



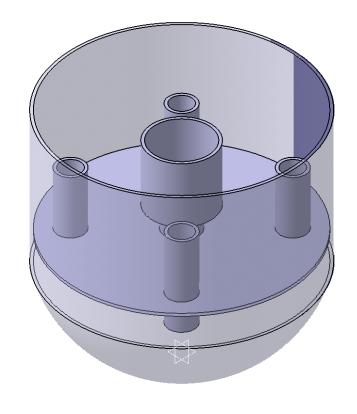
# SIMULATING REACTOR THERMAL-HYDRAULICS IN OPENFOAM

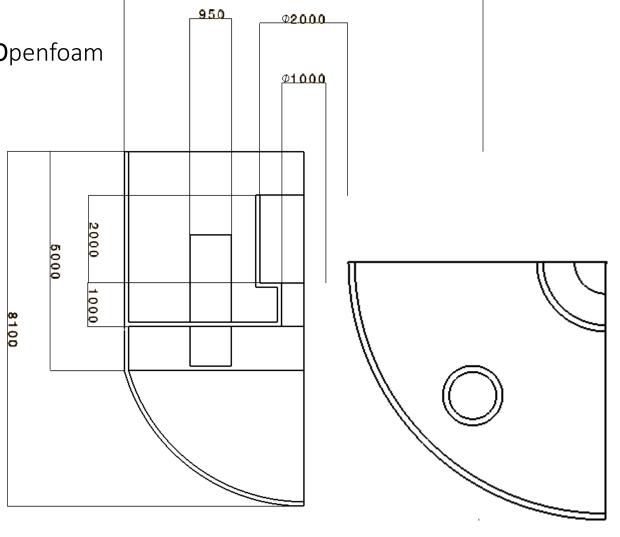
The ESPRESSO test case

Maria Faruoli, Silvania Lopes, Lilla Koloszar, Matilde Fiore

# **ESPRESSO**

Extremely SimPlified REactor Simulation uSing Openfoam



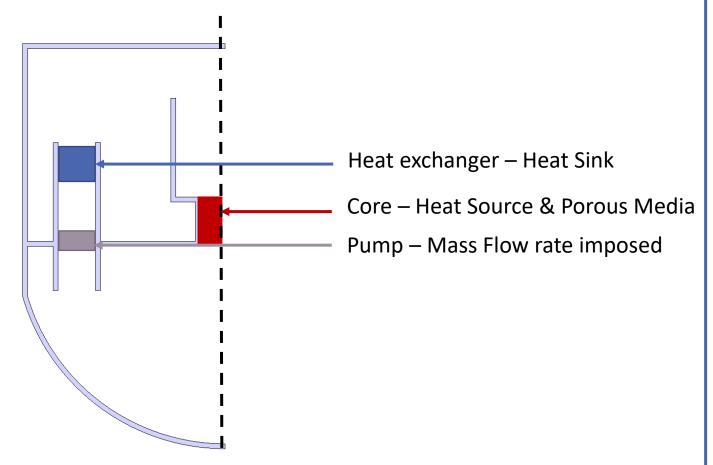


 $\Phi$ 8200



#### **GEOMETRY**

¼ of the entire geometry is simulated, by employing the symmetry boundary conditions



#### Which are the basic features of the flow?

- Constant density fluid (liquid metal):
   INCOMPRESSIBLE
- Viscosity is important to correctly predict the flow: VISCOUS
- Gravity is considered, but assuming conditions of forced convection gravitational effects have limited influence
- Heat exchange is very important (energy generation in the core region/heat sink in the heat exchangers)
- No liquid/gas interfaces modeled:
   SINGLE PHASE FLOW
- Not interested in study the transient (nominal conditions): STEADY state simulation



#### **GENERAL STEPS OF CFD**

- 1. Define the domain of interest
- 2. Discretize the domain
- 3. Physical and numerical setup
- 4. Solve the resulting problem
- 5. Post-process the results





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$$q = h(T - T_{out})$$

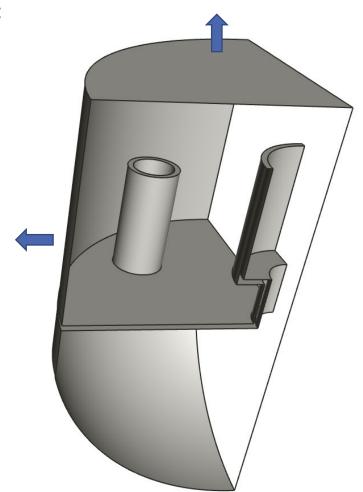
$$h = 10 W/m^2 K$$

$$T_{out} = 165^{\circ} C$$

We will show you how to consider the conduction through the cover without resolving it.

Explicit wall heat flux:

$$q = -150W/m^2$$



**Pumps:** effect on the fluid -> provides the massflow.

In our case prescribed as velocity magnitude in the pumps equivalent to **0.384m/s**.

**HXs:** effect on the fluid -> cools down the fluid after heated up by the core.

In our case constant heat sink of **10MW**, each.

**Core:** effect on the fluid -> heats up the fluid and strong pressure drop of dense structures.

In our case constant heat source of **10MW**. Pressure drop modelled by Darcy-Forchheimer law.

U

#### **GENERAL STEPS OF CFD**

1. Define the domain of interest

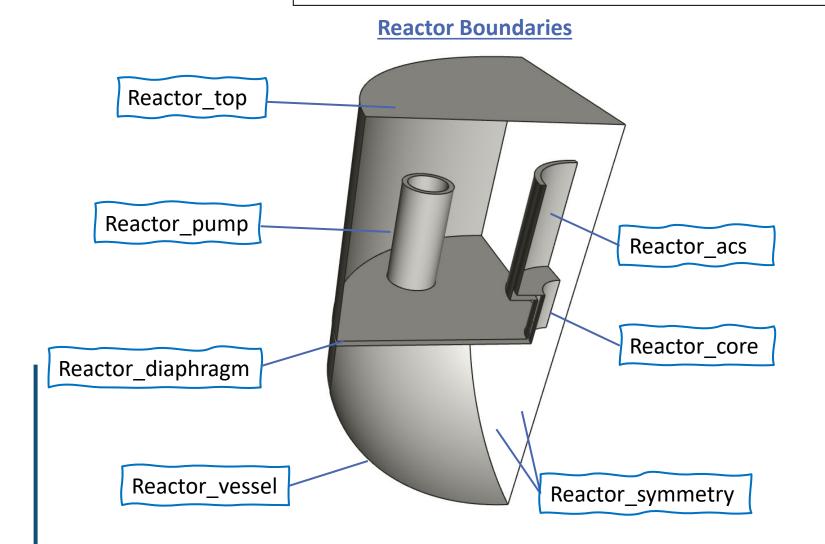
- 2. Discretize the domain
- 3. Physical and numerical setup
- 4. Solve the resulting problem
- 5.Post-process the results

