APPLICATIONS OF PRECONDITIONED NEWTON-KRYLOV METHODS

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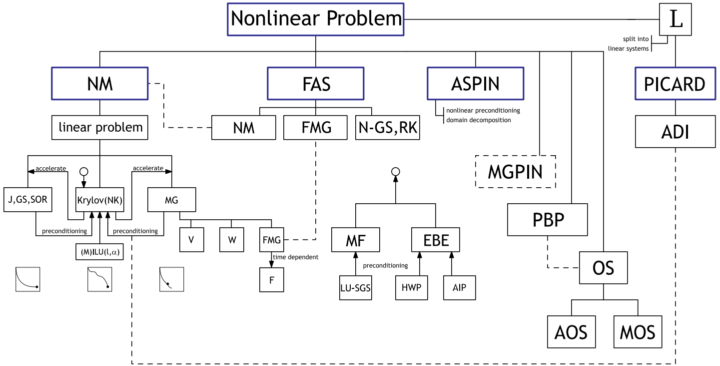
Role of CFD

- Analysis
- Design (Direct and Inverse Approach)
- Optimization

Nonlinear Equations

- Discretization yields a system of nonlinear equations
- Nonlinear-GS (or Jacobi)
- Newton's Method (Inexact NM)
- Full Approximation Scheme (Multigrid)
- Picard - (governing equations one-by-one)

Nonlinear Solver



Newton's Method

Used to linearize the non-linear system of equations.

1. $J(x^k)\Delta x^{k+1} = -f(x^k)$
2. $x^{k+1} = x^k + \Delta x^{k+1}$
3. $J_{ij} = \frac{\partial f_i}{\partial x_j}$

- Quadratically convergent from good starting guesses.
- Not globally convergent
- Requires the solution of the linear steps

Krylov Methods and Preconditioners

Following linear Krylov sub-space solvers are used.

- BiCGSTAB (Bi-conjugate Gradient Stabilized)
- GMRES (Generalized Minimal Residual)

Combined with the preconditioners

- Jacobi
- SGS (Symmetric Gauss-Seidel)
- ILU(l) (Incomplete LU decomposition)

Matrix-free algorithms

Using directional differencing the Jacobian matrix vector multiplications are carried out using only the f vector.

$$Jv = \frac{f(x + \epsilon v) - f(x)}{\epsilon} \tag{1}$$

where

$$\epsilon = \sigma^{1/2}/\|x\|[8] \tag{2}$$

if $\|x\| = 0$, the result of the matrix vector product is set identically to zero.

Matrix-free algorithms

Advantages:

- Low memory requirement
- Faster matrix vector multiplications
- Suitable for using storage schemes and some preconditioners such as Jacobi, SGS.

Disadvantages:

- Preconditioners requiring J explicitly can not be used (ILU).

Compressed Storage Schemes

CCS (Compressed Column Storage):

- Value vector: Stores the subsequent non-zeros of the matrix rows.
- Row indicator: Stores the row indexes of the elements in the value vector.
- Column pointer: Stores the locations in the value vector that start a column.

Grid Generation - 2D

The Winslow Equations

$$g_{22}\frac{\partial^2 x}{\partial \xi^2} - 2g_{12}\frac{\partial^2 x}{\partial \xi \partial \eta} + g_{11}\frac{\partial^2 x}{\partial \eta^2} = -g\left(P\frac{\partial x}{\partial \xi} + Q\frac{\partial x}{\partial \eta}\right) \quad (3)$$

$$g_{22}\frac{\partial^2 y}{\partial \xi^2} - 2g_{12}\frac{\partial^2 y}{\partial \xi \partial \eta} + g_{11}\frac{\partial^2 y}{\partial \eta^2} = -g\left(P\frac{\partial y}{\partial \xi} + Q\frac{\partial y}{\partial \eta}\right) \quad (4)$$

where $g = g_{11}g_{22} - g_{12}g_{12}$ and $P(\xi,\eta)$, $Q(\xi,\eta)$ are suitably selected *control functions*.
A set of possible control functions was proposed by *Thompson*, *Thames*, and *and Mastin* (The *TTM Method*):

$$P(\xi,\eta) = -\sum_{n=1}^{N} a_n \frac{(\xi-\xi_n)}{|\xi-\xi_n|} e^{-c_n|\xi-\xi_n|} - \sum_{i=1}^{I} b_i \frac{(\xi-\xi_i)}{|\xi-\xi_i|} e^{-d_i\left[(\xi-\xi_i)^2+(\eta-\eta_i)^2\right]^{\frac{1}{2}}} \quad (5)$$

$$Q(\xi,\eta) = -\sum_{n=1}^{N} a_n \frac{(\eta-\eta_n)}{|\eta-\eta_n|} e^{-c_n|\eta-\eta_n|} - \sum_{i=1}^{I} b_i \frac{(\eta-\eta_i)}{|\eta-\eta_i|} e^{-d_i\left[(\xi-\xi_i)^2+(\eta-\eta_i)^2\right]^{\frac{1}{2}}} \quad (6)$$

Domain Decomposition Methods

The idea: Divide the problem into regions and solve them separately instead of dealing with it as a whole.
Advantages:

- Geometrical simplicity
- Application of different modeling equations For example; Navier Stoke's at the objects proximity and Euler at the other regions
- Gain in computation speed with parallel processing

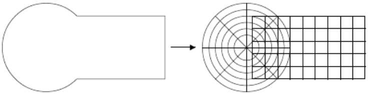


Figure: Splitting of the domain for geometrical simplicity

External Flow: Flow Past an Airfoil

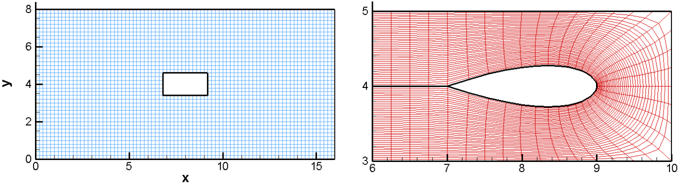


Figure: Seperate domains

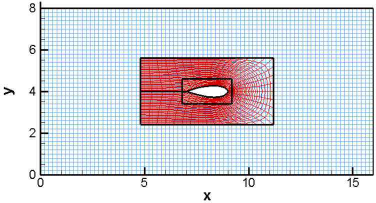


Figure: Overlapping of the domains

Overlapping Domains

- From the cartesian domain to the inner by simple interpolation
- From the inner domain to the cartesian by bilinear interpolation
- Repeat the process until the convergence is achieved

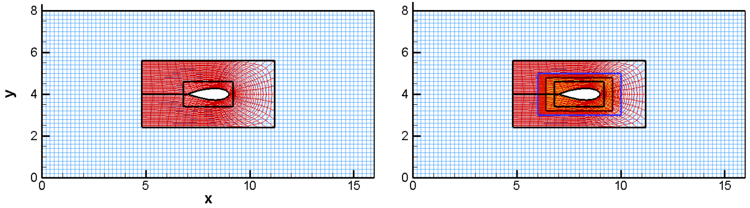


Figure: Adaptive grid

Advantages

- No grid generation in the cartesian domain
- Dealing with complex geometries is easier
- Solving the equations for the cartesian and inner domain separately (parallel computing)
- Calculation of the flow at different angle of attacks

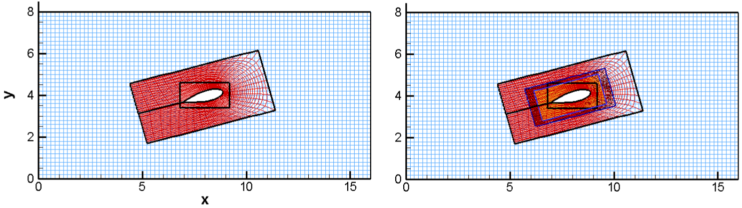


Figure: Different angle of attack

Internal Flow: Flow Between Turbomachinery Blades

- Shock waves
- Turbulent boundary layers and wakes
- Complex geometry

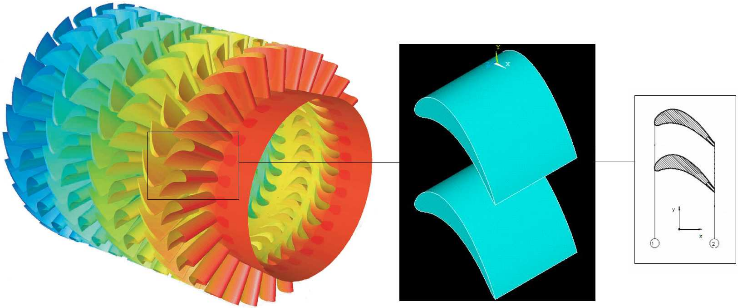


Figure: Problem domains (3D-2D)

