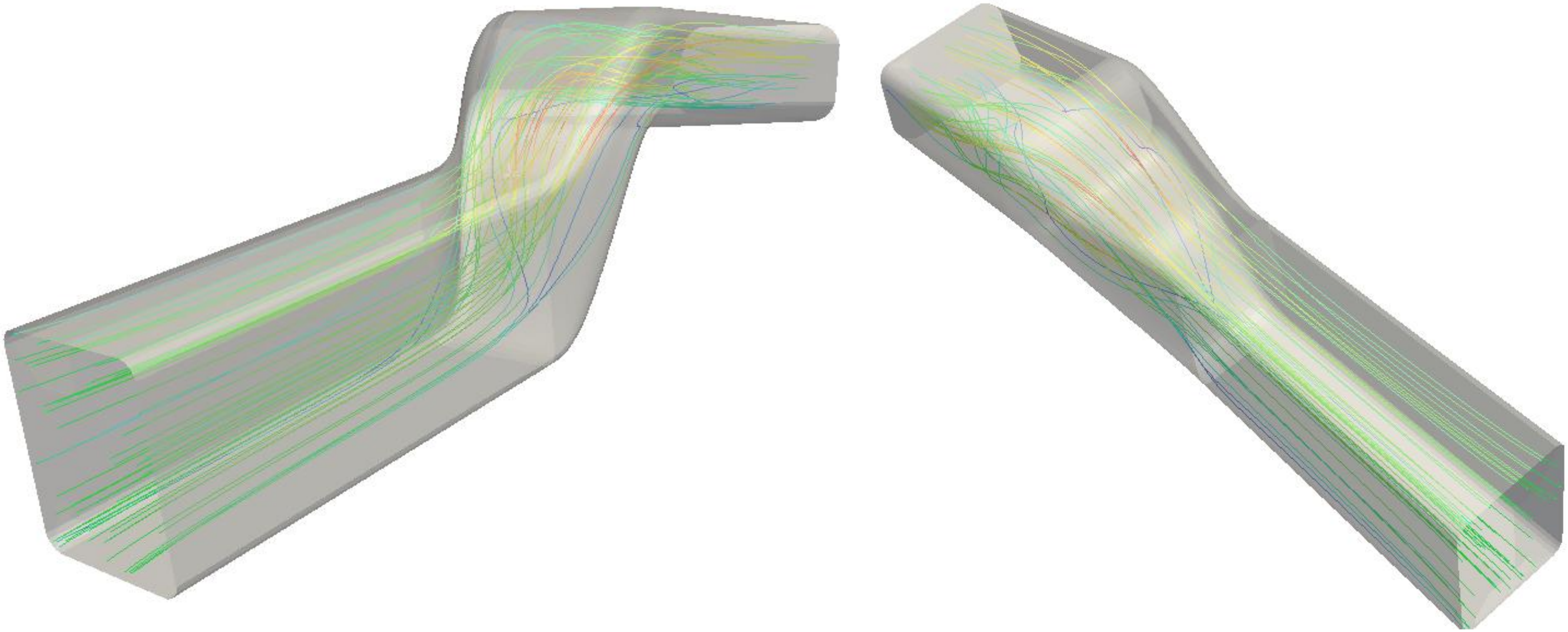
Off-diagonal contributions

$$C_{Pi} \vec{q}_i = \begin{bmatrix} c_{pp} & c_{px} & c_{py} \\ c_{xp} & c_{xx} & 0 \\ c_{yp} & 0 & c_{yy} \end{bmatrix} \begin{bmatrix} p \\ \upsilon_x \\ \upsilon_y \end{bmatrix}$$

