

OpenFOAM

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1 **TODO**

- transport models
- [library up to openfoam 6](#)
- sponge (?)

2 Building

2.1 Pre-reqs

Setup environment

- DANE:

```
module unload intel-classic/2021.6.0-magic mvapich2/2.3.7  
module load gcc/11.2.1 openmpi/4.1.2  
check that cmake exists
```
- Campus Cluster:

```
module load cmake/3.26.3  
module unload gcc/11.2.0  
module load openmpi/.4.1.4-gcc-12.2.0  
src/OpenFOAM/db/Iostreams/hashes/: see link
```
- Local installation:

```
sudo apt install flex
```

openMPI

Install [openMPI](#)

Cantera

```
python3 -m pip install cantera
```

gmsh

```
cd /g/g92/<your-username>  
wget https://gmsh.info/bin/Linux/gmsh-4.13.1-Linux64.tgz  
tar zxv gmsh-4.13.1-Linux64.tgz  
export PATH="$PATH:/g/g92/<your-username>/gmsh-4.13.1-Linux64/bin"
```

2.2 openFOAM

- Build openFOAM:

```
wget -O - http://dl.openfoam.org/third-party/7 | tar -xz  
mv ThirdParty-7-version-7 ThirdParty-7  
wget -O - http://dl.openfoam.org/source/7 | tar -xz  
mv OpenFOAM-7-version-7 OpenFOAM-7  
source <path>/OpenFOAM-7/etc/bashrc  
./Allwmake <-j np>
```

- Add to .bashrc for future use (or as an alias):
source <path>/OpenFOAM-7/etc/bashrc

2.3 PATO

- Build PATO:
 wget https://github.com/nasa/pato/archive/refs/tags/3.1.tar.gz
 tar -zxvf 3.1.tar.gz
 export PATO_DIR=\$(pwd)/PATO/pato-3.1
 source <path>/OpenFOAM-7/etc/bashrc
 source \$PATO_DIR/bashrc
 cd \$PATO_DIR/src/thirdParty/mutation++
 See instruction in 2.4 for mutation++
 ln -s \$(pwd)/thirdparty/eigen/Eigen/ ./install/include
 cd \$PATO_DIR
 ./Allwmake
- Alias in .bashrc

2.4 Mutation++

If outside PATO:

```
git clone https://github.com/mutationpp/Mutationpp.git
```

Build Mutation:

```
cmake -DCMAKE_INSTALL_PREFIX:PATH=<path>/install  
make -j 4 install
```

If installing inside PATO, it is done.

Else, if stand-alone, add to .bashrc:

```
export MPP_DIRECTORY=<path>  
export MPP_DATA_DIRECTORY=$MPP_DIRECTORY/data  
export PATH=$MPP_DIRECTORY/install/bin:$PATH  
export LD_LIBRARY_PATH=$MPP_DIRECTORY/install/lib64:$LD_LIBRARY_PATH
```

Can check just in case:

```
checkmix air_11
```

2.5 TODO: (ignore this)

swak4Foam

[swak4Foam](#)

3 Environment configuration and running

3.1 Dane:

Before running OpenFOAM:

```
module unload intel-classic/2021.6.0-magic mvapich2/2.3.7
module load gcc/11.2.1 openmpi/4.1.2
source /g/g92/<your-username>/openFOAM/OpenFOAM-X/etc/bashrc
cd <path/to/the/case>
```

A whole bunch of configuration (i.e., case-dependent)

```
sh setFields.sh
```

Run with this (add to the queue system file):

```
mpirun -np 3 buoyantReactingFoam -parallel
```


4 Setup

4.1 Basic steps

Steps for running openFOAM simulations:

```
gmshToFoam mesh.msh
> update constant/boundary with wedge if axisymmetric
> update constant/boundary with wall may be necessary
create 0 folder with initial and boundary conditions
> setFields -region flow for non-uniform IC
splitMeshRegions -cellZones -overwrite
> decomposePar -allRegions if running in parallel
```

4.2 Mesh generation

```
gmshToFoam mesh.msh
```

Quads that touch the boundaries with a single node gives trouble and make a new “boundary” (defaultFaces). This may lead to issues on the simulation.

So far, the best I could do was to run mixed meshes, with quads/hexes on well behaved regions (transfinite) and triangles everywhere else.

4.2.1 blockMesh

```
paraFoam -block
```

4.2.2 axisymmetry

Using `writeFormat binary;` in `controlDict` helps depending on openFOAM version

When meshing, add two separate boundaries: front and back

Add wedge as BC for all variables in front and back

in `polyMesh/boundary`, modify from patch to wedge where necessary

[link](#)

PS: I see non-zero Z-velocity on the wedge faces.