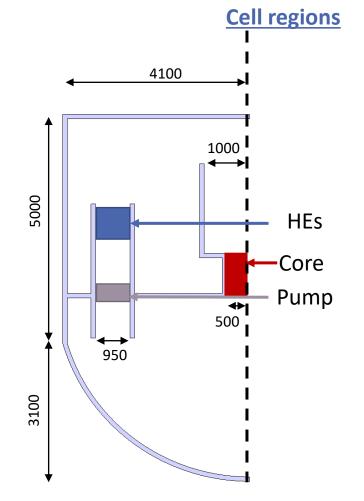




#### **GEOMETRY**

1/4 of the entire geometry is simulated, by employing the symmetry boundary conditions







## WHAT IS SNAPPYHEXMESH?

- Generation of 3-dimensional meshes containing hexahedra
- •Zonal meshing for support of porous media and MRF



```
cd $FOAM_RUN
```

Create a directory named as river

```
mkdir ESPRESSO
```

Enter to this directory

```
cd ESPRESSO
```

Copy the snappyHexMesh/motorBike tutorial directory in your river directory

```
cp -r $FOAM_TUTORIALS/mesh/snappyHexMesh/motorBike/motorbike/* ./
```

```
git clone git@github.com:ofcourse-VKI/ofseminar.git
cd ofseminar/of_seminar_ESPRESSO/tutorial
```



#### **CLEAN TUTORIAL AND COPY NEW GEOMETRY**

Clean the tutorial by removing useless files

```
rm -r constant/geometry/* 0/ Allclean Allrun
```

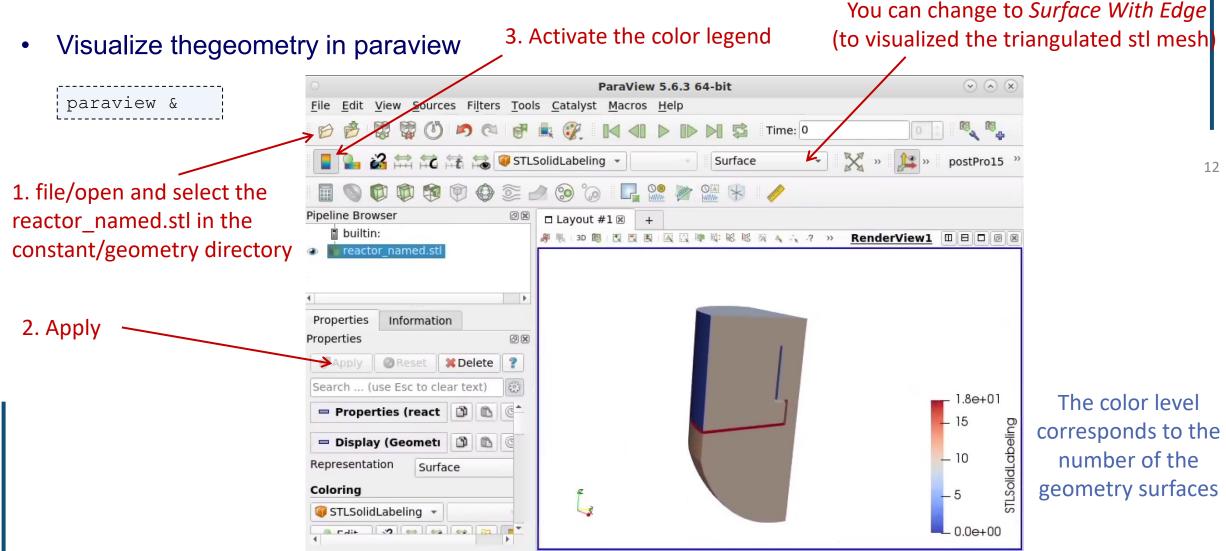
- Check that the .stl CAD files are in the geometry directory
  - reactor named.stl
  - •core region.stl
  - •pump\_region.stl
  - •hx region.stl

```
cp ../results/constant/geometry/* ./constant/geometry/
```

reactor\_named.stl is already separated in different surfaces

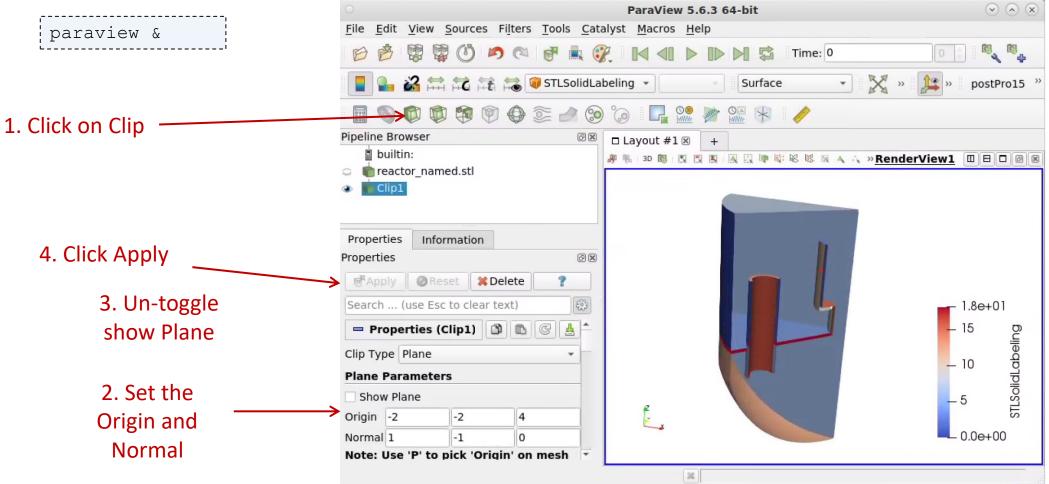


#### **STL** FILES





Create a clip in paraview to visualize the interior of the reactor





#### **STL** UTILITIES

```
cp -r $FOAM_ETC/caseDicts/surface/surfaceFeaturesDict ./system/
```

Edit the surfaceFeaturesDict in system directory

```
surfaces
    "reactor named.stl" "core region.stl" "hx region.stl" "pump region.stl"
// Identify edges when angle between faces < includedAngle
includedAngle
// Include region boundaries as features
geometricTestOnly no;
subsetFeatures
   // Include nonManifold edges (edges with >2 connected faces)
   nonManifoldEdges
                       no;
   // Include open edges (edges with 1 connected face)
    openEdges
                        yes;
// Write features to obj format for visualisation
writeObj
                    yes;
verboseObj
                    no;
```

Run the edge extraction

```
surfaceFeatures
```

This is creating a file "reactor\_named.eMesh" in the "constant/geometry" directory



1 /

#### **STL** UTILITIES

• The STL surface can be first checked using surfaceCheck utility:

surfaceCheck constant/geometry/reactor named.stl >log.surfaceCheck

Open the output file

vi log.surfaceCheck

or use grep to extract informations:

grep 'Bounding Box' log.surfaceCheck

Bounding Box: (-4-40) (2.4349e-1608)