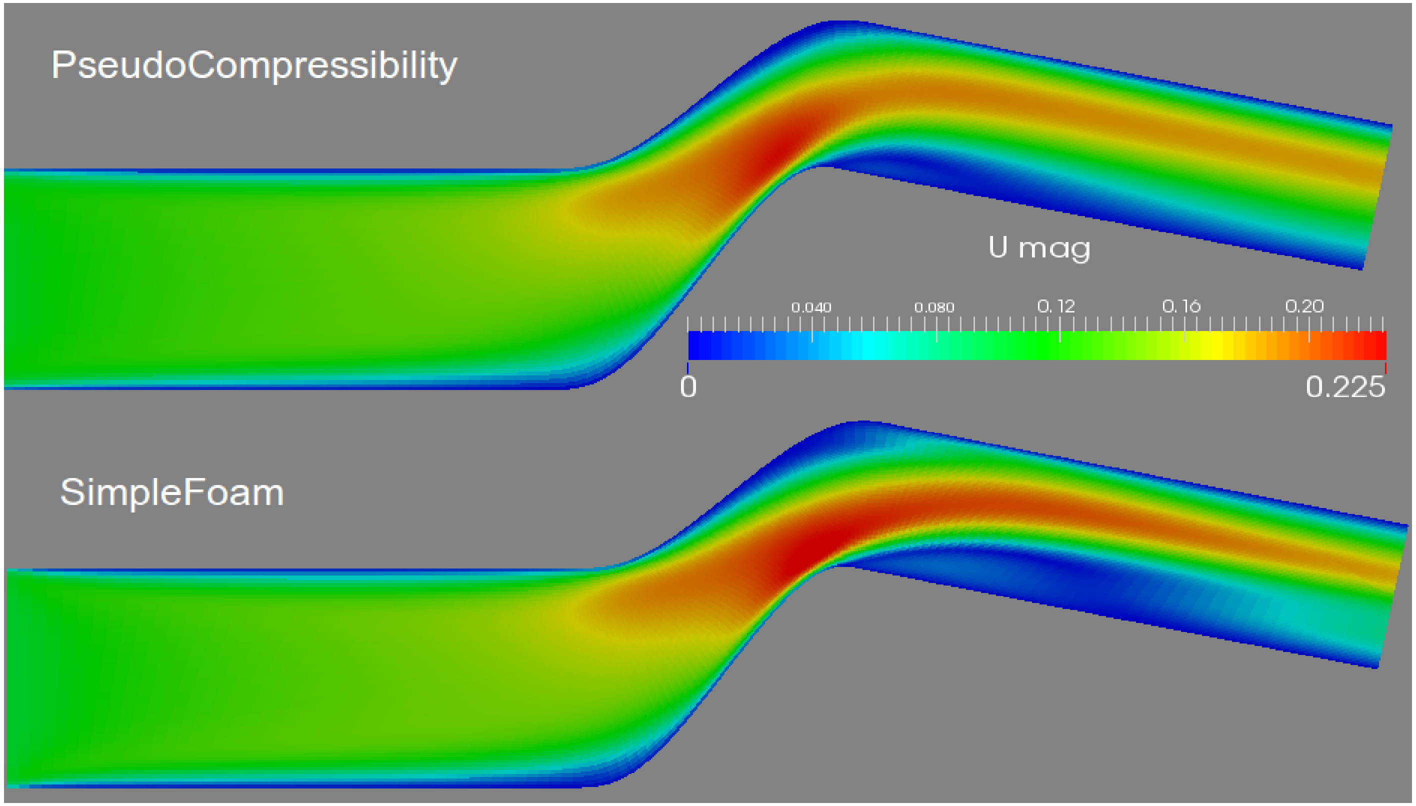
$$\begin{pmatrix} \ddots & & \cdots & & \\ \cdots \begin{bmatrix} c_{pp} & c_{px} & c_{py} \\ c_{xp} & c_{xx} & 0 \\ c_{yp} & 0 & c_{yy} \end{bmatrix}_{PE} & & \begin{bmatrix} \alpha_{pp} & \alpha_{px} & \alpha_{py} \\ \alpha_{xp} & \alpha_{xx} & 0 \\ \alpha_{yp} & 0 & \alpha_{yy} \end{bmatrix}_{P} & & \begin{bmatrix} c_{pp} & c_{px} & c_{py} \\ c_{xp} & c_{xx} & 0 \\ c_{yp} & 0 & c_{yy} \end{bmatrix}_{PW} \cdots \\ & & \cdots & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \begin{bmatrix} p \\ \upsilon_x \\ \upsilon_y \end{bmatrix}_P \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \begin{bmatrix} b_p \\ b_{\upsilon_x} \\ b_{\upsilon_y} \end{bmatrix}_P \\ \vdots \end{pmatrix}$$

Results-Implicit solver in OpenFOAM

- Implicit solver developed in foam-3.1
- Preconditioned ILU GMRES as linear solver
- Laminar and turbulent cases



