Using commercial CFD (Computational Fluid Dynamics) Software

1 Introduction

There are several reasons to buy and use a commercial CFD package.

- No time to write code
- No time for code maintenance
- Need for documentation
- Need for support

Writing your own code takes much time, especially for debugging. The code needs maintenance (bug repair, new models etc.). The code must be documented if other people have to use it. Moreover, if other people use it, you will need support in case of problems. Unless you always have the right people around to do all this for you, you may have to use a commercial CFD package.

Typically you will not get the source code of a commercial CFD package. So, to some extent it is black box.

This has several consequences. It may be exactly what you want, for instance if you have no time to look at the code or if you are not interested to do so. On the other hand, you have no insight in "tricks" that are used in the code. Bugs have to be corrected by the developer. This is nice since you do not have to do it, but you may have to wait for some time before bugs are corrected ("this bug will be fixed in the next release"). If there is a feature that you absolutely need but which is not in the package the same applies: you don't have to add the new feature, but you will have to wait until it is added.

2 Some general packages

Some general packages which are available, together with their websites, are:

- Fluent www.fluent.com
- CFX www-waterloo.ansys.com/cfx
- Flow3d www.flow3d.com
- starcd www.cd-adapco.com
- Numeca www.numeca.com
- Comet www.cd-adapco.com

Fluent is (in number of licenses sold) the biggest package, which is why we use it at ahd. The packages are comparable in price and overall quality. For commercial use count on (say) 20.000 euro for one or two licenses. Academic licenses are much cheaper but the service (helpdesk etc) is accordingly worse.

There are some differences which may be important when choosing a package. It is wothwhile to try a package out before buying it.

CFX 5 (un-structured) has no special 2D feature. If you have a 2D or axi-symmetric problem you need to simulate it 3D with few grid cells in one direction.

CFX 5 has a better grid generator for 3D geometries (IF it works, sometimes it fails).

Fluent has a particle routine which is not reliable.

All packages offer:

- laminar flow
- turbulent flow
- multi-phase flow
- free surface flow
- (conjugate) heat transfer
- chemistry (combustion)

3 How do you use a commercial CFD package

A commercial CFD package consists of a set of tools for doing CFD. It is NOT a solver which always gives the right answer! Tools must be used in the right way, even good tools do not work if you do not know what you are doing. Not everything can be tested! sometimes you have to find out yourself if the CFD package has the right tools for you, meaning: for the flow you want to calculate. A good way to find out is to ask somebody who has used the package for your type of flow. Otherwise, the way to go is as follows: Try to learn about the flow. Test simple examples (learn how to use the tools). Then go to the real problem.

Tools which you have to know are:

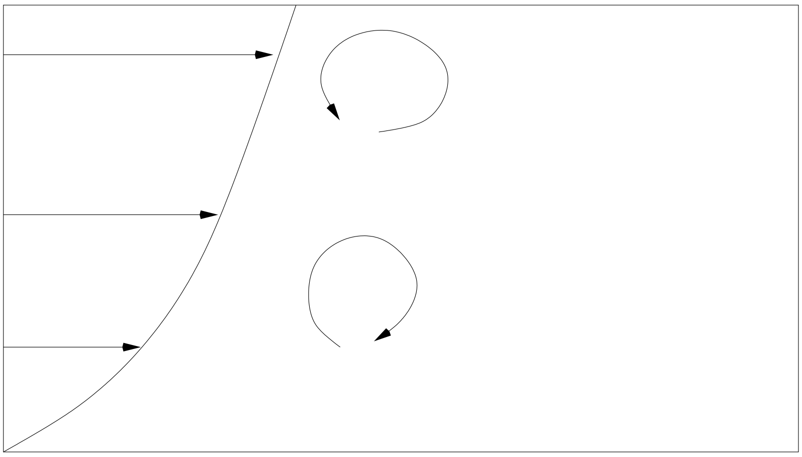
- the flow geometry:
- the boundary conditions: are they applied correctly?
- the grid
  - is the grid of sufficient quality?
  - is the grid of the right type?
  - is the grid fine enough to resolve all details of the flow?
  - is the grid too fine in some regions, leading to excessive CPU usage?
- the physical model: do you know if the physical model is valid?
- the solver: is the discretization scheme appropriate?
- visualization: how do you use the visualization tools for studying the solution and for comparison with other data?

All of the points mentioned above will be discussed in some detail below. Some points of discussion concern just application of common sense or physical intuition. Other points require knowledge of numerics or physical models.

Almost all flow you calculate will be turbulent in practice. Turbulence flows are characterized by:

- high Re
- $Re = UD/\nu$
- lots of vortices, are constantly created and then destroyed
- chaotic, 3D, time-dependent motion
- too expensive to calculate all for high Re
- only interested in mean motion
- equation for mean quantities ($u = \overline{U} + u'$)
- extra terms arise and must be modeled
- extra terms represent influence of vortices on mean flow

- extra terms: look like stress
- gradient hypothesis ("effect of vortices is kind of viscous")
- stress $= \nu \dfrac{\partial U}{\partial y}$
- k, ϵ
- $\nu_T \sim ul$
- velocity scale, length scale



- OR
- more equations for the stresses and...
- more modeling: Reynolds stress model (RSM)

gambit and fluent in a nutshell.

- gambit
  - make geometry outline
  - indicate position BC
  - generate grid
- fluent
  - set appropriate values for BC and physical parameters
  - calculate flow (choose solver, discretization)
  - study results

4 Simplify the geometry as much as you can.

Considerable effort can be saved by making the geometry as simple as possible. Remove any detail which is not important for the flow. Small details require a fine grid if the flow has to be resolved. If the influence of the details is small it mey be better to leave it out and put more grid points at places where they are useful.

The flow you study may be 3D or 2D. If the flow permits, try to model the flow 2D (or axi-symmetric). 2D grids are much easier to generate and check.

5 Make the geometry outline

The first action is to generate the geometry outline, i.e. draw the geometry where the fluid has to flow. Typically, you simulate only a piece of a more complicated, bigger geometry. The part of interest is cut out of the surrounding geometry. As a result, you have to give information at the cuts about the flow which is entering the calculation domain and possibly also some effect of the surroundings on the flow which is leaving the domain.

The exact position where you put the cuts can be very important. Examples are discussed below.

The information required at an inflow boundary depends on the type of flow. For laminar flow, just the velocity is needed. For turbulent flow you would like to know everything about the turbulent flow which is coming in. For the k-epsilon model these are profiles of the velocity, k and *epsilon*. If no profile is available (this is typical) the user must at least supply some information. namely the intensity of the turbulence (u'/U with u' the fluctuation level and U the average velocity) and a typical length scale of the turbulent eddies. For some standard flows there are some extimates for these numbers available, for instance for fully developed channel flow or fully developed pipe flow.

- u'/U 5 % and $l = 0.1D$ channel and pipe
- inflow length laminar $0.06ReD$
- inflow length turbulent $4.4Re^{(1/6)}D$

The inflow length mentioned is the length needed to change from a straight (block) profile at the entrance of a pipe or channel to the position where the flow is fully developed. The inflow length is different for laminar and turbulent flow. As you can see, for high Re flows will not always be fully developed in practice.

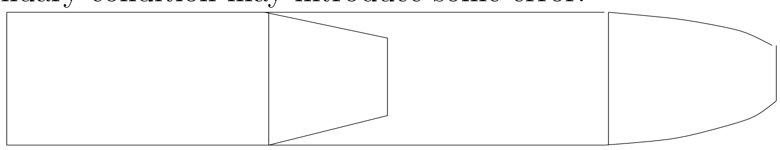
The influence of the inflow conditions on the flow is shown in the examples.

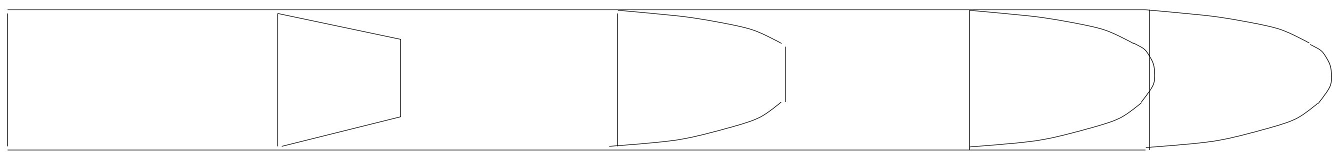
6 The outflow boundary

The outflow boundary of Fluent applies a so-called zero-deriveative condition. It assumes that the flow is fully developed and shows no change any more at the outflow part.

If this is not true for the geometry you study you may have to add some extra part to the geometry to have a well developed flow near the exit.

In the pictures below you see a sketch of a short pipe and a long one for laminar flow. In the long one flow as fully developed at the end: the flow gets a parabolic profile and does not change anymore. The short one is still developing near the outflow boundary, and the Fluent ouflow boundary condition may introduce some error.





The somain in first case too short for proper application of outflow BC.

