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Applications: solvers and utilities – basic workflow





Applications: Solvers and Utilities

- OpenFOAM is first and foremost a C++ library, used primarily to create executables, known as applications. The applications fall into two categories: solvers, that are each designed to solve a specific continuum mechanics problem; and utilities, that are designed to perform tasks that involve data manipulation.
- Special applications for pre- and post-processing are included in OpenFOAM. Converters to/from other pre- and post-processors are available.
- OpenFOAM is distributed with a large number of applications, but soon any advanced user will start developing new applications for his/ her special needs. The basic way to do this is to find and copy an application that almost does what is needed, and then to modify it by copy/paste from other applications that has some features that are needed.

We will now have a look at how to use this in practice. NOTE that the output of the commands in the following slides might not be exactly the same in all versions of OpenFOAM, but the general procedures are the same.





The icoFoam/cavity tutorial

• Basic procedure when running a tutorial, in this case icoFoam/cavity:

```
cp -r $FOAM TUTORIALS/incompressible/icoFoam/cavity/cavity $FOAM RUN
run
```

cd cavity

You have copied the cavity tutorial and moved to \$FOAM_RUN/cavity

• The mesh is defined by a dictionary that is read by the blockMesh utility blockMesh

You have now generated the mesh in OpenFOAM format. Check the output from blockMesh!

• Check the mesh by

checkMesh

You see the mesh size, the geometrical size and some mesh checks (e.g. cell volumes).

• This is a case for the icoFoam solver, so run

icoFoam > & log&

You now ran the simulation in background using the settings in the case, and forwarded the errors and standard output to the \$FOAM_RUN/cavity/log file, where the Courant numbers and the residuals are shown.





Application parameters

Most OpenFOAM applications take parameters. Use the -help flag to get info:

• blockMesh -help (do it and look at the output in the terminal window)

The [-case dir] is the most common one, and with that you can specify the path to the case directory if you do not want to move to that case directory.

- checkMesh -help (do it and look at the output in the terminal window)
- icoFoam -help (do it and look at the output in the terminal window)

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A graphical view of the icoFoam/cavity tutorial

• We will now have a quick look at the results using paraFoam:

paraFoam Click on 'Last Frame': Click Apply. Color by Pressure using Display/Color by Move, rotate and scale the visualization using the mouse

- We will learn how to use paraFoam more further on.
- Exit paraFoam: File/Exit
- The results may also be viewed using third-party products: foamToEnsight etc., type: foamTo[TAB] to see alternatives. There is also a direct reader for Ensight - see the UserGuide.
- For post-processing in Fluent, run: foamMeshToFluent, and foamDataToFluent (controlDict is used to specify the time step, and a foamDataToFluentDict dictionary is required - see the UserGuide).





What did we do?

- We will have a look at what we did when running the cavity tutorial by looking at the case files.
- First of all it should be noted that icoFoam is a Transient solver for incompressible, laminar flow of Newtonian fluids
- The case directory originally contains the following sub-directories: 0, constant, and system. After our run it also contains the output 0.1, 0.2, 0.3, 0.4, 0.5, and log
- The 0* directories contain the values of all the variables at those time steps. The 0 directory is thus the initial condition.
- The constant directory contains the mesh and a transport Properties dictionary for the kinematic viscosity.
- The system directory contains settings for the run, discretization schemes, and solution procedures.
- The icoFoam solver reads the files in the case directory and runs the case according to those settings.





The constant directory

- The constant/transportProperties file is a dictionary for the dimensioned scalar nu
- The polyMesh directory originally contains the blockMeshDict dictionary for the blockMesh mesh generator (in old versions and in FOAMextend, moved to the system directory in recent OpenFOAM versions), and now also the mesh in OpenFOAM format.
- We will now have a quick look at the blockMeshDict dictionary in order to understand what mesh we have used. (we will have a look at it now even if it is in the system directory, since we are looking at mesh generation).





