Supplement Tips and tricks

Where and how should we put more salt



... and as this is kind of a cooking recipe, it comes with a small warning

- 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 cell 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.



Our vertical workflow

- In our simulation vertical workflow, 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.



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. Namely,

\$HOME/OpenFOAM/OpenFOAM-1.6-ext.GPU/etc/bashrc \$HOME/OpenFOAM/OpenFOAM-2.4.0-debug/etc/bashrc \$HOME/OpenFOAM/OpenFOAM-2.4.x/etc/bashrc \$HOME/OpenFOAM/OpenFOAM-1806-adjoint/etc/bashrc \$HOME/OpenFOAM/OpenFOAM-1912/etc/bashrc \$HOME/OpenFOAM/OpenFOAM-2006/etc/bashrc \$HOME/OpenFOAM/OpenFOAM-7/etc/bashrc \$HOME/OpenFOAM/OpenFOAM-8/etc/bashrc \$HOME/OpenFOAM/OpenFOAM-8/etc/bashrc

OpenFOAM® shell environment

- If at any time I want to use a given version of OpenFOAM®, I just source the right OpenFOAM® environment variables suing predefined aliases.
- This is how my .bashrc file looks like,

alias of24x='source /home/joegi/OpenFOAM/OpenFOAM-2.4.x/etc/bashrc' alias of7='source /home/joegi/OpenFOAM/OpenFOAM-7/etc/bashrc' alias of8='source /home/joegi/OpenFOAM/OpenFOAM-8/etc/bashrc' alias ofdev='source /home/joegi/OpenFOAM/OpenFOAM-dev/etc/bashrc' alias of2006='source /home/joegi/OpenFOAM/OpenFOAM-2006/etc/bashrc'

- If I want to start using OpenFOAM® version 8, I just type in the terminal of8.
- You can also have two different versions of OpenFOAM® running together at the same time in different terminals.
- Just open the terminal and source the desired version.

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®

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 SRC -name "*fvPatch*"

This command will locate the files containing the string "*fvPatch*" in the directory \$FOAM_SRC

- 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 argument-r means recursive and -n will output the line number.

- 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 SRC -name "*fvPatch*"

This command will locate the files containing the string "*fvPatch*" in the directory \$FOAM_SRC

Looking for information in OpenFOAM® source code

- 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 argument-r means recursive and -n will output the line number.

- 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"

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
 - \$> find \$WM_PROJECT_DIR -type f | xargs grep -sl 'noParallel'
 - Remember, OpenFOAM® understand REGEX syntax.

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.



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 much faster, and the output files use less space.
- 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

- 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 naive 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.

Naming directories, files and variables

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

•	directory+1!	instead use	directory_1
•	This is a dir	instead use	this_is_a_dir
•	working@home	instead use	working_at_home
•	my/solution!!!	instead use	my_solution
•	#my_file;txt	instead use	my_file.txt
•	my dictionary.dict	instead use	my_dictionary.dict

 Also, I do not recommend you to use underscore as the first character when naming your files or directories

•	_my_dir	instead use	my_dir
•	_my_file	instead use	my_file

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.

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.

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 or paraview to visualize the failed sets.
- 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.

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/p rimitiveMeshCheck.C. Their maximum (or minimum) values are defined as follows:

36	Foam::scalar Foam::primitiveMesh::closedThreshold = 1.0e-6;
37	Foam::scalar Foam::primitiveMesh::aspectThreshold = 1000;
38	Foam::scalar Foam::primitiveMesh::nonOrthThreshold_ = 70; // deg
39	Foam::scalar Foam::primitiveMesh::skewThreshold = 4;
40	<pre>Foam::scalar Foam::primitiveMesh::planarCosAngle_ = 1.0e-6;</pre>

- 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).
- 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.

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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, especially close to the inlets.
- In few words, get a **good quality mesh** at the boundaries.
- Remember, for each single variable you are solving you need to specify a boundary condition.
- 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.

Initial conditions

- First of 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 a good idea of the sensitivity of the mesh quality.
 - If the residuals stall after 2-3 iterations, it means that your meshis sensitive to gradients.
- 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.

Initial conditions

- 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 do that.
- 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.