7 Test case: ventilation of a container

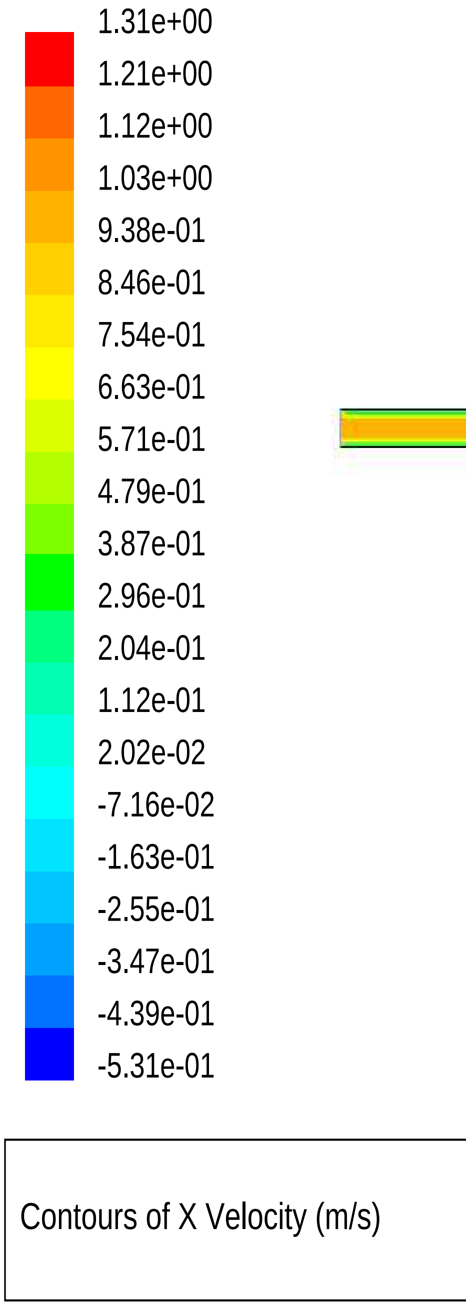
The following example shows the effect of inflow- and outflow BC on the flow in a container. The container (part of a more complicated structure) is modeled as a 2D geometry. There are inflow parts and outlfow parts consisting of plane channel. We try the following cases:

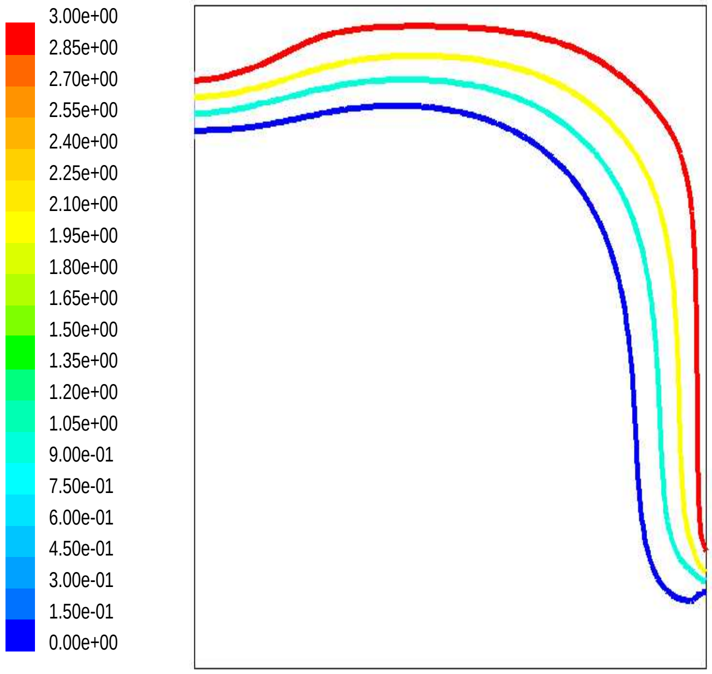
- the geometry with inflow parts and outlfow parts
- the geometry without inflow parts and outlfow parts (BC directly applied at container)

Moreover, the conditions prescribed at the inlet are:

- the default Fluent inflow conditions ($k = 1$ and $\epsilon = 1$)
- developed channel inflow BC applied at container)

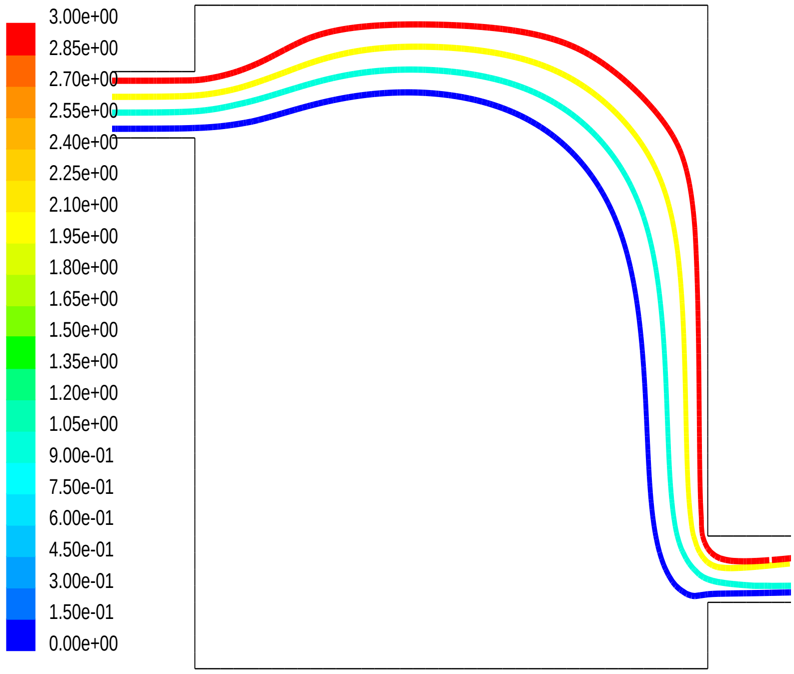
So, in all, we have four calculations (2 geometries and 2 different inflow BC)





Path Lines Colored by Particle ID

Apr 20, 2004
FLUENT 6.1 (2d, segregated, ske)