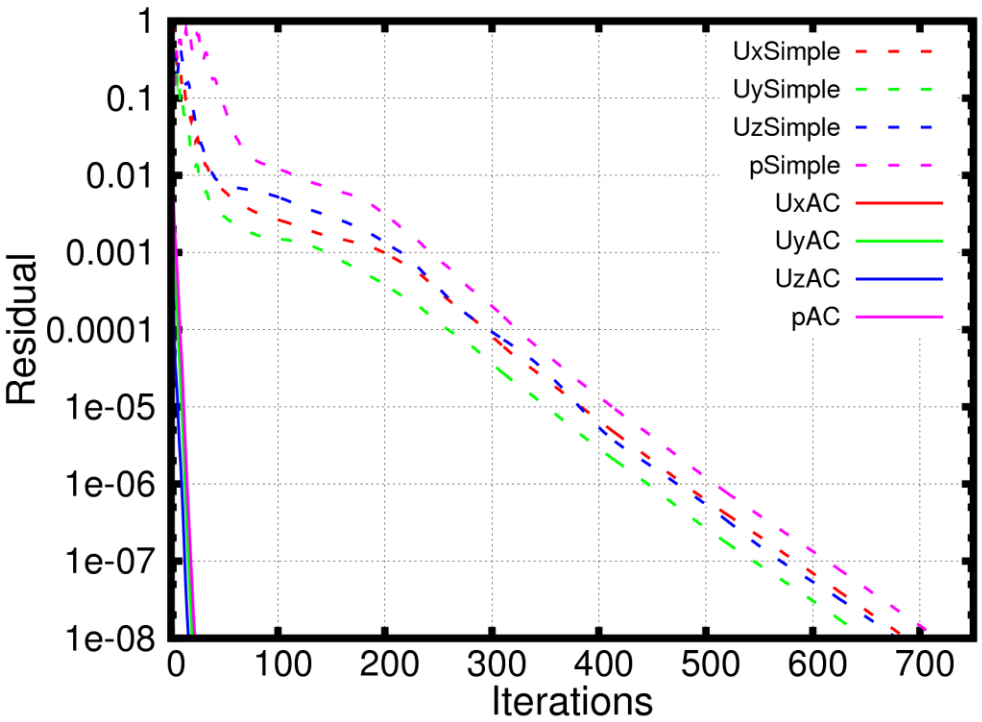
Results-Implicit solver in OpenFOAM



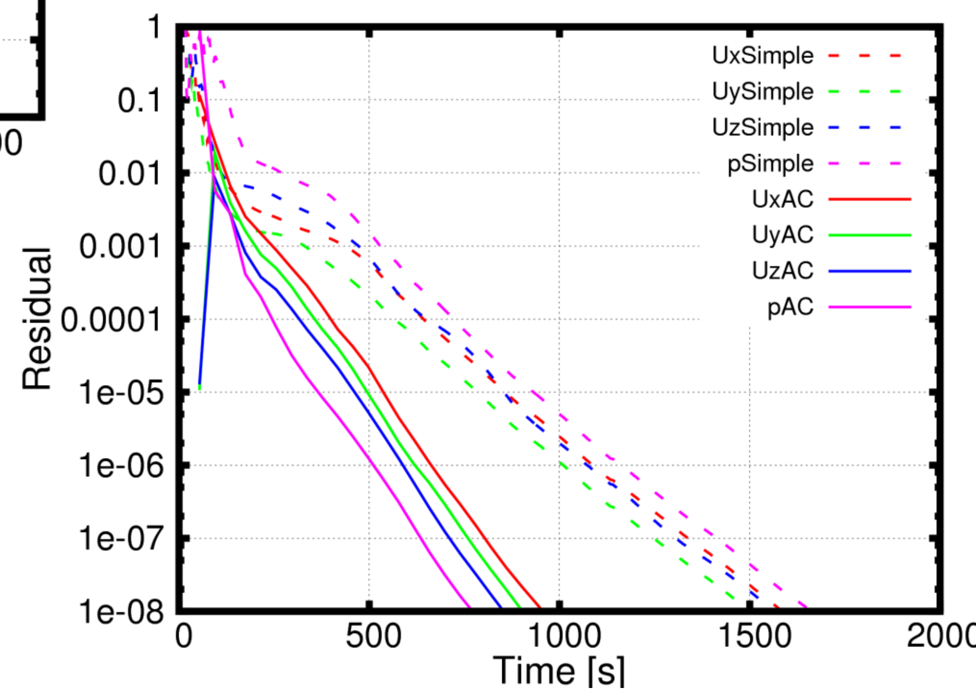
Case features:

- Laminar flow (Re~400)
- Steady flow
- Mesh size ~470k cells
- 6% total pressure losses difference
- Standard AboutFLOW test case

Results-Implicit solver in OpenFOAM



- **Implicit solver:** prec. ILU GMRES
- **Segregated solver:** *GAMG*-pressure, *Gauss-Seidel*-velocity

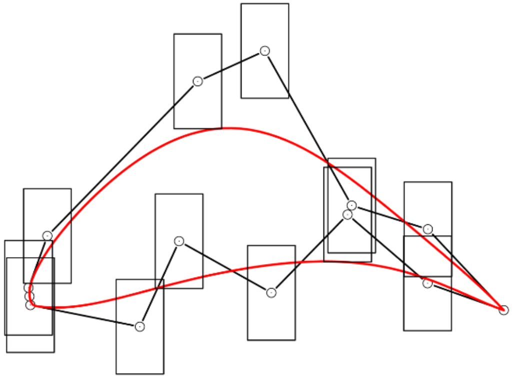


- Less than **40** iterations for deep convergence
- Total execution time gain **2x** (SIMPLE in standard OpenFOAM)