This information is used later to define the background mesh size

Can be also obtained by loading the mesh in paraview

#### **BLOCKMESH**

Edit the blockMeshDict in system/

Bounding Box: (-4 -4 0) (2.4349e-16 0 8)

```
convertToMeters 1;
vertices
   (-4.2)
                           -0.2)
                  -4.2
                           -0.2)
   (0.2
   (0.2
                 0.2
                           -0.2)
                          -0.2)
                 -4.2
   (-4.2)
                           8.1)
   (0.2
                 -4.2
                           8.1)
   (0.2
                 0.2
                           8.1)
   (-4.2
                  0.2
                           8.1)
);
blocks
   hex (0 1 2 3 4 5 6 7) (44 44 83) simpleGrading (1 1 1)
);
edges
defaultPatch
              sides;
       name
              patch;
       type
boundary
                      Remove all the boundaries that they are
                             all defined in the stl file
```

#### **BLOCKMESH**

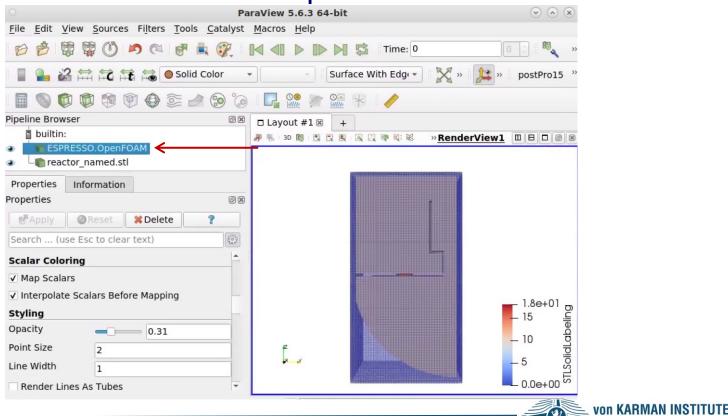
Run blockMesh :

blockMesh

Visualize the background mesh to check correspondence with

CAD file

paraFoam &



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FOR FLUID DYNAMICS

#### SNAPPYHEXMESHDICT- GEOMETRY CONTROLS SECTION

Open and Edit the snappyHexMeshDict

gedit system/snappyHexMeshDict &

```
FoamFile
           ascii;
  format
          dictionary;
  class
          snappyHexMeshDict;
  object
castellatedMesh true;
snap
                true;
                false;
addLayers
geometry
reactor
    type triSurfaceMesh;
    file "reactor named.stl";
```

```
core region
   type triSurfaceMesh;
   file "core region.stl";
 pump region
   type triSurfaceMesh;
   file "pump region.stl";
 hx region
   type triSurfaceMesh;
   file "hx region.stl";
```

```
refinementCylinderP
    type searchableCylinder;
    point1 (-2.1 -2.1 3);
    point2 (-2.1 -2.1 6.3);
   radius 0.5;
refinementCylinderC
    type searchableCylinder;
    point1 (0.0 0.0 3.2);
    point2 (0.0 0.0 5.1);
    radius 0.65;
refinementCylinderA
    type searchableCylinder;
    point1 (0.0 0.0 5.1);
    point2 (0.0 0.0 8.0);
    radius 1.2;
refinementCylinderL
    type searchableCylinder;
    point1 (0.0 0.0 0);
    point2 (0.0 0.0 4);
    radius 4.1;
```



### SNAPPYHEXMESHDICT- GENERAL MESH CONTROL

```
castellatedMeshControls
{
maxLocalCells 100000;

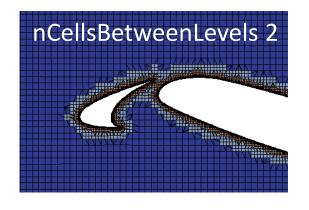
maxGlobalCells 2000000;

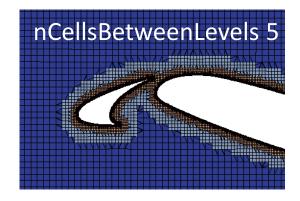
minRefinementCells 10;

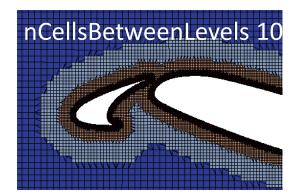
maxLoadUnbalance 0.1;

nCellsBetweenLevels 4;
```

```
features
           file "reactor named.eMesh";
           level 0;
           file "hx region.eMesh";
           level 2;
           file "core region.eMesh";
           level 2;
           file "pump region.eMesh";
           level 2;
```









#### SNAPPYHEXMESHDICT-SURFACE REFINEMENT

```
refinementSurfaces
        reactor
          level (0 0);
          regions
              "symmetry.*"
                level (0 0);
              "diaph.*"
                level (1 1);
              "core.*"
                level (3 3);
```

```
"acs.*"
  level (2 2);
 "acs5*"
  level (3 3);
"vessel.*"
   level (0 0);
 "top. *"
   level (0 0);
 "pump.*"
   level (2 2);
```

```
core region
        level (2 2);
         faceZone core region;
        cellZone core region;
        cellZoneInside inside;
    pump region
       level (1 1);
       faceZone pump region;
        cellZone pump region;
        cellZoneInside inside;
    hx region
      level (1 1);
      faceZone hx region;
        cellZone hx region;
        cellZoneInside inside;
// Resolve sharp angles
resolveFeatureAngle 30;
```

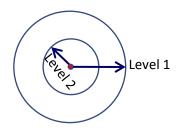
#### SNAPPYHEXMESHDICT-REGION REFINEMENT

```
refinementRegions
       refinementCylinderP
            mode inside:
            levels ((1E15 1));
    refinementCylinderC
            mode inside;
            levels ((1E15 2));
      refinementCylinderA
            mode inside;
            levels ((1E15 2));
      refinementCylinderL
            mode inside;
            levels ((1E15 1));
locationInMesh (-1 -1 5);
allowFreeStandingZoneFaces true;
```

Level of refinement can also be defined by specifying the distance around the edge that will take the level of refinement

```
levels ((0.1 2) (0.2 1) );

Distance in meter
```



```
snapControls
{
    nSmoothPatch 3;

    tolerance 2.0;

    nSolveIter 30;

    nRelaxIter 5;

    nFeatureSnapIter 10;

    implicitFeatureSnap false;

    explicitFeatureSnap true;

    multiRegionFeatureSnap false;
}
```



#### **CREATE THE MESH WITH SHM**

Run snappyHexMesh in the case directory

snappyHexMesh -overwrite

Check the quality of the mesh

checkMesh

Before visualize the mesh, we will create the boundary conditions

~ ~



#### **CREATE BOUNDARY CONDITIONS**

Create patches out of selected boundary faces and change name and type of the boundaries

```
cp $FOAM_ETC/caseDicts/mesh/manipulation/patches/createPatchDict ./system
```