Path Lines Colored by Particle ID

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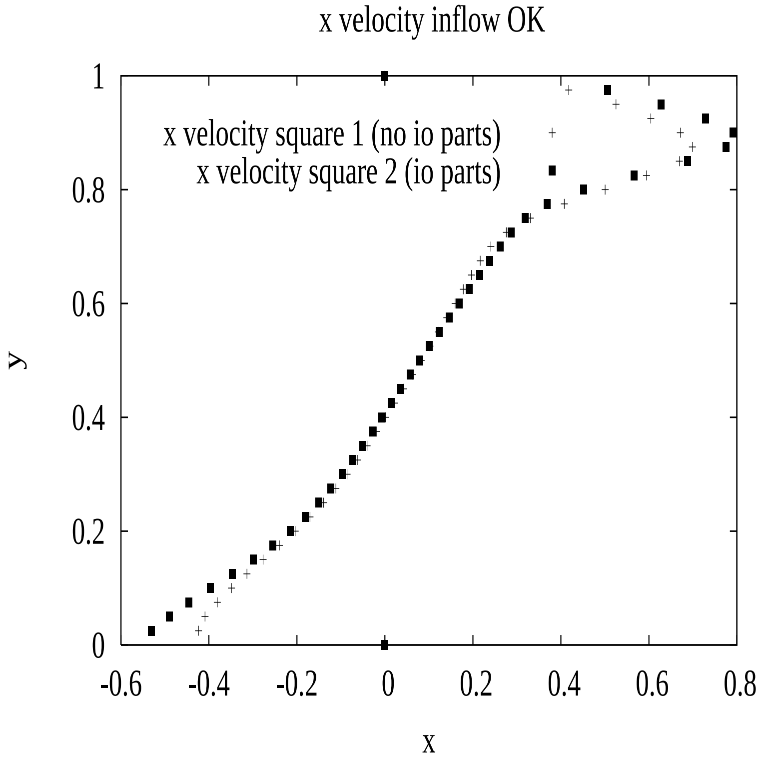
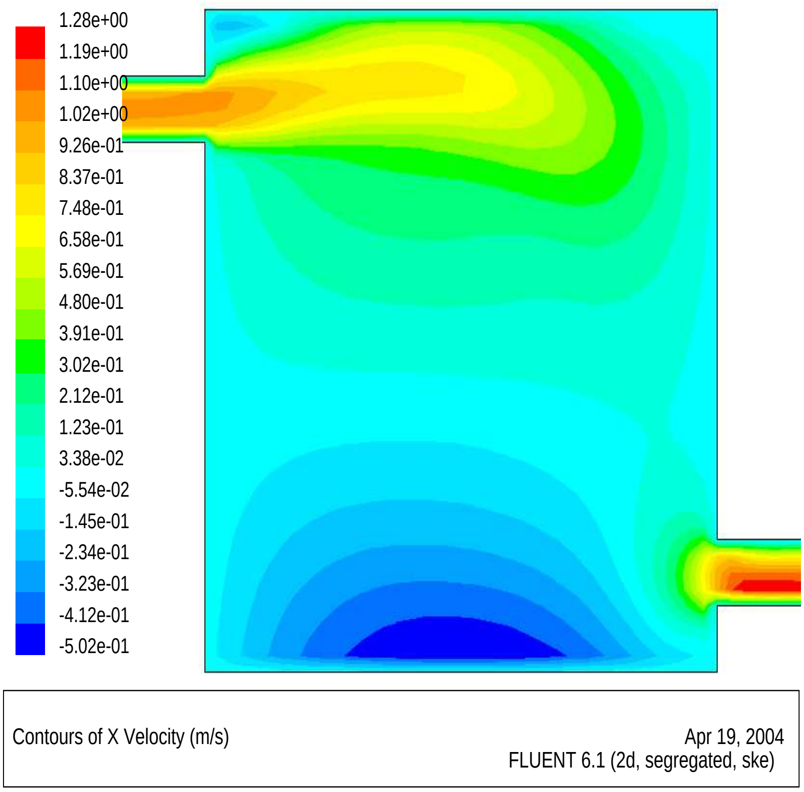
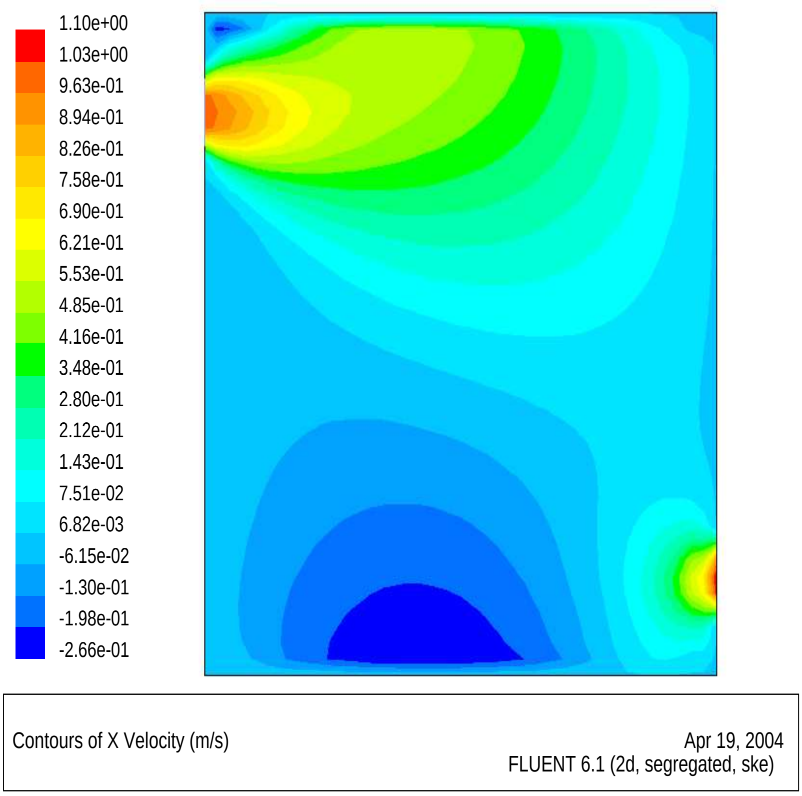
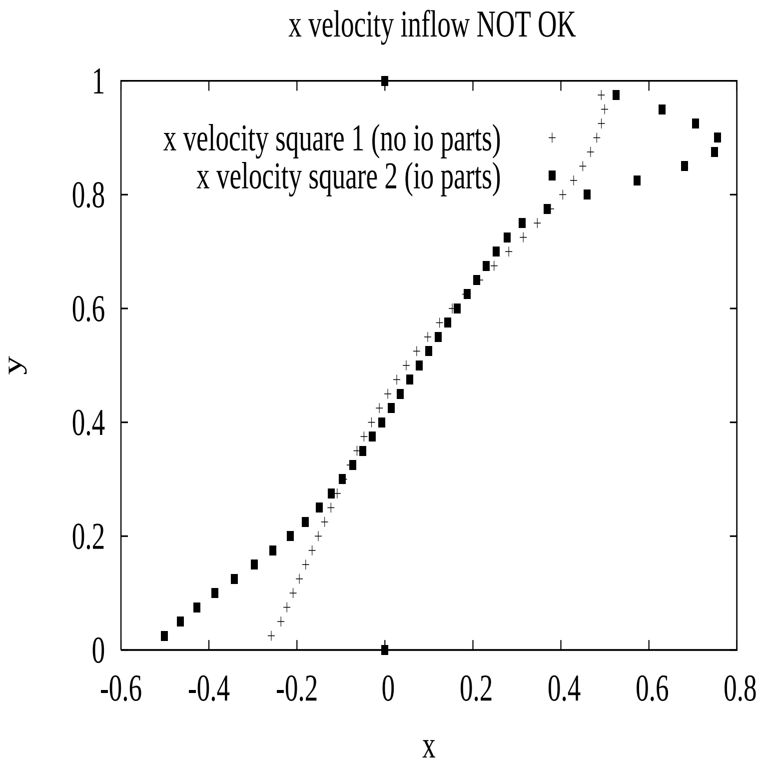


x velocity inflow OK
x velocity square 1 (no io parts)
x velocity square 2 (io parts)
y
x
1
0.8
0.6
0.4
0.2
0
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8

Now with wrong turbulent inflow BC.





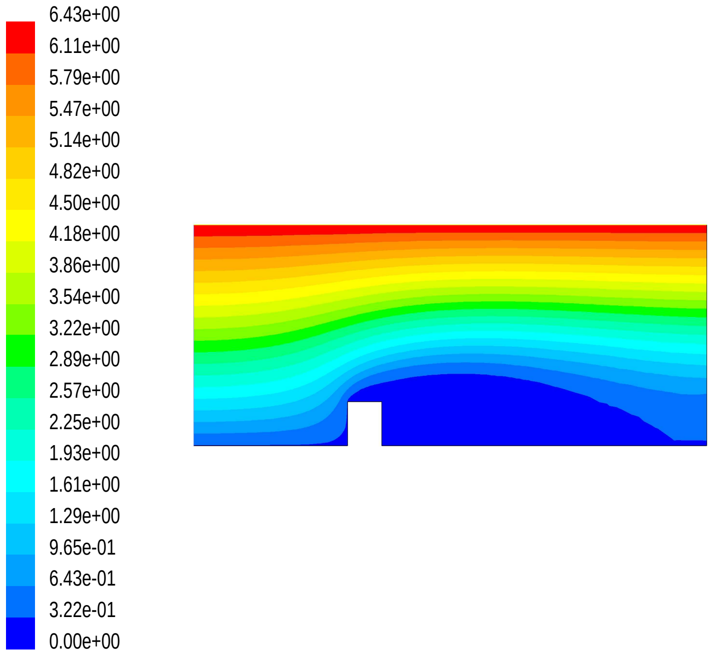


Conclusion:

- extra inlet and outlet pieces give better inlet profile
- also if the inflow condition is not precisely known

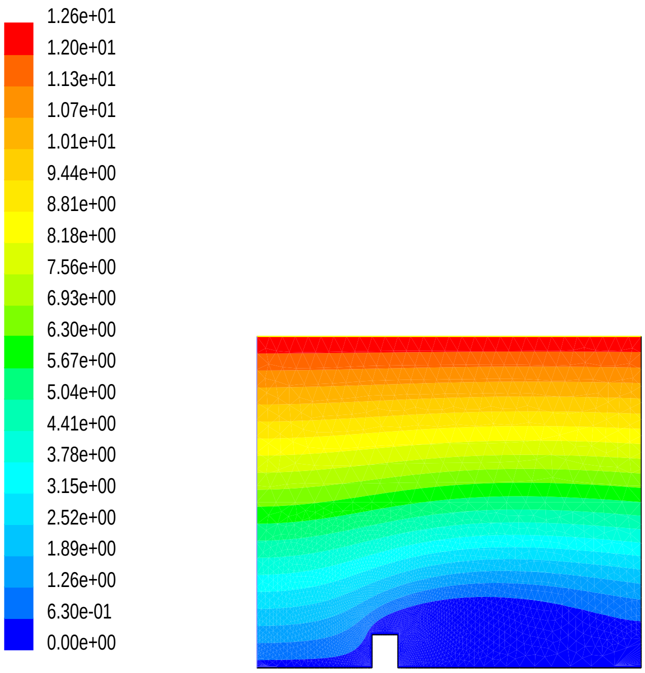
free space, open boundary

- where do you put the open boundary?
- how far is far enough?
- depends on boundary condition
- symmetry
- pressure