Flow Between Turbomachinery Blades

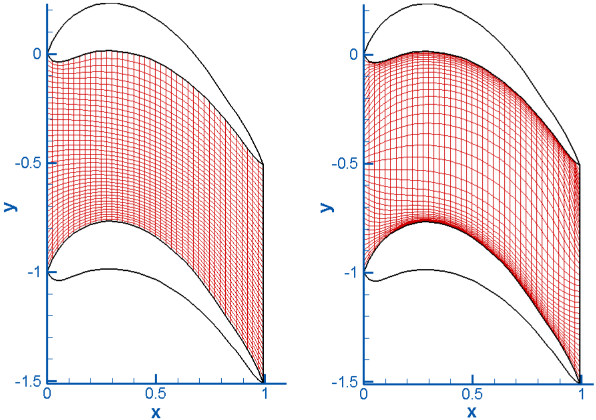


Figure: Controlling grid density

Flow Between Turbomachinery Blades

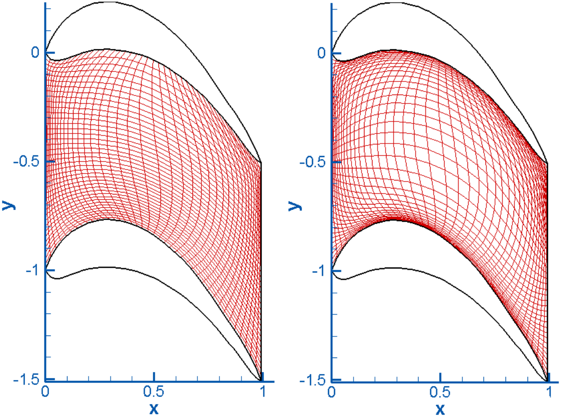


Figure: Controlling grid density

Flow Between Turbomachinery Blades

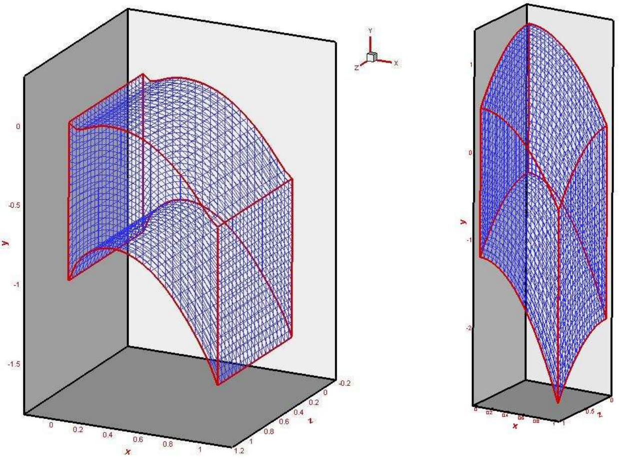


Figure: Problem domains in 3D

Formulations and Assumptions

- Stream Function-Vorticity formulation (2D)
- Velocity-Vorticity formulation (2D - 3D)
- Steady and incompressible (2D - 3D)
- Finite difference discretization (2D - 3D)

Governing Equations in 2D

Stream function - Vorticity:

$$\nabla^2\Psi + \Omega = 0 \tag{7}$$

$$\nabla^2\Omega - Re\left[\frac{\partial\Psi}{\partial y}\frac{\partial\Omega}{\partial x} - \frac{\partial\Psi}{\partial x}\frac{\partial\Omega}{\partial y}\right] = 0 \tag{8}$$

Velocity - Vorticity:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\frac{\partial\Omega}{\partial y} \tag{9}$$

$$\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} = \frac{\partial\Omega}{\partial x} \tag{10}$$

$$u\frac{\partial\Omega}{\partial x} + v\frac{\partial\Omega}{\partial y} = \frac{1}{\mathrm{Re}}\left(\frac{\partial^2\Omega}{\partial x^2} + \frac{\partial^2\Omega}{\partial y^2}\right) \tag{11}$$

Coordinate Transformation

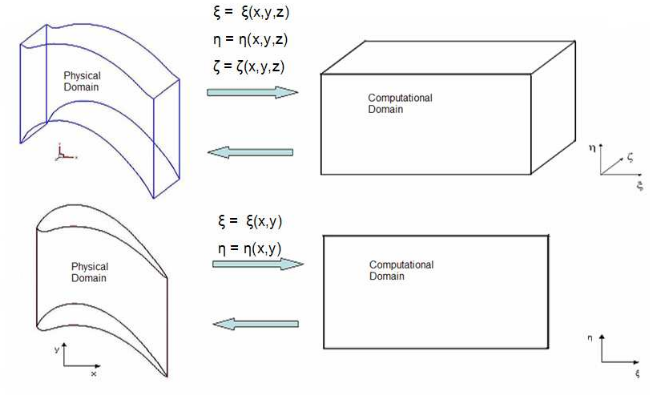


Figure: From Physical to Computational

Transformed Form of The Governing Equations in 2D

Stream Function Equation

$$\frac{\partial\psi}{\partial\eta}\left[\frac{\partial y}{\partial\xi}\left(\frac{\partial^2 x}{\partial\xi^2}\alpha+\frac{\partial^2 x}{\partial\eta^2}\beta-2\frac{\partial^2 x}{\partial\xi\partial\eta}\gamma\right)-\frac{\partial x}{\partial\xi}\left(\frac{\partial^2 y}{\partial\xi^2}\alpha+\frac{\partial^2 y}{\partial\eta^2}\beta-2\frac{\partial^2 y}{\partial\xi\partial\eta}\gamma\right)\right]$$
$$+\frac{\partial\psi}{\partial\xi}\left[\frac{\partial x}{\partial\eta}\left(\frac{\partial^2 y}{\partial\xi^2}\alpha+\frac{\partial^2 y}{\partial\eta^2}\beta-2\frac{\partial^2 y}{\partial\xi\partial\eta}\gamma\right)-\frac{\partial y}{\partial\xi}\left(\frac{\partial^2 x}{\partial\xi^2}\alpha+\frac{\partial^2 x}{\partial\eta^2}\beta-2\frac{\partial^2 x}{\partial\xi\partial\eta}\gamma\right)\right]$$
$$+\frac{\partial^2\psi}{\partial\xi^2}J\alpha+\frac{\partial^2\psi}{\partial\eta^2}J\beta-2\frac{\partial^2\psi}{\partial\xi\partial\eta}J\gamma=-J^3\Omega \tag{12}$$