Edit system/createPatchDict

```
patches
    name diaph;
    patchInfo
      type wall;
    constructFrom patches;
    patches ("reactor diaph.*");
    name acs;
    patchInfo
      type wall;
    constructFrom patches;
    patches ("reactor_acs.*");
```

```
name core;
patchInfo
  type wall;
constructFrom patches;
patches ("reactor core.*");
name vessel;
patchInfo
  type wall;
constructFrom patches;
patches ("reactor vessel.*");
```

```
name pump;
patchInfo
  type wall;
constructFrom patches;
patches ("reactor pump.*");
name top;
patchInfo
  type wall;
constructFrom patches;
patches ("reactor top.*");
```

```
name symmetry1;
patchInfo
 type symmetry;
constructFrom patches;
patches ("reactor symmetry1");
name symmetry2;
patchInfo
 type symmetry;
constructFrom patches;
patches ("reactor symmetry2");
```



#### **CREATE BOUNDARY CONDITIONS**

Run createPatch to create the new BC

createPatch -overwrite

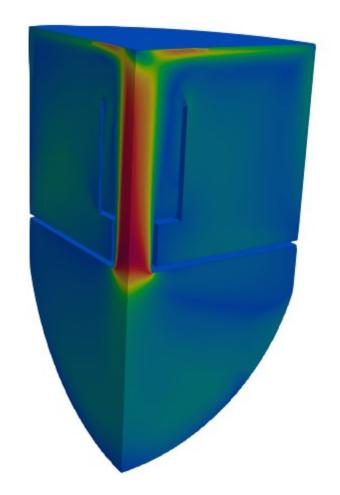
Visualize in paraFoam

paraFoam





- 1. Define the domain of interest
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The RANS module for non-isothermal (buoyant) flows in OpenFoam 11 is called

fluid

And it is approximating this set of equations:

$$\nabla \cdot (\rho \mathbf{u}) = 0$$
 Mass

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \rho \mathbf{g} + \nabla \cdot \left(2\mu_{eff} D(\mathbf{u})\right) - \nabla \cdot \left(\frac{2}{3}\mu_{eff} \nabla \cdot (\mathbf{u})\right) \text{ Momentum}$$

Many of these terms will be nil in our case as a result of the incompressibility

$$\nabla \cdot (\rho \mathbf{u}h) + \nabla \cdot (\rho \mathbf{u}K) = \rho(\mathbf{g} \cdot \mathbf{u}) + \nabla \cdot (\alpha_{eff} \nabla h)$$
 Energy



```
cd $FOAM_RUN
```

Create a directory named as ESPRESSO setup

```
mkdir ESPRESSO_setup
```

Enter to this directory

```
cd ESPRESSO_setup
```

Copy the buoyantCavity tutorial directory in your directory

```
cp -r $FOAM_TUTORIALS/fluid/buoyantCavity/* ./
```

Copy the mesh created previously in your directory

```
cp -r ../ESPRESSO/constant/polyMesh/ ./constant/
```

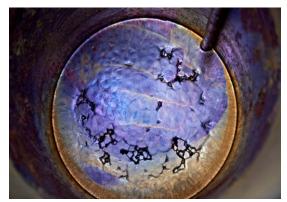
mv 0.orig 0

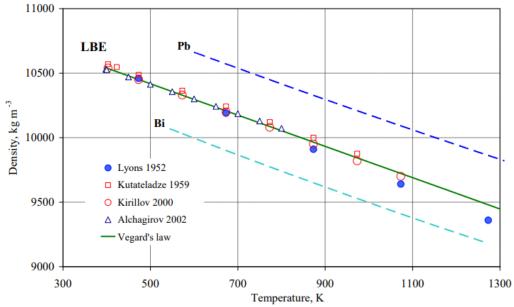




#### **PHYSICAL PROPERTIES**

LBE





```
thermoType
                                                        In case you want to
                                                        account for variable
    type
                       heRhoThermo;
    mixture
                      pureMixture;
                                                       transport properties,
                      polynomial;
    transport
                                                        you can specify the
                      hPolynomial;
    thermo
    equationOfState icoPolynomial;
                                                           coefficients of
    specie
                      specie;
                                                          polynomial laws
                      sensibleEnthalpy;
    energy
mixture
                               Property
                                                                    Formula
    specie
                               Density(\rho) [kg m^3]
                                                                    11096-1.3326T
                                Heat capacity (cp) [Jkq^{-1}K^{-1}]
                                                                   159-2.72 \ 10^{-2}T+7.12 \ 10^{-6}T^2
       molWeight 208.98;
                                                                    3.61+1.517\ 10^{-2}T-1.741\ 10^{-6}T^2
                                Th. conductivity (\lambda) [Wm^{-1}K^{-1}]
                                Cinematic Viscosity (\mu) [kgm^{-1}s-1]
                                                                    4.94 \ 10^{-4} \exp(754.1/T)
    thermodynamics
                                                                   c_p \mu \lambda^{-1}
                                Prandtl number (Pr) [-]
                          0;
       Ηf
        Sf
                          ( 159 0.0272 7.12e-6 0 0 0 0 0);
       CpCoeffs<8>
    equationOfState
        rhoCoeffs<8>
                          ( 11096 -1.3326 0 0 0 0 0 0 );
    transport
```

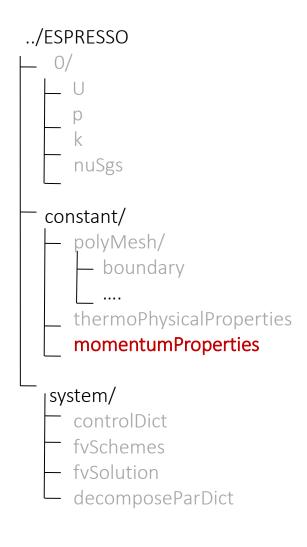
(0.0056 - 1e - 5 5e - 9 0 0 0 0);

( 3.61 1.517e-2 1.741e-6 0 0 0 0 0); }

muCoeffs<8>

kappaCoeffs<8>

#### **TURBULENCE MODELS**



# Several **turbulence models** are available in OpenFoam.

#### laminar

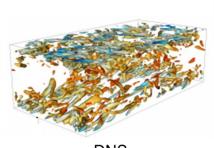
uses no turbulence models;

RAS

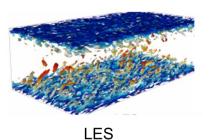
uses Reynolds-averaged simulation (RAS) modelling;

LES

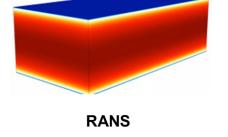
uses large-eddy simulation (LES) modelling.