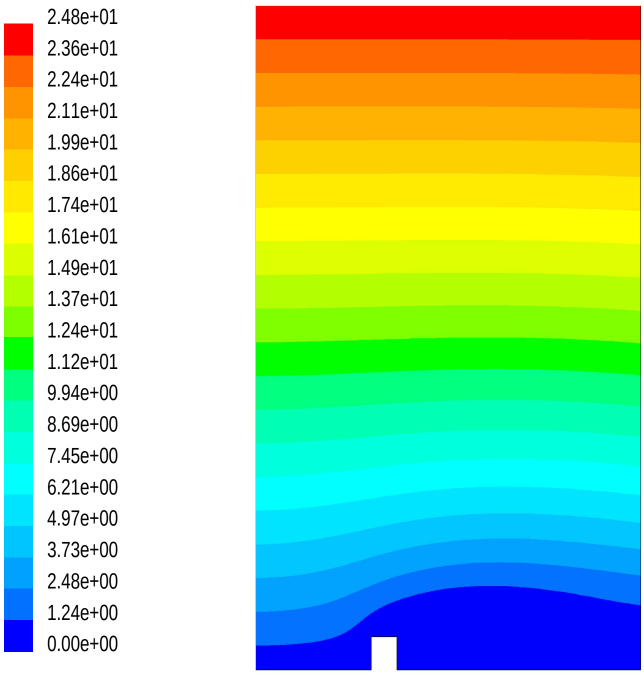
Contours of Stream Function (kg/s)

Apr 20, 2004
FLUENT 6.1 (2d, segregated, ske)



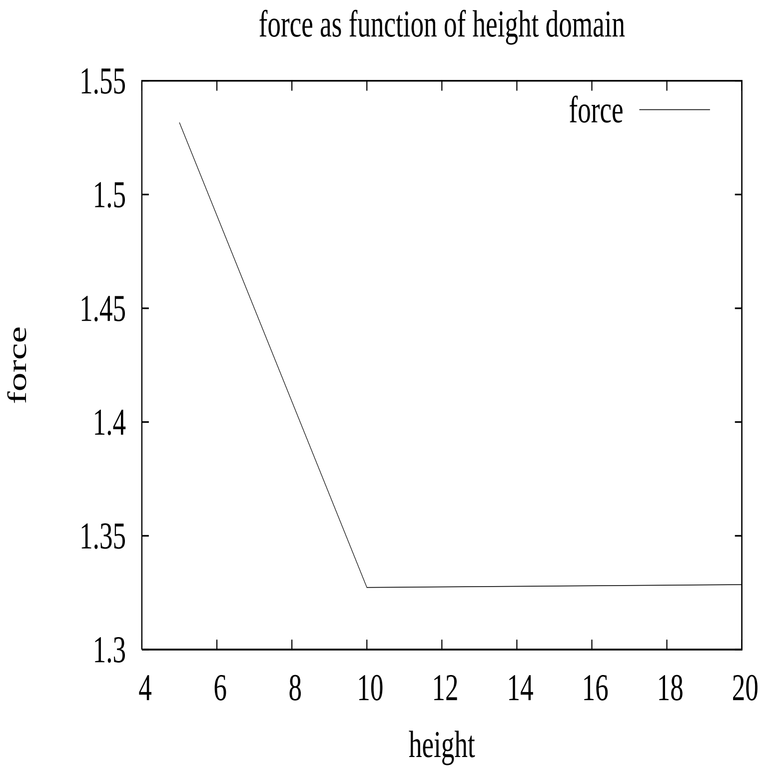
Contours of Stream Function (kg/s)

Apr 20, 2004
FLUENT 6.1 (2d, segregated, ske)



Contours of Stream Function (kg/s)

Apr 20, 2004
FLUENT 6.1 (2d, segregated, ske)

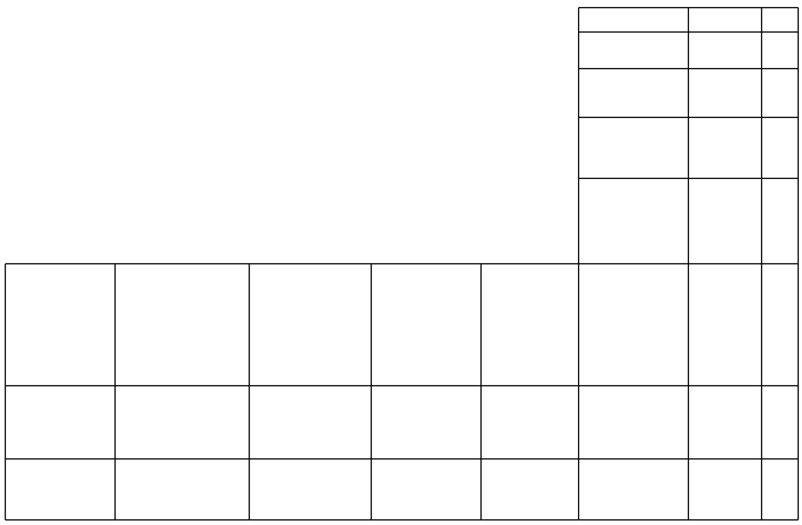

force as function of height domain
force
1.55
1.5
1.45
1.4
1.35
1.3
4
6
8
10
12
14
16
18
20
height
force

Grids.

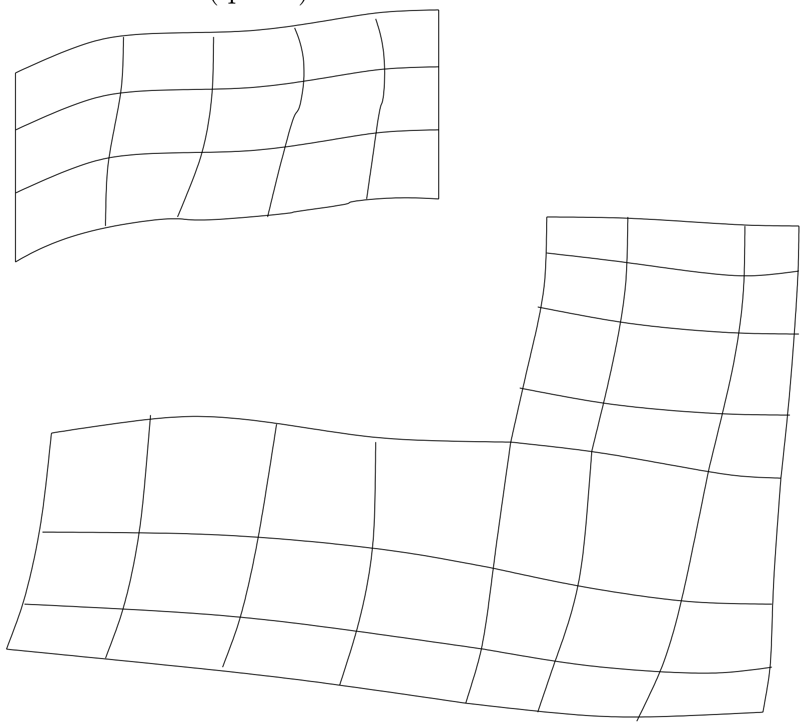
Grids treated so far: Cartesian.
Grids in Fluent
grid quality

cartesian (quads)

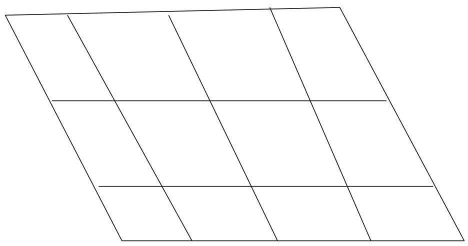
- structured, map
- block-structured, submap

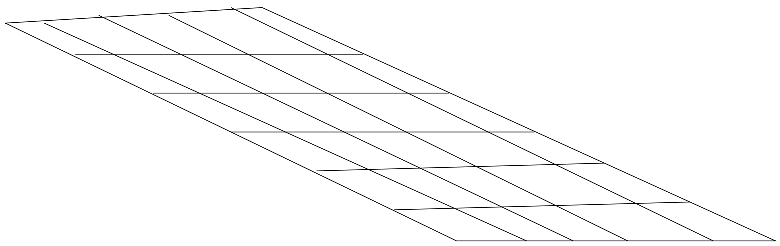


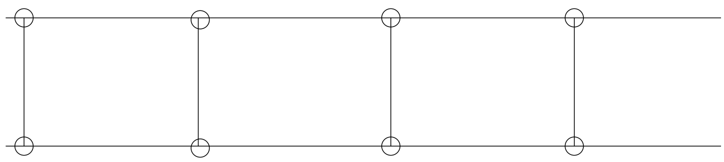
curvilinear (quads)

