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Introductory OpenFOAM® Course

From 16th to 20th February, 2015

University of Genoa, DICCA

Dipartimento di **I**ngegneria **C**ivile, **C**himica e **A**mbientale

1. **Tips and tricks in OpenFOAM®**

Where and how should we
put more salt

… and as this is kind of a cooking recipe, it comes with a small warning
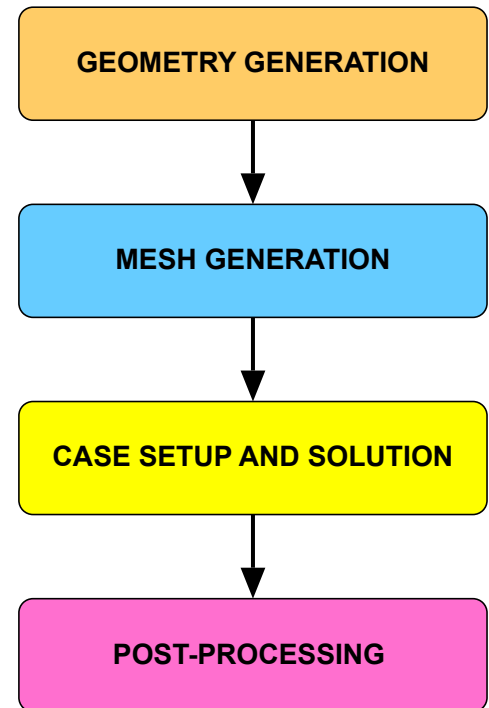
Tips and tricks in OpenFOAM®

- What I am about to show you is based on my personal experience.

- To draw these kind of conclusions or observations, I conducted hundreds of numerical experiments, under different conditions, with different meshes (from good quality meshes to bad quality meshes with different element types), and different physics and models involved.

- Most important of all, before starting this long road, I got familiar with the theory behind the FVM and CFD, the physics behind what I was doing, and OpenFOAM® source code.

- At this point, I highly advise you to conduct similar numerical experiments and draw your own conclusions.

- Please, use these slides as a reference only. I am not responsible for your failures and mistakes.

Tips and tricks in OpenFOAM®

Our vertical workflow

- Do you remember this vertical workflow? I hope so.

- Everything starts with the geometry. So in order to get a good mesh, you need a good geometry.

- When it comes to geometry generation, the only rule you should keep in mind is that by the end of the day you should get a unique clean and watertight geometry.

- Geometry defeaturing can made your life easier. Do not fool yourself, if you have no constraints avoid sharp angles.

- And as for the mesh concerns, try to keep the skewness, orthogonality, aspect ratio, and growth rate low.

- No need to say that if you have a bad geometry, is likely probable that your mesh will be bad as well.

- Always remember: **good mesh – good results.**

```
GEOMETRY GENERATION
        ↓
MESH GENERATION
        ↓
CASE SETUP AND SOLUTION
        ↓
POST-PROCESSING
```

Tips and tricks in OpenFOAM®

OpenFOAM® shell environment

- You can have as many versions of OpenFOAM® as you like living together. You just need to source the right environment variables. For instance, on my workstation I have nine versions living together.   This is how my `.bashrc` file looks like,

```
### OPENFOAM ###

#     source $HOME/OpenFOAM/OpenFOAM-1.6-ext/etc/bashrc
#     source $HOME/OpenFOAM/OpenFOAM-1.6-ext.GPU/etc/bashrc
#     source $HOME/OpenFOAM/OpenFOAM-1.7.1/etc/bashrc
#     source $HOME/OpenFOAM/OpenFOAM-2.0.x/etc/bashrc
#     source $HOME/OpenFOAM/OpenFOAM-2.1.1/etc/bashrc
#     source $HOME/OpenFOAM/OpenFOAM-2.2.0/etc/bashrc
#     source $HOME/OpenFOAM/OpenFOAM-2.2.x/etc/bashrc
#     source $HOME/OpenFOAM/OpenFOAM-2.3.0-debug/etc/bashrc
      source $HOME/OpenFOAM/OpenFOAM-2.3.x/etc/bashrc


### OPENFOAM ###
```

Tips and tricks in OpenFOAM®

OpenFOAM® shell environment

- If at any time I want to use a different version of OpenFOAM®, I just source the right OpenFOAM® environment variables. For instance if I want to switch from version 2.2.0 to version 2.3.x, I modify my `.bashrc` as follows,

Old `.bashrc`

```
### OPENFOAM ###

#    source $HOME/OpenFOAM/OpenFOAM-1.6-ext/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-1.6-ext.GPU/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-1.7.1/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-2.0.x/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-2.1.1/etc/bashrc
     source $HOME/OpenFOAM/OpenFOAM-2.2.0/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-2.2.x/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-2.3.0-debug/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-2.3.x/etc/bashrc

### OPENFOAM ###
```

New `.bashrc`

```
### OPENFOAM ###

#    source $HOME/OpenFOAM/OpenFOAM-1.6-ext/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-1.6-ext.GPU/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-1.7.1/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-2.0.x/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-2.1.1/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-2.2.0/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-2.2.x/etc/bashrc
#    source $HOME/OpenFOAM/OpenFOAM-2.3.0-debug/etc/bashrc
     source $HOME/OpenFOAM/OpenFOAM-2.3.x/etc/bashrc

### OPENFOAM ###
```

- Then open a new terminal, and you can start using the new version. You can also have two different versions of OpenFOAM® running together at the same time in different terminals.

- You can also use aliases to source the OpenFOAM® version.

Tips and tricks in OpenFOAM®

OpenFOAM® shell environment

- When switching from one OpenFOAM® version to another one, it is highly advisable to clear as many OpenFOAM environment settings as possible, to do so you can use the script `unset.sh`. In the terminal type:

  - `unset`

- Be careful, there may be more than one `unset.sh` script. The OpenFOAM® specific script is located in the directory `$WM_PROJECT_DIR/etc/config.`

- You can also use the alias `wmUNSET`, which is set in the OpenFOAM® environment variables. Remember, you can type `alias` in the terminal window to see all the aliases available.

- In the directory `$WM_PROJECT_DIR/etc/config`, you will also find many useful scripts. For instance, you can take a look at the script `aliases.sh`, in this script you will find all the aliases defined in OpenFOAM®

Tips and tricks in OpenFOAM®

Looking for information in OpenFOAM® source code

- To locate files you can use the **find** command. For instance, if you want to locate a file that contains the string `fvPatch` in its name you can proceed as follows,

  - **find $FOAM_SOLVERS -name "*fvPatch*"**

  This command will locate the files containing the string `"*fvPatch*"` in the directory **$FOAM_SOLVERS**

- If you want to find a string inside a file, you can use the command **grep**

  - **grep -r -n LES $FOAM_SOLVERS**

  This command will look for the string LES in all files inside the directory **$FOAM_SOLVERS**. The option `-r` means recursive and `-n` will output the line number.

Tips and tricks in OpenFOAM®

Looking for information in OpenFOAM® source code

- As you might already know, there are a gazillion dictionaries in OpenFOAM®. The easiest way to find all of them is to do a local search in the installation directory as follows,

    - For instance, if you are interested in finding all dictionary files that end with the "Dict" word in the **tutorials** directory, in the terminal type:

        - **find $FOAM_TUTORIALS -name "*Dict"**

        - **find $FOAM_TUTORIALS -iname "*dict"**

Tips and tricks in OpenFOAM®

Looking for information in OpenFOAM® source code

- A few more advanced commands to find information in your OpenFOAM® installation.

  - To find which tutorial files use the boundary condition "`slip`":

    - **`find $FOAM_TUTORIALS -type f | xargs grep -sl 'slip'`**

  - To find where the source code for the boundary condition "`slip`" is located:

    - **`find $FOAM_SRC -name "*slip*"`**

  - To find what applications do not run in parallel

    - **`$WM_PROJECT_DIR -type f  | xargs grep -sl 'noParallel'`**

  - Remember, OpenFOAM® understand REGEX syntax.

Tips and tricks in OpenFOAM®

OpenFOAM® Doxygen documentation

- The best source of information is the source code and the Doxygen documentation.

- The `$WM_PROJECT_DIR/doc` directory contains the Doxygen documentation of OpenFOAM®.

- Before using the Doxygen documentation, you will need to compile it. To compile the Doxygen documentation, from the terminal:

  - `cd $WM_PROJECT_DIR`

  - `./Allwmake doc`

    Note: You will need to install doxygen and graphviz/dot

- After compiling the Doxygen documentation you can use it by typing:

  - `firefox file://$WM_PROJECT_DIR/doc/Doxygen/html/index.html`

- The compilation is time consuming. ⚠️

Tips and tricks in OpenFOAM®

Intensive IO

- If you are doing intensive IO or running big cases, I highly advise you to save the solution in binary format. When using binary format, the IO is a way much faster and the output files use less space.

