SOME IMPLEMENTATION ASPECTS OF TURBULENCE MODELS IN CFD

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Contents:

Reynolds averaged Navier-Stokes equations

The steady-state Navier-Stokes equations for a turbulent incompressible fluid moving in a domain Ω are

$$\begin{aligned}(\boldsymbol{u}\cdot\nabla)\boldsymbol{u}-\nabla\cdot[2\nu\boldsymbol{S}(\boldsymbol{u})+\boldsymbol{\tau}]+\nabla p&=\boldsymbol{f}\\ \nabla\cdot\boldsymbol{u}&=0\end{aligned}$$

where $\boldsymbol{u}$ is the mean velocity field, p is the mean pressure, $\boldsymbol{f}$ is the vector of mean body forces, ν is the kinematic viscosity, $\boldsymbol{S}(\boldsymbol{u})$ is the symmetrical part of the velocity gradient and

$$\boldsymbol{\tau}=-\overline{\boldsymbol{u}'\otimes\boldsymbol{u}'}$$

is the Reynolds stress tensor ($\boldsymbol{u}'$ is the fluctuating velocity and the overbar denotes the Reynolds average).

The boundary conditions for problem are

$$\boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{on } \Gamma_{\mathrm{du}}$$

$$\boldsymbol{n} \cdot \boldsymbol{\sigma} = \bar{\boldsymbol{t}} \quad \text{on } \Gamma_{\mathrm{nu}}$$

$$\boldsymbol{u} \cdot \boldsymbol{n} = \bar{u}_n, \ \boldsymbol{n} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{g}_1 = \bar{t}_1, \ \boldsymbol{n} \cdot \boldsymbol{\sigma} \cdot \boldsymbol{g}_2 = \bar{t}_2 \quad \text{on } \Gamma_{\mathrm{mu}}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\boldsymbol{n}$ is the unit exterior normal to $\partial\Omega$.

The Reynolds stress tensor $\boldsymbol{\tau}$ requires modeling. Two possibilities are the Boussinesq assumption and the use of algebraic stress models (ASM).

Boussinesq assumption: one and two equation models

Boussinesq assumption

The Boussinesq assumption consists in taking $\boldsymbol{\tau}$ as

$$\boldsymbol{\tau} = -\frac{2}{3}k\boldsymbol{I} + 2\nu_t\boldsymbol{S}(\boldsymbol{u})$$

where $\boldsymbol{I}$ is the identity tensor, k is the turbulent kinetic energy, defined as

$$k = \frac{1}{2}\overline{\boldsymbol{u}' \cdot \boldsymbol{u}'},$$

and ν_t is the turbulent (kinematic) viscosity. Different turbulence models are obtained depending on the way in which ν_t is computed.

Spalart Almaras model

In this case, the turbulent viscosity is computed as

$$\nu_t = f_{v_1} \tilde{\nu}$$
$$f_{v_1} = \frac{\chi^3}{\chi^3 + c_{v_1}^3}, \quad \chi := \frac{\tilde{\nu}}{\nu}$$

where $\tilde{\nu}$ is solution of the equation

$$\boldsymbol{u} \cdot \nabla \tilde{\nu} - c_{b_1} \tilde{S} \tilde{\nu} - \frac{1}{\sigma} \nabla \cdot [(\nu + \tilde{\nu}) \nabla \nu]$$
$$= \frac{c_{b_2}}{\sigma} (\nabla \tilde{\nu})^2 - c_{w_1} f_w \frac{\tilde{\nu}^2}{d^2}$$

where d is the shortest distance to the walls, c_{v_1}, c_{b_1}, σ, c_{b_2} and c_{w_1} are constants of the model and f_w is a function of the vorticity of the flow.

The equation and the problems encountered are the same as for the k-ϵ model described next.

k-ϵ model

In this case, ν_t is computed as

$$\nu_t = c_\mu \frac{k^2}{\varepsilon}$$

where c_μ is a constant and ε is rate of turbulent energy dissipation.

The equations for k and ε have to be modeled. In the k-ε model the differential equations for k and ε are

$$(\boldsymbol{u} \cdot \nabla)\varepsilon - \nabla \cdot \left(\frac{\nu_t}{\sigma_\varepsilon} \nabla \varepsilon\right) - \frac{\varepsilon}{k}(C_1 P_k - C_2 \varepsilon) = 0$$

$$(\boldsymbol{u} \cdot \nabla)k - \nabla \cdot \left(\frac{\nu_t}{\sigma_k} \nabla k\right) - P_k + \varepsilon = 0$$

where

$$P_k = 2\nu_t \boldsymbol{S}(\boldsymbol{u}) : \boldsymbol{S}(\boldsymbol{u})$$

is the production term and σ_k, σ_ε, C_1 and C_2 are experimental constants.

Proper boundary conditions have to be added. For the case in which the velocity is prescribed, k is also prescribed (Dirichlet type of boundary condition). The value of the prescription is

$$k = c_{\mathrm{bc}} u^2$$

where c_{bc} is a constant. When k is prescribed, so is ε. The prescription for it is

$$\varepsilon = c_\mu \frac{k^{3/2}}{L}$$

where L is again a constant the physical meaning of which is the characteristic length of the model. On the boundary it must be given, but in the interior of the computational domain the characteristic length (or mixing length) for the k-ε model is

$$L = c_\mu \frac{k^{3/2}}{\varepsilon}$$

so that $\nu_t = \sqrt{k} L$.

On Γ_{nu} the boundary conditions we take are

$$\frac{\partial k}{\partial n} = 0, \quad \frac{\partial \varepsilon}{\partial n} = 0$$

The same boundary condition is prescribed on Γ_{mu} except when a wall law is prescribed there. In this case, the traction on the boundary is given by

$$\boldsymbol{t} = -\rho \frac{U_*^2}{|\boldsymbol{u}|} \boldsymbol{u}$$

where ρ is the fluid density and U_* is the solution of the nonlinear equation

$$\frac{|\boldsymbol{u}|}{U_*} = \frac{1}{\kappa} \log\left(\frac{U_* \Delta}{\nu}\right) + C$$

with $\kappa = 0.41$ (von Kármán constant), $C = 5.5$ and where Δ is the distance from the wall at which the velocity is evaluated.

When a wall law is prescribed for the velocity, k and ε are prescribed to

$$k = \frac{U_*^2}{\sqrt{c_\mu}}, \quad \varepsilon = \frac{U_*^3}{\kappa \Delta}$$

An algebraic stress model

The Boussinesq assumption is inaccurate when the flow has an important swirl.

The alternative is to use the Reynolds stress models, in which differential equations are proposed to model the components of the Reynolds stress tensor. These models can be simplified using some heuristic approximations that lead to closed algebraic expressions for the components of $\boldsymbol{\tau}$.

One of these models is given by

$$\frac{\tau_{ij}}{\rho} = \frac{6(1+\eta^2)\alpha_1 k}{3+\eta^2+6\zeta^2\eta^2+6\zeta^2}\Big[S^*_{ij} + (S^*_{ik}W^*_{kj} + S^*_{jk}W^*_{ki}) \\ -2(S^*_{ik}S^*_{kj} - \frac{1}{3}S^*_{kl}S^*_{kl}\delta_{ij})\Big]$$

where $\alpha_1 = (C_2 - \frac{4}{3})/(C_3 - 2)$ and

$$S^*_{ij} = \frac{1}{2} g\tau(2 - C_3) S_{ij},$$
$$W^*_{ij} = \frac{1}{2} g\tau(2 - C_4) \Big[W_{ij} + \Big(\frac{C_4 - 4}{C_4 - 2}\Big) e_{mji}\omega_m \Big],$$
$$\eta = (S^*_{ij} S^*_{ij}), \quad \zeta = (W^*_{ij} W^*_{ij}),$$

and

$$g = \Big(\frac{1}{2}C_1 + \frac{P_k}{\varepsilon} - 1\Big)^{-1}, \quad \tau = \frac{k}{\varepsilon}.$$

In these equations, P_k is the production term, ω_m is the mth component of the speed of rotation vector, e_{mji} are the components of the permutation tensor and we have used W_{ij} for the components of the skew-symmetric part of the velocity gradient.

The physical constants appearing in this turbulence model are C_1, C_2, C_3 and C_4.

Iterative strategy

General considerations

It is known that it is very difficult to obtain a converged solution in general situations even for the simplest k-ε model.