4.3 Initial conditions

Units: [kg m s K mol A cd]

In an incompressible solver, N-S equation is divided by a uniform density ρ . This causes (1) the dimension of pressure of [0 2 -2 0 0 0 0] and (2) the kinematic viscosity ν in Laplacian

term. In an incompressible solver, pressure is assumed to be relative. The atmosphere will be 0 usually.

In a compressible solver, N-S equation is not divided by density. So, the dimension of pressure is [1 -1 -2 0 0 0 0] as usual. The dynamic viscosity μ appears in Laplacian term. In a compressible solver, the absolute pressure must be provided in p file because the value of pressure will be used to calculate other physical properties. The atmosphere will be O(1e5) usually.

4.4 Boundary conditions

4.4.1 Variable BCs

custom boundary conditions:

[link](#)

[link](#)

4.4.2 Pressure BC + gravity

Walls :: use `fixedFluxPressure` or `fixedFluxExtrapolatedPressure` (instead of `zeroGradient`) or it will give issues.

Outlet :: To satisfy the characteristics and avoid under/over-specification, gotta prescribe U and T (potentially Y) when there is reversed flow in the outlet; pressure is extrapolated by using a zero-gradient BC. For outflow, the internal properties are extrapolated but pressure is prescribed.

See [inletOutlet](#)

See [fixedMeanOutletInlet](#)

Far-field :: Potentially, using the non-reflective `waveTransmissive` may help suppress some weird(-but-small) behavior (which may be waves reflection). This would be useful in the sides/bottom, but **may not** be robust in the outlet. Additionally, the extra source terms (damping and isentropic) can be used in the bottom and right to damp velocity fluctuations and the initial vortex for increased robustness.

```
farfield
{
    type            waveTransmissive;
    gamma           1.4;
    fieldInf        101325.0;
    lInf            0.1;
    value           uniform 101325.0;
}
```

4.4.3 time-dependent BCs

Linear interpolation from t1 to t2

```
inlet
{
    type uniformFixedValue;
    uniformValue table
    (
        (0.0 (0 0.02 0)) // t1 (Ux_1 Uy_1 Uz_1)
        (2.5 (0 0.10 0)) // t2 (Ux_2 Uy_2 Uz_2)
    );
}
```

4.4.4 Robin BC

<https://www.cfd-online.com/Forums/openfoam/219113-how-access-boundary-conditions-species-react>

https://foamingtime2.wordpress.com/wp-content/uploads/2017/07/convection-bc_1.pdf

<https://www.cfd-online.com/Forums/openfoam-pre-processing/225340-mixed-boundary-condition.htm>

<https://www.cfd-online.com/Forums/openfoam/238186-implementation-robin-boundary-condition-op>

<https://www.cfd-online.com/Forums/openfoam-solving/69464-robin-b-c-mixed-b-c.html>

<https://www.cfd-online.com/Forums/openfoam-solving/83194-mixed-boundary-condition.html>

<https://www.cfd-online.com/Forums/openfoam-pre-processing/74593-mixed-bc-heat-transfer-laplacian>

4.4.5 change of BCs

[change BC](#)

foamGetDict

4.5 Chemistry

4.5.1 mechanisms

need yaml2ck from Cantera

```
$>> chemkinToFoam uiuc_20sp.dat thermo-uiuc_20sp.dat ...
```

```
transportProperties ../constant/reactions ...
```

```
../constant/thermo.compressibleGas
```

**This may still present issues with chemkin format (e.g., spacing)
and it may be necessary to fix by hand**

4.5.2 possible mechanism simplification

see Sandia flame example in reactingFoam > RAS

4.6 Radiation

system/flow/fvOptions

```
radiation
{
    type            radiation;
    libs            ("libradiationModels.so");
}
```

4.6.1 viewFactor

faceAgglomerate -region flow

viewFactorsGen -region flow

```
flow_to_solidLeft
{
    type            greyDiffusiveRadiationViewFactor;
    qro             uniform 0;
    emissivityMode  solidRadiation;
    value           uniform 0;
    emissivity      uniform 1.0; // Emissivity of the wall
}
```

4.6.2 P1 model

constant file

fvSolution

G file

[Species coefficients](#)

https://boyaowang.github.io/boyaowang-OpenFOAM.github.io/2020/09/16/P1_model/

<https://www.afs.enea.it/project/neptunius/docs/fluent/html/th/node112.htm>

<https://www.cfd-online.com/Forums/openfoam-solving/219601-adding-radiations-chtmultiregionsimple.html>

<https://www.cfd-online.com/Forums/openfoam/78052-boundary-condition-p1-marshakradiation.html>

<https://www.cfd-online.com/Forums/openfoam-programming-development/135502-understanding-ma.html>