- **The problem**

$$\frac{\delta F}{\delta b_n} = ??$$

F, objective function to be minimized,
$b_n, \quad n \in [1, N]$, design variables



- **The goal**

Compute accurate sensitivity derivatives at a cost independent of N

- **The constraints: flow (or primal) equations**

$$R_i^{\upsilon} = \frac{\partial \upsilon_i}{\partial t} + \frac{\partial (\upsilon_i \upsilon_j)}{\partial x_j} - \frac{\partial}{\partial x_j}\left[(\nu + \nu_t)\left(\frac{\partial \upsilon_i}{\partial x_j} + \frac{\partial \upsilon_j}{\partial x_i}\right)\right] + \frac{\partial p}{\partial x_i} = 0$$

$$R^p = \frac{1}{\beta^2}\frac{\partial p}{\partial t} + \frac{\partial \upsilon_j}{\partial x_j} = 0$$

+ the turbulence model equations

Continuous Adjoint Method

$$F_{aug} = F + \int_{\Omega} qR^p d\Omega + \int_{\Omega} u_i R_i^{\upsilon} d\Omega$$

$$\boxed{\frac{\delta}{\delta b_n}(\cdot)}$$

Leibniz, Green-Gauss

$$\frac{\delta F_{aug}}{\delta b_n} = \frac{\delta F}{\delta b_n} + \int_S BC_{1,i} \frac{\partial \upsilon_i}{\partial b_n} dS + \int_S BC_2 \frac{\partial p}{\partial b_n} dS + \int_S BC_{3,ij} \left[(\nu + \nu_t) \left(\frac{\partial \upsilon_i}{\partial x_j} + \frac{\partial \upsilon_j}{\partial x_i} \right) \right] dS$$

$$+ \int_{\Omega} R_i^u \frac{\partial \upsilon_i}{\partial b_n} d\Omega + \int_{\Omega} R^q \frac{\partial p}{\partial b_n} d\Omega + \int_S \left(u_i R_i^{\upsilon} + qR^p \right) \frac{\delta x_{\kappa}}{\delta b_n} n_{\kappa} dS$$

Field Adjoint Equations

$$R_i^u = \frac{\partial u_i}{\partial t} - \upsilon_j \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{\partial}{\partial x_j} \left[(\nu + \nu_t) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] - \beta^2 \frac{\partial q}{\partial x_i} = 0$$

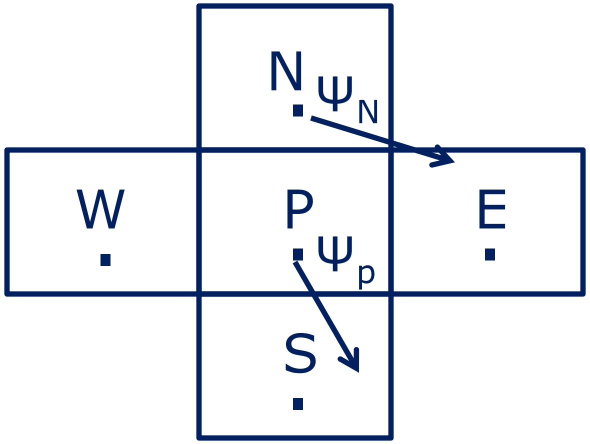
$$R^q = \frac{\partial q}{\partial t} + \frac{\partial u_i}{\partial x_i} = 0$$

Adjoint boundary conditions & sensitivity derivatives

$$BC_{1,i} = \beta^2 q n_i + u_j \upsilon_j n_i + u_i \upsilon_j n_j + (\nu + \nu_t) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) n_j + \frac{\partial F}{\partial \upsilon_i}$$

$$BC_2 = u_i n_i + \frac{\partial F}{\partial p}$$

$$BC_{3,ij} = -u_i n_j + \frac{\partial F}{\partial \tau_{ij}}$$



Discretization for P

$$A_P\vec{\Psi}_P + \sum_i C_{Pi}\vec{\Psi}_i = \vec{b}_P$$

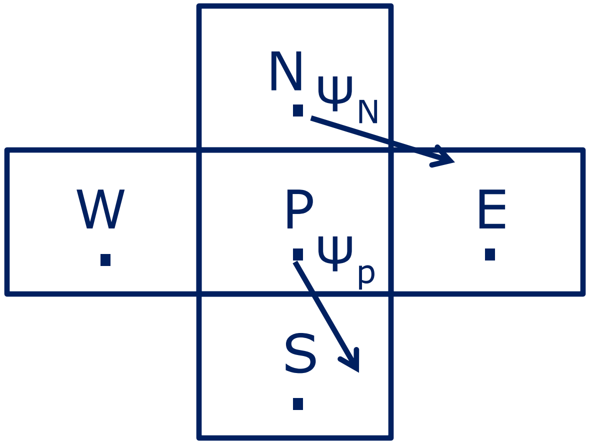
Diagonal contributions

$$A_P\vec{\Psi}_P = \begin{bmatrix} \alpha_{qq} & \alpha_{qx} & \alpha_{qy} \\ \alpha_{xq} & \alpha_{xx} & \alpha_{xy} \\ \alpha_{yq} & \alpha_{yx} & \alpha_{yy} \end{bmatrix} \begin{bmatrix} q \\ u_x \\ u_y \end{bmatrix}$$