The scheme we propose is:

1 Solve the Navier-Stokes equations.

2 Solve for k and ε

2.1 Update production

2.2 Solve for k (until convergence)

2.3 Solve for ε (until convergence)

2.4 Check convergence in terms of L. If not, go to 2.2.

3 Check convergence for $\boldsymbol{u}$. If not, go to 1.

Linearization of the equations for k and ε

Let us consider first a convection-diffusion-production equation of the form

$$(\boldsymbol{u} \cdot \nabla)\phi - \nabla \cdot (\kappa \nabla \phi) + \alpha \phi = f$$

It is known that this equation is 'well behaved' when $\kappa > 0$ and $\alpha > 0$.

The first point of our iterative scheme is that we couple the equations for k and ε iteratively.

Since we do not want to deal with problems with a negative production term (that is, with reaction-like terms), we keep the term P_k constant and also constant

$$P_\varepsilon = -C_1 P_k \frac{\varepsilon}{k}$$

We could express ν_t in terms of k and linearize it (with ε given). However, we keep ν_t constant while iterating for k to avoid the possibility of having a problem with negative diffusion or smaller than the converged one.

In order to avoid keeping ε constant we write it as $c_\mu k^2/\nu_t$ and linearize it using the Newton-Raphson method. Therefore, the innermost iterative loop to be performed is:

Given ν_t and P_k, solve until convergence:

$$(\boldsymbol{u}\cdot\nabla)k_i - \nabla\cdot\left(\frac{\nu_t}{\sigma_k}\nabla k_i\right) - P_k$$
$$+\frac{c_\mu}{\nu_t}\left(2k_{i-1}k_i - k_{i-1}^2\right) = 0$$

Similarly, we also keep constant ν_t in the equation for ε:

Given k, ν_t and P_ε, solve until convergence:

$$(\boldsymbol{u}\cdot\nabla)\varepsilon_i - \nabla\cdot\left(\frac{\nu_t}{\sigma_\varepsilon}\nabla \varepsilon_i\right) - P_\varepsilon$$
$$+\frac{C_2}{k}\left(2\varepsilon_{i-1}\varepsilon_i - \varepsilon_{i-1}^2\right) = 0$$

Iterative scheme for the k-ε model

The global scheme is as follows:

1 Compute P_k and P_ε

2 Repeat until convergence for L:

2.1 Solve for k:

2.1.1 Solve for k

2.1.2 $k_i \leftarrow \gamma k_i + (1-\gamma)k_{i-1}$

2.2 Check convergence for k. If not, go to 2.1

2.3 Update ν_t

2.4 Solve for ε:

2.4.1 Solve for ε

2.4.2 $\varepsilon_i \leftarrow \gamma \varepsilon_i + (1-\gamma)\varepsilon_{i-1}$

2.5 Check convergence for ε. If not, go to 2.4

2.6 Compute L

2.7 Use under-relaxation for L

2.8 Update ν_t

3 Check convergence for L. If not, go to 2.

Iterative scheme for algebraic stress models

The deviatoric part $\boldsymbol{\tau}_{\mathrm{d}} = 2\nu_t \boldsymbol{S}(\boldsymbol{u})$ of the Reynolds stress tensor it can be linearized as

$$\boldsymbol{\tau}_{\mathrm{d}} \approx 2\nu_{t,i-1}\boldsymbol{S}(\boldsymbol{u}_i)$$

However, when a ASM is employed, all the terms of $\boldsymbol{\tau}$ must be evaluated using $\boldsymbol{u}_{i-1}$. This leads to a poor linearization that leads to a poor convergence behavior.

In order to improve it, we use a pre-conditioning of the ASM model with the Boussinesq assumption. Suppose that the convective term of the Navier-Stokes equations is linearized as $(\boldsymbol{u}_{i-1} \cdot \nabla)\boldsymbol{u}_i$. Then the linearization that we use is

$$(\boldsymbol{u}_{i-1} \cdot \nabla)\boldsymbol{u}_i - \nabla \cdot [2(\nu + \nu_{t,i-1})\boldsymbol{S}(\boldsymbol{u}_i)] + \nabla p_i$$
$$= \boldsymbol{f} - \nabla \cdot [2\nu_{t,i-1}\boldsymbol{S}(\boldsymbol{u}_{i-1}) - \boldsymbol{\tau}_{i-1}]$$

where $\boldsymbol{\tau}_{i-1}$ is computed using the unknowns of the iteration $i-1$ and according to the particular ASM employed.

Finite element approximation

Model problem and basic formulation

Once the equations for k and ε have been linearized, both can be considered as convection-diffusion-production equations.

The boundary value problem that we consider is

$$\begin{aligned} -\kappa\Delta\phi + \boldsymbol{u}\cdot\nabla\phi + \alpha\phi &= f \quad \text{in} \quad \Omega \\ \phi &= g \quad \text{on} \quad \partial\Omega \end{aligned}$$

where we assume that $\alpha \geq 0$. The basic finite element formulation for solving the problem can be (for example) the SUPG method. It reads: Find $\phi_h \in \Phi_h$ such that

$$\begin{aligned} &\kappa \int_\Omega \nabla\psi_h \cdot \nabla\phi_h \mathrm{d}\Omega + \int_\Omega \psi_h \boldsymbol{u}\cdot\nabla\phi_h \,\mathrm{d}\Omega \\ &+\alpha \int_\Omega \psi_h\phi_h \mathrm{d}\Omega - \int_\Omega \psi_h f \mathrm{d}\Omega \\ &+\sum_{e=1}^{n_{\mathrm{el}}} \int_{\Omega^e} \boldsymbol{u}\cdot\nabla\psi_h \tau \mathcal{R}(\phi_h)\mathrm{d}\Omega = 0 \end{aligned}$$

for all $\psi_h \in \Psi_h$, where

$$\mathcal{R}(\phi_h) := -\kappa\Delta\phi_h + \boldsymbol{u} \cdot \nabla\phi_h + \alpha\phi_h - f$$

and τ is computed as

$$\tau = \frac{\xi h}{2|\boldsymbol{u}|}, \quad \xi = \min(\mathrm{Pe}/3, 1)$$

where ξ is the upwind function, which depends on the element Péclet number

$$\mathrm{Pe} := \frac{|\boldsymbol{u}|h}{2\kappa}$$

Discontinuity capturing technique

The SUPG or similar techniques do not preclude the presence of overshoots and undershoots in the vicinity of sharp gradients of the solution of problems with a very small diffusion term. A shock-capturing technique is required.

The idea is to introduce a nonlinear numerical scheme in which the diffusion added is given by

$$\kappa_{\mathrm{dc}} = \frac{1}{2}\xi_{\mathrm{c}} h \frac{|\mathcal{R}(\phi_h)|}{|\nabla\phi_h|} \quad \text{for each element}$$

where the parameter ξ_{c} is computed as

$$\xi_{\mathrm{c}} = \max\left\{0, C_{\mathrm{dc}} - \frac{2\kappa}{|\boldsymbol{u}^*|h}\right\},$$

with

$$\boldsymbol{u}^* := \frac{1}{|\nabla\phi_h|^2}\left(\boldsymbol{u}\cdot\nabla\phi_h + \sigma\phi_h - f\right)\nabla\phi_h,$$

and C_{dc} a constant.

Numerical examples

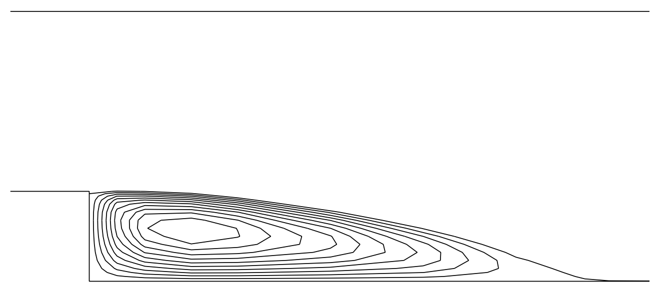

Figure 1: Streamlines for the backward facing step.