- Remember, you can get a performance gain when you save in binary format as you minimize any requirement for parsing.

- If OpenFOAM® binary format is not good enough for you, you can try another format. For instance you can use HDF5 format with OpenFOAM®.

  http://openfoamwiki.net/index.php/Contrib/IOH5Write

Tips and tricks in OpenFOAM®

Intensive IO

- Know your hardware, intensive IO can slow-down your computations or crash your system, even the most powerful supercomputers.

- For big simulations, most of the times the bottleneck is the IO.

- No need to say that eventually you will run out of space if you are working with big files.

- One naïve solution to the IO bottleneck and big datasets space, do not save your solution very often. But be careful, at least save your solution before stopping your solution or reaching the job maximum time.

Tips and tricks in OpenFOAM®

Running in a cluster

- Best advice, familiarize with your hardware.

- Do not get overwhelm when running in a cluster. Running OpenFOAM® in a cluster is not different from running in your workstation or portable computer. The only difference is that you need to schedule your jobs.

- Depending on the system current demand of resources, the resources you request and your job priority, sometimes you can be in queue for hours, even days, so be patient and wait for your turn.

- Consequently, remember to always double or triple check your scripts. It will be a waste of time if after two days in queue, your simulation did not start because there were errors in your scripts.

- For those running on fancy clusters, such as blue gene supercomputers, I have found a processor limit of 512, after that is quite difficult to get any improvement.

- Also, the IO is really time consuming.

Tips and tricks in OpenFOAM®

Running in a cluster

- By the way, I know it looks super cool, but try to avoid spaces or funny characters when naming directories and files, specially if you run in clusters. *e.g.*:

  - `my dictionary.dict`   instead use   `my_dictionary.dict`

  - `#my_file;txt`   instead use   `my_file.txt`

  - `my/solution!!!`   instead use   `my_solution`

  - `working@home`   instead use   `working_at_home`

Tips and tricks in OpenFOAM®

OpenFOAM® mesh quality and checkMesh utility

- Before running a simulation remember to always check the mesh quality using the `checkMesh` utility.

- Remember, **good quality meshes** are of paramount importance to obtain accurate results.

- `checkMesh` will also check for topological errors.

- Have in mind that topological errors must be repaired.

- You will be able to run with mesh quality errors (such as skewness, aspect ratio, minimum face area, and non-orthogonality), but they will severely tamper the solution accuracy and can made the solver run super slow or even blow-up.

- In my personal experience, I have found that OpenFOAM® is very picky when it comes to mesh quality. So if `checkMesh` is telling you that the mesh is bad, you better correct those errors.

- Unfortunately, to correct mesh quality errors you will have to remesh the geometry.

Tips and tricks in OpenFOAM®

OpenFOAM® mesh quality and checkMesh utility

- If for any reason `checkMesh` finds errors, it will give you a message and it will tell you what check failed.

- It will also write a set with the faulty cells, faces, and/or points. These sets are saved in the directory `constant/polyMesh/sets/`

- If at any point you want to visualize the failed faces/cells/points you will need to convert them to VTK format using the utility `foamToVTK`.

- At the end, `foamToVTK` will create a directory named **VTK**, where you will find the failed faces/cells/points in VTK format. At this point you can use `paraFoam/ paraview` to visualize the failed sets.

Tips and tricks in OpenFOAM®

OpenFOAM® mesh quality and checkMesh utility

- I want to emphasize the fact that you will be able to run with mesh quality errors such as skewness, aspect ratio, minimum face area, and non-orthogonality.

- However, they will severely tamper the solution accuracy and can made the solver explode.

Tips and tricks in OpenFOAM®

OpenFOAM® mesh quality and checkMesh utility

- If you want to know the quality metrics hard-wired in OpenFOAM®, just read the file `$WM_PROJECT_DIR/src/OpenFOAM/meshes/primitiveMesh/primitiveMeshCheck/primitiveMeshCheck.C`. Their maximum (or minimum) values are defined as follows:

  - `Foam::scalar Foam::primitiveMesh::closedThreshold_  = 1.0e-6;`

  - `Foam::scalar Foam::primitiveMesh::aspectThreshold_  = 1000;`

  - `Foam::scalar Foam::primitiveMesh::nonOrthThreshold_ = 70;    // deg`

  - `Foam::scalar Foam::primitiveMesh::skewThreshold_    = 4;`

  - `Foam::scalar Foam::primitiveMesh::planarCosAngle_   = 1.0e-6;`

- By the way, if you are not happy with these values, you can just change them and voila, your quality problems are solved (I am kidding of course).

OpenFOAM® mesh quality and renumberMesh utility

- Before running a simulation, I highly recommend you to use the `renumberMesh` utility. This utility will renumber the mesh to minimize its bandwidth, in other words, it will make the linear solver run faster (at least for the first time-steps)

- Summarizing, before running a simulation remember to always check the mesh quality using `checkMesh` and then reduce the mesh bandwidth by using the `renumberMesh.` This is a good standard practice, I always do it (at least for big meshes).

- Before running a simulation, try to always get a good quality mesh. Remember, **garbage in – garbage out**. Or in a positive way, **good mesh – good results**.

Tips and tricks in OpenFOAM®

Boundary conditions

- Boundary conditions should be physically realistic. They must represent the physics involved.

- Minimize grid skewness, non-orthogonality, growth rate, and aspect ratio near the boundaries. You do not want to introduce diffusion errors early in the simulation, specially close to the inlets.

- Get a **good quality mesh** at the boundaries.

- Remember, for each single variable you are solving you need to specify a boundary condition.

Boundary conditions

- Try to avoid large gradients in the direction normal to the boundaries near inlets and outlets. That is to say, put your boundaries far away from where things are happening.

- Do not force the flow at the outflow, use a zero normal gradient for all flow variables except pressure. The solver extrapolates the required information from the interior.

- Be careful with backward flow at the outlets (flow coming back to the domain) and backward flow at inlet (reflection waves), they require special treatment.

Tips and tricks in OpenFOAM®

Initial conditions

- First at all, a good initial condition can improve the stability and convergence rate. On the other hand, unphysical boundary conditions can slow down the convergence rate or can cause divergence.

- As for boundary conditions, for each single variable you are solving you need to specify initial conditions.

- When it is possible, use `potentialFoam` to get an initial solution. It is computational inexpensive.

- `potentialFoam` can also give you an idea of the sensitivity of the mesh quality.

Initial conditions

- You can also get a computational inexpensive solution on a coarse mesh and then interpolate it to a fine mesh. This will be a very good initial solution only if the solution in the coarse mesh is acceptable.

- By the way, do not forget to use a **good quality coarse mesh.**

- Use `mapFields` to map the solution from a coarse mesh to a finer mesh. It also works the other way around, but I do not see any reason to proceed in this way.

Initial conditions

- If you are using a turbulence model, you can initialize the velocity and pressure fields from the solution obtained from a laminar case.

- If you are running an unsteady simulation and if the initial transient is of no interest, you can initialize your flow using the solution obtained from a steady simulation.

- Always try to get initial conditions that are close to the solution (I know this is difficult to achieve as we do not know the solution, if we knew the solution we would not have a job).

- I want to remind you again, initial conditions should be physically realistic.

Tips and tricks in OpenFOAM®

Starting and running a simulation

- Remember, you can change the parameters in the dictionaries `controlDict`, `fvSchemes` and `fvSolution` on the fly. But you will need to set the keyword `runTimeModifiable` to `yes` in the `controlDict` dictionary.

- When starting a simulation and if the initial transient is of no interest, you can start the simulation by using a high value of viscosity (low Reynolds number), and as the simulation runs you can change the value until you reach the desired value.

- If you are working with high Reynolds numbers and you do not like the trick of increasing the viscosity, you can get a very good initial solution using an Euler solver with upwind.

- You can also start the simulation by using a first order scheme and then switch to a high order scheme.

Tips and tricks in OpenFOAM®

Starting and running a simulation

- You can also change the convergence criterion of the linear solvers on the fly.

- For instance, you can start using a not so tight convergence criterion with a robust numerical scheme, and as the simulation runs you can tighten the convergence criterion to increase the accuracy.

- When the simulation starts I usually use more correctors steps (for

- and `PIMPLE` methods), and as the solution advance or stabilizes I decrease the number of corrector steps, but I always use at least one corrector step.

- Remember to always check the time step continuity errors. This number should be small (negative or positive), if it increases in time for sure something is wrong.