<https://www.cfd-online.com/Forums/openfoam/183686-radiation-boundary-conditions-flow-through-b.html>

<https://www.cfd-online.com/Forums/openfoam-solving/240250-p1-model-no-participating-media-heat.html>

<https://www.cfd-online.com/Forums/openfoam-solving/216879-radiation-models-general-p1-implement.html>

4.7 System

4.7.1 fvSchemes

[fvSchemes](#)

4.7.2 fvSolution

PISO - PIMPLE - SIMPLE

convergence:

In some case, if tolerances are too big, the solution may look a bit off, with pressure oscillations and spurious velocity fields

Also, it may happen that the flow won't evolve if it is "converged" due to a high tolerance, with 0 iterations in the system solvers

In both cases, just modify the `fvSolution` files to have smaller tolerances.

PIMPLE:

Looks like 2 (or more) `nCorrectors` loops are key to not screw up pressure-velocity coupling. Additionally, `nNonOrthogonalCorrectors` may help in regions where the mesh is not properly orthogonal. Issues in this regard were observed when solving a finer mesh. Previously, on a coarser mesh, `nCorrectors = 1` and `nNonOrthogonalCorrectors = 0` were used just fine.

4.8 fvOptions

```
limitT
{
    type            limitTemperature;
    active          yes;

    selectionMode   all;
    min             200;
    max             2400;
}
```

[verticalDamping.C](#)

```
verticalDamping
{
    type            verticalDamping;

    selectionMode   all;
```

```

origin          (0 0.35 0); // x y z
direction       (0 1 0);

scale // still unclear what it exactly means
{
    type          halfCosineRamp;
    start         0;
    duration      .05;
}

lambda          [0 0 -1 0 0 0 0] 1000; // Damping coefficient

timeStart       0;
duration        5; // time

writeForceFields true;
}

```

4.9 controlDict

```

/*application    rhoPimpleFoam;*/
startFrom        latestTime;
/*startFrom      startTime;*/
startTime        0;
stopAt           endTime;
endTime          10;
deltaT           5e-5;
writeControl     adjustableRunTime;
writeInterval    0.2;
/*writeControl   timeStep;*/
/*writeInterval  50;*/
purgeWrite       0;
writeFormat      ascii;
/*writeFormat    binary;*/
writePrecision   9;
writeCompression off;
timeFormat       fixed;
timePrecision    6;
runTimeModifiable true;
adjustTimeStep   yes;
maxCo            5.0;

```

4.9.1 functions

```

functions
{

```

```

    ...
}

gradient
{
    type            grad;
    libs            ("libfieldFunctionObjects.so");
    field           T;

    // Optional (inherited) entries
    writePrecision  8;
    writeToFile     true;
    region          flow;
    writeControl    writeTime;
}

wallHeatFlux
{
    type            wallHeatFlux;
    libs            ("libfieldFunctionObjects.so");
    patches         ("solid_to_flow");
    qr              qr;
    writePrecision  8;
    writeToFile     true;
    region          flow;
    writeControl    writeTime;
}

```

PS: may have to modify the constant/boundary with wall patch.
 If coupled domains, using mappedWall, it seems to work.

```

probes
{
    type            probes;
    functionObjectLibs ("libsampling.so");
    writeControl    timeStep;
    writeInterval    5;
    region          flow;
    fields          (T);
    probeLocations (
        ( 0.0001 0.105 0.0)
        ...
    );
}

```

```

patchProbes
{
    type                patchProbes;
    functionObjectLibs ("libsampling.so");

    // Patches to sample (wildcards allowed)
    patchName            wall;

    // Name of the directory for probe data
    //name                patchProbes;

    writeControl          writeTime;
    //writeControl        timeStep;
    //writeInterval        5;

    //region              flow;
    fields                (wallHeatFlux);

    // Locations to probe. These get snapped onto the nearest point
    // on the selected patches
    probeLocations (
        ( 0.0 0.11 0.0)
    );
}

```



```

line
{
    type                sets;
    functionObjectLibs  ("libsampling.so");
    enabled              true;
    writeControl        timeStep;
    writeInterval       10;
    region              flow;
    interpolationScheme  cellPoint;
    setFormat           raw;
    sets
    (
        line1
        {
            type lineUniform;
            axis distance;
            start ( 1e-5 0.105 0 );
            end   ( 0.05 0.105 0 );
            nPoints 10;
        }
    );
    fields ( p T );
}

volAverage
{
    libs                ("libfieldFunctionObjects.so");
    type                volFieldValue;
    operation           volAverage;
    region              porousMat;
    fields              (Ta tau rho_s[1] rho_s[2]);
    writeFields         false;
    writeControl        timeStep;
    writeInterval       5;
}

volIntegrate
{
    libs                ("libfieldFunctionObjects.so");
    type                volFieldValue;
    operation           volIntegrate;
    region              porousMat;
    fields              (rho_s[1] rho_s[2]);
    writeFields         false;
    writeControl        timeStep;
    writeInterval       5;
}