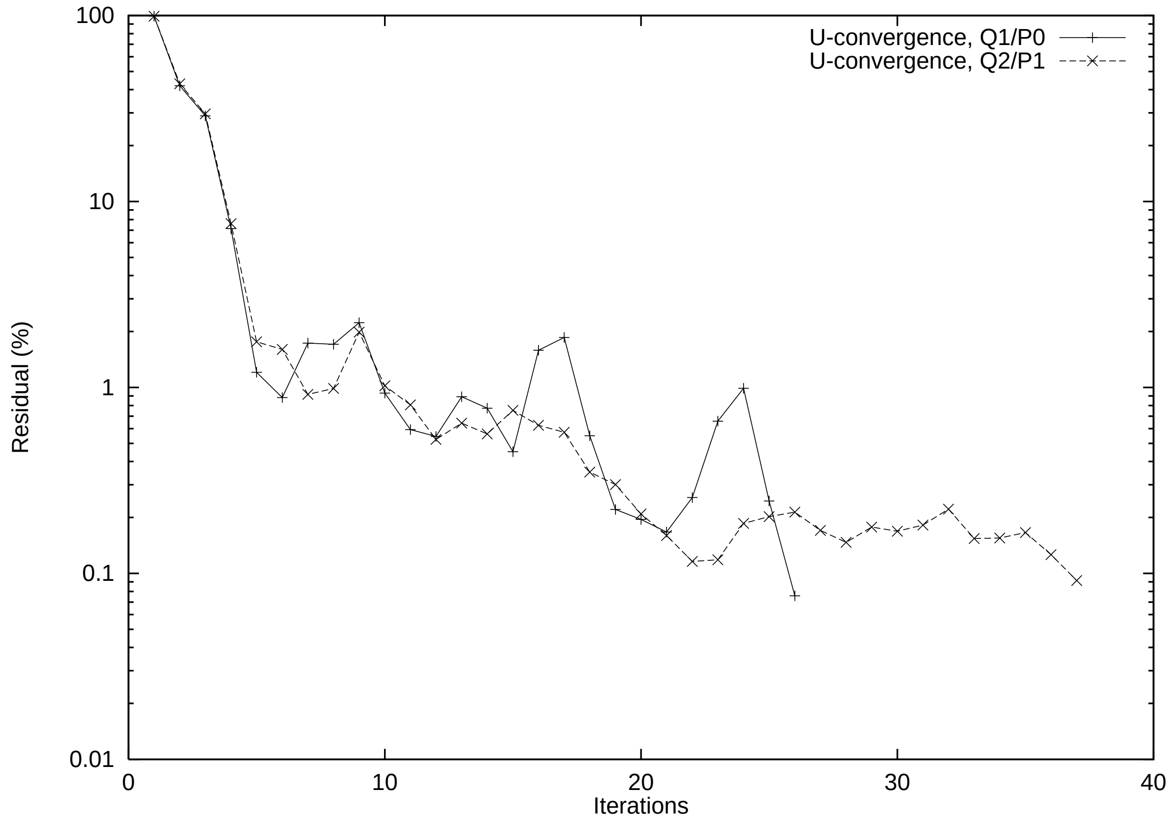

Figure 2: Velocity convergence for the flow over a backward facing step.

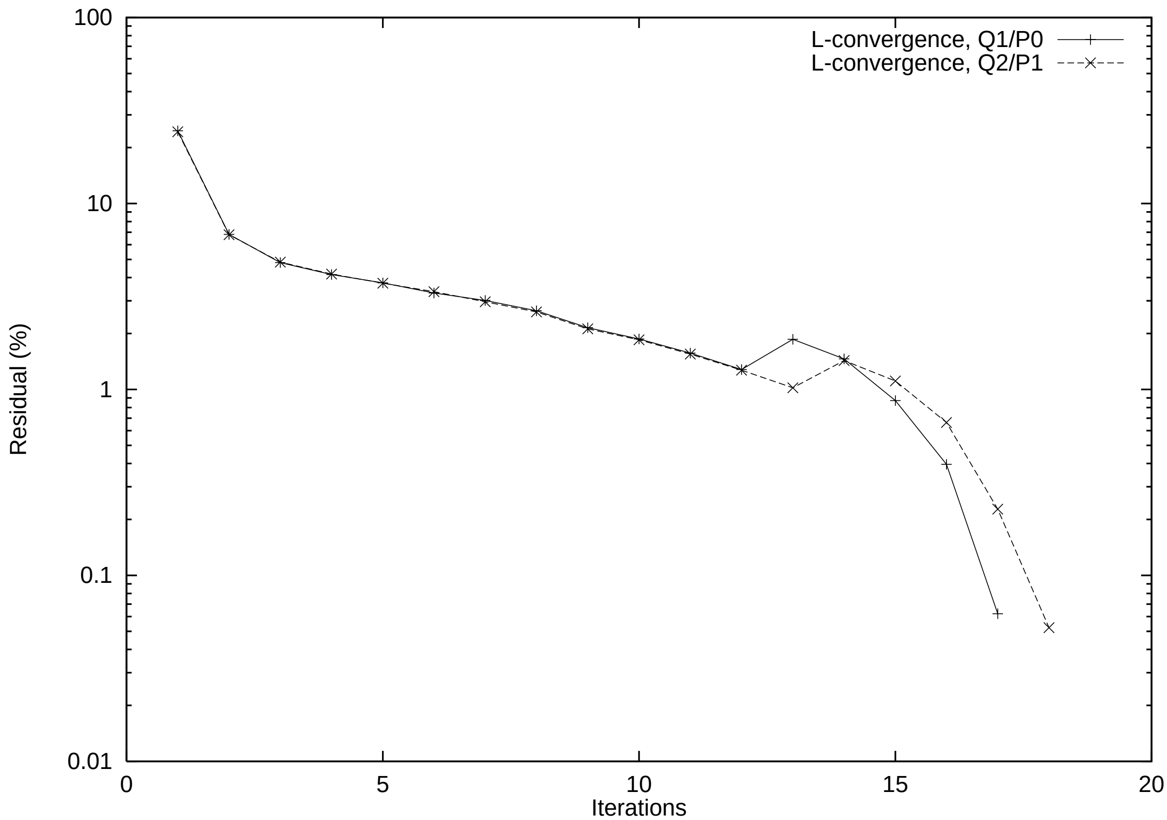

Figure 3: Convergence of L for the flow over a backward facing step. First iteration of $\boldsymbol{u}$.

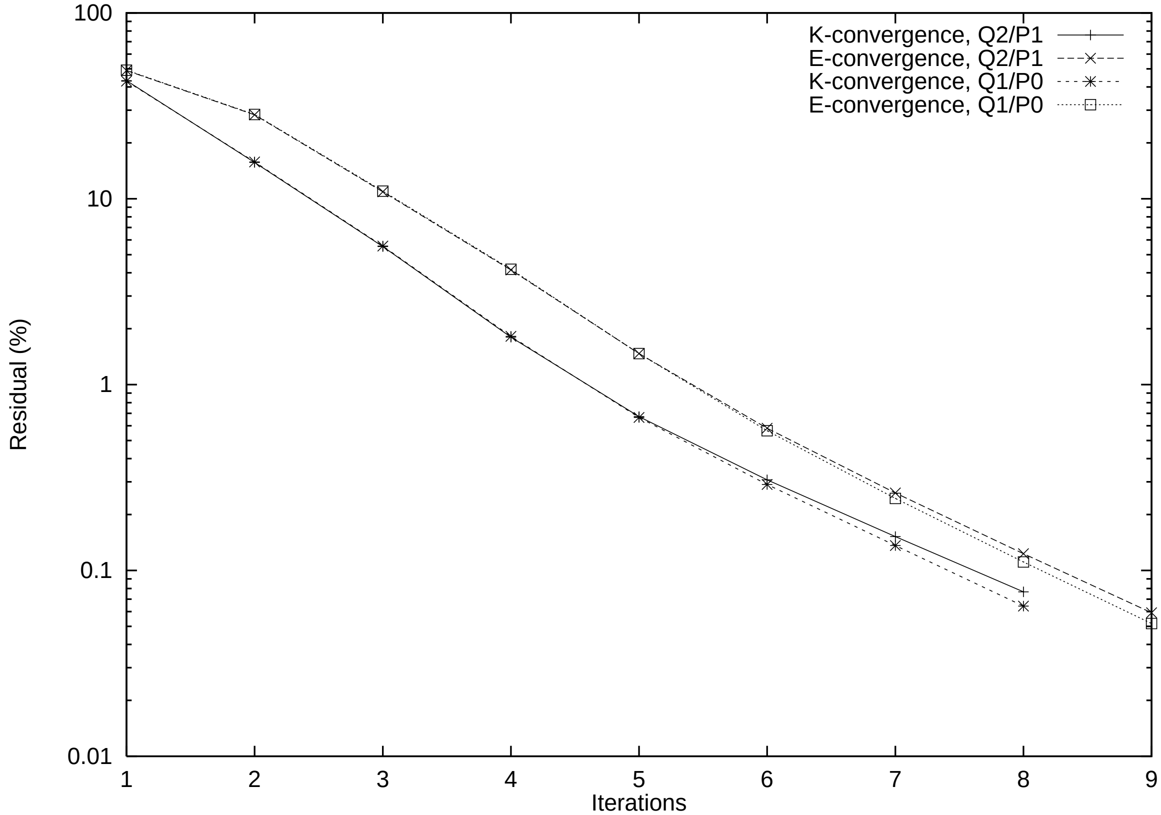

Figure 4: Convergence of k and ε for the flow over a backward facing step. First iteration of $\boldsymbol{u}$ and first iteration of L.

