



# HPC enabling of OpenFOAM<sup>(R)</sup> for CFD applications



### How to submit an OpenFOAM job to the cluster

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### Objectives and Topics

2 Case directory structure

③ Run the icoFoam cavity tutorial in your shell

④ Run the icoFoam cavity tutorial via batch job

**5** Run the pitzDaily tutorial via batch job in parallel







- Objective Show how to set-up and submit your OpenFOAM job in HPC environment:
- Topics
  - Case directory structure
  - Run the icoFoam cavity tutorial in your shell
  - Run the icoFoam cavity tutorial via batch job
  - Run the icoFoam pitzDaily tutorial via batch job in parallel







1 Objectives and Topics

### 2 Case directory structure

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# **OpenFOAM** environment



Check that OpenFOAM is loaded in your shell environment with the command [a08tra89@node343 ~]\$ module list if not, loaded it

[a08tra89@node343 ~]\$ module load autoload openfoam/2.3.0-gnu-4.7.2

Test the path to the icoFoam executable:

which icoFoam

You will see the full path to the selected executable.

Check that your  $M_PROJECT_USER_DIR and your run <math display="inline">M_PROJECT_USER_DIR/run exists$ 

```
echo WM_PROJECT_USER_DIR
/plx/usertrain/a08tra89/OpenFOAM/a08tra89-2.3.0
echo $WM_PROJECT_USER_DIR/run
/plx/usertrain/a08tra89/OpenFOAM/a08tra89-2.3.0/run
```

- Use the predefined alias foam and tut to go, respectively, to the \$WM\_PROJECT\_USER\_DIR and your tutorial directory, where there are complete set-ups of cases for all the solvers.
- Make a copy of the tutorial to your \$WM\_PROJECT\_USER\_DIR/run directory before running. You have the permission only to read the installed tutorial directory.
- There is no specific tutorials for the utilities, but some solver tutorials also show how to use the utilities.





### Case directory structure



- We will use the icoFoam cavity tutorial as a general example of case directory structure, how to set up and run the applications in OpenFOAM.
- Start by copying the tutorial to your run directory

```
cp -r $FOAM_TUTORIALS/incompressible/icoFoam/cavity $FOAM_RUN
cd $FOAM_RUN/cavity
```

Go to your FOAM\_RUN and have a look to the case directory structure, as follow

```
(case)
                     system
              -controlDict (control parameters; time step, grid spacing, max Courant number)
              |-fvSchemes (discretization schemes for grad, div, laplacian, time integration, interpolation)
              I-fySolution (linear algebra solvers for the discretized linear system)
                     constant
              -transportProperties (viscosity, gravity, etc.)
                          polyMesh (mesh generation files by BlockMeshDict)
                    -blockMeshDict
                    -points
                    -cells
                   I-faces
                   -boundary
                     time directories (initial 0 and boundary conditions)
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```





Objectives and Topics

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### 3 Run the icoFoam cavity tutorial in your shell

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Remember: interactive job in your shell max 10 minutes. Use with caution. Do not overload the login with memory intensive operations (it is not our case)

 The mesh is defined by a dictionary that is read by the blockMesh utility. Create the mesh by typing

[a08tra89@node343 ~]\$ blockMesh

You have now generated the mesh in OpenFOAM format.

Check the mesh by typing

[a08tra89@node343 ~]\$ checkMesh

You will see the mesh size, the geometrical size and some checks.

• This is the case for the icoFoam solver, so run it with the command

[a08tra89@node343 ~]\$ icoFoam > icofoam.log&

You will run the simulation, using 1 proc, in background in the login2 node, using the settings specified in the case dir. The log file reports the Courant numbers and the residuals

• You will see in your working dir, the new time directories. [a08tra89@node343 cavity]\$ 1s

0 0.1 0.2 0.3 0.4 0.5 constant icofoam.log system





We have a look at what we did when running the cavity tutorial by looking inside the case files

- First of all, remember that the solver 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 the run it also contains the output directories: 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. Hence the 0 directory is the initial condition.
  - The constant directory contains the mesh and dictionaries for the thermophysical and turbulence models.
  - 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.

In the next slides we will have a quick look the the dictionaries files to better understand how we have set the test case.







The constant directory has the following structure:

	constant
	-transportProperties
	I
	- polyMesh
	-blockMeshDict
	-points
	1
	-cells
	I
	-faces
	I
	-boundary

• The transportProperties file is the dictionary for the dimensioned scalar kinematic viscosity  $\nu$  ( $m^2/s$ , in SI system)

FoamFile			
version	2.0;		
format	ascii;		
class	dictionary;		
location	"constant";		
object	transportProperties;		
-			
* * * * * * *	* * * * * * * * * * * * * * * * * * * *		
nu	nu [ 0 2 -1 0 0 0 0 ] 0.01;		
		. ***	
		* *	
*******	************************	🥥 PRACE ★	CINEC



# The blockMeshDict file



The blockMeshDict dictionary is used to set-up the mesh generation utility blockMesh. First of all, it contains a numbers of vertices:

```
FoamFile
   version
             2.0:
   format
             ascii:
   class
             dictionary;
   obiect
             blockMeshDict:
convertToMeters 0.1; It applies a scaling factor for the vertex coordinates. Scales to dm.
vertices There are eight vertices definining a 3D block. OpenFOAM always uses a 3D meshes
even if the simulation is 2D
(
   (0 0 0)
           // vertex number 0
   (1 0 0) // vertex number 1
           // vertex number 2
   (1 \ 1 \ 0)
   (0 1 0) // vertex number 3
   (0 0 0.1) // vertex number 4
   (1 0 0.1) // vertex number 5
   (1 1 0.1) // vertex number 6
   (0 1 0.1) // vertex number 7
);
```





# The blockMeshDict file



Secondly, it defines a block and the mesh for the vertices

- hex means that is a structured hexahedral mesh
- (0 1 2 3 4 5 6 7) is the list of the vertices used to define the block. The order is important, they have to form a right-hand side system (see the User-Guide)
- (20 20 1) is the number of mesh cells in each direction
- simpleGrading is the cell expansion ratio, in this case equidistant. The expansion ratio enables the mesh to be graded, or refined, in specified directions. The ratio  $ex_r = \frac{\delta_e}{\delta_s}$  is that of the width of the end cell  $\delta_e$  along one edge of a block to the width of the start cell  $\delta_s$  along that edge. There are other grading system as edgeGrading (see User-Guide for more info).





### The blockMeshDict file



Finally, the boundary of the mesh is given in a list named boundary.

```
boundary
(
  movingWall // patch name (user choice) It contains two sub-dictionary
       type wall; // the patch type, either a generic patch or a particular geometric condition
                  // a list of block faces that make up the patch. The order in which the vertices are given
       faces
       must be such that, looking from inside the block and starting with any vertex,
        the face must be traversed in a clockwise direction to define the other vertices.
            (3762)
       ):
   fixedWalls // patch name (user choice)
       type wall;
       faces
            (0 4 7 3)
           (2651)
           (1540)
       ):
    frontAndBack // patch name (user choice)
       type empty: // 2 dimensional geometry
        faces
            (0 3 2 1)
           (4567)
       ):
):
```

The boundary is broken into patches (regions), in the example movingWall, fixedWalls and frontAndBack, where each patch in the list has its name as the keyword, which is the choice of the user. It is recommend something that conveniently identifies the patch, e.g.inlet; the name is used as an identifier for setting boundary conditions in the field data files. More info at User-Guide.





# The blockMeshDict file: summary



To sum up, the **blockMeshDict** dictionary generates a block with:

- x/y/z dimensions 0.1/0.1/0.1 m
- 20  $\times$  20  $\times$  1 cells
- boundary conditions type: 1 movingWall faces, 3 fixedWall face, 2 empty frontAndBack faces
- the type empty tells OpenFOAM that is a 2 dimensional case.

OpenFOAM supports natively two mesh generators:

- The mesh generation utility **blockMesh** to generate simple meshes of blocks of hexahedral cells.
- P The mesh generation utility snappyHexMesh for generating complex meshes of hexahedral and split-hexahedral cells automatically from triangulated surface geometries

For more info, please have a look to the Mesh generation and conversion User Guide. There are different options available for conversion of a mesh that has been generated by a third-party product into that of OpenFOAM can read (fluentMeshToFoam, starToFoam, gambitToFoam, ideasToFoam, cfx4ToFoam). Moreover there are commerical mesh generator tools that write the mesh directly in OpenFOAM format (ex: PointWise<sup>(R)</sup>).







The system directory has the following structure:



- The controlDict contains general instructions on how to run the case
- The fvSchemes contains instructions on which discretization schemes that should be used for different terms in the equations.
- The fvSolution contains instructions on how to solve each discretized linear equation system. It also contains instructions for the PISO pressure-velocity coupling





### The controlDict dictionary



The controlDict dictionary consist of the following lines:

```
FoamFile
    version
               2.0;
   format
               ascii;
   class
               dictionary;
   location
               "system":
               controlDict:
   object
}
// * * * * * *
                           icoFoam: // names of the application the tutorial is set up for
application
startFrom
               startTime:
startTime
               0:
                         // These lines tells icoFoam to start at startTime=0.
stopAt
               endTime:
                         // and stop at the endTime=0.5 with a TimeStep deltaT=0.005
endTime
               0.5:
deltaT
               0.005:
writeControl
               timeStep:
                         // These lines telles icoFoam to write the results in separate directories
writeInterval
                         // (purgeWrite=0) every 20 timeSteps, and that they should be written in
               20:
purgeWrite
               0:
                         // uncompressed ascii format with write precision 6.
writeFormat
               ascii:
writePrecision 6:
writeCompression off:
timeFormat
                         // timeFormat and timePrecision are used for the format
               general:
timePrecision
               6:
                         // of the naming of the time directories
runTimeModifiable true:
                         // Allows you to make modifications to the case while is running
```

The OpenFOAM solvers begin all runs by setting up a database. The controlDict dictionary sets input parameters essential for the creation of the database Only the time control and writeInterval entries are truly compulsory. For more info, please have a look to the Time and data I/O control User Guide.



# The fvSchemes dictionary



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The fvSchemes dictionary defines the discretization schemes, in particular the time marching scheme and the convection scheme for the spatial discretization

```
FoamFile
{
    version
                 2.0:
    format
                 ascii:
    class
                 dictionary:
    location
                 "system":
                 fvSchemes:
    object
// * * * *
ddtSchemes
                    Euler;
    default
divSchemes
    default
                     none;
    div(phi,U)
                      Gauss linear:
```

- We use the Euler implicit temporal discretization, and the linear (central-difference) scheme for convection.
- none means that the scheme must be explicitly specified.
- There are more than 50 alternatives for the convection scheme, and the number is increasing.

The terms that must typically be assigned a numerical scheme in fvSchemes range from derivatives, e.g. gradient and interpolations of values from one set of points to another. The aim in OpenFOAM is to offer an unrestricted choice to the user. For more info, please have a look to the Numerical Scheme User Guide.





The **fvSolution** dictionary defines the solution procedure. The equation solvers, tolerances and algorithms are controlled by this dictionary.

The solution of the pressure p linear equation system required for the icoFoam solver looks like:

```
solvers
{
    P
    {
        solver PCG;
        preconditioner DIC;
        tolerance ie-06;
        relTol 0;
    }
```

- The p linear equation system is solved using the Preconditioned Conjugate Gradient solver PCG, with the preconditioner DIC Diagonal incomplete-Cholesky (symmetric).
- The solution is considered converged when the residual has reached the tolerance, or if it has been reduced by relTol at each time step.
- Have a look yourself the the solution of the U linear equation system.

For more info, please have a look to the Solution and algorithm control User Guide and cite Benzi.







Most fluid dynamics solver applications in OpenFOAM use the

- Pressure-Implicit Split-Operator PISO algorithm, for transient problems.
- Semi-Implicit Method for Pressure-Linked Equations SIMPLE algorithm for steady-state problems.
- These algorithms are iterative procedures for solving equations for velocity and pressure. Both algorithms are based on evaluating some initial solutions and then correcting them.