Vorticity Transport Equation

$$\mathrm{Re}\frac{\partial\psi}{\partial\eta}\frac{\partial\Omega}{\partial\xi}J\left(\frac{\partial x}{\partial\xi}\frac{\partial y}{\partial\eta}-\frac{\partial y}{\partial\xi}\frac{\partial x}{\partial\eta}\right)+\mathrm{Re}\frac{\partial\psi}{\partial\xi}\frac{\partial\Omega}{\partial\eta}J\left(\frac{\partial x}{\partial\eta}\frac{\partial y}{\partial\xi}-\frac{\partial y}{\partial\eta}\frac{\partial x}{\partial\xi}\right)=$$
$$+\frac{\partial\Omega}{\partial\eta}\left[\frac{\partial y}{\partial\xi}\left(\frac{\partial^2 x}{\partial\xi^2}\alpha+\frac{\partial^2 x}{\partial\eta^2}\beta-2\frac{\partial^2 x}{\partial\xi\partial\eta}\gamma\right)-\frac{\partial x}{\partial\xi}\left(\frac{\partial^2 y}{\partial\xi^2}\alpha+\frac{\partial^2 y}{\partial\eta^2}\beta-2\frac{\partial^2 y}{\partial\xi\partial\eta}\gamma\right)\right]$$
$$+\frac{\partial\Omega}{\partial\xi}\left[\frac{\partial x}{\partial\eta}\left(\frac{\partial^2 y}{\partial\xi^2}\alpha+\frac{\partial^2 y}{\partial\eta^2}\beta-2\frac{\partial^2 y}{\partial\xi\partial\eta}\gamma\right)-\frac{\partial y}{\partial\eta}\left(\frac{\partial^2 x}{\partial\xi^2}\alpha+\frac{\partial^2 x}{\partial\eta^2}\beta-2\frac{\partial^2 x}{\partial\xi\partial\eta}\gamma\right)\right]$$
$$+\frac{\partial^2\Omega}{\partial\xi^2}J\alpha+\frac{\partial^2\Omega}{\partial\eta^2}J\beta-2\frac{\partial^2\Omega}{\partial\xi\partial\eta}J\gamma \tag{13}$$

Governing Equations in 3D

Equations for the velocity components in vector form:

$$\nabla^2 \bar{u} = -\bar{\nabla} \times \bar{\Omega} \tag{14}$$

The three-component vorticity transport equation,:

$$\left(\bar{u}.\bar{\nabla}\right)\bar{\Omega} - \left(\bar{\Omega}.\bar{\nabla}\right)\bar{u} - \frac{1}{\mathrm{Re}}\nabla^2\bar{\Omega} = 0 \tag{15}$$

Boundary conditions

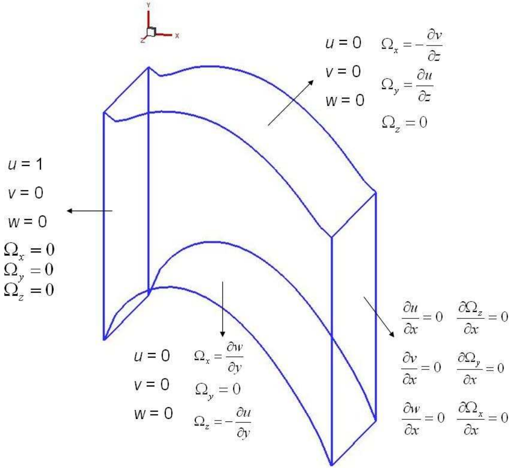
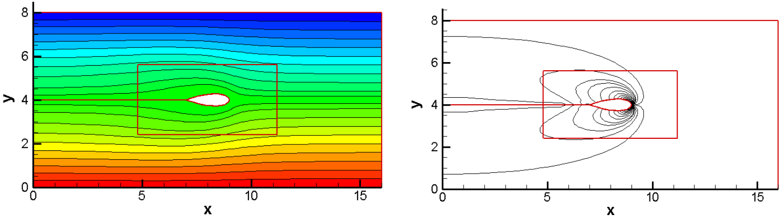


Figure: Boundary conditions

Flow Past an Airfoil

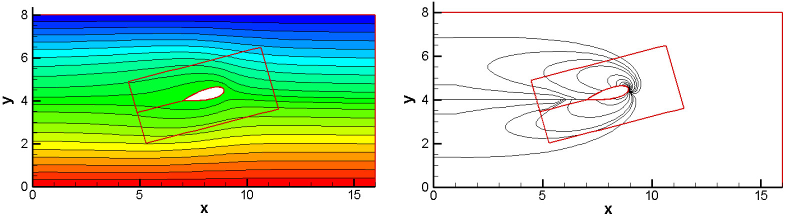


(a) Stream function contours

(b) Vorticity contours

Figure: Flow Past an Airfoil (Re=50)

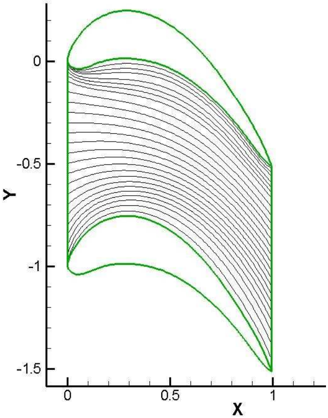
Flow Past an Airfoil



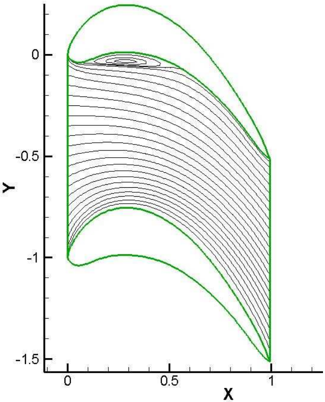
(a) Stream function contours (b) Vorticity contours