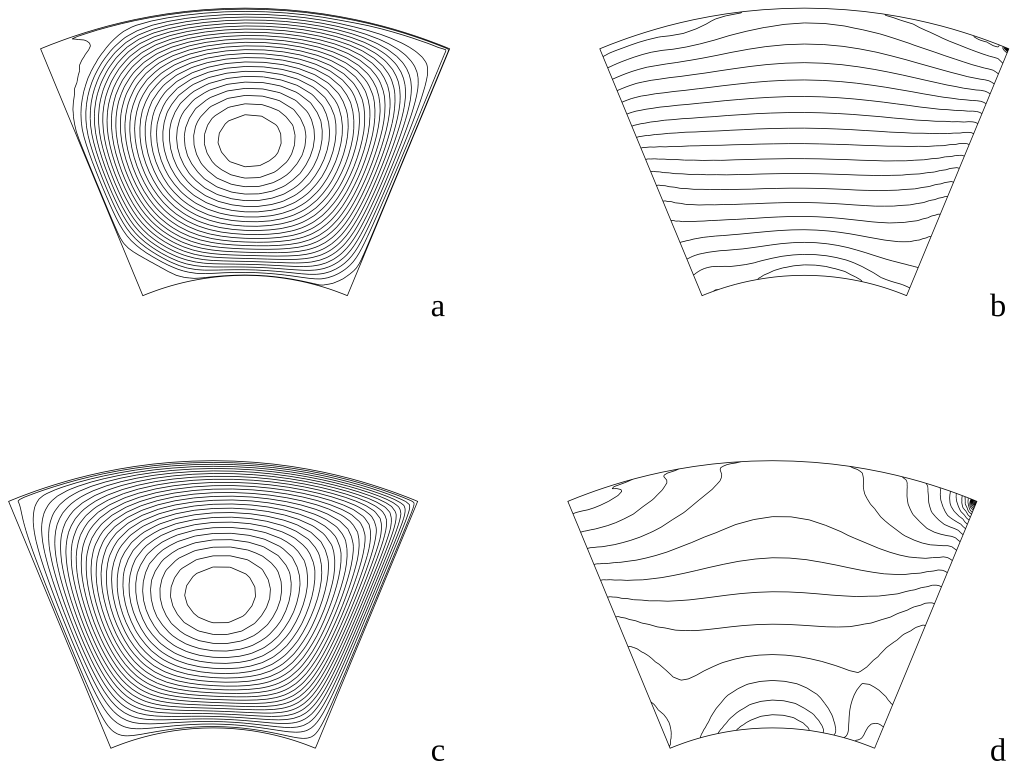

Figure 5: (a): Streamlines using the ASM. (b): Pressure contours using the ASM. (c): Streamlines using the k-ε model. (d): Pressure contours using the k-ε model.

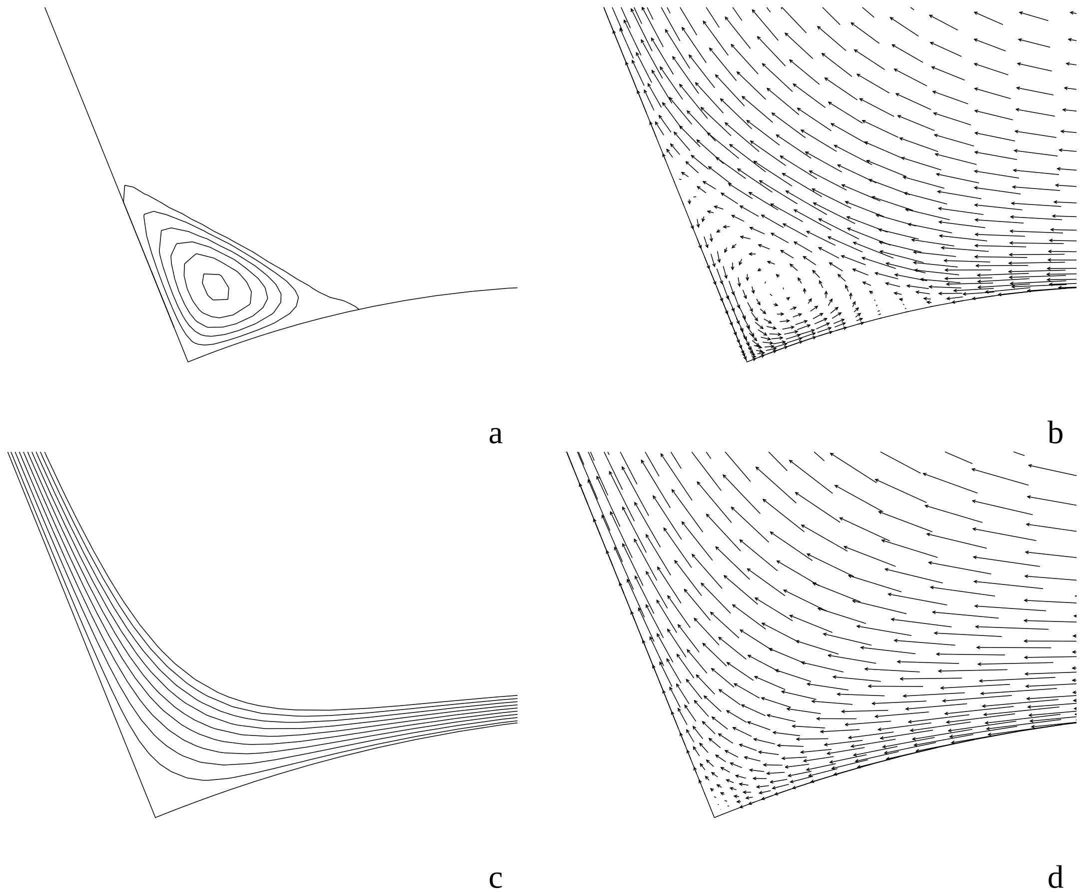

Figure 6: (a): Detail of the streamlines using the ASM. (b): Detail of the velocity vectors using the ASM. (c): Detail of the streamlines using the k-ε model. (d): Detail of the velocity vectors using the k-ε model.

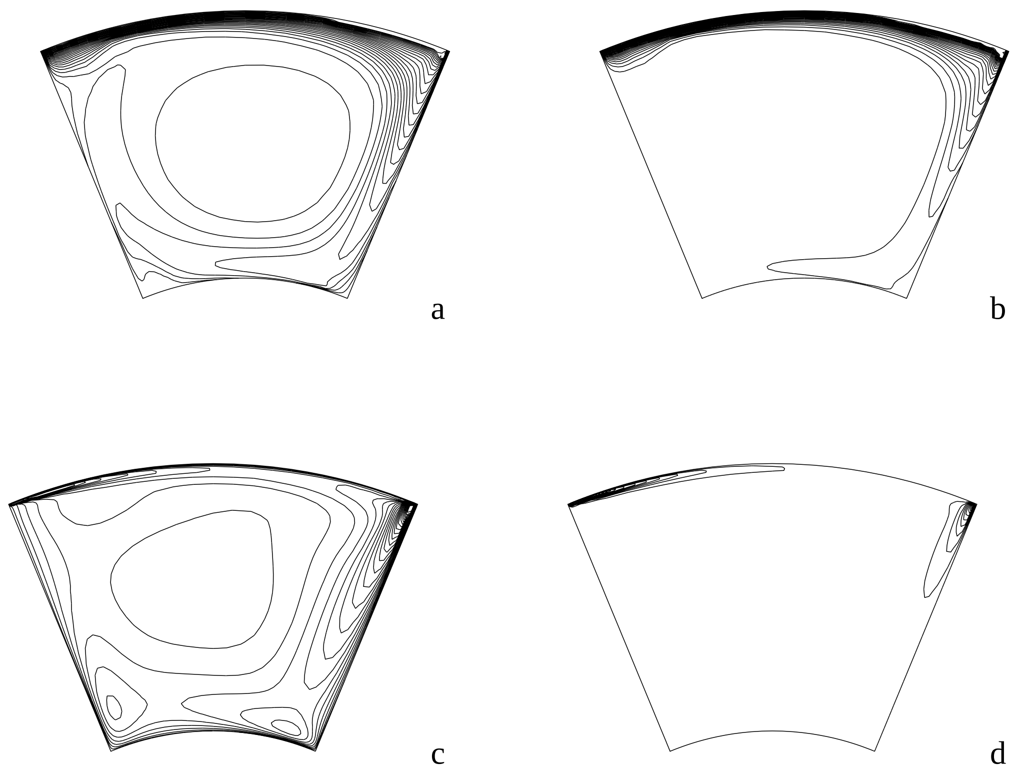

Figure 7: (a): Contours of k using the ASM; max = 0.03. (b): Contours of ε using the ASM; max = 0.05. (c): Contours of k using the k-ε model; max = 0.38. (d): Contours of ε using the k-ε model; max = 9.25.