Off-diagonal contributions

$$C_{Pi}\vec{\Psi}_i = \begin{bmatrix} c_{qq} & c_{qx} & c_{qy} \\ c_{xq} & c_{xx} & c_{xy} \\ c_{yq} & c_{yx} & c_{yy} \end{bmatrix} \begin{bmatrix} q \\ u_x \\ u_y \end{bmatrix}$$

Adjoint implicit solver



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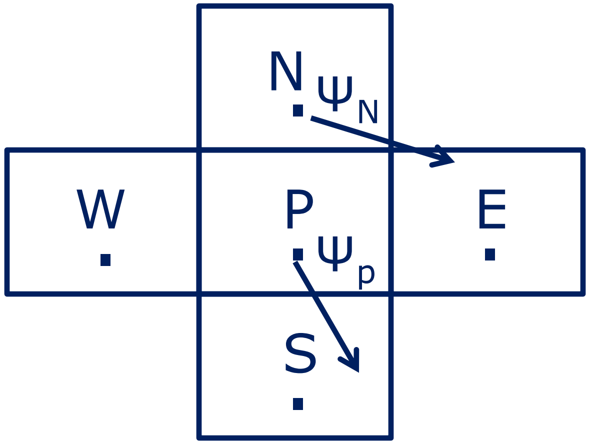
Adjoint Transpose Convection

Adjoint implicit solver



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Adjoint Transpose Convection

Adjoint invicid equations

$$R_{\Psi_n} = -A_{mnk} \frac{\partial \Psi_m}{\partial x_k} = 0$$

analytically ⟺

$$R_x^u = -\upsilon_x \frac{\partial u_x}{\partial x} - \upsilon_y \frac{\partial u_y}{\partial x} + \ldots$$

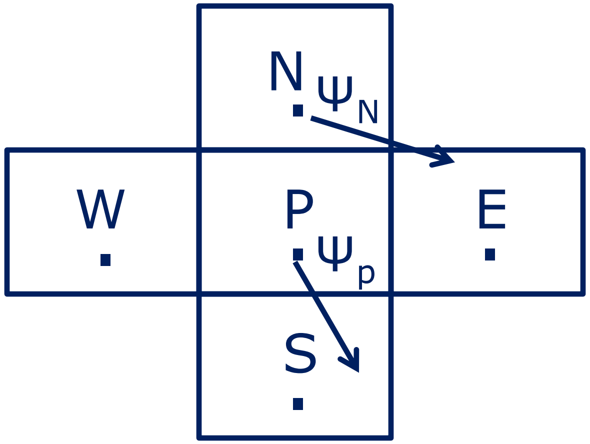
$$R_y^u = -\upsilon_x \frac{\partial u_x}{\partial y} - \upsilon_y \frac{\partial u_y}{\partial y} + \ldots$$

Adjoint invicid fluxes

$$\Phi_n^{adj,Pi} = -\frac{1}{2} A_{mnk}^P \left(\Psi_n^P + \Psi_n^i\right) n_k - \frac{1}{2} \left|A_{mnk}^{Pi}\right| \left(\Psi_n^R - \Psi_n^L\right) n_k$$

$$\Phi_n^{adj,iP} = \frac{1}{2} A_{mnk}^i \left(\Psi_n^P + \Psi_n^i\right) n_k + \frac{1}{2} \left|A_{mnk}^{Pi}\right| \left(\Psi_n^R - \Psi_n^L\right) n_k$$

Adjoint implicit solver



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Off-diagonal contributions

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analytically ⟺

$$R_x^u = -\upsilon_x \frac{\partial u_x}{\partial x} - \upsilon_y \frac{\partial u_y}{\partial x} + \dots$$

$$R_y^u = -\upsilon_x \frac{\partial u_x}{\partial y} - \upsilon_y \frac{\partial u_y}{\partial y} + \dots$$