• The blockMeshDict dictionary first of all contains a number of vertices:

```
convertToMeters 0.1;
vertices
      (0 \ 0 \ 0)
      (1 \ 0 \ 0)
      (1 \ 1 \ 0)
      (0 \ 1 \ 0)
      (0 \ 0 \ 0.1)
      (1 \ 0 \ 0.1)
      (1 \ 1 \ 0.1)
      (0\ 1\ 0.1)
);
```

- There are eight vertices defining a 3D block. OpenFOAM always uses 3D meshes, even if the simulation is 2D.
- convertToMeters 0.1; multiplies the coordinates by 0.1.





• The blockMeshDict dictionary secondly defines a block and the mesh from the vertices:

```
blocks
    hex (0 1 2 3 4 5 6 7) (20 20 1) simpleGrading (1 1 1)
);
```

- hex means that it is a structured hexahedral block.
- (0 1 2 3 4 5 6 7) is the vertices used to define the block. The order of these is important - they should form a right-hand system! See the UserGuide.
- (20 20 1) is the number of mesh *cells* in each direction.
- simpleGrading (1 1 1) is the expansion ratio, in this case equidistant. The numbers are the ratios between the end cells along three edges. See the UserGuide.





The blockMeshDict dictionary finally defines three patches:

```
boundary
    movingWall
        type wall;
        faces
             (3762)
        );
    fixedWalls
        type wall;
        faces
             (0 \ 4 \ 7 \ 3)
             (2 6 5 1)
             (1 5 4 0)
        );
```

```
frontAndBack
         type empty;
         faces
              (0 \ 3 \ 2 \ 1)
              (4 5 6 7)
         );
);
```





- Each patch defines a type, a name, and a list of boundary faces
- Let's have a look at the fixedWalls patch:

```
fixedWalls{
    type wall;
    faces
          (0 \ 4 \ 7 \ 3)
          (2 6 5 1)
          (1 5 4 0)
    );}
```

- wall is the type of the boundary.
- fixedWalls is the name of the patch.
- The patch is defined by three sides of the block according to the list, which refers to the vertex numbers. The order of the vertex numbers is such that they are marched clock-wise when looking from inside the block. This is important, and unfortunately checkMesh will not check this.





• There are two empty sub-dictionaries in the icoFoam/cavity tutorial:

```
edges();
mergePatchPairs();
```

- edges (); is used to define shapes of the edges if they are not straight - polySpline, polyLine, line, simpleSpline, arc. We will use arc later on.
- (The following not in the blockMeshDict of this case anymore. You can figure out yourself if it works to add again)

mergePatchPairs(); is used to stitch two blocks that are not connected, but share the same physical surface at a patch of each block. This means that both blocks have a patch which is defined with four vertices in the same location as the corresponding patch in the neighbouring block, but the vertices are not the same in both blocks. It should be possible to stitch non-conformal meshes so the number of nodes and the distribution of the nodes do not have to be the same on both sides. This can also be done for two separate meshes, using the stitchMesh utility. We will do that later.





- \bullet To sum up, the blockMeshDict dictionary generates a block with: x/y/z dimensions 0.1/0.1/0.01
 - $20 \times 20 \times 1$ cells

```
wall fixedWalls patch at three sides
wall movingWall patch at one side
empty frontAndBack patch at two sides
```

• The type empty tells OpenFOAM that it is a 2D case, i.e. the equations will not be solved for in the direction of the empty patches. In fact, the discretization will explicitly neglect the third direction, which makes the numerical problem purely 2D.

- Read more about blockMesh yourself in the UserGuide.
- You can also convert mesh files from third-party products see the User-Guide. If you use ICEM, a good procedure is to write a Fluent mesh file (*.msh) and convert it with fluentMeshToFoam or fluent3DMeshToFoam.



The mesh files

• blockMesh uses the blockMeshDict to generate some files in the constant/polyMesh directory:

neighbour owner boundary faces points

• In the following slides we will discuss them...





The boundary file

• The boundary file shows the definitions of the patches, for instance:

```
movingWall
        type
                       wall;
        inGroups
                       1 (wall);
                       20;
        nFaces
                        760;
        startFace
```

- The faces are numbered, starting with the internal faces, following with the boundary faces. That is why the first patch starts with face 760.
- The movingWall patch has 20 faces, and the next patch starts at face 780.
- Each patch can be put inGroups for pre- and post-processing purpose. Each patch can thus be in several groups. The patchGroup generated by this makes e.g. setting of boundary conditions easier. A patch boundary condition definition takes precedence over a patchGroup boundary condition. The patchGroups are also listed in paraFoam.