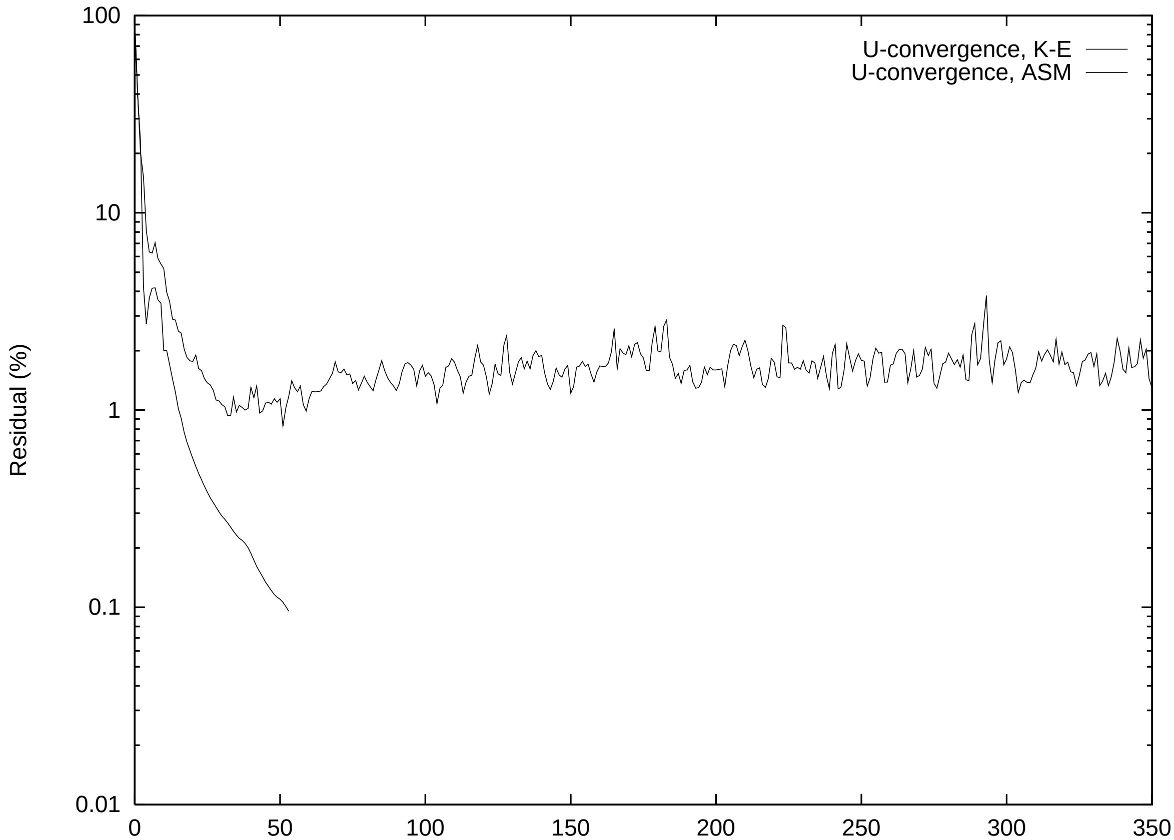

Figure 8: Velocity convergence for the flow in a polar cavity.

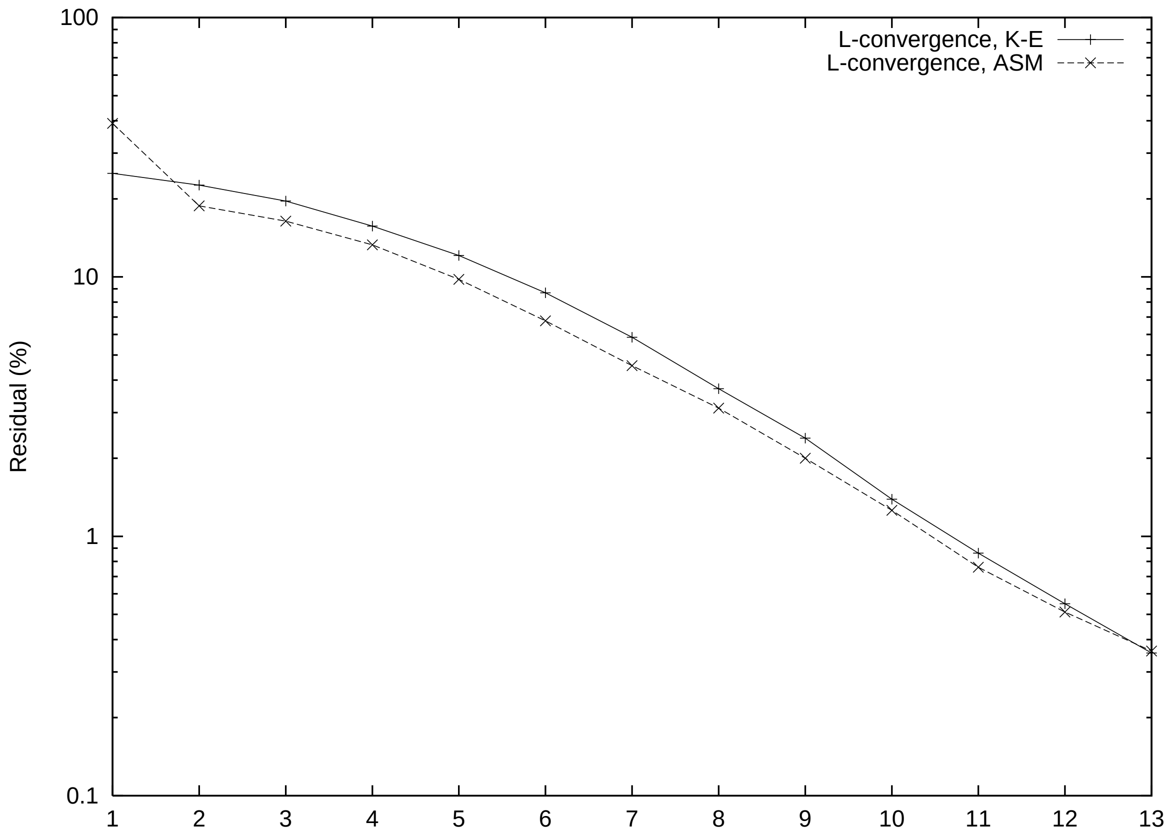

Figure 9: Convergence of L for the flow in a polar cavity. First iteration of $\boldsymbol{u}$.