- If you want to know how the continuity errors are computed just type in the terminal `find $FOAM_SRC -iname *continuity*`, and open any of the files.

Discretization schemes

- Never get a final solution using first order schemes. They are too diffusive, which means they will under predict the forces and smear the gradients. In the other side, first order schemes are extremely robust, so you might be tented to use them as they will always give you a solution.

- You can start using a first order scheme, and then switch to a high order scheme. Remember, you can change the parameters on the fly.

- **This means, start robustly and end with accuracy.**

- By the way, an accurate numerical scheme needs a **good quality mesh**.

- Bad quality meshes will add numerical oscillations and reduce the accuracy of the numerical solution.

Tips and tricks in OpenFOAM®

Discretization schemes

- If you have a **good mesh and a good initial solution**, you can start immediately with a high order scheme, but be careful, remember to always check the stability of the solution.

- If at one point your solution starts to oscillate, you can switch to upwind and let the simulation stabilize, then you can switch back to high order accuracy.

- Have in mind that this behavior is telling you that something is happening so you better adjust other parameters, such as, solver tolerances, non-orthogonal corrections, number of correctors, gradient discretization and so on.

- **Try to always use a good quality mesh. Avoid the GIGO syndrome.**

- In the next slides I will show you how I usually setup the discretization schemes.

Discretization schemes – Convective terms

- A robust numerical scheme but too diffusive,

```
divSchemes

{

    div(phi,U)                        Gauss upwind;

    div(phi,omega)                    Gauss upwind;

    div(phi,k)                        Gauss upwind;

    div((nuEff*dev(T(grad(U)))))   Gauss linear;

}
```

Discretization schemes – Convective terms

- An accurate and stable numerical scheme,

```
divSchemes

{

    div(phi,U)                         Gauss linearUpwind grad(U);

     div(phi,omega)                    Gauss linearUpwind default;

    div(phi,k)                         Gauss linearUpwind default;

    div((nuEff*dev(T(grad(U)))))   Gauss linear;

}
```

Discretization schemes – Convective terms

- An even more accurate but oscillatory scheme,

```
divSchemes
{
    div(phi,U)                       Gauss linear;
    div(phi,omega)                   Gauss linearUpwind default;
    div(phi,k)                       Gauss linearUpwind default;
    div((nuEff*dev(T(grad(U)))))   Gauss linear;
}
```

Discretization schemes – Diffusive terms

- For the discretization of the diffusive terms, you can use a fully orthogonal scheme,

```
laplacianSchemes
{
    default        Gauss linear corrected;
}
```

- You can also use a scheme that uses a blending between a fully orthogonal scheme and a non-orthogonal scheme,

```
laplacianSchemes
{
    default        Gauss linear limited  ψ;
}
```

Discretization schemes – Diffusive terms

- The method you use highly depends on the quality of the mesh.

- For meshes with low non-orthogonality you can use the `corrected` scheme or the `limited 1` scheme.

- For meshes with high non-orthogonality you can use the `limited` ψ scheme. The higher the non-orthogonality the lower the value of the blending factor ψ.

$$\psi$$

0 ←————————————→ 1

- Bad quality mesh
- Non-orthogonal correction
- Bounded on low quality meshes

- Good quality mesh
- Orthogonal correction
- Unbounded on low quality meshes

Discretization schemes – Diffusive terms

- An accurate numerical scheme on orthogonal meshes (**this is a very good quality mesh with uniform cell size**, this is what we want),

```
laplacianSchemes
{
        default             Gauss linear orthogonal;
}


snGradSchemes
{
        default             orthogonal;
}
```

Discretization schemes – Diffusive terms

- An accurate numerical scheme on orthogonal meshes (with non-orthogonal corrections),

```
laplacianSchemes

{

        default         Gauss linear limited 1;

}



snGradSchemes

{

        default         limited 1;

}
```

Discretization schemes – Diffusive terms

- A less accurate numerical scheme valid on non-orthogonal meshes (with non-orthogonal corrections),

```
laplacianSchemes

{

        default             Gauss linear limited 0.5;

}



snGradSchemes

{

        default             limited 0.5;

}
```

Discretization schemes – Gradient terms

- Let us talk about the `gradSchemes`, this entry defines the way we compute the gradients.

- The gradients can be computed using the Gauss method or the least squares method. The keywords are:

    - `Gauss linear;`

    - `leastSquares;`

- In practice, the `leastSquares` method is more accurate, however, I have found that it tends to be more oscillatory on tetrahedral meshes.

Discretization schemes – Gradient terms

- You can also use gradient limiters.

- Gradient limiters will avoid over and under shoots on the gradient computations. There are four available,

      `cellMDLimited`   **Less diffusive**

      `cellLimited`

      `faceMDLimited`

      `faceLimited`   **More diffusive**

- The following entry corresponds to the `leastSquares` method using gradient limiters

      `cellMDLimited leastSquares 1.0;`

Discretization schemes – Gradient terms

- Gradient limiters avoid over and under shoots on the gradient computations.

- The gradient limiter implementation in OpenFOAM®, uses a blending factor ψ.

```
gradSchemes
{
    default      cellMDLimited Gauss linear  ψ;
}
```

$$\psi$$

0 ⟵━━━━━━━━━━━━━━⟶ 1

Accuracy
Limiter off

Stability
Limiter on
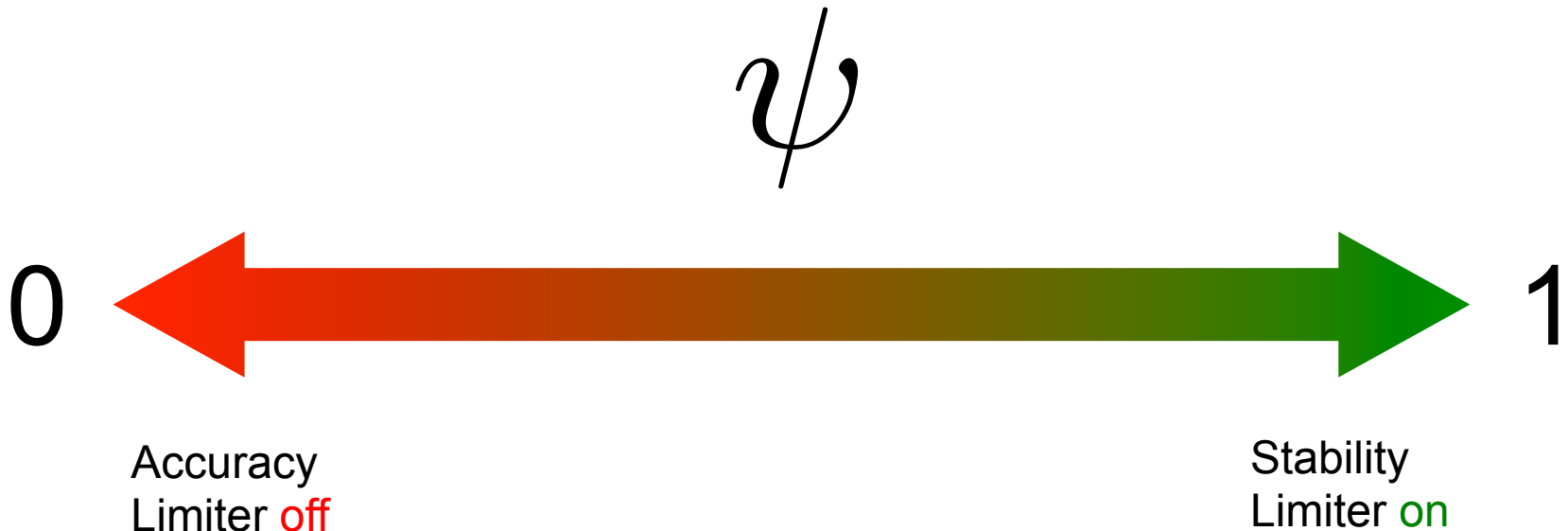
Discretization schemes – How to choose the schemes

- If after checking the mesh quality, the non-orthogonality is higher than 80, I prefer to redo the mesh and improve the quality.

- By the way, if you are running LES simulations, do not even think about running in highly non-orthogonal meshes. Better spend more time in getting a **good quality mesh**, maybe with non-orthogonality less than 60.

- Do not try to push too much the numerical scheme on highly non-orthogonal meshes. You already know that the quality is low, so this highly influence the accuracy and stability of the solution. Specially the gradient computations.

- I do not like to run simulations on highly orthogonal meshes, but if I have to, I often use the following numerical scheme.