DNS (Direct Navier-Stokes simulation)

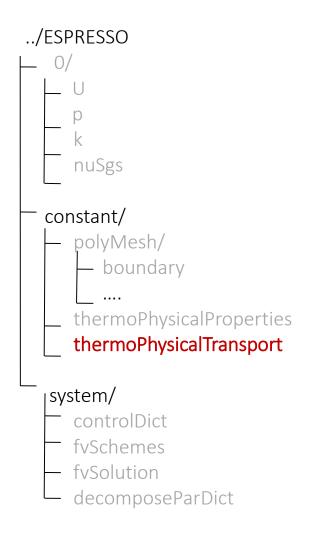


(Reynolds Averaged Navier-Stokes simulation)





cp -r \$FOAM TUTORIALS/fluid/cavity/constant/thermophysicalTransport constant/



```
RAS
{
    model eddyDiffusivity;

Prt 2;
}
```

The value of  $P_{r,T}=0.85$  is the default one, but for forced convection in liquid metals the value of  $P_{r,T}=2.0$  is recommended

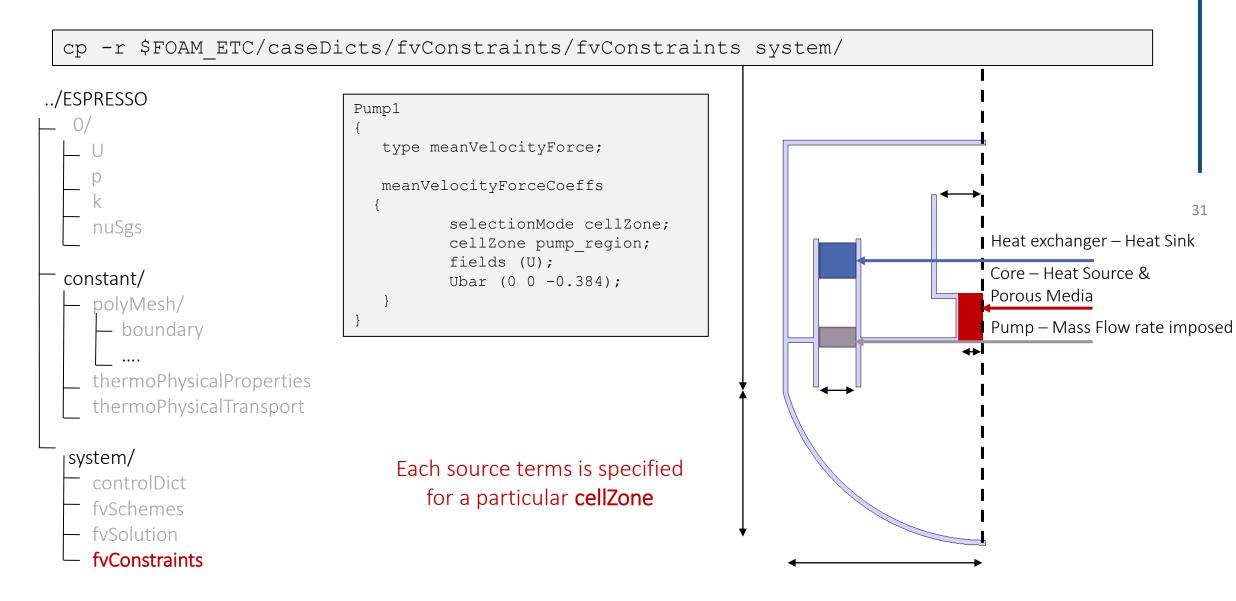
The **Reynolds' Analogy** is the only thermal turbulence model currently implemented in the released version of OpenFoam 9

$$q_{T,j} = -\alpha_T \frac{\partial T}{\partial x_i} \qquad \alpha_T = \frac{v_T}{P_{r,T}}$$

For liquid metal turbulent simulations, we implemented other thermal turbulence models (ThermophysicalTransportModels library): Kays Correlation, Manservisi  $k_{\theta} - \varepsilon_{\theta}$ , etc.



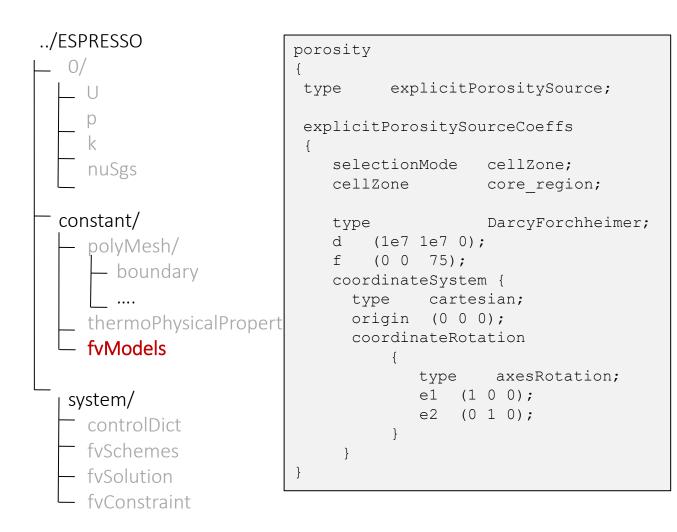
#### **SOURCE TERMS**





#### **Source Terms**

cp -r \$FOAM\_ETC/caseDicts/fvModels/fvModels constant/



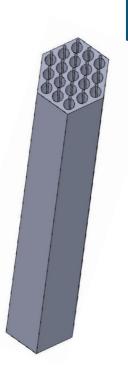
The flow trough the fuel assemblies is modelled as a **porous medium** 

Darcy-Forchheimer Law

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot \mathbf{\sigma} + \mathbf{S}_m$$

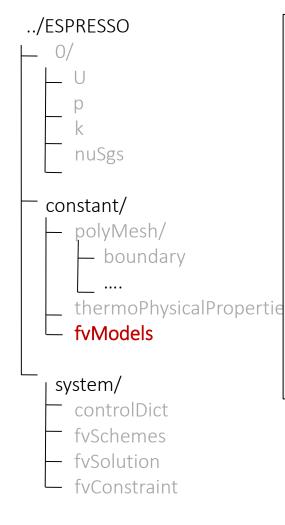
$$\mathbf{S}_m = -\left(\mu \mathbf{D} + \frac{1}{2}\rho \ tr(\mathbf{u} \cdot \mathbf{I})\mathbf{F}\right)\mathbf{u}$$

We must specify the coefficients **D** and **F** (directional dependent)