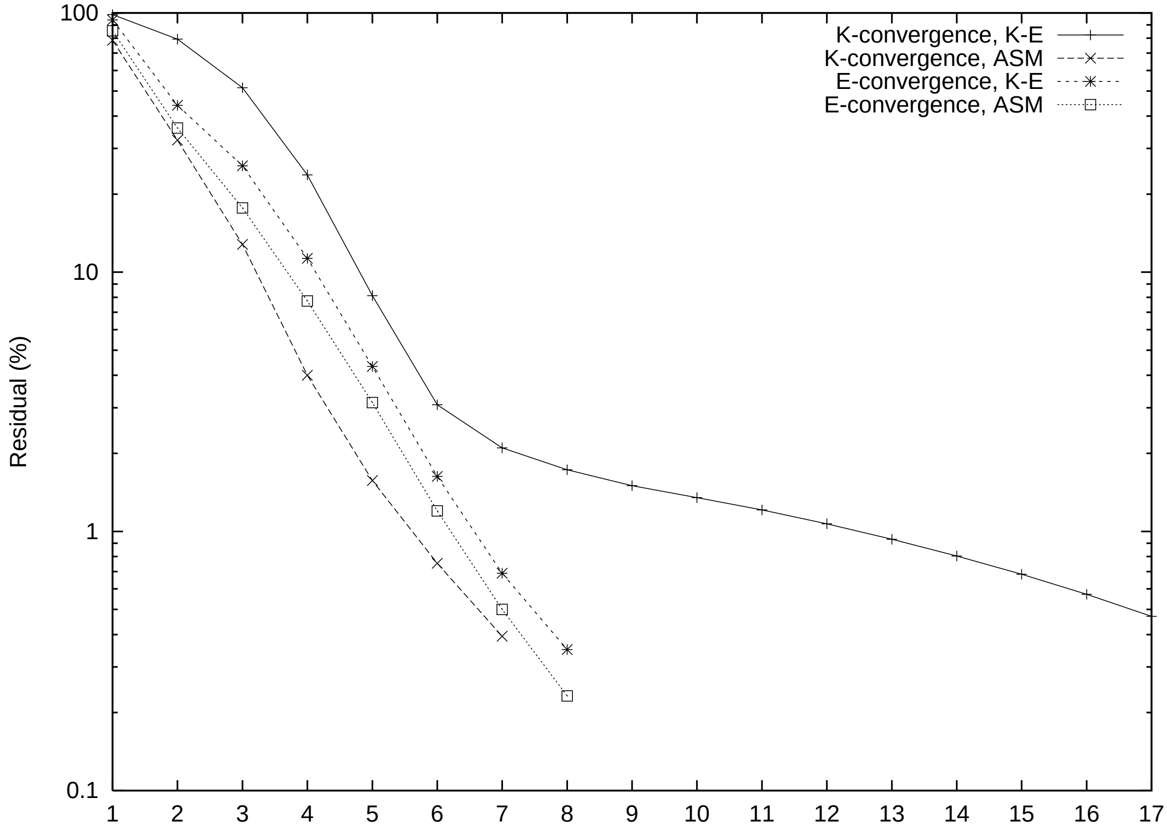

Figure 10: Convergence of k and ε for the flow in a polar cavity. First iteration of $\boldsymbol{u}$ and first iteration of L.

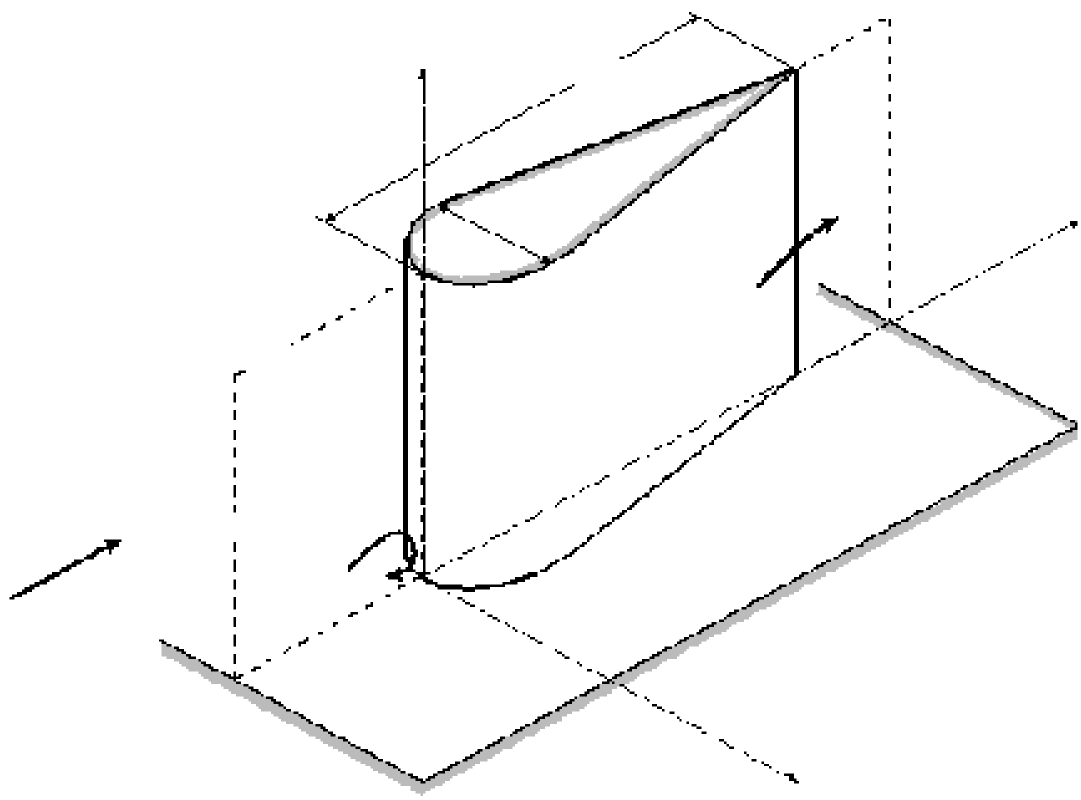

Figure 11: Flow over a wing: Problem set-up.

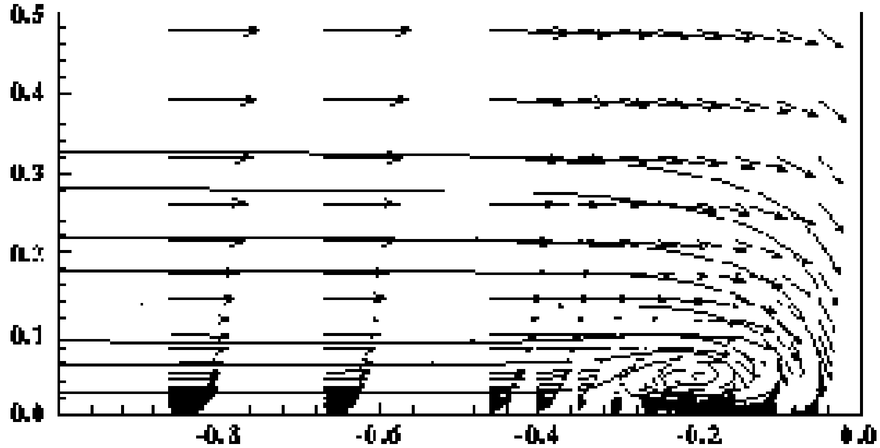

Figure 12: Experimental flow pattern at the symmetry plane for the flow over a wing.

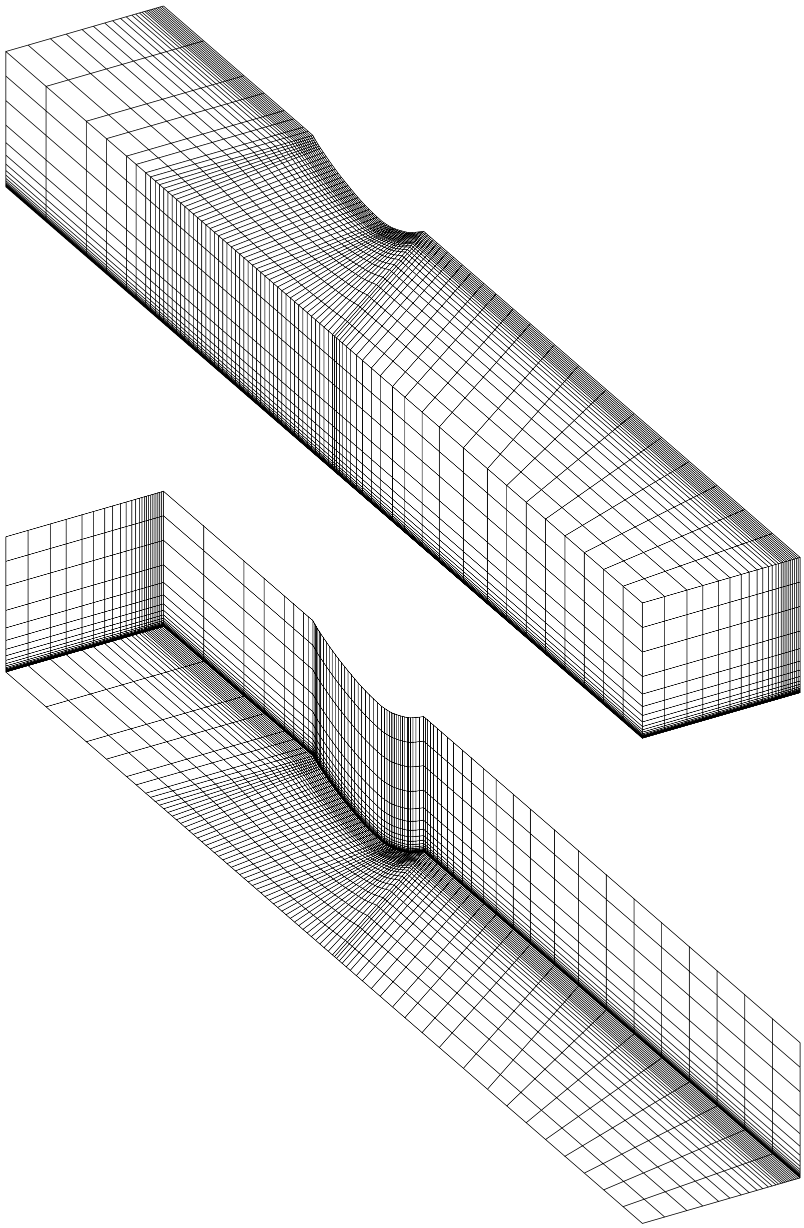

Figure 13: Surface mesh for the flow over a wing (37296 Q_1/P_0 elements, 41250 nodal points) (a): Upper and frontal walls. (b): Bottom and rear walls.