```
PISO
{
    nCorrectors
                     2:
    nNonOrthogonalCorrectors 0:
    pRefCell
                     0:
    pRefValue
                     0:
}
SIMPLE
    nNonOrthogonalCorrectors 0:
    pRefCell
                     0;
    pRefValue
                     0:
```

• SIMPLE only makes 1 correction (keyword ncorrectors) whereas PISO requires more than 1, but typically not more than 4.

**...** 

 nNonOrthogonalCorrectors add correctors for non-orthogonal meshes, which may sometimes influence the solution, specially for very skewed (bad quality) meshes.







The 0 directory contains the dimension, the initial and boundary conditions for all primary variables. In this case p and U. As example, see below the U field

```
* * * * * * * * * * *
dimensions
                [0 1 -1 0 0 0 0]; // state the dimensions of U m/s
                uniform (0 0 0); // sets the U field to zero internally
internalField
boundarvField
{
    movingWall
                        fixedValue:
        type
        value
                        uniform (1 0 0):
    fixedWalls
                         fixedValue:
        type
        value
                        uniform (0 \ 0 \ 0):
    frontAndBack
        type
                         empty;
```

- The boundaryPatches movingWall and fixedWall are given the type fixedValue; Values uniform  $U_x = 1$  m/s and  $U_x = 0$ , respectively.
- The frontAndBack patch is given type empty, indicating that no solution is required in the that direction since the case is 2D.
- You can have a look yourself to the 0/p directory.





To visual the mesh and the global fields use RCM.

- The Remote Connection Manager (RCM) is an application that allows HPC-users to perform remote visualization on Cineca HPC clusters.
- Open a session from your local workstation

cd run cd cavity touch cavity.openFOAM

- Open with ParaView and select data format OpenFOAM.
- You do not need to use paraFoam that is a parser to a specific version of ParaView.
- In this case you can use your version of openFOAM with the selected version of ParaView.

More details, in tomorrow presentation.







Objectives and Topics

2 Case directory structure

③ Run the icoFoam cavity tutorial in your shell

**4** Run the icoFoam cavity tutorial via batch job

**5** Run the pitzDaily tutorial via batch job in parallel





### Run tutorial in your batch



We will run the cavity tutorial via batch script. This tutorial is a serial job, we require only 1 cpu.

In the following batch script, we will execute the pre-processing blockMesh and the executable icoFoam.

- Copy the batch script in your \$FOAM\_RUN/cavity
   [a08tra89@node343 ~]\$ cp \$FOAM\_CINECA\_SCRIPT/serial.pbs \$FOAM\_RUN/cavity
- Move to the working dir and remove the time directories, if presents [a08tra89@node343 ~]\$ cd \$FOAM\_RUN/cavity [a08tra89@node343 ~]\$ rm -rf 0.\*
- Now have a look to the script
- And modify it, according to your account and the selected queue





# Serial batch script 1/2



```
#!/bin/bash
#PBS -1 walltime=05:00
#PBS -1 select=1:ncpus=1:mpiprocs=1
## .lob name
#PBS -N foam serial
#### Standard output and error
#PBS -o serial.out
#PBS -e serial.err
#### Submission queue
#PBS -q private -W group_list=train_copf2014
#PBS -A train_copf2014
# redirect stdout and stderr
# -0 log
# -e log.err
#PBS -j oe
#PBS -m bea
#PBS -M i.spisso@cineca.it
#### end PBS directivies
```

This part of script includes the PBS directives that begins with the symbol  $\frac{4}{7}$ . Please note that  $\frac{4}{7}$  is a comment for PBS job scheduler





# Serial batch script 2/2



```
module load autoload/0.1/verbose
module load openfoam/2.3.0-gnu-4.7.2
# move to directory where the case has been submitted
cd $PBS_0_WORKDIR
## set the solver
solver=icoFoam
blockMesh >blockMesh.$PBS_JOBID
checkMesh > checkMesh.$PBS_JOBID
$solver > run.$PBS_JOBID
```

- The blue section load the module and move to the working dir
- The red section create the mesh with blockMesh, check it with checkMesh and execute the solver icoFoam in serial using the same cpu.
- The suffix \$PBS\_JOBID will append the jobid to the name of the logfile. After the execution, you will see something like run.1595057.node351.plx.cineca.it

Submit the job in queue system