Figure: Flow Past an Airfoil (Re=50)

Stream function contours



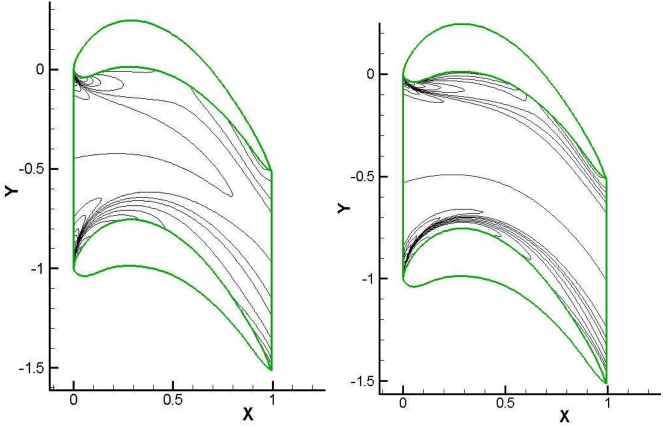
(a) Re=100



(b) Re=500

Figure: Stream function contours

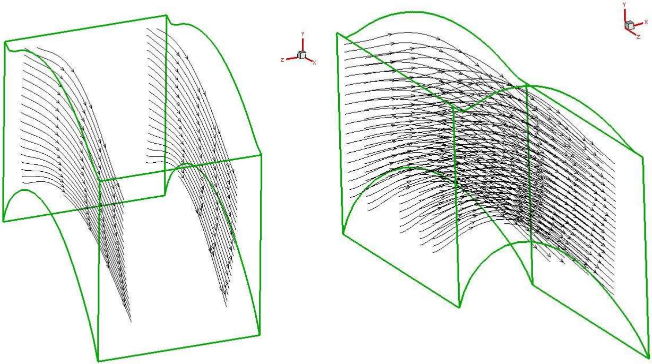
Vorticity contours



(a) Re=100 (b) Re=500

Figure: Vorticity contours

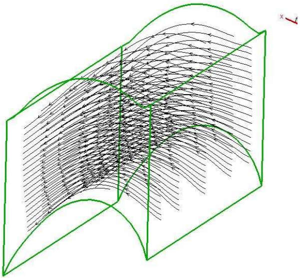
Streamtrace contours



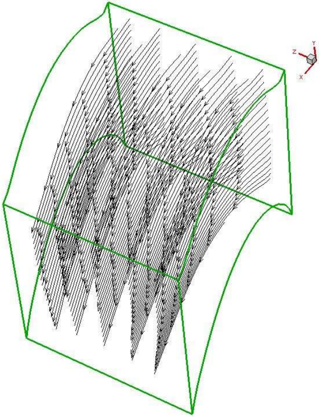
(a) Streamtrace contours (b) Streamtrace contours