Starting and running a simulation

- Remember, you can change the parameters in the dictionaries *controlDict*, *fvSchemes* and *fvSolution* on-the-fly (and most of the dictionaries in the case directory).
- 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 slowly 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.
- Scaling the inlet velocity values can help to improve the convergence rate.
- That is to say, increase slowly the inlet velocity until you reach the desired value.
- By proceeding in this way, the body will not see the maximum instantaneous velocity at the first iteration.

Starting and running a simulation

- To accelerate the iterative convergence, you can 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 **PISO** 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. T
- 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.
- However, 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, high-order and high-resolution schemes need a **good quality mesh**.
- Bad quality meshes will add numerical oscillations and reduce the accuracy of the numerical solution.
- If you have a **good mesh and a good initial solution**, you can start immediately with a highorder scheme, but be careful, remember to always check the stability of the solution.

Discretization schemes

- 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 (first order accurate),



Discretization schemes – Convective terms

• An accurate and stable numerical scheme (second order accurate),

```
divSchemes
{
    div(phi,U) Gauss linearUpwind grad(U);
    div(phi,omega) Gauss linearUpwind grad(omega);
    div(phi,k) Gauss linearUpwind grad(omega);
    div((nuEff*dev2(T(grad(U))))) Gauss linear;
```

Discretization schemes – Convective terms

• An even more accurate but oscillatory scheme (second order accurate),

```
divSchemes
{
    div(phi,U) Gauss linear;
    div(phi,omega) Gauss limitedLinear 1;
    div(phi,k) Gauss limitedLinear 1;
    div((nuEff*dev2(T(grad(U))))) Gauss linear;
}
```

Discretization schemes – Convective terms

- By the way, do not get lost with all the convective terms implemented in OpenFOAM®.
- Last time I checked there were more than 50.
- These are the convective discretization schemes that you will use most of the times:
 - **upwind**: first order accurate.
 - **linearUpwind**: second order accurate, bounded.
 - **linear:** second order accurate, unbounded.
 - A good TVD scheme (vanLeer or Minmod): TVD, second order accurate, bounded.
 - **limitedLinear**: second order accurate, unbounded, but more stable than pure linear. Recommended for LES simulations (kind of similar to the Fromm method).
- Remember,
 - First order methods are bounded and stable but diffusive.
 - Second order methods are accurate, but they might become oscillatory.
 - At the end of the day, we always want a second order accurate solution.

Discretization schemes – Diffusive terms

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

laplacianSc	laplacianSchemes	
{ default }	Gauss linear corrected;	

• You can also use a scheme that uses a blending between a fully orthogonal scheme and a nonorthogonal scheme,

laplacianSo	laplacianSchemes			
{ default ک	Gauss linear limited ψ ;			
J				

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 $~\psi~$.



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

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

Discretization schemes – Diffusive terms

- In summary:
 - By setting the blending factor equal to 0 is equivalent to using the **uncorrected** method. You give up accuracy but gain stability (not so much though).
 - If you set the blending factor to 0.5, you get the best of both worlds. In this case, the nonorthogonal contribution does not exceed the orthogonal part. You give up accuracy but gain stability.
 - For meshes with non-orthogonality less than 70, you can set the blending factor to 1.
 - For meshes with non-orthogonality between 70 and 85, you can set the blending factor to 0.5
 - For meshes with non-orthogonality more than 85, it is better to get a better mesh. But if you definitely want to use that mesh, you can set the blending factor to 0.333-0.5, and increase the number of non-orthogonal corrections.
 - If you are doing LES or DES simulations, use a blending factor of 1 (this means that you need good 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),



Discretization schemes – Diffusive terms

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



Discretization schemes – Diffusive terms

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



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.
- By the way, there more methods implemented in OpenFOAM®, but these are the most commonly used.
- Also, all of the gradient discretization schemes are at least second order accurate.

Discretization schemes – Gradient terms

- You can also use gradient limiters.
- Gradient limiters will avoid over and under shoots on the gradient computations. They increase the stability of the method but add diffusion due to clipping.
- There are four available,



 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 $\,\psi$.