The points file

• The points file shows the positions of all the points in the mesh:

```
882
(0 \ 0 \ 0)
(0.005\ 0\ 0)
(0.01\ 0\ 0)
(0.015 \ 0 \ 0)
```

- There are 882 points in this case.
- The points have an internal number: 0, 1, 2, ..., 881





The faces file

• The faces file shows the definitions of the faces in the mesh:

```
1640
4 (1 22 463 442)
4 (21 462 463 22)
4 (2 23 464 443)
4 (22 463 464 23)
```

- There are 1640 faces in the mesh.
- The faces have an internal number: 0, 1, 2, ..., 1639
- The first 759 faces are internal (remember from the boundary file!)
- The numbers in the brackets correspond to the numbers of the points that form each face.





The owner file

• The owner file defines which cell owns each face:

```
1640
(0
0
1
1
```

- There are 1640 faces in the mesh, so each line corresponds to a face.
- face 0 is owned by cell 0 (the number on that line) face 1 is owned by cell 0 (the number on that line) face 2 is owned by cell 1 (the number on that line) face 3 is owned by cell 1 (the number on that line) ...
- The face area vector is defined to point out of the owner cell.





The neighbour file

• The neighbour file defines which cell is the neighbour of the owner of each face:

```
760
2.0
2.
21 ...
```

- There are 760 internal faces in the mesh. The boundary faces only have an owner cell.
- face **0** is owned by cell 0 (as before), and cell **1** is the neighbouring cell face 1 is owned by cell 0 (as before), and cell 20 is the neighbouring cell face **2** is owned by cell 1 (as before), and cell **2** is the neighbouring cell face 3 is owned by cell 1 (as before), and cell 21 is the neighbouring cell
- The face area vector is defined to point into the neighbour cell.





The system directory

• The system directory consists of three set-up files:

```
controlDict fvSchemes
                          fySolution
(also blockMeshDict in recent versions of OpenFOAM)
```

- controlDict contains general instructions on how to run the case.
- fySchemes contains instructions on which discretization schemes that should be used for different terms in the equations.
- fysolution contains instructions on how to solve each discretized linear equation system. It also contains instructions for the PISO pressurevelocity coupling.
- In OFv2112 there is also decomposeParDict and PDRblockMeshDict. We will look at parallel processing later (decomposeParDict), and PDRblockMeshDict is left for you to examine by yourself (or for our discussions).





• The controlDict dictionary consists of the following lines:

```
application
                  icoFoam;
startFrom
                  startTime;
startTime
                  0;
stopAt
                  endTime;
endTime
                  0.5;
deltaT
                  0.005;
writeControl
                  timeStep;
writeInterval
                  20;
purgeWrite
                  0;
writeFormat
                  ascii;
writePrecision
                  6;
writeCompression
                  off;
timeFormat.
                  general;
timePrecision
                  6;
runTimeModifiable true;
```



- application icoFoam; Was previously used to tell the GUI FoamX in OpenFOAM-1.4.1 (and earlier) to use the set-up specifications of the icoFoam solver. Is used for the Allrun scripts in the tutorials directory, but it will not influence the solution as long as you manually start the case with the correct solver.
- The following lines tells icoFoam to start at startTime=0, and stop at endTime=0.5, with a time step deltaT=0.005:

```
startFrom
                    startTime;
startTime
                    0;
                    endTime;
stopAt
endTime
                    0.5;
deltaT
                    0.005;
```



• The following lines tells icoFoam to write out results in separate directories (purgeWrite 0;) every 20 timeStep, and that they should be written in uncompressed ascii format with writePrecision 6. timeFormat and timePrecision are instructions for the names of the time directories.

```
writeControl
                   timeStep;
writeInterval
                   20;
purgeWrite
                   0;
writeFormat
                   ascii;
writePrecision
                   6;
writeCompression
                   off;
timeFormat.
                   general;
timePrecision
                   6;
```

I recommend the use of writeCompression on; and writeFormat ascii;, which does not fill up your hard drive, and you can still open the files with vim. For fine dynamic meshes, it is recommended to use the binary format, to avoid deterioration of the mesh.