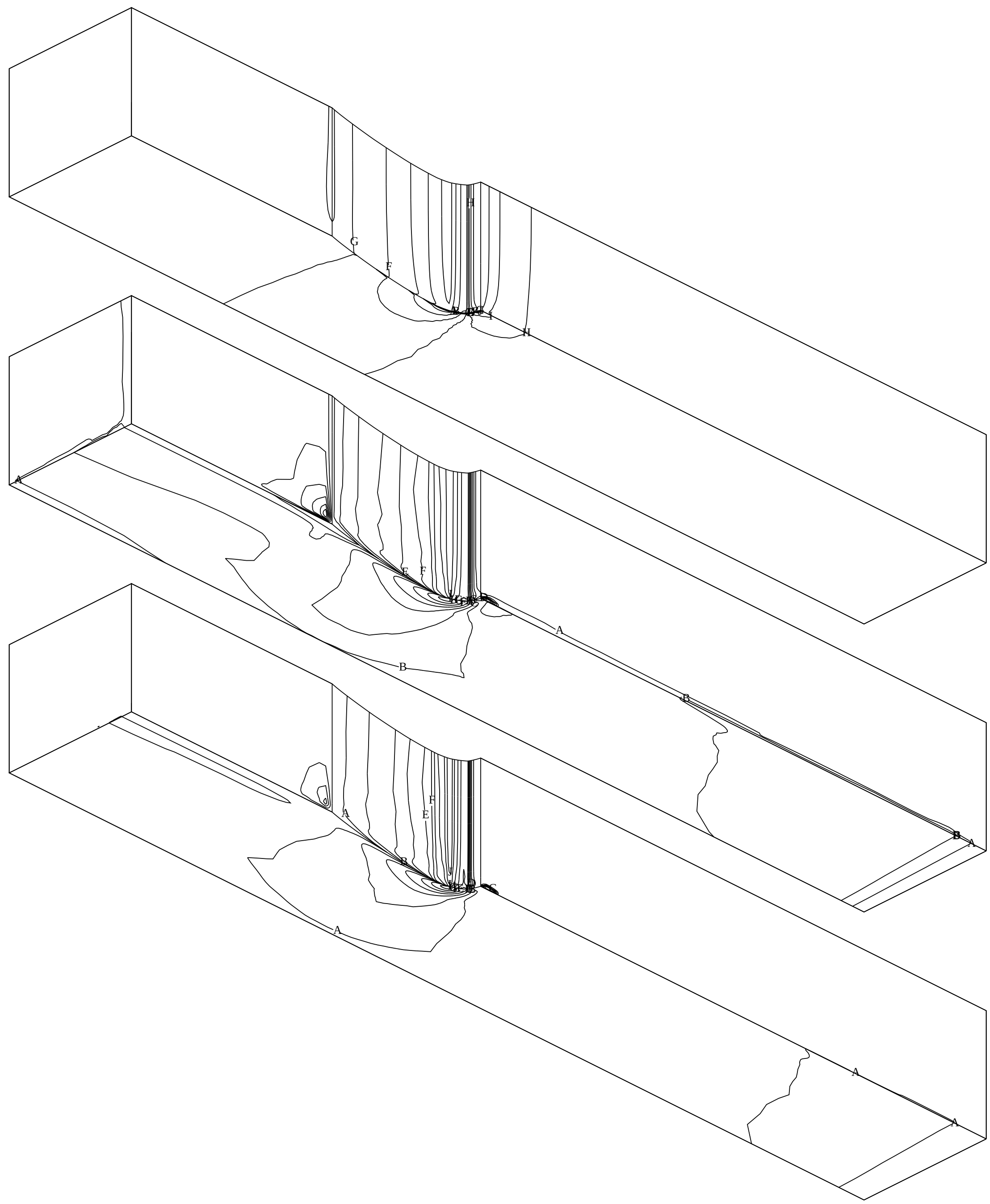

Figure 14: Results for the flow over a wing. Pressure contours. Contours of k. Contours of ε.

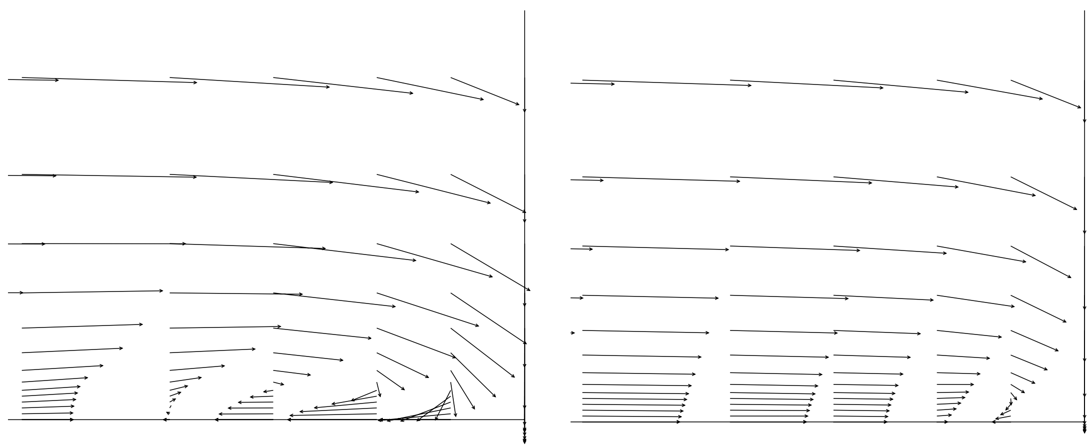

Figure 15: Detail of the vortex before the wing on the symmetry plane. (a): $\Delta = 2$ mm. (b): $\Delta = 7$ mm.