```
[a08tra89@node343 ~]$ qsub serial.pbs
```







1 Objectives and Topics

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A Run the icoFoam cavity tutorial via batch job

**5** Run the pitzDaily tutorial via batch job in parallel







The method of parallel computing used by OpenFOAM is based on the standard Message Passing Interface (MPI) using the strategy of domain decomposition. The geometry and the associated fields are broken into pieces and allocated to separate processors for solution.

A convenient interface, Pstream, is used to plug any Message Passing Interface (MPI) library into OpenFOAM

• The first step is to decompose the computational domain using the decomposePar utility, which is set-up by the corresponding decomposeParDict dictionary located in the system directory of the case.

The parallel running uses the public domain openMPI implementation of the standard Message Passing Interface (MPI). In your case your have \$FOAM\_MPI=openmpi-system which use the openmpi/1.6.3--gnu--4.7.2 library.
Each processor run a copy of the solver with one separate part of the domain mesh.

• Finally the solution is reconstructed with the reconstructPar utility, to obtain the final result.





# pitzDaily at a glance









Run the pitzDaily tut in parallel



We will run the pitzDaily tutorial via batch script. This tutorial is a **parallel** job. In this tutorial we will:

- execute the pre-processing, which include decomposePar, according to the selected domain decomposition strategy.
- execute the job batch in parallel

Reconstruct the fields with reconstructPar

• Make a copy of the pitzDaily case to your run directory

cp -r \$FOAM\_TUTORIALS/incompressible/simpleFoam/pitzDaily \$FOAM\_RUN/.

• copy into the system directory the decomposeParDict file available in the pitzDailyExptInlet directory

cp \$FOAM\_TUTORIALS/incompressible/simpleFoam/pitzDailyExptInlet/system/decomposeParDict \$FOAM\_RUN/pitzDaily/system/.

• Move to the case directory

[a08tra89@node343 ~]\$ cd \$FOAM\_RUN/pitzDaily

• Now have a look to the decomposeParDict Dictionary.





The geometry and fields are broken up according to a set of parameters specified in the decomposeParDict dictionary, which must be located in the system directory of the case of interest.

```
FoamFile
    version
                2.0;
    format
                ascii:
    class
                dictionary:
    location
                "system":
    object
                decomposeParDict:
numberOfSubdomains 4: // The user must set the number of domains which the case has to be decompose into
it corresponds to the number of cores available for the computations
method
               hierarchical: // the user has the choice of six mothods of decomposition, specified by method.
For each method there are a set of coefficients specified in a sub-dictionary, named <method>Coeffs,
used to instruct the decomposition process
simpleCoeffs
    n
                    (211):
    delta
                    0.001:
hierarchicalCoeffs
                    (221): // where n is the number os sub-domains in the x.v and z directions
    delta
                    0.001:
                               // delta is the cell skew factor
    order
                    xyz;
                               // order is the order of decomposition xyz/yzx/zxy....
manualCoeffs
                    •••
    dataFile
                no; // Data files may be distributed if local disks are used in order to improve I/O performace.
distributed
roots
                ( ); Data may be distributed among different machines.
```



Domain decomposition method



#### method simple/hierarchical/scotch/manual

- simple Simple geometric decomposition in which the domain is split into pieces by direction, e.g. 2 pieces in the x direction, 1 in y direction.
- hierarchical Hierarchical geometric decomposition which is the same as simple except the user specifies the order in which the directional split is done, e.g. first in the y direction, then the x direction
- scotch Scotch decomposition which requires no geometric input from the user and attempts to minimise the number of processor boundaries. The user can specify a weighting for the decomposition between processors, through an optional processorWeights keyword.
- manual Manual decomposition, where the user directly specifies the allocation of each cell to a particular processor.

It is possible to plug METIS that requires no geometric input from the user and attempts to minimize the number of processor boundaries. You will need to install METIS as it is not distributed with OpenFOAM. METIS and parMetis are not free for commercial use.

For more info, please have a look to the Decomposition of mesh User Guide. \*



Run the pitzDaily tut in parallel



- Check that you are in your case directory
   [a08tra89@node343 ~]\$ pwd
   /plx/usertrain/a08tra89/OpenFOAM/a08tra89-2.3.0/run/pitzDaily
- Generate the mesh with the blockMesh utility

#### [a08tra89@node343 ~]\$ blockMesh

The end of the output lookslike





# Run the pitzDaily tut in parallel

• Execute the decomposePar utility, to decompose the domain according to the selected strategy.

#### [a08tra89@node343 ~]\$ decomposePar

The output lookslike