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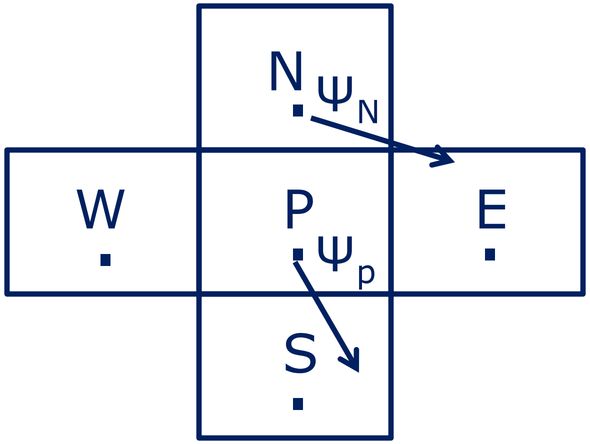
Diagonal terms

Off-diagonal terms

Adjoint implicit solver



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Off-diagonal contributions

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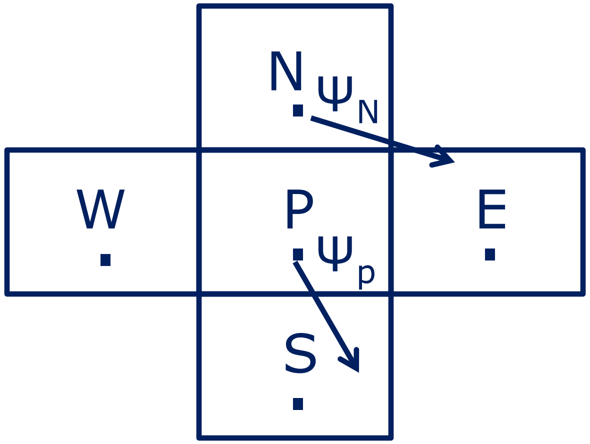
$$\begin{pmatrix} \ddots & & \cdots & \\ \cdots & \begin{bmatrix} c_{qq} & c_{qx} & c_{qy} \\ c_{xq} & c_{xx} & c_{xy} \\ c_{yq} & c_{yx} & c_{yy} \end{bmatrix}_{PE} \begin{bmatrix} \alpha_{qq} & \alpha_{qx} & \alpha_{qy} \\ \alpha_{xq} & \alpha_{xx} & \alpha_{xy} \\ \alpha_{yq} & \alpha_{yx} & \alpha_{yy} \end{bmatrix}_{P} \begin{bmatrix} c_{qq} & c_{qx} & c_{qy} \\ c_{xq} & c_{xx} & c_{xy} \\ c_{yq} & c_{yx} & c_{yy} \end{bmatrix}_{PW} & \cdots \\ & \cdots & & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ \begin{bmatrix} q \\ u_x \\ u_y \end{bmatrix}_P \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ \begin{bmatrix} b_q \\ b_{u_x} \\ b_{u_y} \end{bmatrix}_P \\ \vdots \end{pmatrix}$$

Adjoint implicit solver



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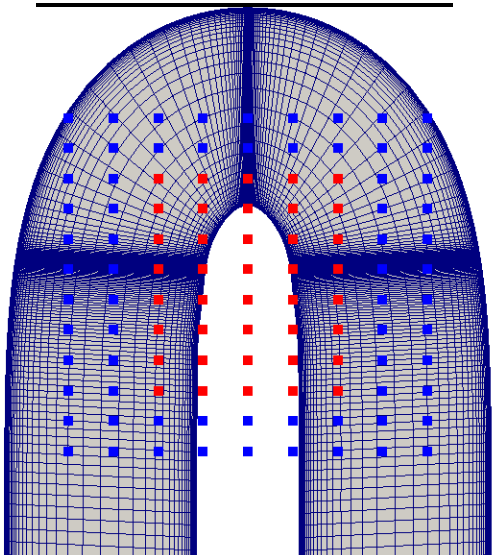
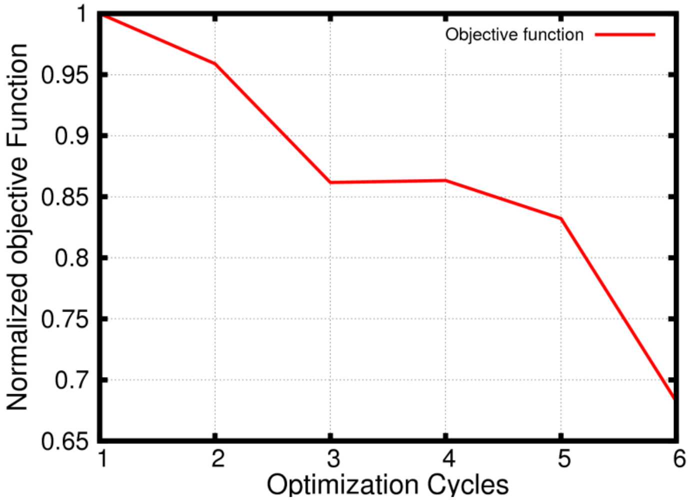
Results- Optimization