Figure: Velocity-Vorticity Approach

Streamtrace contours



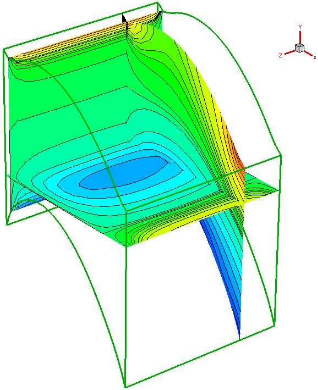
(a) Streamtrace contours



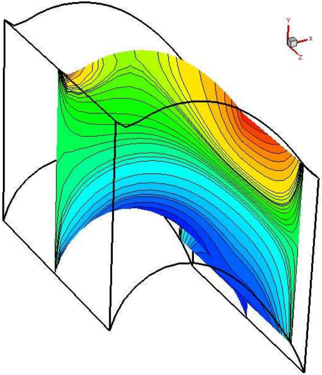
(b) Streamtrace contours

Figure: Velocity-Vorticity Approach

Vorticity contours



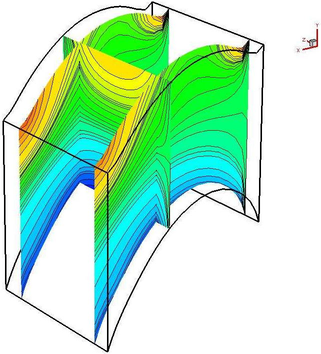
(a) Vorticity contours



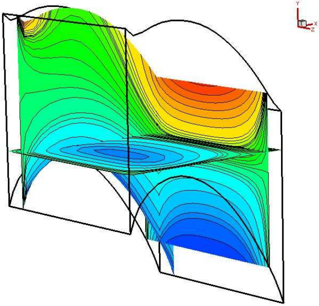
(b) Vorticity contours

Figure: Velocity-Vorticity Approach

Vorticity contours



(a) Vorticity contours

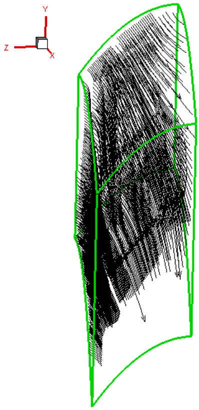


(b) Vorticity contours

Figure: Velocity-Vorticity Approach

Streamtrace contours

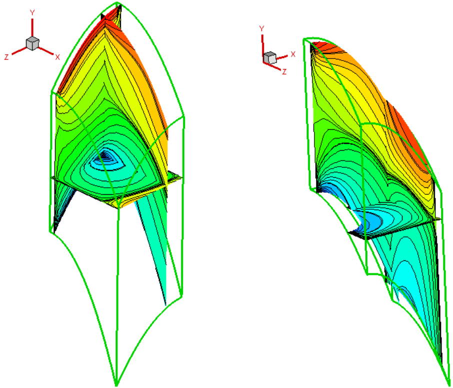
(a) Streamtrace contours



(b) Streamtrace contours

Figure: Velocity-Vorticity Approach

Streamtrace contours



(a) Vorticity contours (b) Vorticity contours

Figure: Velocity-Vorticity Approach

Performance

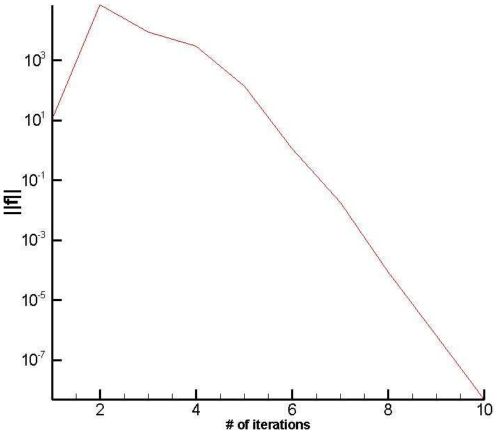


Figure: Typical non-linear convergence history for Re=100

Comparison of the Solvers and the Preconditioners

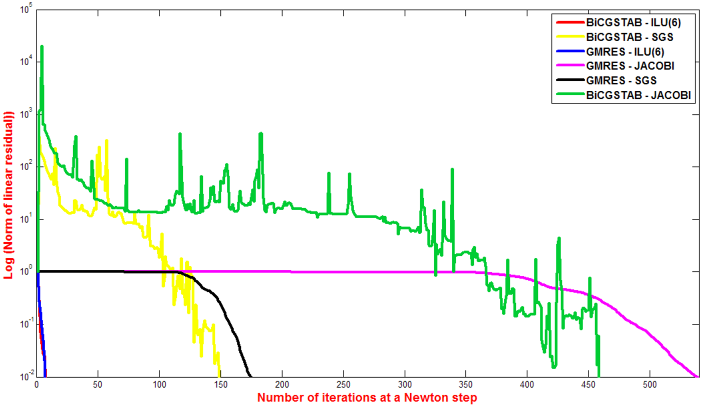


Figure: Comparison of the Solvers and the Preconditioners

Comparison of the Solvers and the Preconditioners

- Implementation of an effective preconditioner is crucial.
- Jacobi does not have a major effect on the convergence pattern.
- BiCGSTAB has a more stable pattern than GMRES and is the fastest solver by means of iteration steps and computation time.
- GMRES is the most stable solver, enables a continuous residual reduction.
- In GMRES the computational work increases linearly with the iteration$\Rightarrow$ Restartable GMRES(m)

Fluid-Structure Interaction

The idea:

- Extract grid points on the blade surface from ANSYS to an aerodynamic code
- Generate grid, execute fluid analysis and achieve the velocity, vorticity and pressure fields
- Transfer pressure values to ANSYS, execute solid analysis and acquire displacements
- With storing displacements from ANSYS, finish first step of FSI
- By using displacements from ANSYS, update geometry and start second step

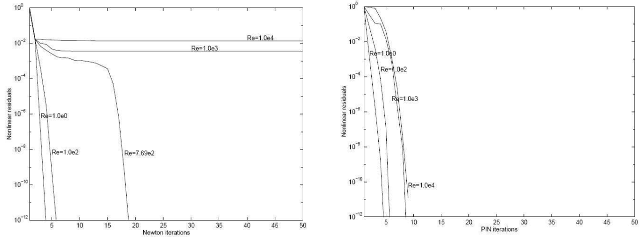
Future Works

- Parallel Computing
- Nonlinear Preconditioning
- Multigrid/Multilevel Techniques

- Schobeiri, M., *Turbomachinery Flow Physics and Dynamic Performance*, Springer, 2005
- Hoffman, K.A., *Computational Fluid Dynamics for Enginners - Volume I*, Engineering Education System, Kansas, 1997.
- Saad, Y., *Iterative Methods for Sparse Linear Systems*, PWS Publishing Company, Boston, 1996.
- Barrett, R., Berry, M., Chan, T.F., Demmel, J., Donato, J., Dongarra, J., Eijkhout, V., Pozo, R., Romine, C. and Van der Vorst, H., *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods, 2nd Edition*, SIAM, Philadelphia, PA, 1994.
- Roache, P.J., *Fundamentals of Computational Fluid Dynamics*, Hermosa Pub., USA, 1998
- http://www.ansys.com
- Cai, X.C., Keyes, D.E., *Nonlinearly preconditioned inexact Newton algorithms*, SIAM J.SCI.COMPUT., Vol.24, No.1, pp.183-200
- Ning Qin, David K. Ludlow and Scott T. Shaw, "A matrix-free preconditioned Newton:GMRES method for unsteady NavierStokes solutions" *International Journal for Numerical Methods in Fluids*, Vol. 33, pp. 223248, 2000

Thank You...