• runTimeModifiable true; allows you to make modifications to the case while it is running.





Specifying a maximum Courant number and varying time steps

• Some solvers, like the interFoam solver allows a varying time step, based on a maximum Courant number. Some extra entries should then be added to the controlDict dictionary:

```
adjustTimeStep
                 on;
maxCo
                 0.5;
maxAlphaCo
                 0.2;
maxDeltaT
                 1;
```

• The solver is then told to adjust the time step so that the output still occurs at specific times using:

```
writeControl adjustableRunTime;
writeInterval
               0.05;
```



A dictionary hint

• If you don't know which entries are available for a specific key word in a dictionary, just use a dummy and the solver will list the alternatives, for instance:

```
stopAt
                    dummy;
```

When running icoFoam you will get the message:

```
dummy is not in enumeration
endTime
writeNow
noWriteNow
nextWrite
```

and you will know the alternatives.

This does not work for all entries for some reason. In some cases, a message is written and a default value is used. Check the log file!





More dictionary hints

• You may also use C++ commenting in the dictionaries:

```
// This is my comment
/* My comments, line 1
  My comments, line 2 */
```

- Dictionary expansion mechanism:
 - Include another file:

```
#include "boundaryConditions"
```

- Define parameters:

```
velocity1
                  1;
```

- Use parameters:

```
$velocity1
```





The fvSchemes dictionary

• The fvSchemes dictionary defines the discretization schemes, in particular the time marching scheme and the convections schemes:

```
ddtSchemes
    default.
                     Euler;
divSchemes
    default
                     none;
    div(phi,U)
                     Gauss linear;
```

- Here we use the first-order Euler implicit temporal discretization, and the second-order linear (central-difference) scheme for convection.
- default none; means that schemes must be explicitly specified.
- Find the available convection schemes using a 'dummy' dictionary entry.



The fvSolution dictionary

- The fvSolution dictionary defines the solution procedure.
- The solutions of the p linear equation systems is defined by:

```
pFinal
solver
                PCG;
preconditioner DIC;
                                      relTol
                                                 0;
                1e-06;
tolerance
                0.05;
relTol
```

- The p linear equation system is solved using PCG (see later), with the DIC preconditioner (see later).
- The solution is considered converged when the residual has reached the tolerance, or if it has been reduced by relTol each time the p equation is solved. The pFinal setting copies the settings for p (\$p) but changes relTol to zero at the final corrector.
- relTol is here set to zero at the final corrector since we use the PISO algorithm. The PISO algorithm only solves each equation once per time step, and we should thus solve the equations to tolerance 1e-06 at each time step. relTol 0; disables relTol. See log file, first time step.





The fvSolution dictionary

• The solutions of the *U* linear equation systems is defined by:

```
IJ
    solver
                      smoothSolver;
    smoother
                      symGaussSeidel;
    tolerance
                      1e-05;
    relTol
                      0;
```

- The *U* linear equation system in solved using smoothSolver (see later), with the symGaussSeidel smoother (see later).
- The solution is considered converged when the residual has reached the tolerance 1e-05 for each time step.
- relTol is again set to zero since we use the PISO algorithm. relTol 0; disables relTol.



Main linear solvers

See:

http://www.tfd.chalmers.se/~hani/kurser/OS CFD 2008/TimBehrens/tibeh-report-fin.pdf http://www-users.cs.umn.edu/~saad/books.html

and descriptions using:

emacs \$FOAM SRC/OpenFOAM/matrices/lduMatrix/solvers/*/*.H

Note that the list below is old, so please refer to the descriptions you find in the code. In OFv2112 there are GAMG, PBiCGStab, PCG, PPCG, PPCR and smoothSolver.

