A modified version of the reactingFoam tutorial for LES

PhD course in CFD with OpenSource software, december 2009
Outline

- change the reactingFoam solver from RAS to LES
- download the original tutorial from the openWiki:
- change the chemkin reaction mechanism
- run

Creating a new solver

This tutorial works on version 1.5.x, thus we have to source it

```
export FOAM_INST_DIR=/chalmers/sw/unsup/OpenFOAM;
. /chalmers/sw/unsup/OpenFOAM/OpenFOAM-1.5.x/etc/bashrc
```

```
cp -r $FOAM_APP/solvers/combustion/reactingFoam/ reactingFoamLES
cd reactingFoamLES
```

Then we copy some files from the course repository that will be necessary in the following:

```
cp ~/pieroRepository/tutFiles.tar.gz .
tar xzf tutFiles.tar.gz
rm tutFiles.tar.gz
```

Modifying the source file

In particular we change the line

```
#include "compressible/RASModel/RASModel.H"
```

into

```
#include "compressible/LESModel/LESModel.H"
```

and we add the line: (all the LES solvers, i.e. *coodles* have this line in the source file)

```
#define divDevRhoReff divDevRhoBeff
```

Modifying creatFields.H

again in `createFields.H` we substitute RAS with LES in lines 61-63 and we also comment lines 72-74:

```
Info << "Creating turbulence model.\n" << nl;
autoPtr<compressible::RASModel> turbulence
(
    compressible::RASModel::New
    (
        rho,
        U,
        phi,
        thermo()
    )
);

Info<< "Creating field DpDt\n" << endl;
volScalarField DpDt =
fvc::DDt(surfaceScalarField("phiU", phi/fvc::interpolate(rho)), p);
```

```
Info << "Creating turbulence model.\n" << nl;
autoPtr<compressible::LESModel> turbulence
(
    compressible::LESModel::New
    (
        rho,
        U,
        phi,
        thermo()
    )

//Info<< "Creating field DpDt\n" << endl;
//volScalarField DpDt =
//    fvc::DDt(surfaceScalarField("phiU", phi/fvc::interpolate(rho)), p);
```

Compiling

We then change the file `Make/files` into:

```
reactingFoamLES.C

EXE = $(FOAM_USER_APPBIN)/reactingFoamLES
```

In the file `Make/files` again we change the RAS libraries with the LES ones, and add `-I$(LIB_SRC)/turbulenceModels/LES/LESdeltas/lnInclude\`

```
EXE_INC = \
    -I../XiFoam \
    -I$(LIB_SRC)/finiteVolume/lnInclude \
    -I$(LIB_SRC)/turbulenceModels/RAS \
    -I$(LIB_SRC)/thermophysicalModels/specie/lnInclude \
 |
 |
EXE_LIBS = \
    -lcompressibleRASModels \
    -lcombustionThermophysicalModels\
```

```
EXE_INC = \
    -I../XiFoam \
    -I$(LIB_SRC)/finiteVolume/lnInclude \
    -I$(LIB_SRC)/turbulenceModels/LES \
    -I$(LIB_SRC)/turbulenceModels/LES/LESdeltas/lnInclude \
|
|
EXE_LIBS = \
    -lcompressibleLESModels \
    -lcombustionThermophysicalModels \
```

We are now ready to compile:

```
wclean
rm -r Make/linuxGccDP*
wmake
```

Set up the case

A tutorial file for *reactingFoam* is found on the OpenWiki
We can download directly from the webpage

```
http://openfoamwiki.net/index.php/Tut_reactingFoam_firstTutorial
```

or we get it typing directly in the shell:

```
wget http://openfoamwiki.net/images/b/b6/ReactingFoamCase.tar.gz
```