Non-linear & Linear Preconditioning



(a) Newton iterations (b) PIN iterations

Figure: Nonlinear residual history for the flow problem with different Reynolds number [7]

Solid Analysis

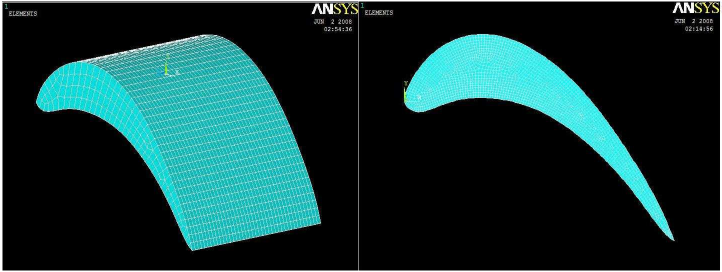
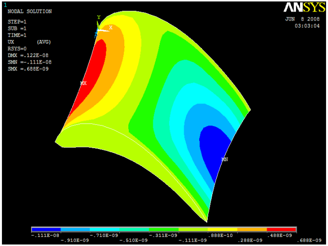


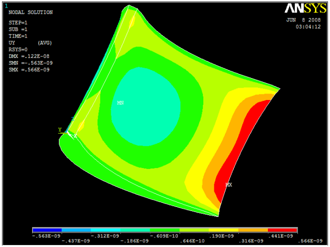
Figure: Blade mesh in ANSYS (3D-2D)

- Hexahedral - Quadrilateral
- MMB: Linear - Elastic - Isotropic

Deformation Under Aerodynamic Loads



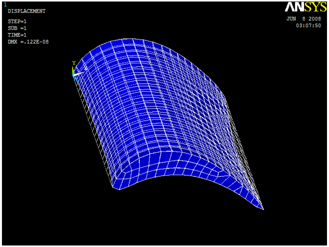
(a) x-component of displacement



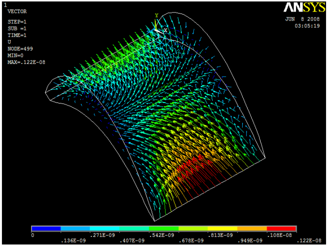
(b) y-component of displacement

Figure: Solid Analysis

Deformation Under Aerodynamic Loads



(a) Deformed shape with undeformed edge



(b) Vector plot of translation

Figure: Solid Analysis

Transformation Terms

$$
\begin{aligned}
\alpha &= \left(\frac{\partial x}{\partial \eta}\right)^2 + \left(\frac{\partial y}{\partial \eta}\right)^2 \\
\beta &= \left(\frac{\partial x}{\partial \xi}\right)^2 + \left(\frac{\partial y}{\partial \xi}\right)^2 \\
\gamma &= \frac{\partial x}{\partial \xi}\frac{\partial x}{\partial \eta} + \frac{\partial y}{\partial \xi}\frac{\partial y}{\partial \eta} \\
J &= \frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi}\frac{\partial x}{\partial \eta}
\end{aligned}
\tag{16}
$$

Governing Equations in 3D

x-component of velocity :

$$\nabla^2 u = \frac{\partial \Omega_y}{\partial z} - \frac{\partial \Omega_z}{\partial y} \quad (17)$$

y-component of velocity :

$$\nabla^2 v = \frac{\partial \Omega_z}{\partial x} - \frac{\partial \Omega_x}{\partial z} \quad (18)$$

z-component of velocity :

$$\nabla^2 w = \frac{\partial \Omega_x}{\partial y} - \frac{\partial \Omega_y}{\partial x} \quad (19)$$

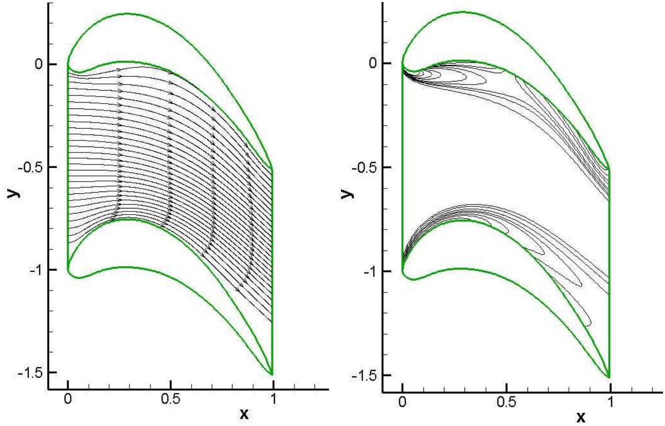
vorticity transport :

$$\nabla.\left(u\Omega\right) - \left(\Omega.\nabla\right)u - \frac{1}{\mathrm{Re}}\nabla^2\Omega = 0 \quad (20)$$