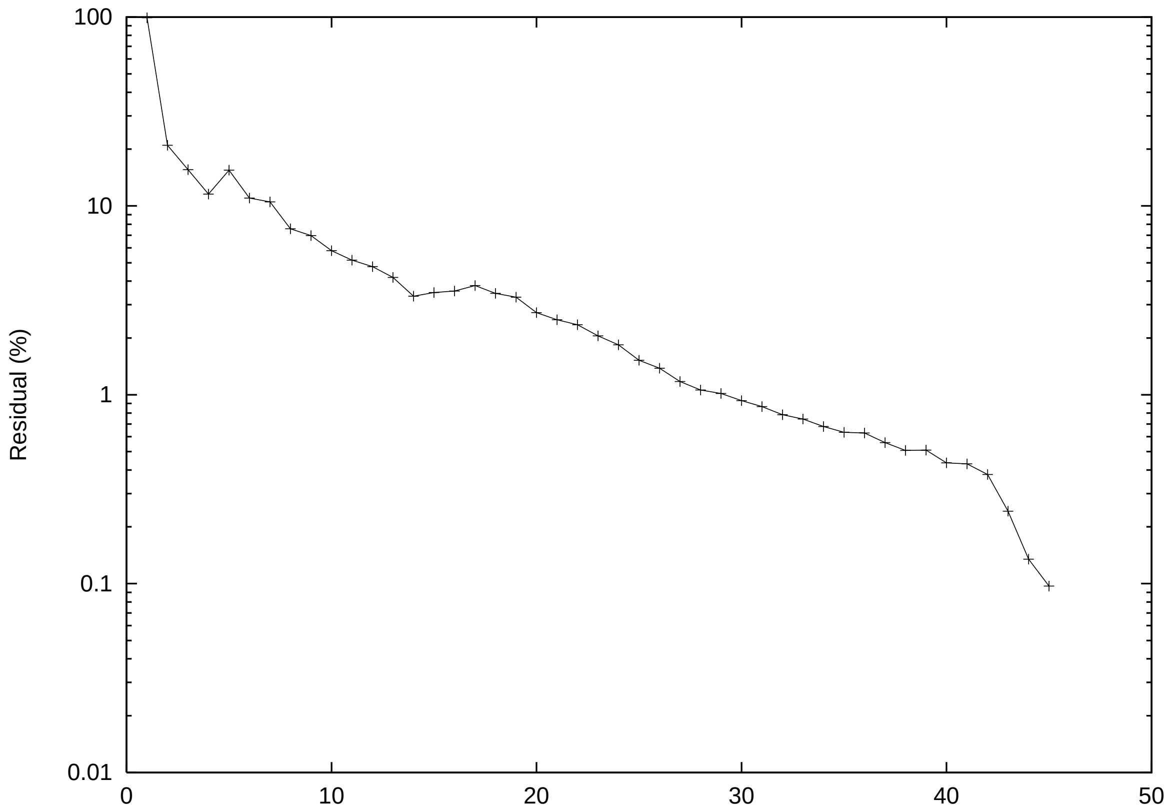

Figure 16: Velocity convergence for the flow over wing.

Large eddy simulation

Smagorinsky, gradient and mixed models

After using arguments of filtering of the Navier-Stokes equations one is led to the introduction of a "stress-like" tensor:

$$\boldsymbol{\tau} = -\overline{\boldsymbol{u} \otimes \boldsymbol{u}} + \bar{\boldsymbol{u}} \otimes \bar{\boldsymbol{u}}$$

where now the overbar denotes filtering and $\boldsymbol{u}$ is the total velocity.

In the case of the Smagorinsky model:

$$\boldsymbol{\tau} \approx \boldsymbol{\tau}_S = 2\nu_t S(\bar{\boldsymbol{u}}) = 2C_S^2 \Delta^2 I_2(S(\bar{\boldsymbol{u}}))S(\bar{\boldsymbol{u}})$$

where Δ is the filter width, which is $\Delta \sim h$ in a FEM calculation.

The gradient (or Clark) model is obtained by taking a Taylor expasion of $\boldsymbol{u}$ around the support of the filter and taking the filter of this expansion. It is found that

$$\boldsymbol{\tau} \approx \boldsymbol{\tau}_C = -\sum_{k=1}^{n} C_k \left(\partial_k \bar{\boldsymbol{u}} \otimes \partial_k \bar{\boldsymbol{u}} - \frac{1}{n} \partial_k \bar{\boldsymbol{u}} \cdot \partial_k \bar{\boldsymbol{u}} \, \boldsymbol{I} \right)$$

The gradient model has extremely poor convergence properties in a CFD application. Often, mixed models are used:

$$\boldsymbol{\tau} \approx \alpha \boldsymbol{\tau}_C + \beta \boldsymbol{\tau}_S$$

$\boldsymbol{\tau}_C$ may introduce negative dissipation into the scheme; $\beta > 0$ is required.

Dynamic models: filtering

In the dynamic models, the "constants" C_S and C_k depend on $\bar{\boldsymbol{u}}$. The dynamic version of Smagorinsky's model is called Germano-Lilly model. If $\tilde{}$ denotes another filter, of width $\tilde{\Delta}$, define

$$T_{ij} = -\widetilde{\overline{u_i u_j}} + \tilde{\bar{u}}_i \tilde{\bar{u}}_j$$

The tensor

$$L_{ij} := \tilde{\tau}_{ij} - T_{ij} = \widetilde{\bar{u}_i \bar{u}_j} - \tilde{\bar{u}}_i \tilde{\bar{u}}_j$$

is computable in terms of the CFD unknown $\tilde{\boldsymbol{u}}$.

Applying Smagorinsky's model to both τ_{ij} and T_{ij} we obtain the computable tensors

$$\tau_{ij}^S = 2C_S^2 \Delta^2 I_2(S(\bar{\boldsymbol{u}}))S_{ij}(\bar{\boldsymbol{u}})$$
$$T_{ij}^S = 2C_S^2 \tilde{\Delta}^2 I_2(S(\tilde{\bar{\boldsymbol{u}}}))S_{ij}(\tilde{\bar{\boldsymbol{u}}})$$

Let

$$L_{ij}^S := \tilde{\tau}_{ij}^S - T_{ij}^S =: C_S^2 M_{ij}$$

Imposing that the difference between L_{ij} and L_{ij}^S

be minimum, it is found that

$$C_S^2 = \frac{M_{ij} L_{ij}}{M_{ij} M_{ij}}$$

The problem is how to compute the filter of a function f, defined as

$$\tilde{f}(x) = \int_\Omega G(x-r) f(r) dr$$

Classical filters G are the Gaussian filter and the "top hat". However, the problem is how to define a filter in terms of finite element functions. Two possibilities are:

- Top hat filter

$$\tilde{f}^a = \frac{1}{\text{meas}\Omega^a} \int_{\Omega^a} N^b f^b \, \mathrm{d}\Omega$$

- Filtering with the shape functions:

$$\tilde{f}^a = \frac{1}{\int_\Omega N^a \, \mathrm{d}\Omega} \int_\Omega N^a N^b f^b \, \mathrm{d}\Omega$$

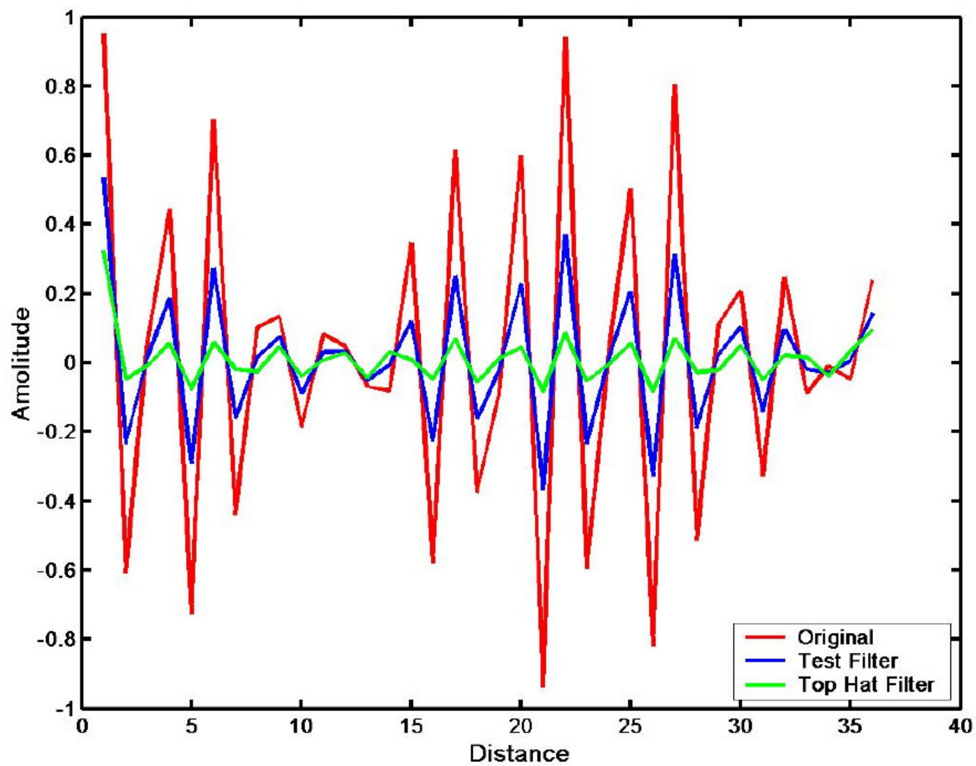

Figure 17: Comparison of the top hat filter and the filtering with the shape function.

Conclusions

The main ideas presented related to the finite element implementation of turbulence models are the following:

- Special care is needed in the design of the iterative scheme. It is important to solve at each iteration convection-diffusion-reaction equations with positive reaction coefficients and as high as possible diffusion coefficients.
- Shock capturing techniques are often necessary to deal with sharp gradients of the solution and to ensure positivity of the unknowns ($\tilde{\nu}$, k-ε, etc).
- Special care is needed to introduce positive dissipation in the Navier-Stokes equations in the iterative process
- Analytical filters have to be reconsidered in FEM approximations of LES calculations