Discretization schemes – How to choose the schemes

- Non-orthogonality more than 80. I do not waste my time. I prefer to go back and get a better mesh. But if you want, you can try something like this,

```
gradSchemes

{

    default    faceLimited leastSquares 1.0;

    grad(U)    faceLimited leastSquares 1.0;

}

divSchemes

{

    div(phi,U)              Gauss linearUpwind grad(U);

    div(phi,omega)          Gauss upwind;

    div(phi,k)              Gauss upwind;

    div((nuEff*dev(T(grad(U)))))   Gauss linear;

}
```

```
laplacianSchemes

{

        default   Gauss linear limited 0.333;

}

snGradSchemes

{

    default    limited 0.333;

}
```

Discretization schemes – How to choose the schemes

- Non-orthogonality between 70 and 80

```
gradSchemes                                laplacianSchemes

{                                          {

    default    cellLimited leastSquares 1.0;    default    Gauss linear limited 0.5;

    grad(U)    cellLimited leastSquares 1.0;  }

}

divSchemes                                 snGradSchemes

{                                          {

    div(phi,U)           Gauss linearUpwind grad(U);    default    limited 0.5;

    div(phi,omega)       Gauss upwind;      }

    div(phi,k)           Gauss upwind;

    div((nuEff*dev(T(grad(U)))))  Gauss linear;

}
```

Discretization schemes – How to choose the schemes

- Non-orthogonality between 60 and 70

```
gradSchemes
{
    default    cellMDLimited Gauss linear 0.5;

    grad(U)    cellMDLimited Gauss linear 0.5;
}
divSchemes
{
    div(phi,U)          Gauss linearUpwind grad(U);

    div(phi,omega)      Gauss linearUpwind default;

    div(phi,k)          Gauss linearUpwind default;

    div((nuEff*dev(T(grad(U)))))  Gauss linear;
}
```

```
laplacianSchemes
{
    default    Gauss linear limited 0.777;
}

snGradSchemes
{
    default    limited 0.777;
}
```

Discretization schemes – How to choose the schemes

- Non-orthogonality between 40 and 60

```
gradSchemes

{

    default    cellMDLimited Gauss linear 0.5;

    grad(U)    cellMDLimited Gauss linear 0.5;

}

divSchemes

{

    div(phi,U)           Gauss linearUpwind grad(U);

    div(phi,omega)       Gauss linearUpwind default;

    div(phi,k)           Gauss linearUpwind default;

    div((nuEff*dev(T(grad(U)))))  Gauss linear;

}
```

```
laplacianSchemes

{

    default Gauss linear limited 1.0;

}

snGradSchemes

{

    default limited 1.0;

}
```

Discretization schemes – How to choose the schemes

- I guess at this point you know how to adjust the numerical scheme for meshes with non-orthogonality less than 40.

Discretization schemes – How to choose the schemes

- Additionally, I also change the number of non-orthogonal corrections.

  - Non-orthogonality between 70 and 80:

    nNonOrthogonalCorrectors 3;

  - Non-orthogonality between 50 and 70:

    nNonOrthogonalCorrectors 2;

  - Non-orthogonality less than 50:

    nNonOrthogonalCorrectors 1;

- I always like to do at least one correction.

Under-relaxation factors

- Because of the non-linearity of the equations being solved, it is necessary to control the change of ϕ. This is achieved by under-relaxation as follows,

$$\phi_P^n = \phi_P^{n-1} + \alpha(\phi_P^{n^*} - \phi_P^{n-1})$$

here α is the relaxation factor,

$\alpha < 1$ Means under-relaxation. This will slow down the convergence rate but increases the stability.

$\alpha = 1$ Means no relaxation at all. We simple use the predicted value of ϕ.

$\alpha > 1$ Means over-relaxation. It can sometimes be used to accelerate convergence rate but will decrease the stability.

- In plain English, this means that the new value of the variable ϕ depends upon the old value, the computed change of ϕ, and the under-relaxation factor α.

Tips and tricks in OpenFOAM®

Under-relaxation factors

- Under-relaxation factors are typical of steady solvers using the `SIMPLE` method.

- To find out what are and how to change the under-relaxation factors requires experience and understanding.

- In general, under-relaxation factors are there to suppress oscillations.

- Small under-relaxation factors will significantly slow down convergence. Sometimes to the extent that the user thinks the solution is converged when it really is not.

- The recommendation is to always use under-relaxation factors that are as high as possible, without resulting in oscillations or divergence.

Tips and tricks in OpenFOAM®

Under-relaxation factors

- I highly recommend you to use the default under-relaxation factors.

- If you have to change the under-relaxation factors, start by decreasing the values of the under-relaxation factors in order to improve the stability of the solution.

- Remember, low under-relaxation factors will slow down the solver while high under-relaxation factors will speed up the computation, but you will give up stability.

- In order to find the optimal under-relaxation factors for your case, it will take some trial and error.

Under-relaxation factors

- These are the under-relaxation factors I often use (which by the way are the commonly used).

```
relaxationFactors
{
    p              0.3;
    U              0.7;
    k              0.7;
    omega          0.7;
}
```

- According to the physics involved you will need to add more under-relaxation factors.

- If you do not define the new under-relaxation factors, they will be set to 1.0 by default.

Tips and tricks in OpenFOAM®

Linear solvers

- The linear solvers are defined in the `fvSolution` dictionary. You will need to define a solver for each variable you are solving.

- The solvers can be modified on the fly.

- The GAMG solver (generalized geometric-algebraic multigrid solver), can often be the optimal choice for solving the pressure equation. However, I have found that when using more than 1024 processors is better to use Newton-Krylov type solvers.

Linear solvers

- When solving multiphase problems, I have found that the GAMG solver might give problems when running in parallel, so be careful. The problem is mainly related to `nCoarsestCells` keyword, so usually I have to set a high value of cells (in the order 1000).

- The utility `renumberMesh` can dramatically increase the speed of the linear solvers, specially during the firsts iterations.

- I usually start by using a not so tight convergence criterion and as the simulation runs, I tight the convergence criterion.

Tips and tricks in OpenFOAM®

Linear solvers

- These are the linear solvers I often use.

- For the pressure equation I usually start with a tolerance equal to 1e-5 and relTol equal to 0.01. After a while I change these values to 1e-6 and 0.001 respectively.

```
p
{
        solver                      GAMG;
        tolerance                   1e-5;
        relTol                      0.01;
        smoother                    GaussSeidel;
        nPreSweeps                  0;
        nPostSweeps                 2;
        cacheAgglomeration          on;
        agglomerator                faceAreaPair;
        nCellsInCoarsestLevel       1000;
        mergeLevels                 1;
}
```

Tips and tricks in OpenFOAM®

Linear solvers

- These are the linear solvers I often use.

- For the pressure equation I usually start with a tolerance equal to 1e-5 and relTol equal to 0.01. After a while I change these values to 1e-6 and 0.001 respectively.

```
p
{
        solver                      GAMG;
        tolerance                   1e-6;
        relTol                      0.001;
        smoother                    GaussSeidel;
        nPreSweeps                  0;
        nPostSweeps                 2;
        cacheAgglomeration          on;
        agglomerator                faceAreaPair;
        nCellsInCoarsestLevel       1000;
        mergeLevels                 1;
}
```

Linear solvers

- These are the linear solvers I often use.

- If I do not use the GAMG solver for the pressure, I often use the PCG solver.

- For the pressure equation I usually start with a tolerance equal to 1e-5 and relTol equal to 0.01. After a while I change these values to 1e-6 and 0.001 respectively.

- If the speed of the solver is too slow, I change the convergence criteria to 1e-4 and relTol equal to 0.05. I usually do this during the first iterations.

```
p
{
    solver                  PCG;
    preconditioner          DIC;
    tolerance               1e-4;
    relTol                  0.05;
}
```

Linear solvers

- These are the linear solvers I often use.

- For the velocity equation I always use a tolerance equal to 1e-8 and relTol equal to 0.0

```
U
{
    solver                      PBiCG;
    preconditioner              DILU;
    tolerance                   1e-8;
    relTol                      0.0;
}
```

Linear solvers

- I like to set the minimum number of iterations to three, especially for the pressure.

- If your solver is doing too much iterations, you can set the maximum number of iterations. But be careful, if the solver reach the maximum number of iterations it will stop, we are talking about unconverged iterations.

- You can set the maximum number of iterations specially during the first time-steps where the solver takes longer.

- I use `minIter` and `maxIter` on symmetric and asymmetric matrix solvers.

```
p
{
    solver                      PCG;
    preconditioner              DIC;
    tolerance                   1e-4;
    relTol                      0.01;
    minIter                     3;
    maxIter                     100;
}
```

Tips and tricks in OpenFOAM®

Linear solvers

- The default option is the conventional segregated solution. That is, you first solve for velocity component x, then velocity component y and finally velocity component z.