Coordinate Transformation

- The chain rule of partial differentiation
  1. $\frac{\partial}{\partial x} = \xi_x \frac{\partial}{\partial \xi} + \eta_x \frac{\partial}{\partial \eta} + \zeta_x \frac{\partial}{\partial \zeta}$
  2. $\frac{\partial}{\partial y} = \xi_y \frac{\partial}{\partial \xi} + \eta_y \frac{\partial}{\partial \eta} + \zeta_y \frac{\partial}{\partial \zeta}$
  3. $\frac{\partial}{\partial z} = \xi_z \frac{\partial}{\partial \xi} + \eta_z \frac{\partial}{\partial \eta} + \zeta_z \frac{\partial}{\partial \zeta}$
- $J = \frac{\partial(\xi,\eta,\zeta)}{\partial(x,y,z)}$

Streamtrace contours



(a) Streamtrace contours (b) Vorticity contours

Figure: Velocity-Vorticity Approach

Preconditioning and Matrix-free Approach

$$P_L^{-1} J(\bar{x})\bar{v} = P_L^{-1} \frac{\bar{f}(\bar{x} + P_R^{-1}\bar{y}) - \bar{f}(\bar{x})}{\varepsilon} = \bar{z} \tag{21}$$

$$P_R \epsilon \bar{v} = \bar{y} \tag{22}$$

$$P_L \bar{z} = J\bar{v} \tag{23}$$

Comparison of the Solvers and the Preconditioners

Table: Comparison of the solvers and preconditioners by means of iteration number and computation time

Method	# of iterations per Newton Step (average)	Time (sec.)
Jacobi-BiCGSTAB	490.5	25.7
SGS-BiCGSTAB	108.8	23.1
ILU(6)-BiCGSTAB	16.2	187.8
Jacobi-GMRES(100)	313.6	26.1
SGS-GMRES(100)	97.7	22.7
ILU(6)-GMRES(100)	12.5	182.14

Coordinate Transformation

Second derivative of an arbitrary variable in the transformed form

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial \xi}\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial u}{\partial \eta}\frac{\partial^2 \eta}{\partial x^2} + \frac{\partial u}{\partial \zeta}\frac{\partial^2 \zeta}{\partial x^2} + \frac{\partial^2 u}{\partial \xi^2}\left(\frac{\partial \xi}{\partial x}\right)^2 + \frac{\partial^2 u}{\partial \eta^2}\left(\frac{\partial \eta}{\partial x}\right)^2 + \frac{\partial^2 u}{\partial \zeta^2}\left(\frac{\partial \zeta}{\partial x}\right)^2 + 2\frac{\partial^2 u}{\partial \xi \partial \eta}\frac{\partial \xi}{\partial x}\frac{\partial \eta}{\partial x} + 2\frac{\partial^2 u}{\partial \xi \partial \zeta}\frac{\partial \xi}{\partial x}\frac{\partial \zeta}{\partial x} + 2\frac{\partial^2 u}{\partial \zeta \partial \eta}\frac{\partial \zeta}{\partial x}\frac{\partial \eta}{\partial x}$$

Blade Shape

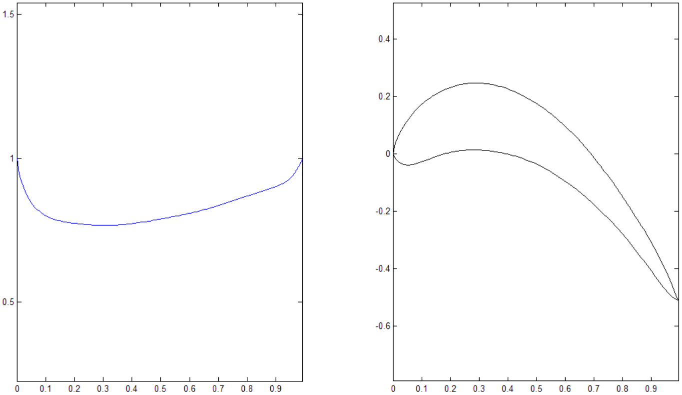
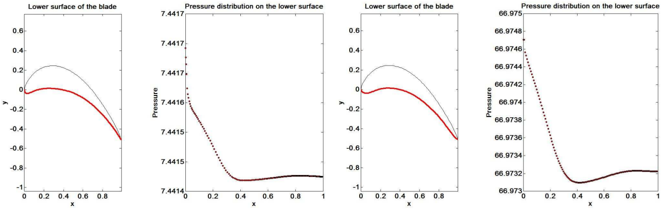


Figure: Blade geometry

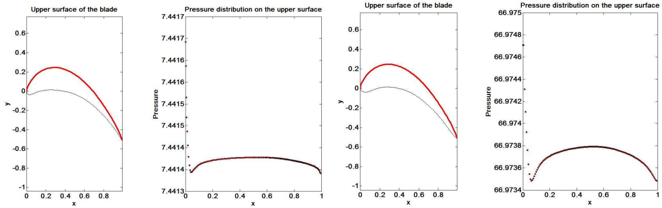
Effect of Reynolds Number



(a) Re=100 (b) Re=300

Figure: Pressure distribution

Effects of Reynolds Number



(a) Re=100 (b) Re=300

Figure: Pressure distribution

Effects of Reynolds Number

- Pressure distribution
  distribution character ⇒ slightly
  values ⇒ extensively
- Vortex generation (bottom surface of upper blade)