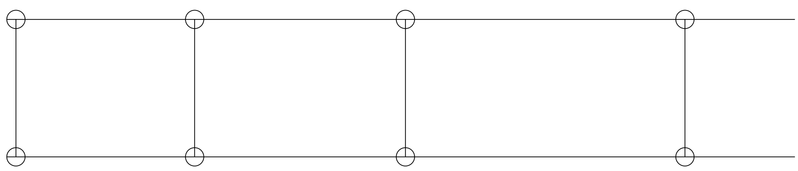


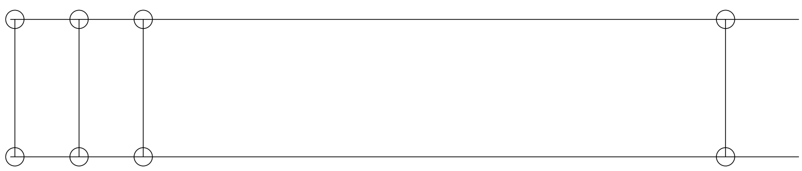
deterioration





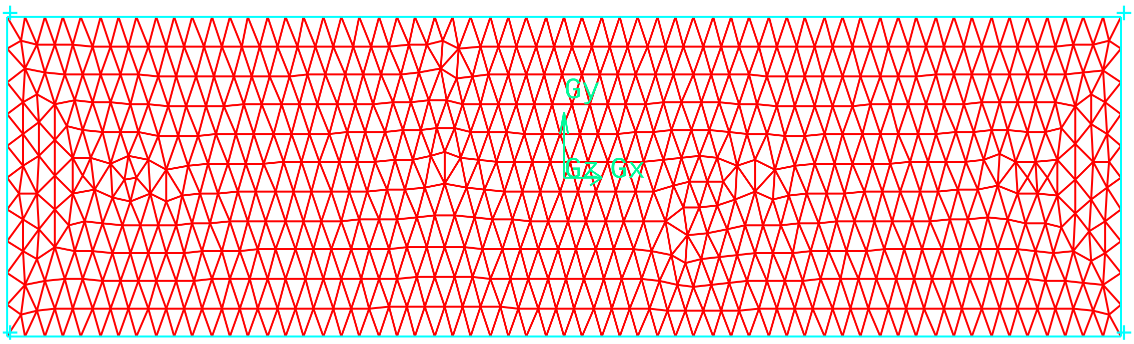


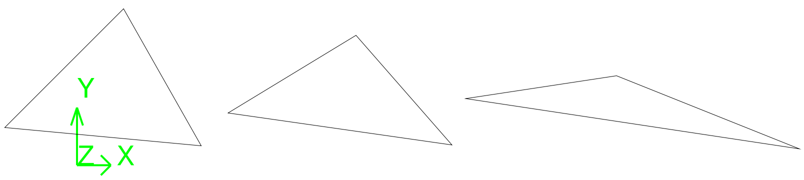




- angles close 90 degrees (larger then 20)
- stretch between 1 and 1.3

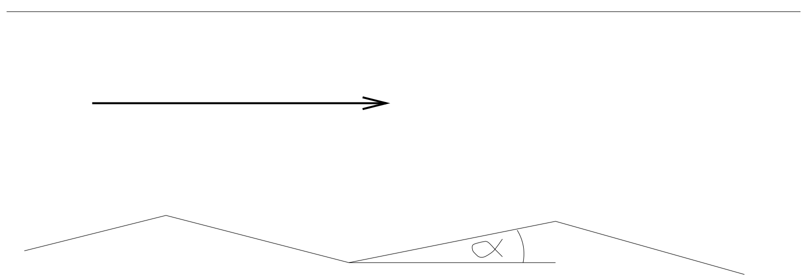
triangular (tri)





- angles close to 60 degrees (larger then 20)
- edge ratio not too big or small

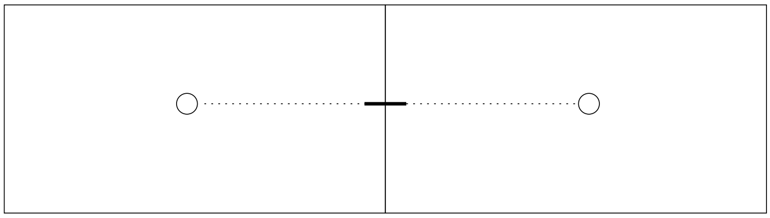
Sometimes compromise necessary:
shallow riblet on surface

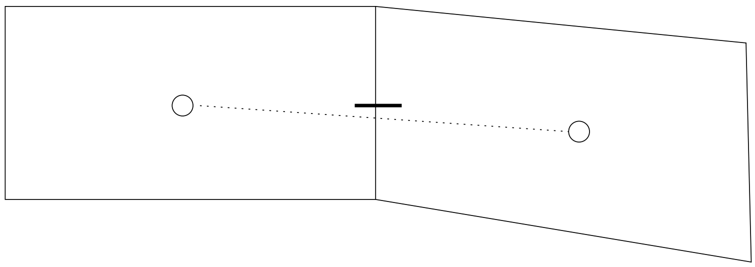


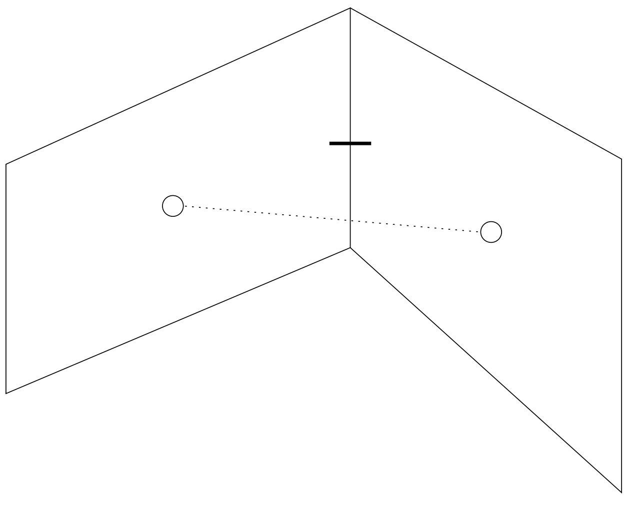
Difficulties with distorted grids:

- less accurate
- slower convergence

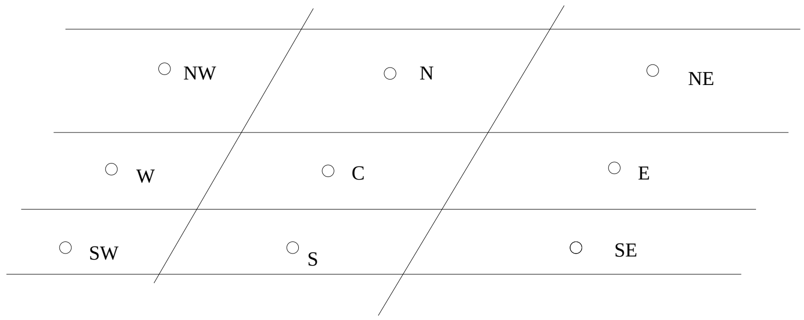
interpolation less accurate







convergence: treatment of extra neighbors



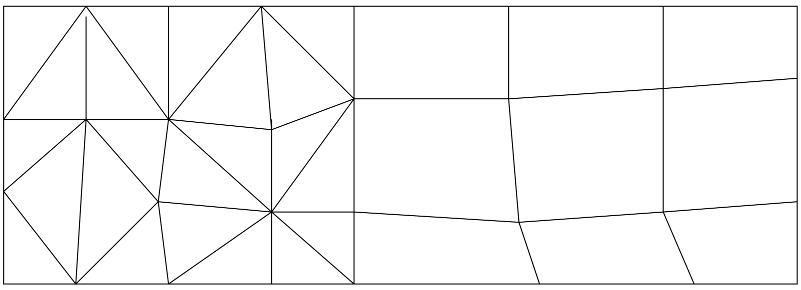
quads

- more accurate
- more difficult to make a grid

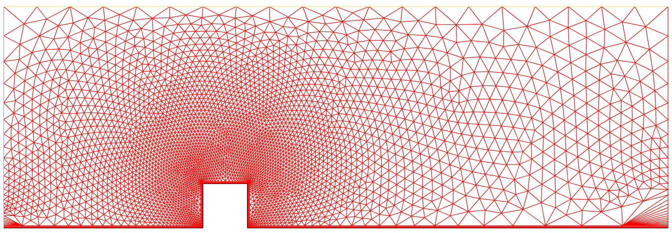
tri's

- less accurate
- more expensive
- less difficult to make a grid

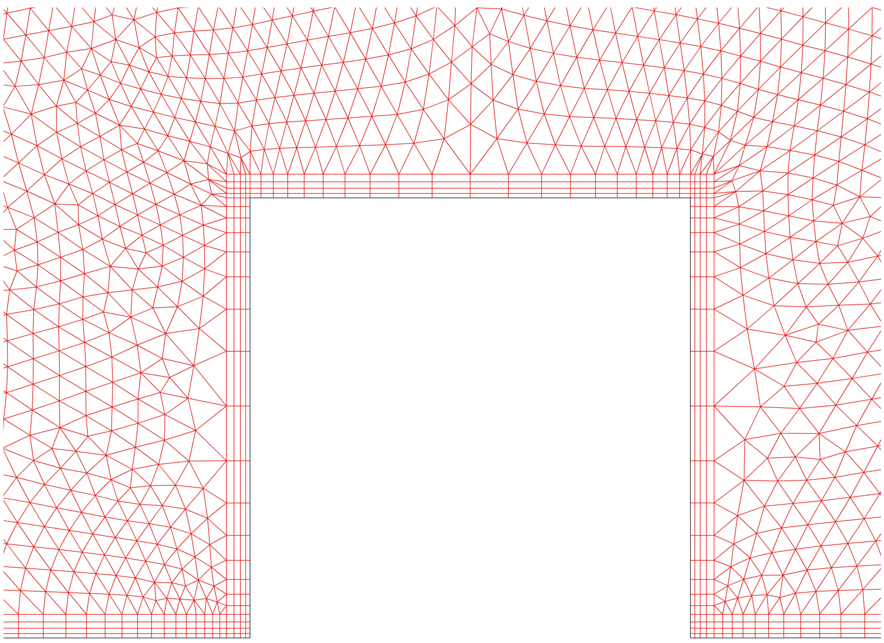
combination possible (mixed)
normally quads where high gradients are



The boundary layer grid feature



Grid Apr 20, 2004
FLUENT 6.1 (2d, segregated, ske)



Grid Apr 20, 2004
FLUENT 6.1 (2d, segregated, ske)

Solver. Discretization method.