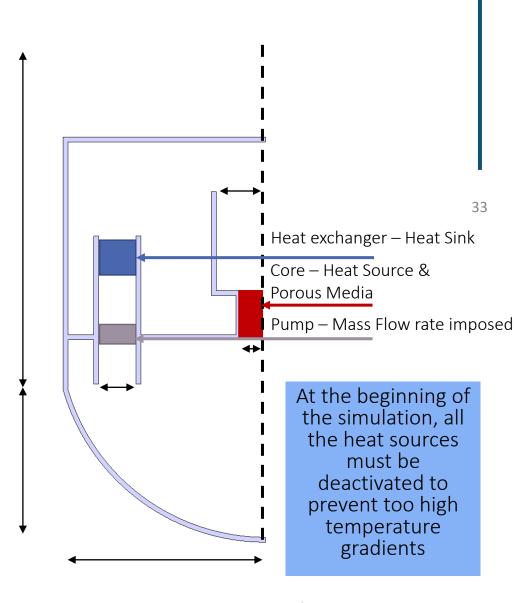




### **SOURCE TERMS**

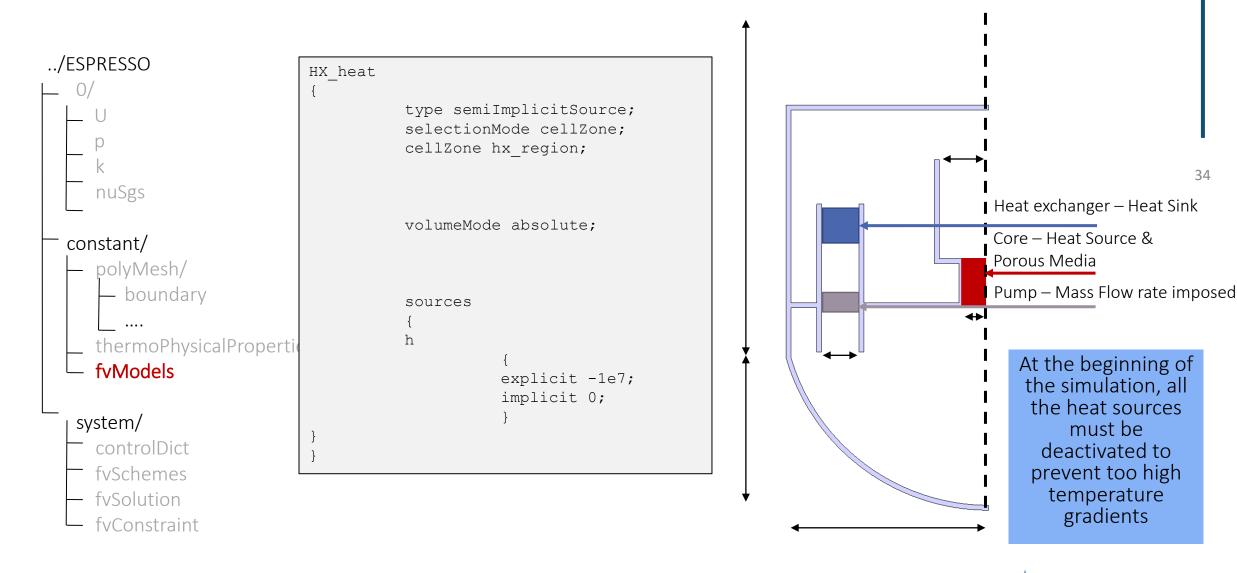


```
Core heat
          type semiImplicitSource;
          selectionMode cellZone;
          cellZone core region;
          volumeMode absolute;
          sources
                    explicit 1e7;
                    implicit 0;
```





### **SOURCE TERMS**





### **INITIAL CONDITIONS**

#### Initialization with constant values

```
../ESPRESSO
 constant/
    polyMesh/
     boundary
    thermoPhysicalProperties
    fvModels
  system/
    controlDict
    fvSchemes
    fvSolution
    fvConstraint
```

```
object
         alphat;
// *************
dimensions [1 -1 -1 0 0 0 0];
internalField uniform 0;
```

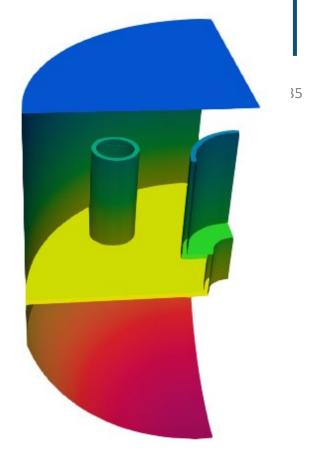
$$\alpha_t = 0.0$$
  $\nu_t = 0.0$   $k = 0.000375$ 

$$k = 0.000375$$

$$0.12 p = 1$$

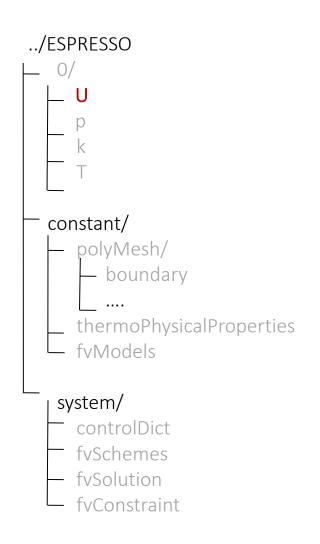
$$\omega = 0.12$$
  $p = 1 \cdot 10^5$   $\mathbf{u} = [0.0, 0.0, 0.0]$ 

$$p_{rgh} = 1 \cdot 10^5 \quad T = 493$$

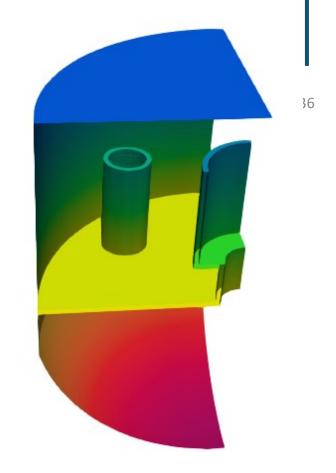




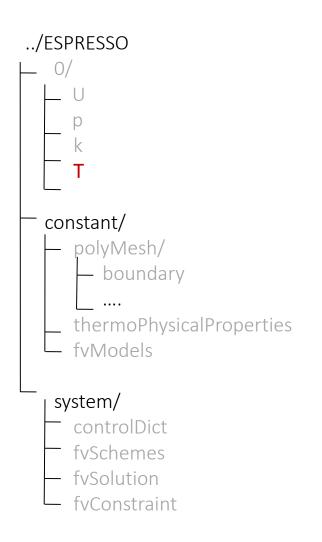
#### **BOUNDARY CONDITIONS**



U





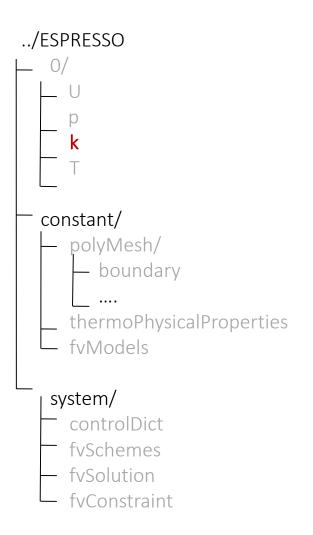


```
T
```

```
- fixed heat flux: supply q
boundaryField
                                                               - fixed heat transfer
                                                            coefficient: supply h and
"(diaph|core|acs|pump)"
                                                                       Ta
                                          zeroGradient;
                     type
vessel
                                          externalWallHeatFluxTemperature;
                     type
                                          flux;
                     mode
                                          uniform -150.0;
                     q
                                          $internalField;
                     value
top
                                          externalWallHeatFluxTemperature;
                     type
                     mode
                                                     coefficient;
                                                     constant 450.0;
                     Τа
                                                     uniform 10.0;
                     thicknessLayers
                                           (0.1);
                                                     (45);
                     kappaLayers
                                                     $internalField;
                     value
"symmetry.*"
                     type
                                                     symmetry;
```