More accuracy but less stability Limiter off More stability but less accuracy Limiter on – Very aggressive

Discretization schemes – Gradient terms

- When running steady simulations, sometimes it may happen that the residuals get stalled.
- This is a well documented behavior related to the nature of non-differentiable slope limiters, as the one implemented in OpenFOAM® (Minmod).
- Sometimes it might help using a differentiable slope limiter.
- In OpenFOAM®, you have the following options:
 - grad(U) cellLimited<Venkatakrishnan> Gauss linear 1;
 - grad(U) cellLimited<cubic> 1.5 Gauss linear 1;
- In general, the cubic slope limiter is preferred over the Venkatakrishnan one.
- Finally, be carefully not to be too aggressive with the pressure gradient as it might add some diffusion to your solution. You will see this effect when computing the forces.
- It is a good idea to use the following setup for pressure gradient,
 - grad(p) Gauss linear 0.5;

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.
- 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 75.
- 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 use a mesh with high non-orthogonality, I often use the following numerical scheme.

Discretization schemes – How to choose the schemes

- Non-orthogonality more than 85. I do not waste my time, I prefer to go back and get a better mesh.
- I do not like to run simulations on highly orthogonal meshes, but if I have to use a mesh with high non-orthogonality, I often use the following numerical scheme.

gradSchemes					laplacianSchemes		
{					{		
	default	cellLimited Gauss	inear 0.5;			default	Gauss linear limited 0.333;
	grad(U)	faceLimited Gaus	s linear 1.0;		}		
}							
divSc	hemes			snGradSchemes			
{					{		
	div(phi,U)		Gauss linearUpwind grad(U);			default	limited 0.333;
	div(phi,ome	ega)	Gauss upwind;		}		
	div(phi,k)		Gauss upwind;				
	div((nuEff*c	dev(T(grad(U)))))	Gauss linear;				
}							

Discretization schemes – How to choose the schemes

Non-orthogonality between 70 and 85 •

				_			
grad {	Schemes default grad(U)	cellLimited Gaus	s linear 0.5; s linear 1.0;		lapla { }	cianSchemes default	s Gauss linear limited 0.5;
}							
divSchemes					snGradSchemes		
{					{		
	div(phi,U)		Gauss linearUpwind grad(U);			default	limited 0.5;
	div(phi,om	ega)	Gauss linearUpwind default;		}		
	div(phi,k)		Gauss linearUpwind default;				
	div((nuEff*	dev(T(grad(U)))))	Gauss linear;				
٦							

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Discretization schemes – How to choose the schemes

• Non-orthogonality between 60 and 70

gradSchemes				lapla	cianScheme	5
{				{		
de	efault cellM	IDLimited Gau	ıss linear 0.5;		default	Gauss linear limited 0.777;
gr	rad(U) cellM	IDLimited Gau	ıss linear 0.5;	}		
}						
<pre>gradSchemes { default celIMDLimited Gauss linear 0.5; grad(U) celIMDLimited 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; }</pre>				snGr	adSchemes	
{				{		
di	iv(phi,U)		Gauss linearUpwind grad(U)		default	limited 0.777;
di	iv(phi,omega)		Gauss linearUpwind default;	}		
di	iv(phi,k)		Gauss linearUpwind default;			
di	iv((nuEff*dev(T(g	grad(U)))))	Gauss linear;			
}						

Discretization schemes – How to choose the schemes

• Non-orthogonality between 40 and 60

				_			
gradSchemes					lapla	cianScheme	S
{					{		
	default	cellMDLimited Ga	auss linear 0;			default	Gauss linear limited 1.0;
	grad(U)	celIMDLimited Ga	auss linear 0.333;		}		
}							
divS	chemes				snGi	adSchemes	
{					{		
	div(phi,U)		Gauss linearUpwind grad(U);			default	limited 1.0;
	div(phi,om	ega)	Gauss linearUpwind default;		}		
	div(phi,k)		Gauss linearUpwind default;				
	div((nuEff*	dev(T(grad(U)))))	Gauss linear;				
}							

Discretization schemes – How to choose the schemes

- I guess at this point you know how to adjust the numerical scheme for meshes with nonorthogonality less than 40.
- Additionally, I also change the number of non-orthogonal corrections.
 - Non-orthogonality between 70 and 85:

nNonOrthogonalCorrectors 3;

• Non-orthogonality between 60 and 70:

nNonOrthogonalCorrectors 2;

• Non-orthogonality less than 60:

nNonOrthogonalCorrectors 1;

• I always like to do at least one non orthogonal correction.