- first order (upwind)
- second order (second order upwind)
- second order upwind more accurate but...
- second order upwind less stable
- central differences: YES but...
- all methods except 1st order upwind have limiter
- choice of method in Fluent ONLY for the advection part
- diffusion part is always the same

Solver.

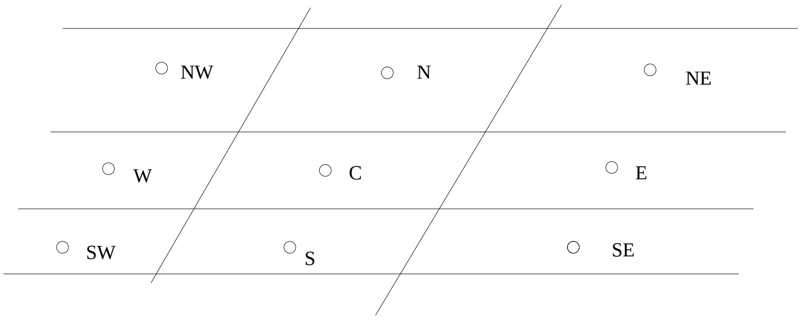
- u equation
- v equation
- p equation

For each equation u, v, w we do:

- linearize
  - equation $\frac{\partial u}{\partial t} + \frac{\partial uu}{\partial x} + \frac{\partial vu}{\partial y} + ..$
  - equation $\frac{\partial u}{\partial t} + \frac{\partial Uu}{\partial x} + \frac{\partial Vu}{\partial y} + ..$
  - U, V constant for this iteration
- solve matrix equation $Ax = b$ by iteration
- after iterations $r = Ax - b$
- residual $=$ max $|r|$
- how small must residual be?

An old problem... extra neighbors

- matrix with no extra neighbors: 5 diagonals
- matrix with extra neighbors: 9 diagonals (4 extra)
- diagonal contribution to right hand side
- update right hand side every so-many iterations
- slower convergence



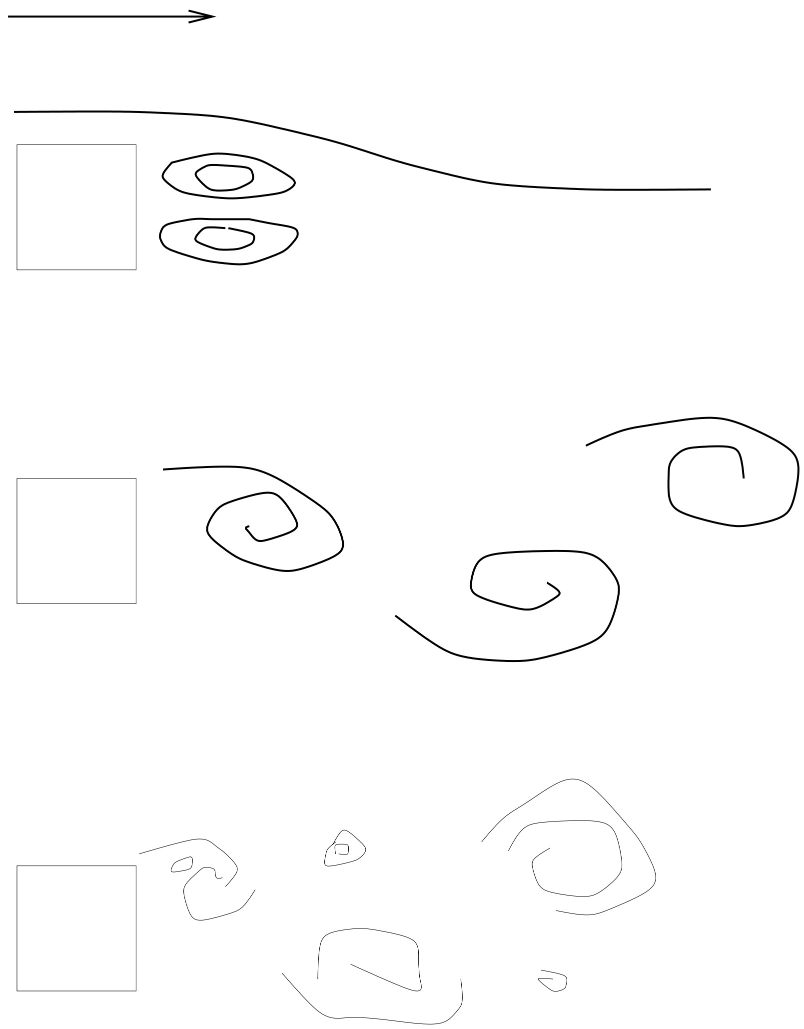
No convergence. Now what?

- is problem physical?
- smaller relaxation factors
- better initialization, start with LO, continue with HO
- time-dependent calculation
- better grid

physical: flow regime

- stationary/in-stationary
- laminar/turbulent
- multiple phase (cavitation)

Example: square cylinder at different flow speeds



relaxation factors

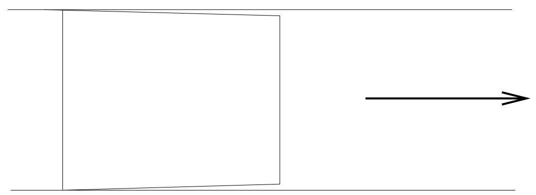
- after each iteration update of variable (say u becomes u_{new})
- relax update: $u = \omega u_{new} + (1 - \omega) u_{old}$
- $\omega < 1$
- more stable but...
- slower convergence

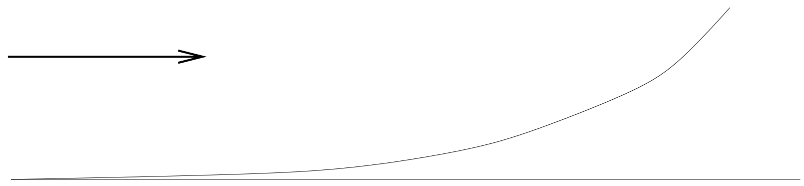
Turbulent flows and the grid.

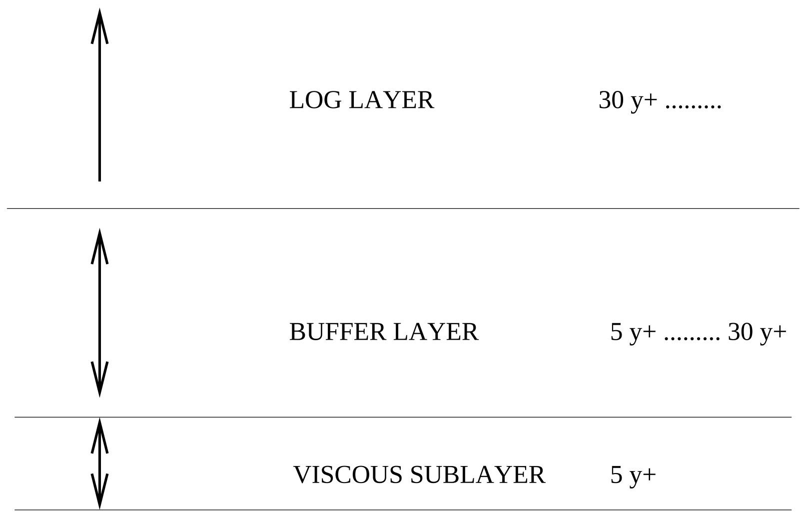
- grid quality?
- model applied correctly?

TURBULENT $\rightarrow k - \epsilon$, wall law

$k - \epsilon$: recirculation?
Wall law: applicable?