- You can get some improvement in terms of stability and turn around time by using the coupled matrix solver for vectors and tensors, *i.e.*, if you are solving the velocity field, you solve all the velocity components at once.

- To select the coupled solver you need to use the keyword **coupled** in the **fvSolution** dictionary.

- In the coupled matrix solver you set tolerance as a vector (absolute and relative)

```
U
{
    type              coupled;
    solver            cPBiCCCG;
    preconditioner  DILU;
    tolerance         (1e-08 1e-08 1e-08);
    relTol            (0 0 0);
    minIter           3;
}
```

Linear solvers

- Remember, you must do at least one corrector step when using `PISO` solvers.

- When you use the `PISO` and `PIMPLE` solvers, you also have the option to set the tolerance for the final corrector step (`.*Final`).

- By proceeding in this way, you can put all the computational effort only in last corrector step (`.*Final`).

```
pFinal
{
    solver                  GAMG;
    tolerance               1e-06;
    relTol                  0.0;
    smoother                GaussSeidel;
    nPreSweeps              0;
    nPostSweeps             2;
    cacheAgglomeration      on;
    agglomerator            faceAreaPair;
    nCellsInCoarsestLevel     1000;
    mergeLevels             1;
}
```

Linear solvers

- By proceeding in this way, you can put all the computational effort only in last corrector step (`.*Final`).

- For all the intermediate corrector steps, you can use a more relaxed convergence criterion.

- For example, you can use the following solver and tolerance criterion for all the intermediate corrector steps (**p**), then in the final corrector step (**pFinal**) you tight the solver tolerance.

```
p                                              pFinal
{                                              {
    solver                  GAMG;                  solver                  GAMG;
    tolerance               1e-05;                 tolerance               1e-06;
    relTol                  0.05;                  relTol                  0.0;
    smoother                GaussSeidel;           smoother                GaussSeidel;
    nPreSweeps              0;                     nPreSweeps              0;
    nPostSweeps             2;                     nPostSweeps             2;
    cacheAgglomeration      on;                    cacheAgglomeration      on;
    agglomerator            faceAreaPair;          agglomerator            faceAreaPair;
    nCellsInCoarsestLevel   1000;                  nCellsInCoarsestLevel   1000;
    mergeLevels             1;                     mergeLevels             1;
}                                              }
```

Tips and tricks in OpenFOAM®

Transient simulations and time-step selection

- Remember, the fact that we are using an implicit solver (unconditionally stable), does not mean that we can choose a time step of any size.

- The time-step must be chosen in such a way that it resolves the time-dependent features and it maintain the solver stability.
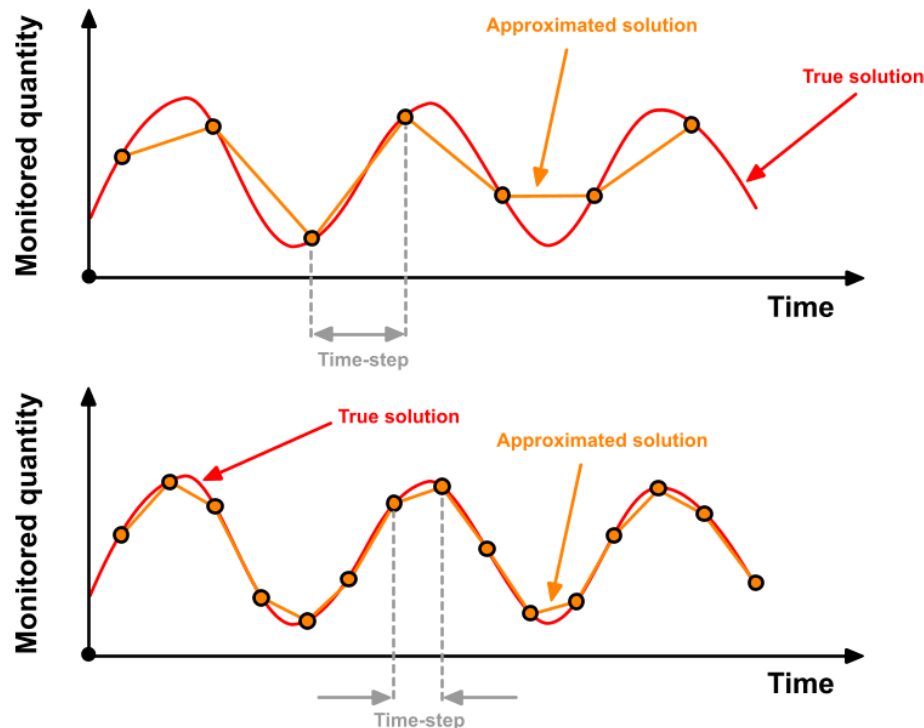
Tips and tricks in OpenFOAM®

Transient simulations and time-step selection

- In my personal experience, I have been able to go up to a CFL = 5.0 while maintaining the accuracy. To achieve this I had to increase the number of corrector steps in the `PIMPLE` solver, decrease the under-relaxation factors and tightening the convergence criteria; and this translates into a higher computational cost.

- I have managed to run with CFL numbers up to 40, but this highly reduces the accuracy of the solution. Also, is quite difficult to maintain the stability of the solver.

- As I am often interested in the unsteadiness of the solution, I usually use a CFL number not larger than 1.0.

Tips and tricks in OpenFOAM®

Transient simulations and time-step selection

- If accuracy is the goal (e.g., predicting forces), definitively use a CFL less than 1.0.

- If you are doing LES simulations, I highly advice you to use a CFL less than 0.6 and if you can afford it, less than 0.3

- If you are doing LES or you are interested in the accurate prediction of forces, definitely you need **high quality meshes**, preferable made of hexahedral elements.

- I usually use the `PIMPLE` solver. In the `PIMPLE` solver you have the option to limit your time-step to a maximum CFL number, so the solver automatically choose the time-step. This is a very cool feature.

- In the `PISO` solver you need to give the time-step size. So basically you need to choose your time-step so it does not exceed a target CFL value.

Tips and tricks in OpenFOAM®

Transient simulations and time-step selection

- You can easily also modify the `PISO` solver so it automatically choose the time-step according to a maximum CFL number, you just need to add one line of code.

- Remember, setting the keyword **nOuterCorrectors** equal to 1 in the `PIMPLE` solver is equivalent to use the `PISO` solver.

- The `PIMPLE` solver is a solver specially formulated for large time-steps. So in order to increase the stability you will need to add more corrector steps (**nOuterCorrectors** and **nCorrectors**).

- A smaller time-step may be needed in the first iterations to maintain solver stability. Have in mind that the first time steps may take longer to converge, do not be alarmed of this behavior, it is perfectly normal.

Tips and tricks in OpenFOAM®

Transient simulations and time-step selection

- If you are interested in the initial transient, you should start using a high order discretization scheme, with a tight convergence criterion, and the right flow properties.

- If you start from an approximate initial solution obtained from an steady simulation, the initial transient will not be accurate.

- If the solution is not converging or is taking too long to converge, try to reduce your time-step.

- If you use the first order Euler scheme, try to use a CFL number less than 1.0 and preferably in the order of 0.6-0.8, this is in order to keep temporal diffusion to a minimum. Yes, numerical diffusion also applies in time.

Transient simulations and time-step selection

- In order to speed up the computation and if you are not interested in the initial transient, you can start using a large time-step (high CFL).

- When you are ready to sample the quantity of interest, reduce the time-step to get a CFL less than one and let the simulation run for a while before doing any sampling.

- My recommendation is to always monitor your solution, and preferably use the `PIMPLE` solver.

- When using the `PIMPLE` or `PISO` solver (with maximum CFL feature enable), the solver will use as a time-step for the first iteration the value set by the keyword **deltaT** in the **controlDict** dictionary. So if you set a high value, is likely that the solver will explode.

Tips and tricks in OpenFOAM®

Transient simulations and time-step selection

- My advice is to set a low `deltaT` and then let the solver gradually adjust the time-step until the desired maximum CFL is reached.

- Some fancy high order numerical schemes (such as the vanLeer, vanAlbada, superbee, MUSCL, OSPRE – cool names no –), are hard to start. So it is better to begin with a small time-step and increase it gradually.

- And by small time-step I mean a time-step that will give a CFL about 0.1.

- Remember, you can change the temporal discretization on the fly. As for the spatial discretization, first order schemes are robust and second order schemes are accurate.

Tips and tricks in OpenFOAM®

Transient simulations and temporal discretization schemes

- The temporal discretization schemes are set in the `fvSchemes` dictionary. To select the schemes you need to use the keyword `ddtSchemes`.

- Euler is a first order implicit scheme (bounded).

- Backward is a second order implicit scheme (unbounded). Similar to the linear multistep Adams-Moulton scheme.