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FOR FLUID DYNAMICS

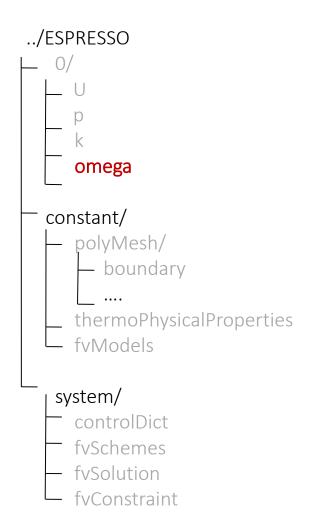
- fixed power: supply Q



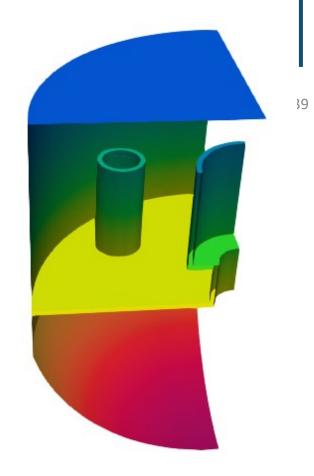
k







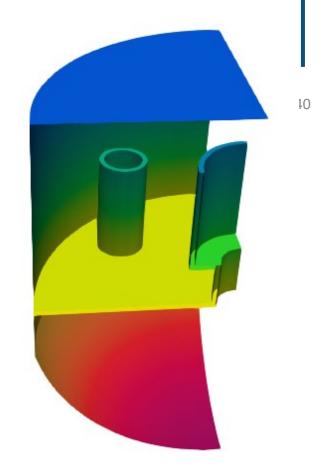
```
ω
```





## ../ESPRESSO omega constant/ polyMesh/ boundary thermoPhysicalProperties fvModels system/ controlDict fvSchemes fvSolution fvConstraint

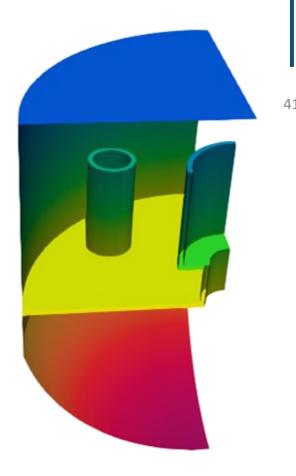
#### nut



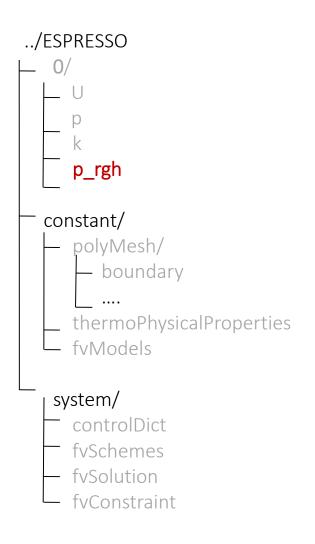


## ../ESPRESSO omega constant/ polyMesh/ boundary thermoPhysicalProperties fvModels system/ controlDict fvSchemes fvSolution fvConstraint

#### alphat



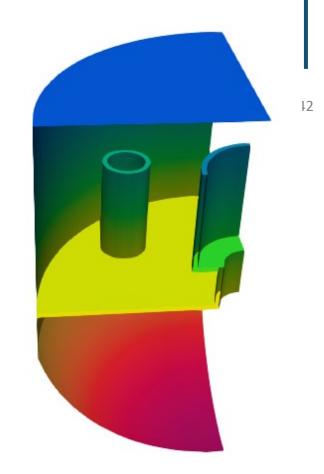




#### $p_{rgh}$

```
boundaryField
{
    "(top|diaph|core|acs|vessel|pump)"
    {
        type             fixedFluxPressure;
        value             $internalField;
    }

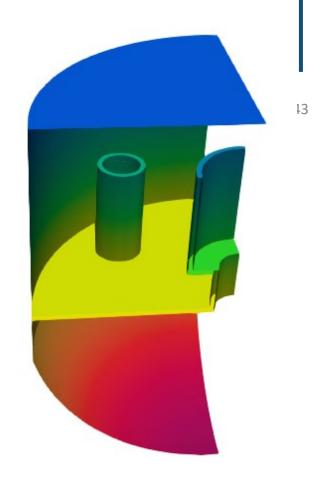
    "symmetry.*"
    {
        type             symmetry;
    }
}
```





```
../ESPRESSO
 constant/
    polyMesh/
     boundary
     thermoPhysicalProperties
    fvModels
  system/
    controlDict
    fvSchemes
    fvSolution
    fvConstraint
```

```
p
```





#### **SIMULATION CONTROLS**

```
../ESPRESSO
    nuSgs
 constant/
    polyMesh/
     boundary
     thermoPhysicalProperties
    fvModels
  system/
    controlDict
    fvSchemes
    fvSolution
     fvConstraint
```

```
application
                foamRun;
solver
                fluid;
startFrom
                startTime;
startTime
                0;
stopAt
                endTime;
endTime
                10000;
deltaT
                1;
writeControl
                timeStep;
writeInterval
                100;
purgeWrite
                2;
writeFormat
                ascii;
writePrecision 8;
writeCompression off;
timeFormat
                general;
timePrecision
runTimeModifiable true;
```

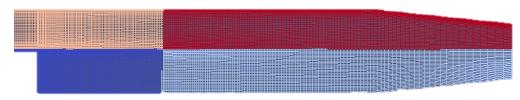


```
../ESPRESSO
 constant/
    polyMesh/
      boundary
     thermoPhysicalProperties
     fvModels
  system/
    controlDict
     fvSchemes
    fvSolution
    decomposeParDict
```

```
numberOfSubdomains 2;
                    scotch;
method
// method
                    hierarchical;
// method
                    simple;
// method
                    manual;
simpleCoeffs
                 (2 \ 1 \ 1);
    delta
                 0.001;
hierarchicalCoeffs
                 (2 \ 1 \ 1);
    n
    delta
                 0.001;
    order
                 xyz;
```

#### Decomposition methods:

- o **Simple**: split in equal parts along directions
- Hierarchical: same as simple, but with specified order of directions
- o Manual: each cell is assigned to a processor
- Scotch: minimizes the communication between processors







#### **RUNNING THE SOLVER**

In serial, run the case by typing on the terminal:

And visualize the output file evolution with:

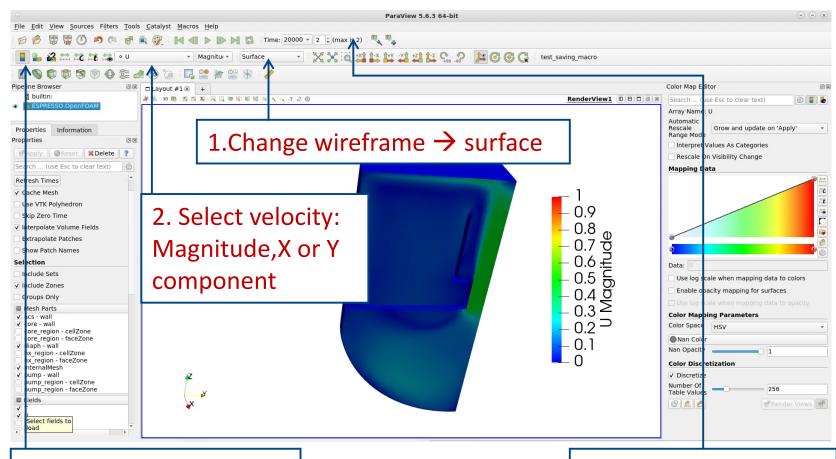
To run in parallel, you should first decompose the case (decomposeParDict specifies 2 processors)