```

4.10 setFields

Non-uniform IC, specified in `setFieldDict` inside `system/<region>`

```
setFields
```

```
setFields -region fluid
```

4.11 parallel

Define `system/decomposeParDict`

```
numberOfSubdomains <n>;  
method              scotch;
```

to partition the mesh and IC, run:

```
decomposePar <-allRegions>
```

run openFOAM with mpi:

```
mpirun -np <n> <foamSolver> -parallel
```

Combine results with

```
reconstructPar <-allRegions>
```

where additional options can be used, such as:

`-latestTime` :: select the latest time

`-newTimes` :: only reconstruct new times (i.e. that do not exist already)

Depending on the version (7 vs 10), each sub-domain (fluid, wall, porous material etc) will need its own `decomposeParDict` in `system`

To modify parameters in a parallel simulation, may be easier to recombine the latest solution file; modify then re-decompose

5 Solvers

5.1 chtMultiRegionFoam

Put all BCs in “0/” (including the wall as fluid_to_solid and solid_to_fluid)

`splitMeshRegions -overwrite` plus:

`-cellZones` :: the usual, where the domains will be split

`-cellZonesOnly` :: in case one of the domains is disjoint, i.e., no shared nodes. Otherwise, it will be split.

May need to copy a `regionProperties` to constant

6 postProcess

[postProcessing](#)

```
postProcess -func "grad(T) "  
postProcess -func writeCellVolumes -region porousMat  
postProcess -list
```

6.1 foamToVTK

Useful in case paraFoam misbehaves (aka Segmentation Fault)

If parallel simulation, first run `reconstructPar`.

```
foamToVTK  
-region flow
```

Older versions :: `-region <fluid> then -region <solid>`

Newer versions :: `-allRegions`

```
-nearCellValue  
-fields '(p p_rgh T U CO2 H2O CO N2)'
```

Specify initial time for conversion :: `-time 5.0:`

6.2 solver-dependent

7 Formulation

7.1 Pressure

For buoyant solvers, pressure is computed with

$$\rho gh + P' = P \quad (7.1)$$

$$-\nabla(\rho gh) - \nabla P' = -\nabla P \quad (7.2)$$

$$-\cancel{\rho h \nabla g} - \rho g \nabla h - gh \nabla \rho - \nabla P' = -\nabla P \quad (7.3)$$

$$-\rho g - gh \nabla \rho - \nabla P' = -\nabla P \quad (7.4)$$

where $\nabla h = \mathbf{I}$.

[link](#)

[link](#)

[link](#)

7.2 Energy equation

$$C_P(T) = \sum_i c_i T^i = \frac{\partial e}{\partial T} \quad (7.5)$$

$$\kappa \nabla T = \kappa \frac{C_P}{C_P} \nabla T \quad (7.6)$$

$$\kappa \nabla T = \frac{\kappa}{C_P} \frac{\partial e}{\partial T} \nabla T \quad (7.7)$$

$$\kappa \nabla T = \frac{\kappa}{C_P} \nabla e \quad (7.8)$$

$$\kappa \nabla T = \alpha_{\text{eff}} \nabla e \quad \text{where} \quad \alpha_{\text{eff}} = \kappa / c_p \quad (7.9)$$

7.3 Species equation

See `openFOAM-10` `unityLewisFourier.H`

$$Le = \frac{\alpha}{D} \quad (7.10)$$

$$Le = \frac{\kappa}{\rho C_p} \frac{1}{D} = \frac{\alpha_{\text{eff}}}{\rho D} \quad (7.11)$$

```

virtual tmp<scalarField> DEff
(
    const volScalarField& Yi,
    const label patchi
) const
{
    return
        this->thermo().kappa().boundaryField()[patchi]
        /this->thermo().Cp().boundaryField()[patchi];
}

```

7.4 Transport model

The individual species viscosity is given by

$$\mu_i = A_{s,i} \frac{\sqrt{T}}{1 + \frac{T_{s,i}}{T}} \quad (7.12)$$

with mixture value given by weighted sum of individual viscosities by the respective mass fractions:

$$\mu = \sum_i Y_i \mu_i \quad (7.13)$$

The thermal conductivity is given by the Eucken correlation as

$$\kappa = \mu c_v \left(1.32 + 1.77 \frac{R}{c_v} \right) \quad (7.14)$$

Species diffusivity based on unitary **Lewis** or **Schmidt** number (may depend on openFOAM version)

[transport model](#)