- Crank-Nicolson is a second order implicit scheme (bounded).

Transient simulations and temporal discretization schemes

- It you do not know what temporal discretization scheme to use, go for the Crank-Nicolson.

- The Crank-Nicolson as it is implemented in OpenFOAM®, uses a blending factor ψ. FYI, you can change the blending on the fly.

- Setting ψ equal to 0 is equivalent to running a pure Euler scheme (robust but first order accurate). By setting the blending factor equal to 1 you use a pure Crank-Nicolson (accurate but oscillatory, formally second order accurate). If you set the blending factor to 0.5, you get something in between first order accuracy and second order accuracy, or in other words, you get the best of both worlds.

```
ddtSchemes
{
    default         CrankNicolson ψ;
}
```

Transient simulations and temporal discretization schemes

- The Crank-Nicolson as it is implemented in OpenFOAM®, uses a blending factor ψ.

```
ddtSchemes
{
    default        CrankNicolson ψ;
}
```

$$\psi$$

0 ←————————————→ 1

Pure Euler
1st order, bounded

Pure Crank-Nicolson
2nd order, bounded
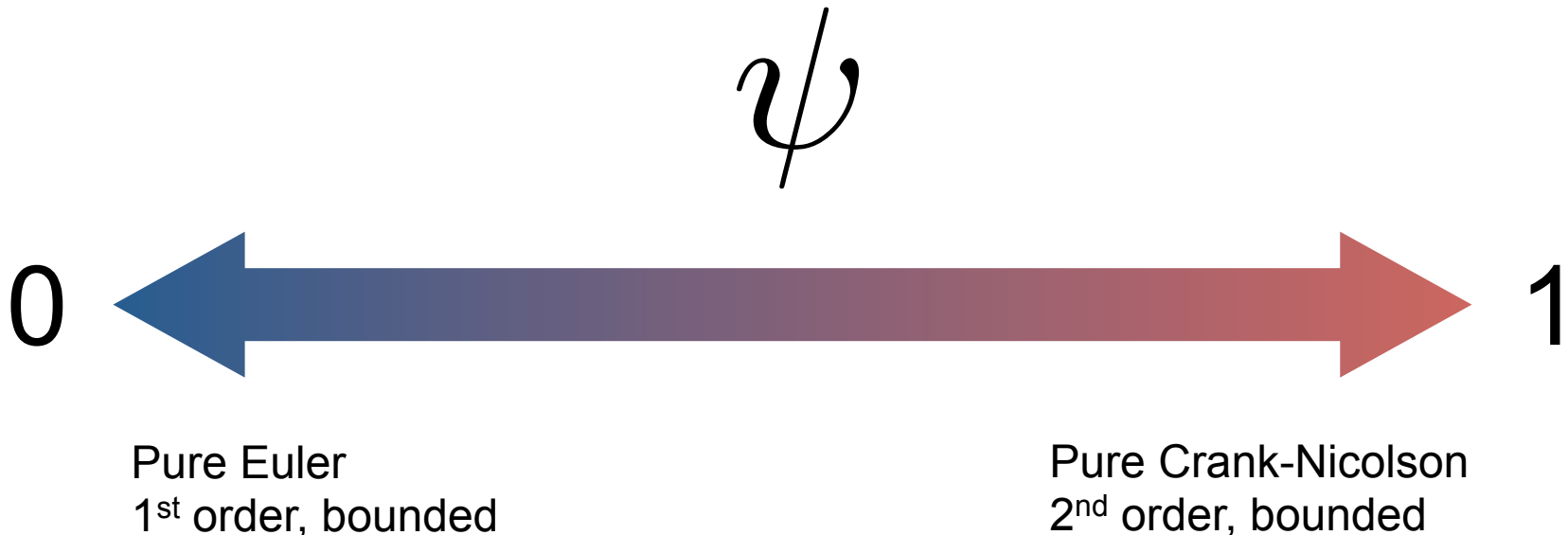
Notes on convergence

- Determining when the solution is converged can be really difficult.

- Solutions can be considered converged when the flow field and scalar fields are no longer changing, but usually this is not the case for unsteady flows. Most flows in nature and industrial applications are highly unsteady.

- It is a good practice to monitor the residuals. But be careful, residuals are not always indicative of a converged solution. The final residuals will reach the tolerance criterion in each iteration, but the flow field may be continuously changing from instant to instant.

- In order to properly assess convergence, it is also recommended to monitor a physical quantity. If this physical quantity does not change in time you may say that the solution is converge.

Tips and tricks in OpenFOAM®

Notes on convergence

- But be careful, it can be the case that the monitored quantity exhibit a random oscillatory behavior or a periodic oscillatory behavior, in the former case you are in the presence of a highly unsteady and turbulent flow with no periodic behavior; in latter case you may say that you have reached a converged periodic unsteady solution.

- Remember, for unsteady flows you will need to analyze/sample the solution in a given time window. Do not take the last saved solution as the final answer.

- If your goal is predicting forces (e.g., drag prediction).   You should monitor the forces, and use them as your convergence criterion.

- The convergence depends on the mesh quality, so a **good quality mesh** means faster convergence and accurate solution.

Tips and tricks in OpenFOAM®

Notes on convergence

- In general, overall mass balance should be satisfied. Remember, the method is conservative. What goes in, goes out.

- Residuals are not your solution. Low residuals do not automatically mean a correct solution, and high residuals do not automatically mean a wrong solution.

- Initial residuals are often higher with higher order discretization schemes than with first order discretization. That does not mean that the first order solution is better.

- Always ensure proper convergence before using a solution. A not converged solution can be misleading when interpreting the results.

Notes on convergence
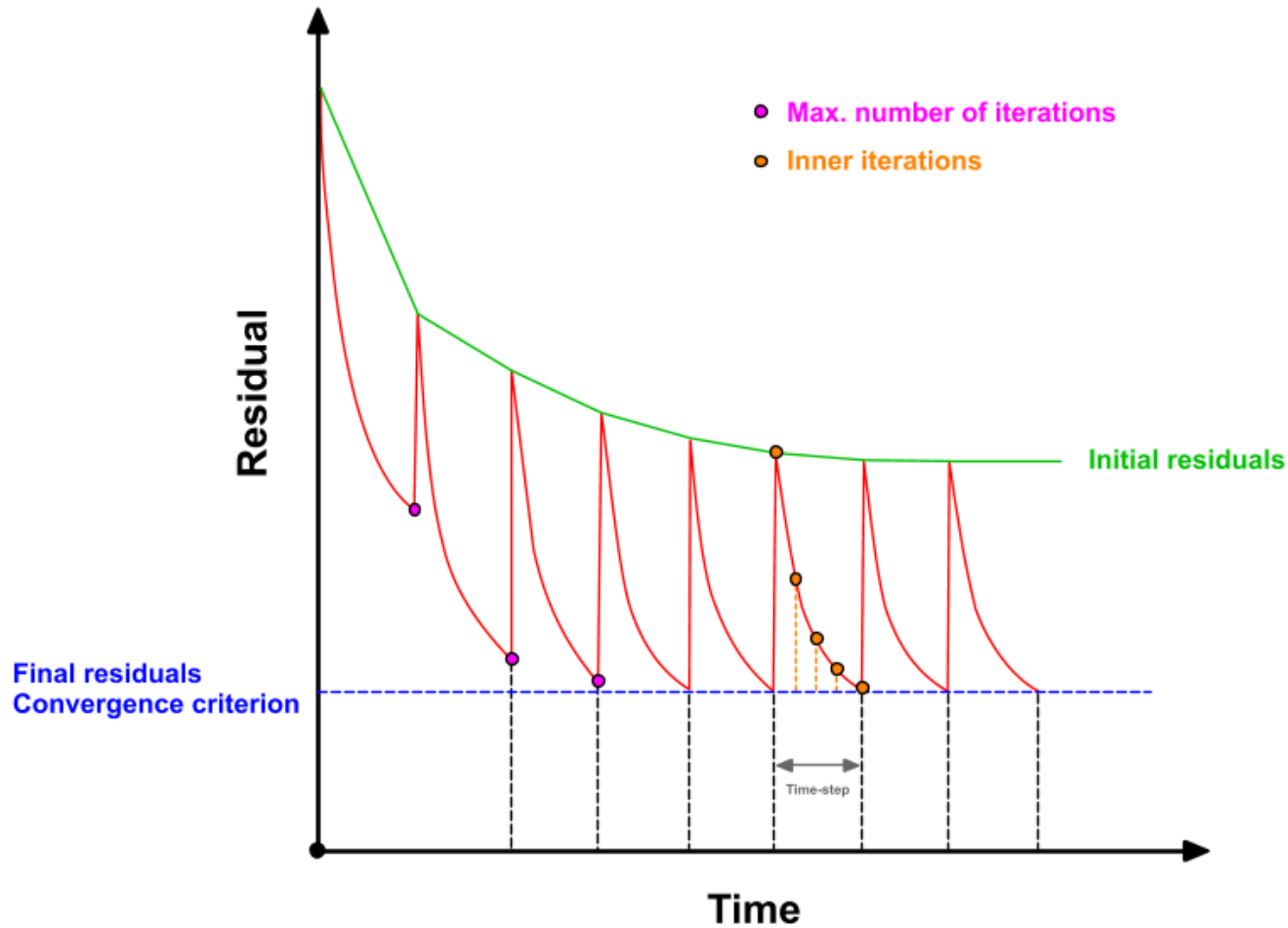
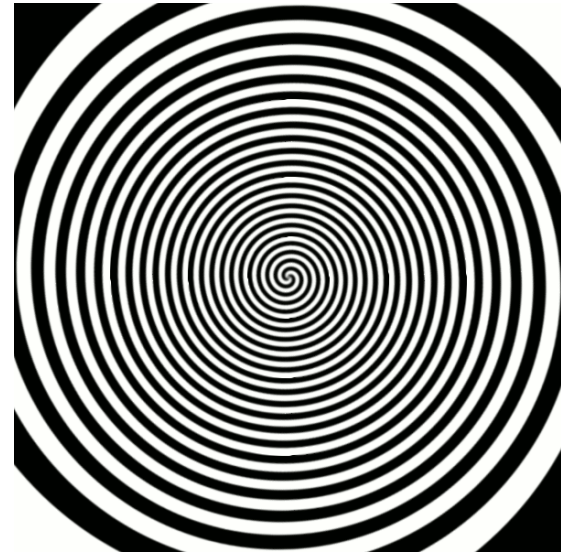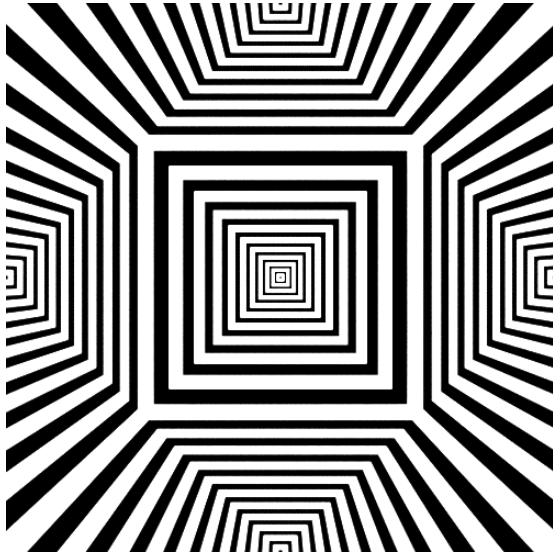# Tips and tricks in OpenFOAM®