Then you run the decomposed case by using:

should first run the first 100 iterations with inactive heat sources (by commenting the corresponding lines in the fvModels file). Then you active the heat sources and continue the run until reaching 10000 iterations



#### PARAFOAM — PLOT VELOCITY CONTOUR

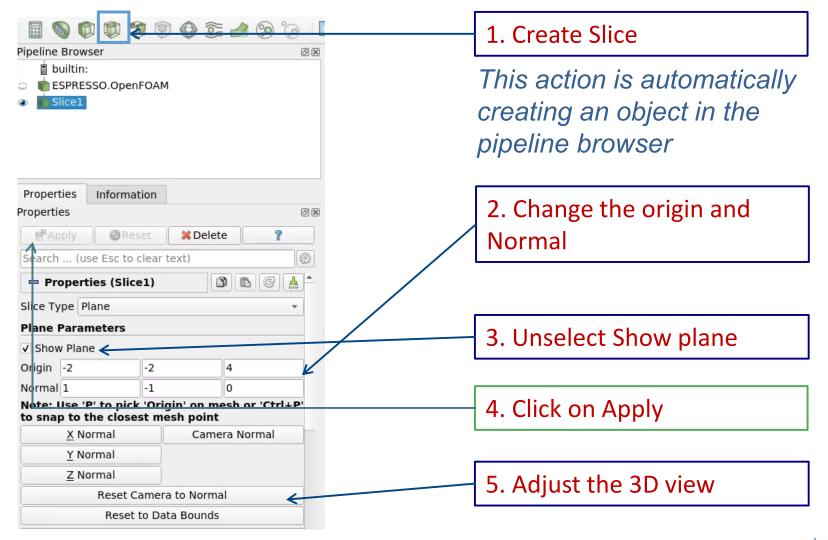


4.Toggle On Color legend

3. Select another time Ex: 1, t=10000



#### PARAFOAM – 2D SLICE

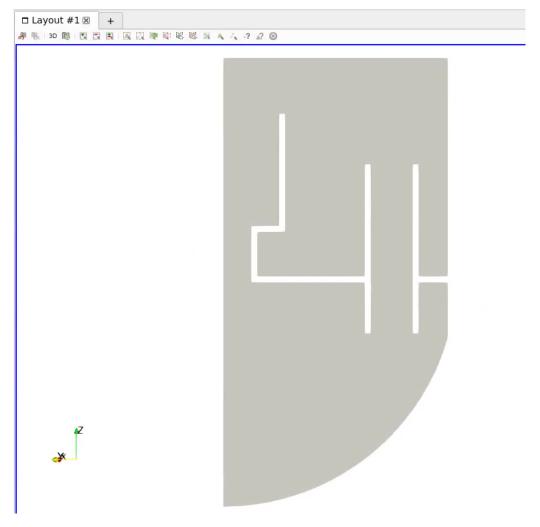


/19



#### PARAFOAM – 2D SLICE

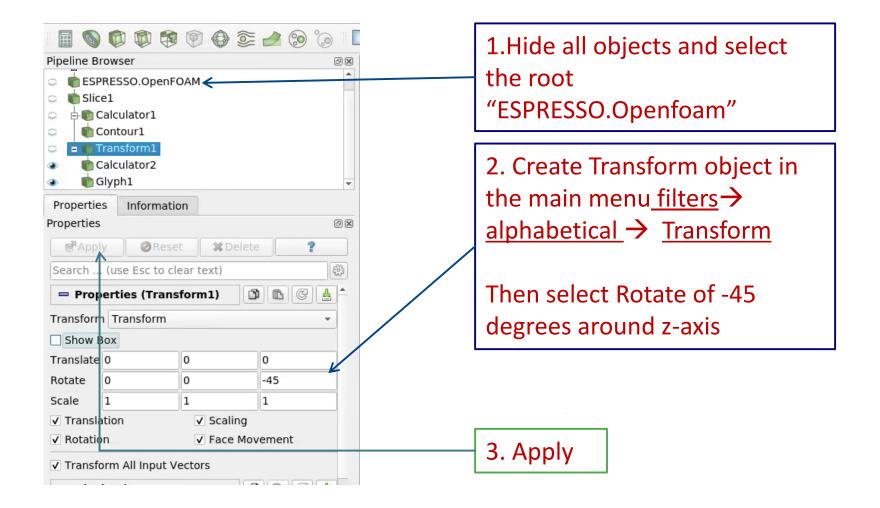




/10

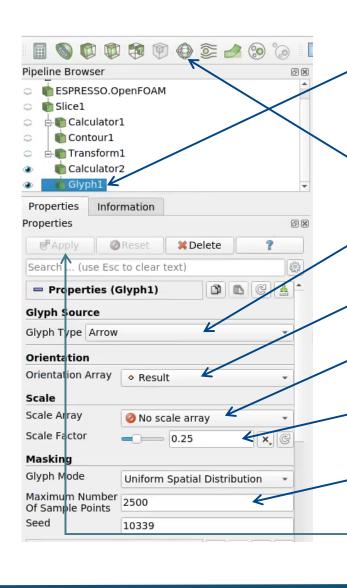


#### PARAFOAM — PLOT VECTORS





#### PARAFOAM — PLOT VECTORS



1. Create new field with the projected velocity on the slice with Calculator with the formula

U\_X\*iHat+U\_Z\*kHat+0\*jHat

2. Create a Gliph object

3. Select Arrow

4. Select the new field

Select "No scale array"

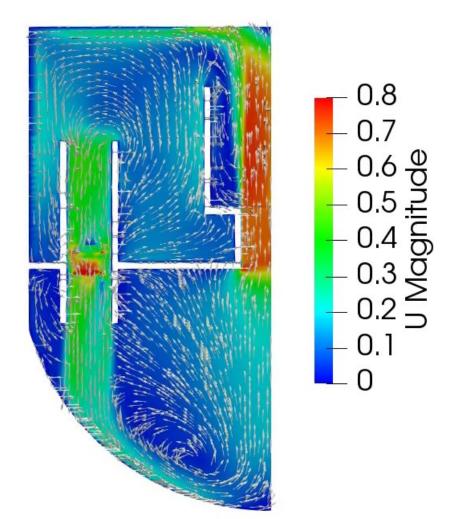
6. Change scale factor to 0.25

7. Change number of points

8. Apply



#### PARAFOAM — PLOT VECTORS







# Questions?