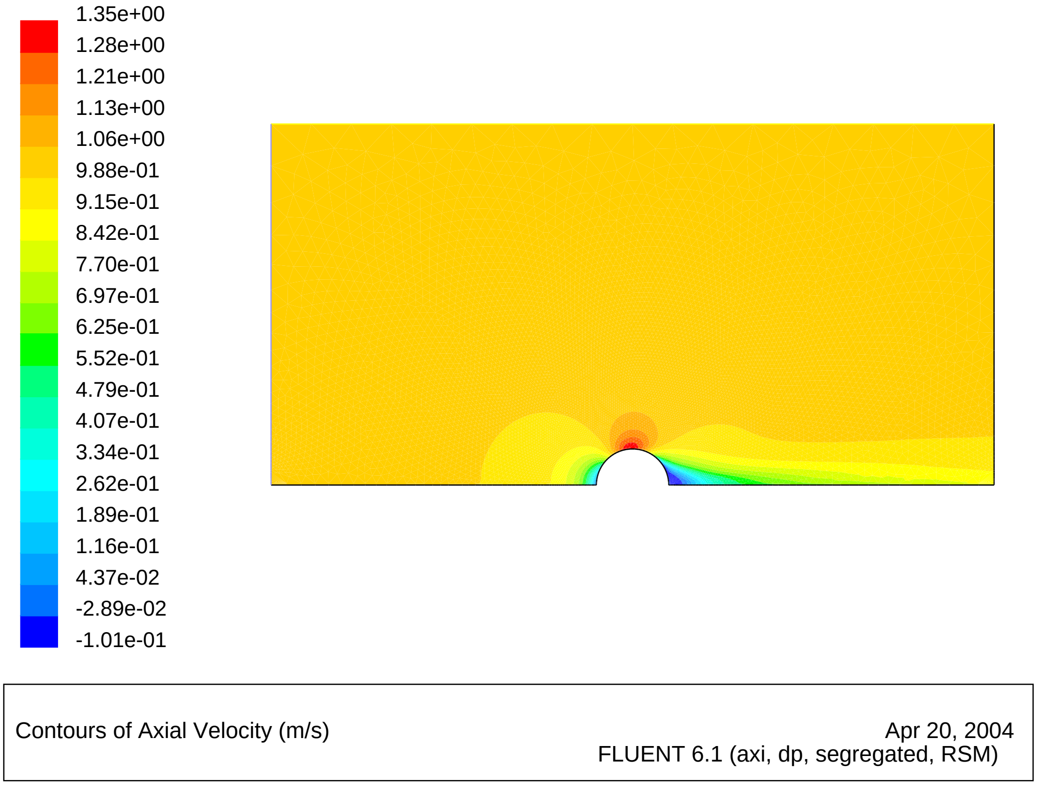




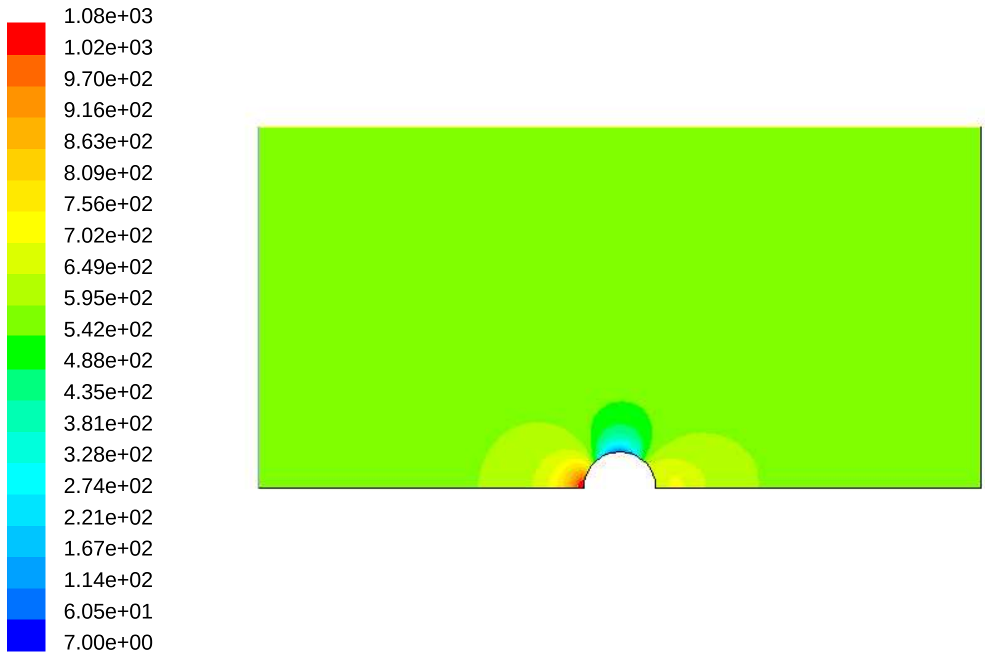
Wall law: Y+ OK?
$U/U+ = (1/k)log(Y/Y+)$

- turbulent case
- axi-symmetric calculation of flow around a sphere
- Re=1000000

axial U

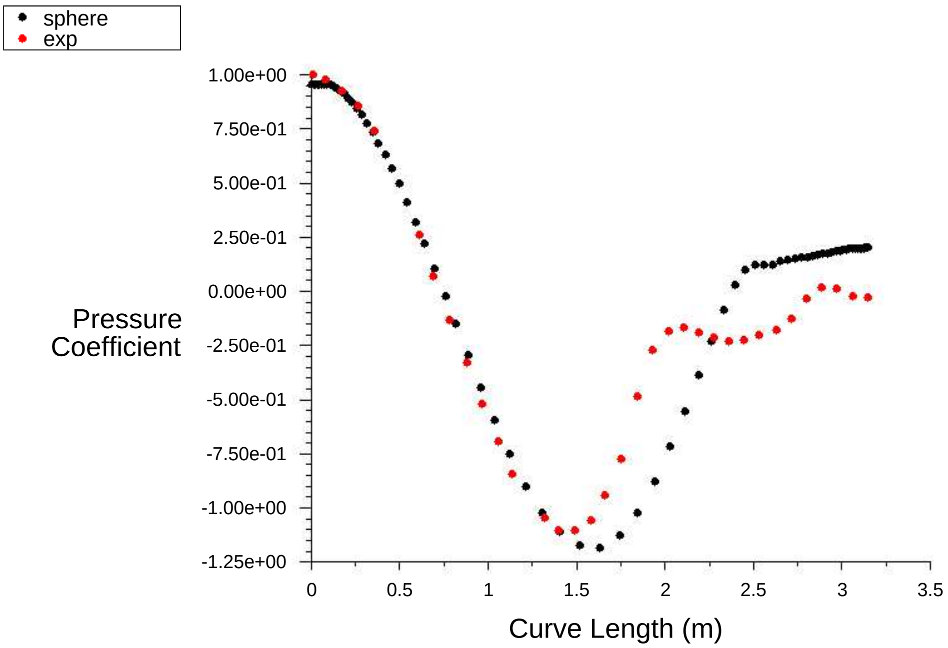


pressure



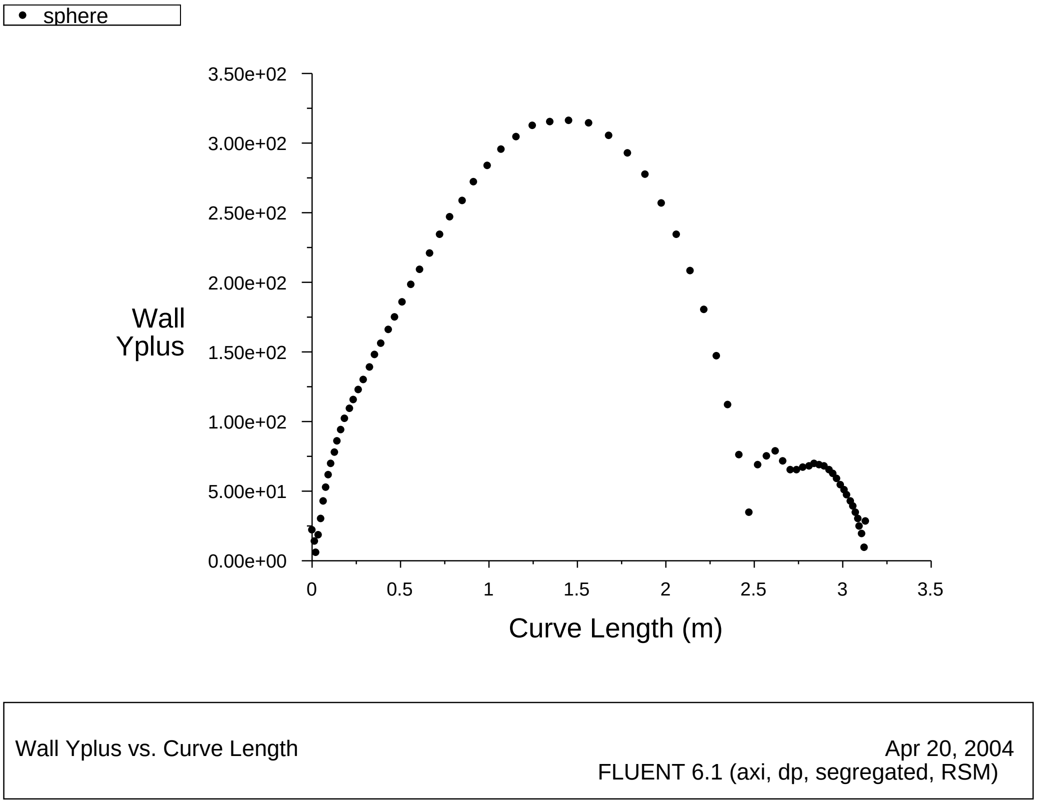
Contours of Static Pressure (pascal) Apr 20, 2004
FLUENT 6.1 (axi, dp, segregated, RSM)