Notes on convergence
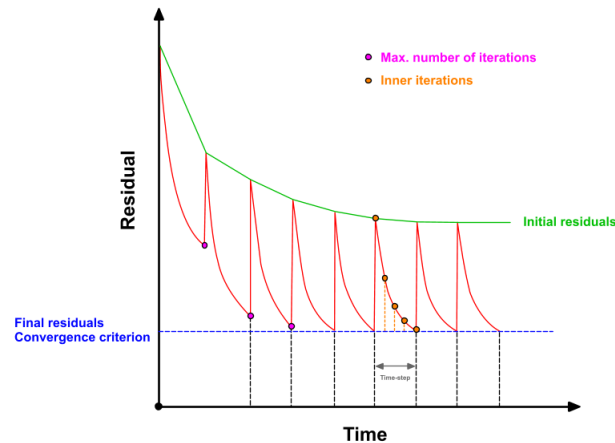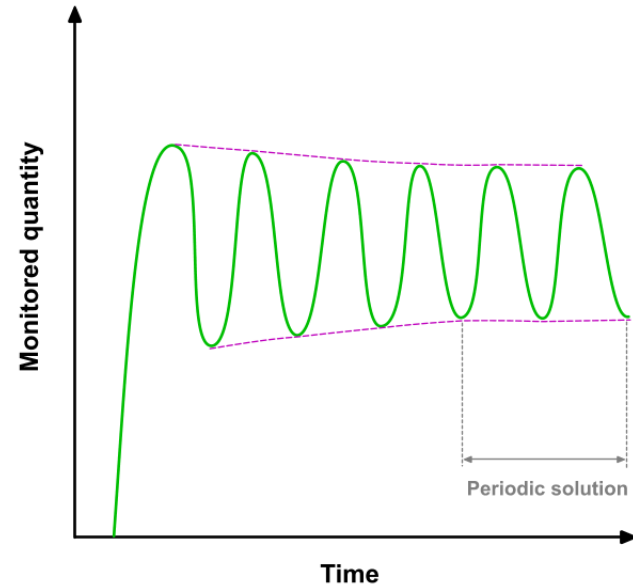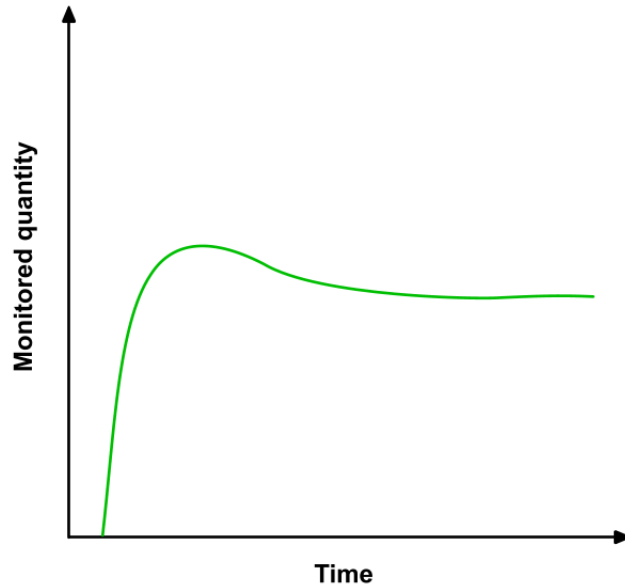
Tips and tricks in OpenFOAM®

Monitoring minimum and maximum values of field variables

- I always monitor the minimum and maximum values of the field variables. For me this is the best indication of stability and accuracy. For this, I use `functionObject`.

- If at one point of the simulation, velocity is higher that the speed of light (believe me, that can happen), you know that something is wrong.

- And believe me, using upwind you can get solutions at velocities higher that the speed of light, you can even do coffee if you want.

- You can also see an oscillatory behavior of the minimum and maximum values of the monitored quantity. This is also an indication that something is going bananas.

- For some variables (*e.g.* volume fraction), the method must be bounded. This means that the values should not exceed some predefined minimum or maximum value (usually 0 and 1).

Tips and tricks in OpenFOAM®

Again, our friend mesh quality
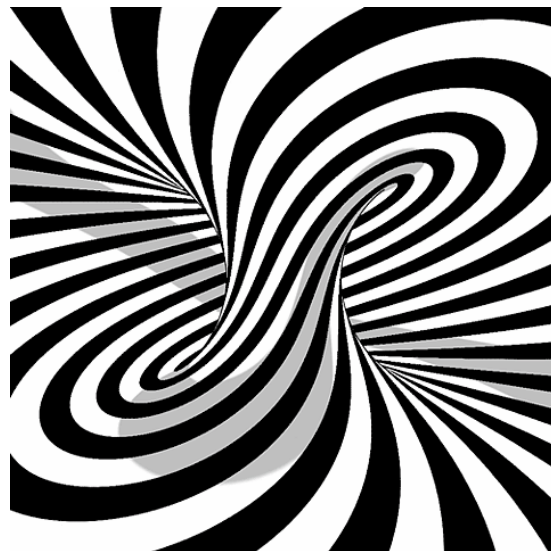
Tips and tricks in OpenFOAM®

Mesh quality and cell type

- **I do not know how much to stress this, but try to always use a good quality mesh. Remember, garbage in - garbage out.**

- Or in a positive way, **good mesh – good results**.

- Use hexahedral meshes whenever is possible, specially if high accuracy in predicting forces is your goal (e.g., drag prediction).

- For the same cell count, hexahedral meshes will give more accurate solutions, especially if the grid lines are aligned with the flow.

- But this does not mean that tetra mesh are no good, by carefully choosing the numerical scheme, you can get the same level of accuracy. The problem with tetra meshes are mainly related to the way gradients are computed.

Tips and tricks in OpenFOAM®

Mesh quality and cell type

- Tetra meshes normally need more computing resources during solving stage. But his can be easily offset by the time saved during the mesh generation stage.