Under-relaxation factors

- Because of the non-linearities 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.
- lpha=1 Means no relaxation at all. We simple use the predicted value of ϕ .
- $\alpha > 1 \quad \underset{\rm convergence \ rate \ but \ will \ decrease \ the \ stability.}{\rm Means \ over-relaxation.} \ {\rm It \ can \ sometimes \ be \ used \ to \ accelerate \ the \ stability.}$
- 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 .

Under-relaxation factors

- Under-relaxation factors (URF) are typical of steady solvers using the SIMPLE family of methods.
- To find out what are and how to change the URF requires experience and understanding.
- In general, URF are there to suppress oscillations.
- Small URF will significantly slow down convergence. Sometimes to the extent that the user thinks the solution is converged when in reality is not.
- The recommendation is to always use URF that are as high as possible, without resulting in oscillations or divergence.
- I highly recommend you to use the default URF (industry standard).
- If you have to change the URF, start by decreasing the values of the URF (one at a time) 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 URF for your case, it will take some trial and error.

Under-relaxation factors

• The under-relaxation factors are bounded between 0 and 1.



relaxationFactors

• Selecting the under-relaxation factors it is kind of equivalent to selecting the right time step.

Under-relaxation factors

• These are the under-relaxation factors I often use (which by the way are the industry standard).

SIM	PLE	SIMPLE	C
р	0.3;	р	1; Usually does not require under-relaxing
U	0.7;	U	0.9;
k	0.7;	k	0.9;
omega	0.7;	omega	0.9;

- According to the physics involved you will need to add more under-relaxation factors.
- Finding the right URF involved experience and some trial and error.
- Selecting the URF it is kind of equivalent to selecting the right time step
- If you do not define the URF, they will be set to 1.0 by default. That is, no under-relaxation.
- It is a good idea to start a steady simulation with low URF (about 0.1), and then increase them slowly until reaching the desired value.

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

- These are the linear solvers I often use.
- For the pressure equation I usually start with a **tolerance** equal to **1e-6** and **reIToI** equal to **0.01**. After a while I change these values to **1e-6** and **0.0** respectively.



- These are the linear solvers I often use.
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- 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-6** and **reIToI** equal to **0.01**. After a while I change these values to **1e-6** and **0.0** 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;
}		

- These are the linear solvers I often use.
- For the velocity equation I always use a **tolerance** equal to **1e-8** and **relTo**I equal to **0.0**



- I like to set the minimum number of iterations to three, especially for the pressure.
- If your solver is doing too many 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.

р		
{		
-	solver	PCG;
	preconditioner	DIC;
	tolerance	1e-6;
	relTol	0.01;
	minlter	3;
	maxIter	100;
}		

- 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);
	minlter	3;
}		

- 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 the last corrector step (.*Final).

1	
solver	GAMG;
tolerance	1e-06;
relTol	0.0;
smoother	GaussSeidel;
nPreSweeps	0;
nPostSweeps	2;
cacheAgglomeration	on;
agglomerator	faceAreaPair;
nCellsInCoarsestLevel	1000;
meraeLevels	1:

- 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.

р {			pFinal {	
-	solver	GAMG;	solver	GAMG;
	tolerance	1e-04;	tolerance	1e-06;
	relTol	0.01;	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;
}	-		}	

Additional notes on the *fvSolution* dictionary

For the *fvSolution* dictionary:



- 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.



Transient simulations and time-step selection

Comparison of PISO with non-iterative time-advancement (PISO-NITA) against PISO with Iterative time-advancement (PISO-ITA)





PISO-ITA (PIMPLE in OpenFOAM®)

PISO-NITA

- 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 outer 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 1000, but this highly reduces the accuracy of the solution. Also, it 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 4.0.
- 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 timestep 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.
- You can easily 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**).
- Remember, you need to do add least one **nCorrector** when using the **PISO** method.
- 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.
- 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 a 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 2.0 and preferably in the order of 0.6-0.9, this is in order to keep temporal diffusion to a minimum.
- Yes, numerical diffusion also applies in time.
- 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 with no under-relaxation.
- 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.
- 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.