$$Cp = p - pref/1/2\rho U^2$$

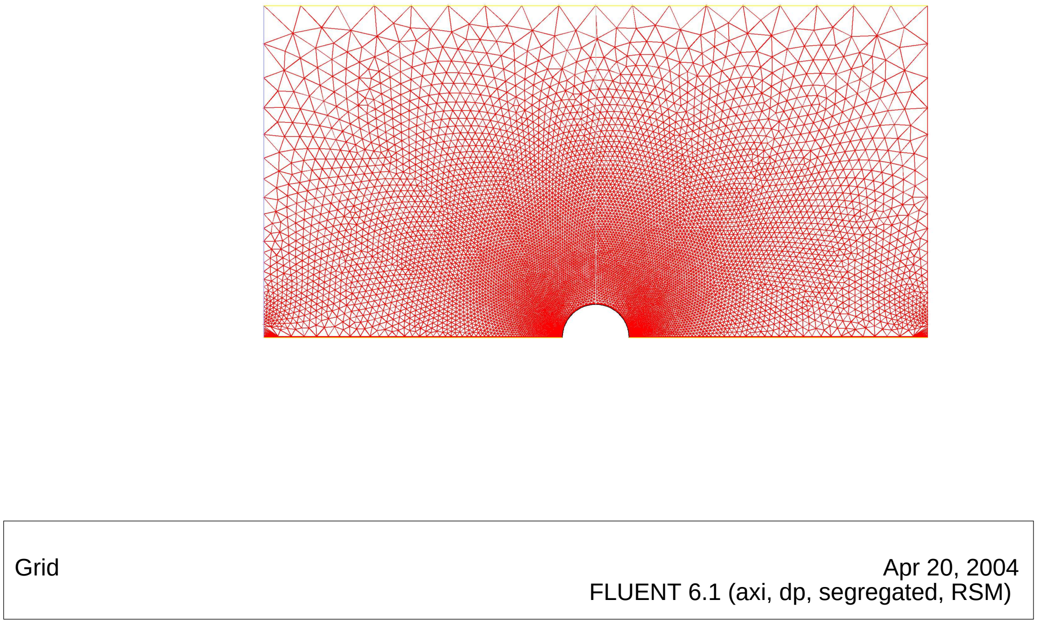


Pressure Coefficient vs. Curve Length Apr 20, 2004
FLUENT 6.1 (axi, dp, segregated, RSM)

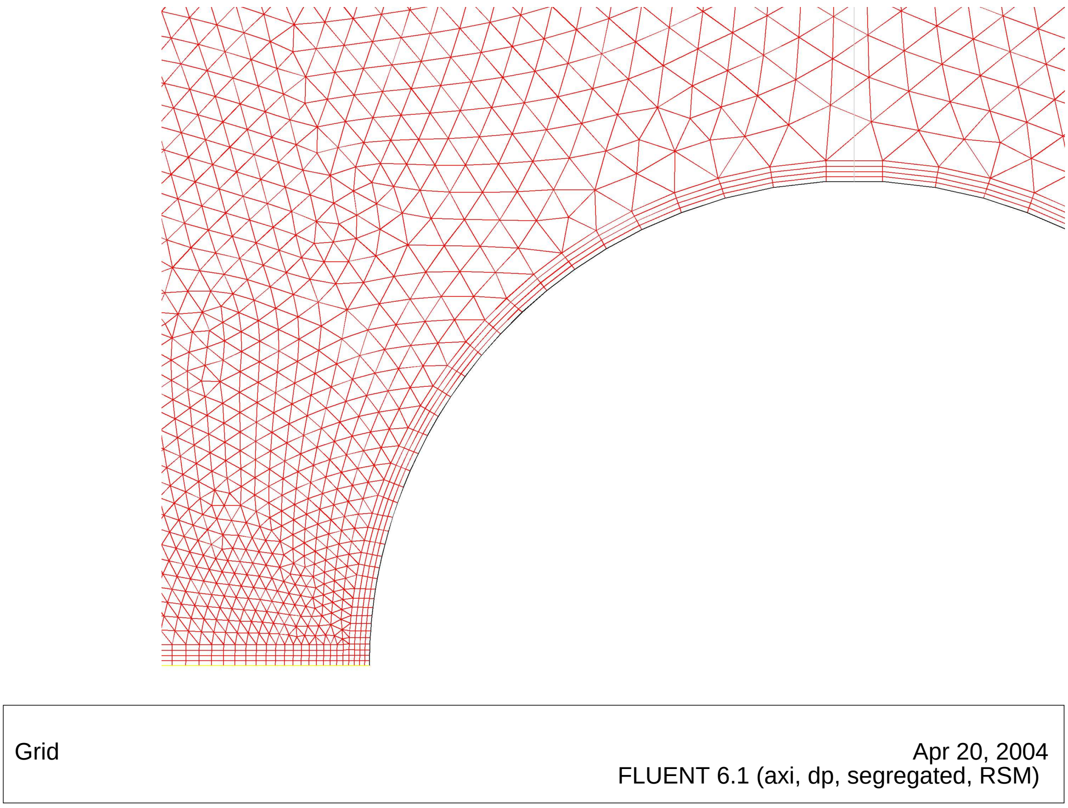
Yplus


sphere
3.50e+02
3.00e+02
2.50e+02
2.00e+02
1.50e+02
1.00e+02
5.00e+01
0.00e+00
Wall Yplus
0
0.5
1
1.5
2
2.5
3
3.5
Curve Length (m)
Wall Yplus vs. Curve Length
Apr 20, 2004
FLUENT 6.1 (axi, dp, segregated, RSM)

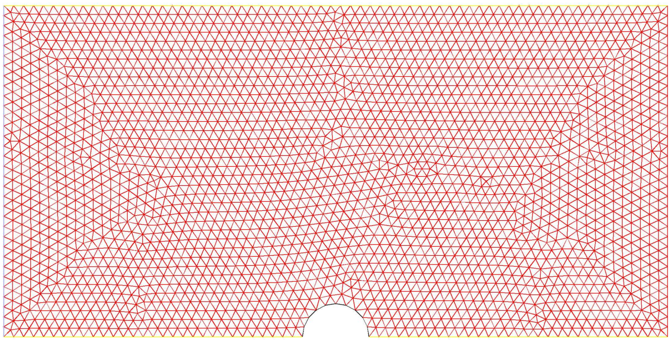
grid sphere



zoom grid sphere

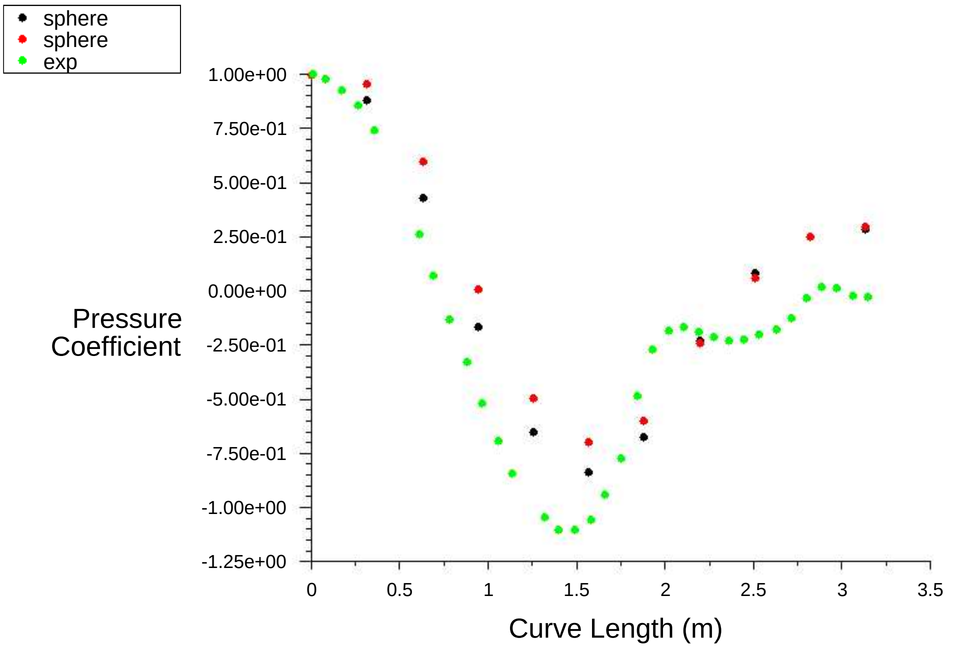


test grid sphere



Grid Apr 20, 2004 FLUENT 6.1 (axi, dp, segregated, ske)

results test grid sphere



Pressure Coefficient vs. Curve Length Apr 20, 2004 FLUENT 6.1 (axi, dp, segregated, ske)

- relevant flow features (stagnation points, separation points)
- Yplus (grid OK? discuss why if and if not)
- compare with experiment if possible

Discussion and summary

- Testing, testing, testing.....
- model makes problem simpler but...
- is physics right (time-dependent, 2D, 3D)
- geometry outline and grid part of the problem
- where inlet and outlet boundary?
- where free boundary?
- where grid refinement?
- turbulence model choice.
  - RSM
  - strongly rotating flow
  - streamline curvature