- If the geometry is slightly complicated, it is just a waste to spend time on hex meshing. Your results will not be better, most of time, if not always. With todays advances in HPC and numerical methods, the computing time saved with hex mesh is marginal compared with time wasted in mesh generation.

- Increasing the cells count will likely improve the solution accuracy, but at the cost of a higher computational cost.

- But attention, finer mesh does not mean a good or better mesh.

- Very often when you refine your mesh (specially when it is done automatically), the overall quality of the mesh is reduced due to clustering and stretching of the mesh.

Tips and tricks in OpenFOAM®

Mesh quality and cell type

- Change in cell size should be smooth.

- In boundary layers, quad, hex, and prism/wedge cells are preferred over triangles, tetrahedras, or pyramids.

- The mesh density should be high enough to capture all relevant flow features. A good mesh should be done in such a way that it resolve the physics of interest and it is adequate for the models used, and not in the fact that the more cells we use the better the accuracy.

- A good mesh resolve physics, and does not need to follow the CAD model. We are talking about geometry defeaturing, you do not need to resolve all features of your CAD model.

Mesh quality and cell type

- There is a new type of meshes in town, polyhedral meshes.

- Many meshing guys and CFDers claim that polyhedral meshes are the panacea of meshing.

- In polyhedral meshes the cells have more neighbors than in tetrahedral and/or hexahedral meshes, hence the gradients are approximated better on polyhedral meshes.

- But attention, this does not mean that this kind of meshes are the solution to all meshing problems, is just a new religion in the meshing and CFD community, you need to become a true believer.

Mesh quality and cell type

- Another interesting property of polyhedral meshes is that they reduce the cell count. But there is a catch, they increase the number of faces so you need to compute more fluxes (diffusive and convective).

- Polyhedral meshes are not easy to generate, most of the times you need to start from tetrahedral meshes.

- In my personal experience, polyhedral meshes inhered the same quality problems of the starting tetrahedral mesh, sometimes they made things worst.

- Are polyhedral meshes better than hex or tet meshes? You need to conduct your own numerical experiments.

Tips and tricks in OpenFOAM®

Mesh quality and cell type

- Just to end for good the meshing talk:

  - A good mesh is a mesh that serves your project objectives.

  - So, as long as your results are physically realistic, reliable and accurate; your mesh is good.

  - At the end of the day, the final mesh will depend on the physic involve.

  - Know your physics and generate a mesh able to resolve that physics, **without over-doing**.

  - At this point, I think you got the idea of the relevance of the mesh.

Mesh quality and cell type

> # Who owns the mesh, owns the solution

Tips and tricks in OpenFOAM®

My simulation is always exploding

- If after choosing the numerical scheme, linear solvers, and time step, your simulation always crash, you can try this.

  - Set the discretization scheme of the convective terms to `upwind`.

  - Set the discretization scheme of the diffusive terms to `Gauss linear limited 0.5`

  - Set the discretization scheme of the gradient terms to `cellLimited Gauss linear 1.0`

  - Set the temporal discretization scheme to `euler`.

  - Use the `PISO` method, and set `nCorrectors 3`, and `nNonOrthogonalCorrectors 2`.

  - Use a high value of viscosity.

  - Use Newton-Krylov type linear solvers (do not use multigrid), and set the minimum number of iterations to 5 (`minIter 5`) for all variables.

  - Use a CFL number of the order of 0.2 and set `deltaT` to a low value in order to avoid jumps during the first iteration.

My simulation is always exploding

- This is one of a hell stable numerical scheme. However is first order accurate.

- If this does not work, you should check your boundary conditions, initial conditions, physical properties and model properties.

- You should also know the limitations of the solver you are trying to use, maybe the solver is not compatible or can not solve the physics involve.

functionObject

- When using utilities (*e.g.* `mirrorMesh`), do not use `functionObject` as they might cause some problems. Yon can run the utility as follows,

  - `utility_name -noFunctionObjects`

  Do this only if you are not interested in computing the actual `functionObject`

- If you forget to use a `functionObject`, you do not need to re-run your simulation. You can use the utility `execFlowFunctionObjects`, this utility will compute the `functionObject` values from the saved solutions. Do not forget to add the new `functionObject` to your `controlDict` before using `execFlowFunctionObjects`.

- Remember, `functionObject` can be temporarily disabled by launching the solver (or utility) with the option `-noFunctionObjects`.

Tips and tricks in OpenFOAM®

On the incompressible solvers

- I am going to be really loud on this.

- For those using the incompressible solvers (`icoFoam`, `simpleFoam`, `pisoFoam`, `pimpleFoam`), I want to remind you that the pressure used by these solvers is the modified pressure or

$$P = \frac{p}{\rho}$$

So when visualizing your results do not forget to multiply the pressure by the density in order to get the physical pressure. This will not made much different if you are working with air, but if you are working with water, you will notice the difference.

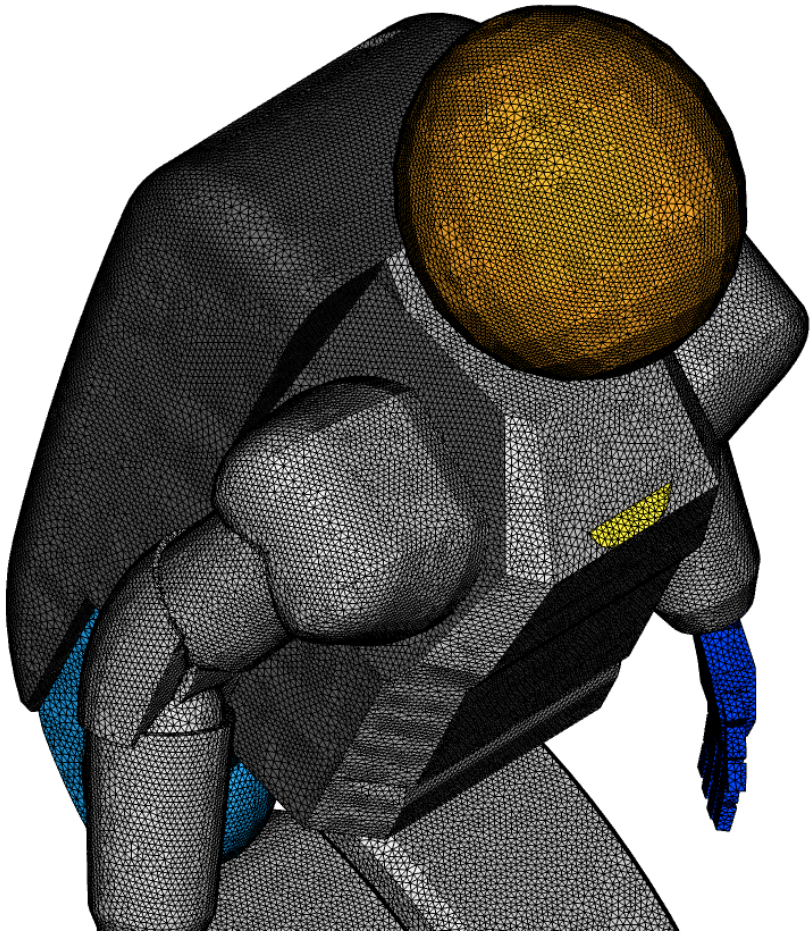# Tips and tricks in OpenFOAM®

Updating OpenFOAM®

- For those who like to always get the latest version of OpenFOAM®, I will give you a word of advise.

- Before changing to the newest version, run a series of test cases just to check the consistency of the results.

- It has come to my attention (and maybe yours as well), that the guys of OpenFOAM® might change (and will change) something in the new releases and you might not get the same results.

- No need to say that very often the syntax change from version to version.

- Personally speaking, I have a test matrix of five cases (involving different physics and models). So before deploying the new version, I always check if I get the same results. This is part of the continuous and arduous task of verification and validation.

- A new version of OpenFOAM® not necessary is a guarantee of innovation, and an old version of OpenFOAM® is no guarantee of efficiency.
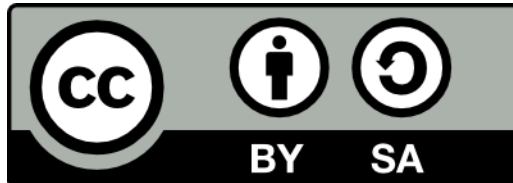
Best tip ever (and totally free)

- I know I sound like a broken record on this, but try to always get a good quality mesh.

- Use accurate and robust numerical schemes (in time and space).

- At this point we all know what is a good quality mesh and what is an accurate numerical scheme, if not, please read the theory. You do not do CFD without understanding the theory and the physics involve.