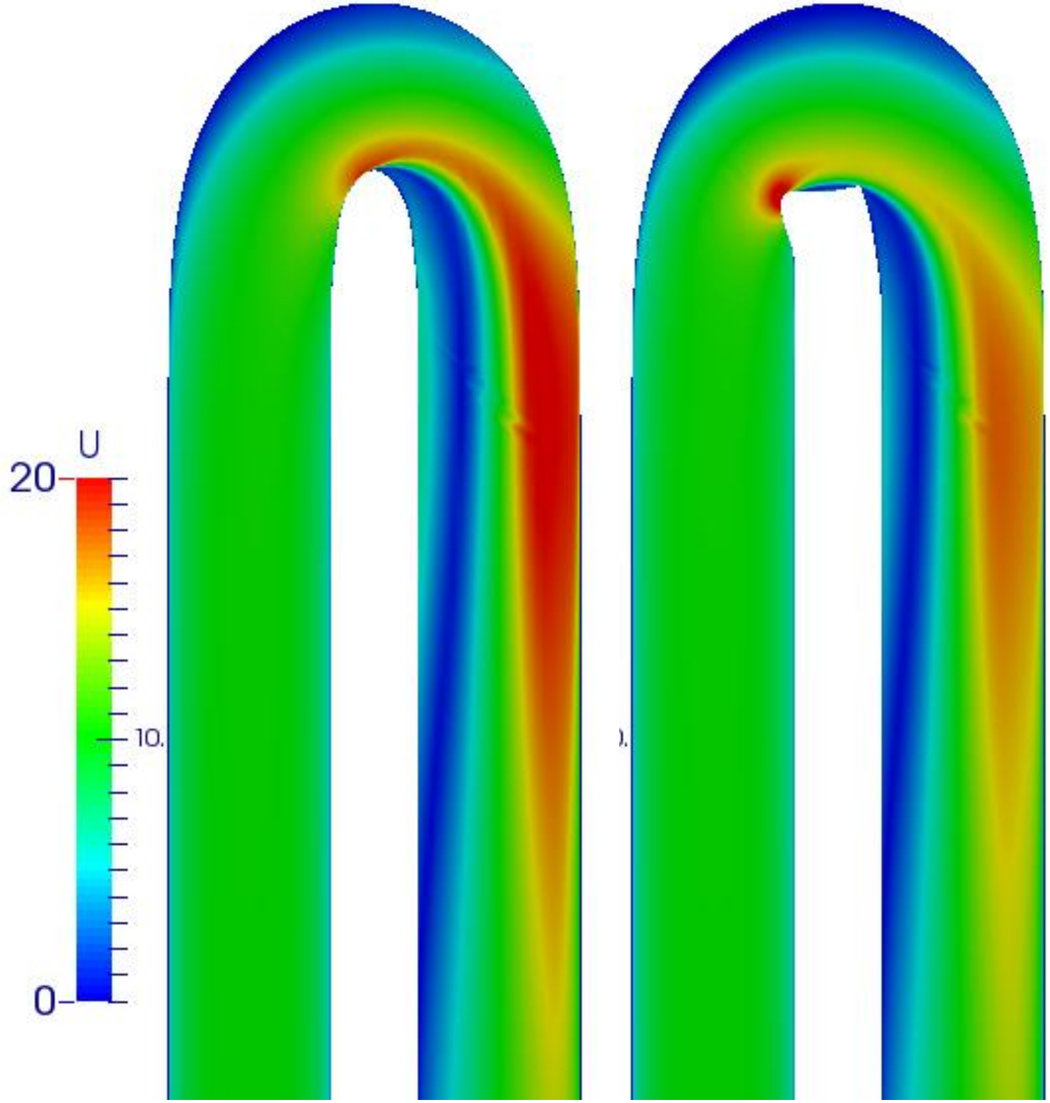
Parameterization



Optimization convergence

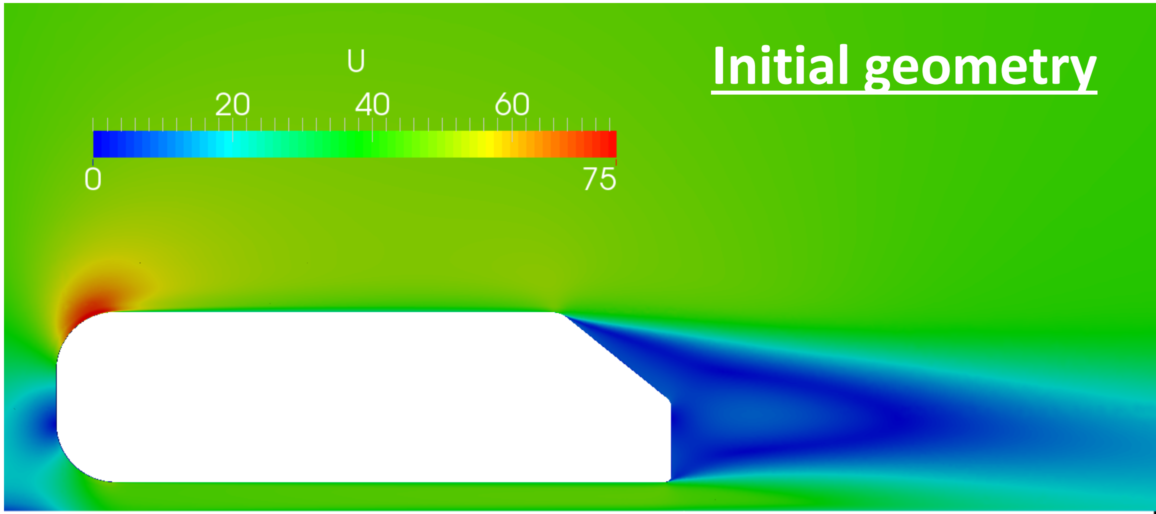


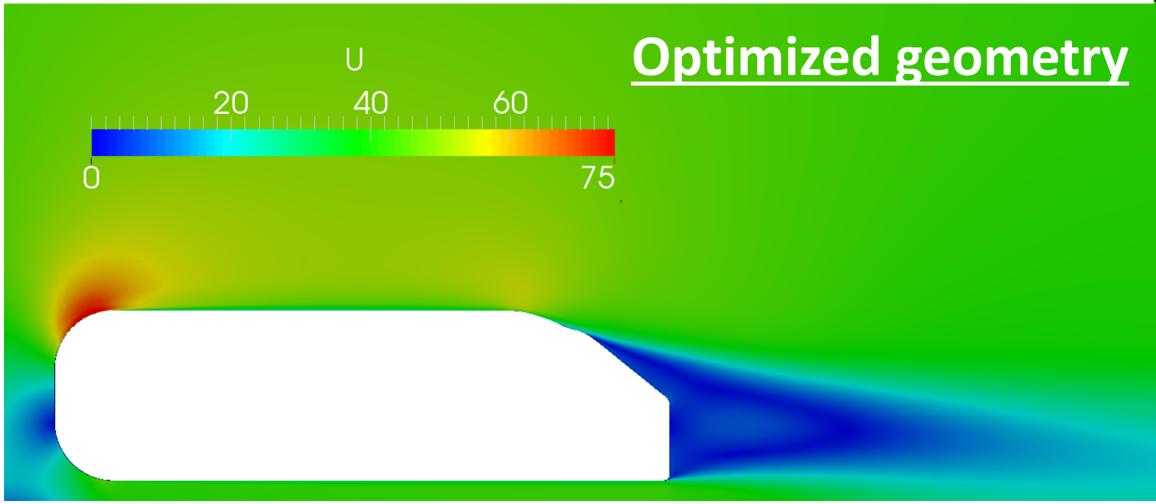
Initial geometry **Optimized geometry**



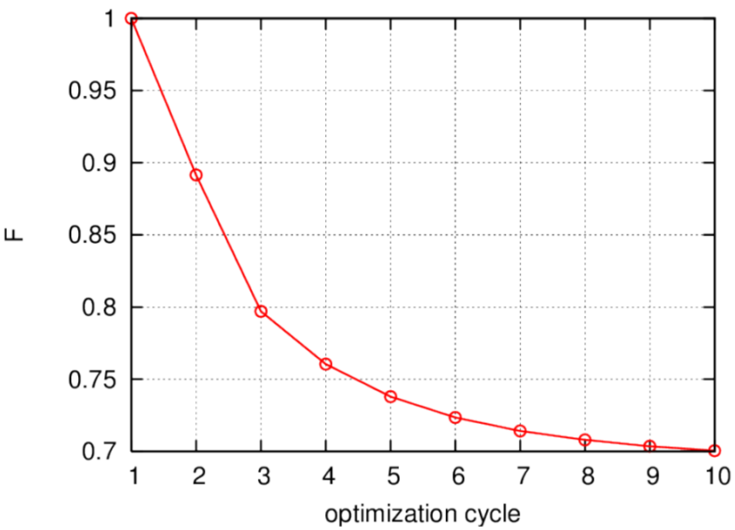
Results- Optimization

- Fully differentiated S-A turbulence model
- 210 design parameters
- Re~ 2.9×10^6
- Slant angle 30^o
- 3×10^6 cells





Optimization convergence



Conclusions/Discussion

- ß -dependence
- Very promising initial results
- Increased memory requirements
- Ongoing work (e.g., linear solver, memory management)
- Extension with previously developed models (fully differentiated turbulence models-wall functions)

ABOUTflow

Adjoint-based optimization of industrial and unsteady flows

http://aboutflow.sems.qmul.ac.uk/

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