```
Create time
Decomposing mesh region0
Create mesh
Calculating distribution of cells
Selecting decompositionMethod hierarchical
Finished decomposition in 0 s
Calculating original mesh data
Distributing cells to processors
Distributing faces to processors
Distributing points to processors
Constructing processor meshes
Processor 0
    Number of cells = 3056
Processor 3
    Number of cells = 3057
Max number of faces between processors = 148 (4,59364% above average 141,5)
Time = 0
Processor 0: field transfer
Processor 1. field transfer
Processor 2: field transfer
Processor 3: field transfer
End.
```

• Remember: This is a **serial** process, which has decomposed the mesh for your next parallel run



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 On completion, a set of subdirectories have been created, one for each processor, in the case directory

Run the pitzDaily tut in parallel

```
[a08tra89@mode343 run]$ tree -L 1 pitzDaily/
pitzDaily/
|-- 0
|-- constant
|-- processor0
|-- processor1
|-- processor2
|- processor3
'-- system
```

- The directories are named processorN where N=0,1.... represents a processor number and a time directory, containing the decomposed filed description, and a constant/polyMesh directory containing the decomposed mesh description.
- Copy the batch script to run in parallel in your case directory \$FOAM\_RUN/pitzDaily/

cp \$FOAM\_CINECA\_SCRIPT/parallel.pbs \$FOAM\_RUN/pitzDaily

- Now have a look to the script
- And modify it, according to your account and the selected queue





# Parallel batch script 1/2



```
#!/bin/bash
#PBS -1 walltime=05:00
#PBS -1 select=1:ncpus=4:mpiprocs=4
## .lob name
#PBS -N foam_par
#### Standard output and error
#PBS -o par4.out
#PBS -e par4.err
#### Submission queue
#PBS -q private -W group_list=train_copf2014
#PBS -A train_copf2014
# redirect stdout and stderr
# -0 log
# -e log.err
#PBS -j oe
#PBS -m bea
##PBS -M i.spisso@cineca.it
#### end PBS directivies
```

Please note that PBS -1 select=1:ncpus=4:mpiprocs=4 is now set up for a pure MPI job with 4 cores.



\*\*\*\*





# Parallel batch script 2/2



```
module load autoload/0.1/verbose
module load openfoam/2.3.0-gnu-4.7.2
# move to directory where the case has been submitted
cd $PBS_0_WORKDIR
## set the solver
solver=simpleFoam
# set the number of procs
np=4
mpirun -np $np $solver -parallel > run_par.$PBS_JOBID
```

- The blue section loads the module and move to the working dir
- The red section selects the solver, the number of procs to run the parallel job, and execute the solver simpleFoam in parallel using the specified number of cpus.
- The suffix \$PBS\_JOBID will append the jobid to the name of the logfile. After the execution, you will see something like run\_par.1595057.node351.plx.cineca.it

Submit the job in queue system

```
[a08tra89@node343 ~]$ qsub parallel.pbs
```





• After the run, have a look the the processor\* directories, ex. processor1

```
[a08tra89@node343 run]$ tree -L 1 processor1/
processor1/
I-- 0
I-- 100
I-- 150
|-- 200
1-- 250
1-- 300
1-- 350
1 - - 400
1-- 450
1-- 50
I-- 500
I-- 550
I-- 600
I-- 650
I-- 700
I-- 750
I-- 800
I-- 825
'-- constant
```

• We can now reconstruct the entire field with the reconstructPar utility, by typing

reconstructPar





Reconstruct the fields: reconstruct Pr

· After a while, you will have the output

```
Create time
Reconstructing fields for mesh region0
Time = 50
Reconstructing FV fields
    Reconstructing volScalarFields
        p
        nut
        epsilon
    Reconstructing volVectorFields
    Reconstructing surfaceScalarFields
        phi
Reconstructing sets:
Time = 825
Reconstructing point fields
No point fields
No lagrangian fields
Reconstructing sets:
End.
```

 And the reconstructed fields in your case directory ready for post-processing and/or visualization.

Try to load yourself the reconstructed case and visualize the time variation of the U field  $% \left( {{U_{\mathrm{s}}}} \right) = 0$ 