- GAMG Geometric agglomerated algebraic multigrid solver (also named Generalised geometric-algebraic multi-grid in the manual)
- PBicg Preconditioned bi-conjugate gradient solver for asymmetric ldu-Matrices using a run-time selectable preconditioner
- PCG Preconditioned conjugate gradient solver for symmetric lduMatrices using a run-timeselectable preconditioner
- smoothSolver Iterative solver using smoother for symmetric and asymmetric matrices which uses a run-time selected smoother, e.g. Gauss-Seidel.





Preconditioners (1/2)

See:

http://www.tfd.chalmers.se/~hani/kurser/OS CFD 2008/TimBehrens/tibeh-report-fin.pdf and descriptions using:

emacs \$FOAM SRC/OpenFOAM/matrices/lduMatrix/preconditioners/*/*.H Note that the list below is old, so please refer to the descriptions you find in the code.

- diagonal Preconditioner Diagonal preconditioner for both symmetric and asymmetric matrices. This preconditioner actually does not help with faster propagation through the grid, but it is very easy and can be a good first step. Note: The reciprocal of the diagonal is calculated and stored for reuse because on most systems multiplications are faster than divisions.
- DICPreconditioner Simplified diagonal-based incomplete Cholesky preconditioner for symmetric matrices (symmetric equivalent of DILU). The reciprocal of the preconditioned diagonal is calculated and stored.
- DILUPreconditioner Simplified diagonal-based incomplete LU preconditioner for asymmetric matrices. The reciprocal of the preconditioned diagonal is calculated and stored.



Preconditioners (2/2)

- FDICPreconditioner Faster version of the DICPreconditioner diagonalbased incomplete Cholesky preconditioner for symmetric matrices (symmetric equivalent of DILU) in which the reciprocal of the preconditioned diagonal and the upper coeffcients divided by the diagonal are calculated and stored.
- GAMGPreconditioner Geometric agglomerated algebraic multigrid preconditioner (also named Generalised geometric-algebraic multi-grid in the manual).
- noPreconditioner Null preconditioner for both symmetric and asymmetric matrices.





Smoothers (1/2)

See:

http://www.tfd.chalmers.se/~hani/kurser/OS CFD 2008/TimBehrens/tibeh-report-fin.pdf and descriptions using:

emacs \$FOAM SRC/OpenFOAM/matrices/lduMatrix/smoothers/*/*.H Note that the list below is old, so please refer to the descriptions you find in the code.

- DIC Simplified diagonal-based incomplete Cholesky smoother for symmetric matrices.
- DICGaussSeidel Combined DIC/GaussSeidel smoother for symmetric matrices in which DIC smoothing is followed by GaussSeidel to ensure that any "spikes" created by the DIC sweeps are smoothed-out.
- DILU Simplified diagonal-based incomplete LU smoother for asymmetric matrices. ILU smoothers are good smoothers for linear multigrid methods.
- DILUGaussSeidel Combined DILU/GaussSeidel smoother for asymmetric matrices in which DILU smoothing is followed by GaussSeidel to ensure that any "spikes" created by the DILU sweeps are smoothed-out.





Smoothers (2/2)

Note that the list below is old, so please refer to the descriptions you find in the code.

- GaussSeidel The GaussSeidel method is a technique used to solve a linear system of equations. The method is an improved version of the Jacobi method. It is defined on matrices with non-zero diagonals, but convergence is only guaranteed if the matrix is either diagonally dominant, or symmetric and positive definite.
- symGaussSeidel, nonBlockingGaussSeidel, FDIC





The fvSolution dictionary

• The settings for the PISO algorithm are specified in the PISO entry:

```
PISO
    nCorrectors
                      2;
    nNonOrthogonalCorrectors 0;
    pRefCell
                      0;
    pRefValue
                      0;
```

- nCorrectors is the number of PISO correctors. You can see this in the log file since the p equation is solved twice, and the pressure-velocity coupling is thus done twice.
- nNonOrthogonalCorrectors adds corrections for non-orthogonal meshes, which may sometimes influence the solution (see plateHole tutorial).
- The pressure is set to prefvalue 0 in cell number prefcell 0. This is over-ridden if a constant pressure boundary condition is used for the pressure.
- We will have a closer look at the PISO algorithm later.