Transient simulations and temporal discretization schemes

- Some fancy high-resolution 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 you a CFL about 0.5.
- 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.
- The temporal discretization schemes are set in the *fvSchemes* dictionary. To select the schemes you need to use the keyword **ddtSchemes**.
 - **Euler:** time dependent first order (implicit/explicit), bounded.
 - **backward:** time dependent second order (implicit), bounded/unbounded. Similar to the linear multistep Adams-Moulton scheme.
 - CrankNicolson: time dependent second order (implicit), bounded/unbounded.

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 .
- 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.



• Most of the time, a value of 0.7 is a good compromise.

Transient simulations and temporal discretization schemes

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



On turbulence modeling

- Compute Reynolds number and determine whether the flow is turbulent.
- Try to avoid using turbulent models with laminar flows.
- Choose the near-wall treatment and estimate y normal distance before generating the mesh.
- Run the simulation for a few time steps and get a better prediction of y⁺ and correct your initial prediction of y.
- The realizable $k-\epsilon$ or $k-\omega$ SST models are good choices for general applications.
- The standard $k \epsilon$ model is very reliable, you can use it to get initial values for more sophisticated models.
- Remember, OpenFOAM® implementation force you the use of wall functions.
- If you are interesting in resolving the large eddies and the inertial range, and modeling the smallest eddies, DES or LES are the right choice.
- If you do not have any restriction in the near wall treatment method, use wall functions.
- Avoid strong oscillations of the turbulent variables.

On turbulence modeling

- If you are doing LES or DES, remember that these models are intrinsically 3D and unsteady.
- In LES you should choose your time-step in such a way to get a CFL of less than 1 and preferably of about 0.5 for LES.
- DES simulations can use larger CFL values (up to 4 for reasonable accuracy).
- If you are doing RANS, it is perfectly fine to use upwind to discretize the turbulence closure equations.
- After all, turbulence is a dissipative process. However, some authors may disagree with this, make your own conclusions.
- On the other hand, if you are doing LES you should keep numerical diffusion to the minimum, so you should use second order methods.
- LES methods can be sensitive to mesh element type; it is highly recommended to use hexahedral meshes.
- Avoid the use of adaptive time-stepping and adaptive save intervals, as they may introduce oscillations in your solution.
- Many times RANS simulation can mysteriously explode, if this is your case, try reducing the URF of the turbulent quantities to something around 0.5 or even less.

- Determining when the solution is converged can be really difficult, especially if you are new to CFD.
- 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.
- 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.
- In general, overall mass balance should be satisfied.
- Remember, the method is conservative. What goes in, goes out (unless you have source terms).
- However, the method is not bounded, so to avoid spurious oscillation remember to use limiters.
- 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.




Monitoring minimum and maximum values of field variables

- I always monitor the minimum and maximum values of the field variables (you can do this using functionObjects).
- For me this is the best indication of stability and accuracy.
- 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, with 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).

- 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.
- Tetra meshes normally need more computing resources during the solution 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 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.
- 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.

- 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.
- 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.
- 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

A good mesh might not lead to the ideal solution, but a bad mesh will always lead to a bad solution.

P. Baker – Pointwise

Who owns the mesh, owns the solution.

H. Jasak – Wikki Ltd.

Garbage in – garbage out. As I am a really positive guy I prefer to say, good mesh – good results.

J. G. – WD

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**.
 - Do not use adaptive time-stepping.
 - 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 0.5 and set **deltaT** to a low value in order to avoid jumps during the first iteration.
- This is one of a hell stable numerical scheme. However it 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
- Remember, functionObject can be temporarily disabled by launching the solver (or utility) with the option -noFunctionObjects.
- If you forget to use a **functionObject**, you do not need to re-run your simulation.
- The solution to this problem is to use the solver with the option -postProcess. This will only compute the new functionObject, it will not rerun the simulation.
- For instance, let us say that you forgot to use a given **functionObject**. Open the dictionary *controlDict*, add the new **functionObject**, and type in the terminal,
 - \$> name_of_the_solver -postProcess -dict dictionary_location
- Do not forget to set all your **functionObjects** before launching your simulation.

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,



- So when visualizing or post processing the results do not forget to multiply the pressure by the density in order to get the physical pressure.
- This will not make much different if you are working with air, but if you are working with water, you will notice the difference.
- By the way, you should also multiply the wall shear stresses by the density.

Updating OpenFOAM®

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