The time directories

• The 0 directory contains the dimensions, and the initial and boundary conditions for all primary variables, in this case p and U. U-example:

```
dimensions [0 \ 1 \ -1 \ 0 \ 0 \ 0];
internalField uniform (0 0 0);
boundaryField
    movingWall
                          fixedValue;
        type
        value
                          uniform (1 \ 0 \ 0);
    fixedWalls
                          noSlip;
        type
    frontAndBack
        type
                          empty;
    } }
```





The 0 directory

- dimensions [0 1 -1 0 0 0 0]; states that the dimension of U is m/s. We will have a further look at this later on.
- internalField uniform (0 0 0); sets U to zero internally.
- The boundary patches movingWall and fixedWalls are given the type fixedValue; value uniform (1 0 0); and (0 0 0) respectively, i.e. $U_x = 1m/s$, and U = 0m/s respectively.
- The frontAndBack patch is given type empty;, indicating that no solution is required in that direction since the case is 2D.
- You should now be able to understand 0/p also.
- The resulting 0.* directories are similar but the internalField is now a nonuniform List<vector> containing the results. Some boundary condition types also give nonuniform List. There is also a phi file, containing the resulting face fluxes that are needed to give a perfect restart. There is also some time information in 0.*/uniform/time. The 0.*/uniform directory is used for uniform information in a parallel simulation.





The log file

• If you followed the earlier instructions you should now have a log file. That file contains mainly the Courant numbers and residuals at all time steps:

```
Time = 0.09
Courant Number mean: 0.220582 max: 0.851424
smoothSolver: Solving for Ux, Initial residual = 0.000444982,
                       Final residual = 6.03872e-06, No Iterations 8
smoothSolver: Solving for Uy, Initial residual = 0.000969729,
                       Final residual = 7.57907e-06, No Iterations 9
DICPCG: Solving for p, Initial residual = 0.000971271,
                       Final residual = 4.7532e-07, No Iterations 26
time step continuity errors : sum local = 3.92322e-09,
                       global = -5.12852e-21, cumulative = -2.64764e-18
DICPCG: Solving for p, Initial residual = 0.000742827,
                       Final residual = 9.70686e-07, No Iterations 25
time step continuity errors : sum local = 7.98147e-09,
                       global = -5.01685e-19, cumulative = -3.14932e-18
ExecutionTime = 0.05 \text{ s} ClockTime = 0 \text{ s}
```





The log file

Looking at the Ux residuals

- smoothSolver: Solving for Ux, Initial residual = 0.000444982, Final residual = 6.03872e-06, No Iterations 8
- We see that we used the smoothSolver solver.
- The Initial residual is calculated before the linear equation system is solved, and the Final residual is calculated afterwards.
- We see that the Final residual is less than our tolerance in fvSolution (tolerance 1e-05;).
- The solver used 8 iterations to reach convergence.

Looking at the rest

- The pressure residuals and continuity errors are reported twice each time step. That is due to nCorrectors 2; for the PISO entry in fvSolution.
- The ExecutionTime is the elapsed CPU time, and the ClockTime is the elapsed wall clock time for the latest time step (approximate!!!).



Plot residuals

- It is of interest to have a graphical representation of the residual development.
- The foamLog utility is basically a script using grep, awk and sed to extract values from a log file. See \$WM_PROJECT_DIR/bin/foamLog for the source code.
- foamLog uses a database (foamLog.db) to know what to extract. The foamLog.db database can be modified if you want to extract any other values that foamlog doesn't extract by default. (find \$WM PROJECT DIR -iname "*foamLog.db*", or see the top of the output of foamLog, and make your own copy to modify directly in a case, or in \$HOME/.OpenFOAM/4.x/foamLog.db, which will be used automatically. Instructions are available in the foamLog.db file.)
- foamLog is executed on the cavity case with log-file log by: foamLog log
- A directory logs has now been generated, with extracted values in ascii format in two columns. The first column is the Time, and the second column is the value at that time.
- Type foamLog -h for more information.
- The graphical representation is then given by Matlab, xmgrace -log y Ux_0 p_0 or gnuplot: Type set logscale y then plot "Ux_0" w 1, "Uy_0" w 1, "p_0" w 1
- You can also use the user-contributed pyFoam to plot residuals on-the-fly.