Once downloaded we extract the files in the folder ReactingFoamCase:

```
mkdir ReactingFoamCase
mv ReactingFoamCase.tar.gz ReactingFoamCase
cd ReactingFoamCase
tar xzf ReactingFoamCase.tar.gz
rm ReactingFoamCase.tar.gz
```

chemkin folder

The files **inp** contain the chemical reaction mechanisms, with the chemical elements, the species involved and all the chemical reactions in the mechanism. For example the file *chem.inp* contains a simple one step reaction mechanism for heptane (C7H16):

```
ELEMENTS
 H   O    C N
END
SPECIE
C7H16 O2 N2 CO2 H2O
END
REACTIONS
 C7H16 + 11O2            => 7CO2 + 8H2O        5.00E+8  0.0   15780.0! 1
        FORD    / C7H16 0.25 /
        FORD    / O2 1.5 /
END
```

chemkin folder

The file therm.dat instead contains for each species coefficients to compute heat capacity, hentalpy, enthropy, heat of reactions. For example:

```
THERMO ALL
   200.000  1000.000  5000.000
(CH2O)3            70590C   3H   6O   3     G  0200.00   4000.00  1500.00      1
 0.01913678E+03 0.08578044E-01-0.08882060E-05-0.03574819E-08 0.06605143E-12    2
-0.06560876E+06-0.08432507E+03-0.04662286E+02 0.06091547E+00-0.04710536E-03    3
 0.01968843E-06-0.03563271E-10-0.05665404E+06 0.04525265E+03                   4
(CH3)2SICH2        61991H   8C   3SI  1     G  0200.00   2500.00  1500.00      1
 0.01547852E+03 0.01065700E+00-0.01234345E-05-0.01293352E-07 0.02528715E-11    2
-0.06693076E+04-0.05358884E+03 0.02027522E+02 0.04408673E+00-0.03370024E-03    3
 0.01484466E-06-0.02830898E-10 0.03931454E+05 0.01815821E+03                   4
AL                 62987AL  1               G  0200.00   5000.00  0600.00      1
 0.02559589E+02-0.01063224E-02 0.07202828E-06-0.02121105E-09 0.02289429E-13    2
 0.03890214E+06 0.05234522E+02 0.02736825E+02-0.05912374E-02-0.04033938E-05    3
 0.02322343E-07-0.01705599E-10 0.03886795E+06 0.04363880E+02                   4
```

The chemkin directory should be contained in *constant*:

```
mv chemkin/ constant/
```

constant folder

In the `constant/thermophysicalProperties` file we change the path of the chemical files:

```
/* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * */

thermoType hMixtureThermo<reactingMixture>;

CHEMKINFile                  "/cluster/samples/reactingFoam/chemkin/chem.inp";
CHEMKINThermoFile            "/cluster/samples/reactingFoam/chemkin/therm.dat";

inertSpecie                  N2;

becomes  -------->

/* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * */

thermoType hMixtureThermo<reactingMixture>;

CHEMKINFile                  "chemkin/chem.inp";
CHEMKINThermoFile            "chemkin/therm.dat";

inertSpecie                  N2;
```

constant folder

From the tutFiles directory we copy the *chemistryProperties* file

```
cp ../reactingFoamLES/tutFiles/chemistryProperties constant/
```

where the sequential solver is selected:

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

chemistry               on;

turbulentReaction off;
Cmix                Cmix [ 0 0 0 0 0 0 0 ] 1.0 ;

//chemistrySolver         ODE;
//chemistrySolver       EulerImplicit;
chemistrySolver       sequential;

initialChemicalTimeStep     1.0e-8;
```

constant folder

We also need a file for the LES properties, we take it from a LES tutorial, for example *coodles*:

```
cp /chalmers/sw/unsup/OpenFOAM/OpenFOAM-1.5.x/tutorials/coodles \
/pitzDaily/constant/LESProperties constant/
```

And we choose the Smagorinsky for the turbulence model:

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

LESModel            Smagorinsky;

printCoeffs         off;

delta               cubeRootVol;
```

system folder

In the file `system/controlDict` file we change the name of the application to `reactingLESFoam`

0/ directory and boundary conditions

We remove the latest directory, and we recall that the Smagorinsky model needs a muSgs file in the *0/* directory. The right dimensions should be assigned to the turbulent viscosity:

```
rm -r 0.055/
cp 0/k 0/muSgs
```

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
dimensions          [ 1 -1 -1 0 0 0 0 ];

internalField       uniform 0.0;

boundaryField
{
    inlet
    {
        type            fixedValue;
        value uniform 0.0;
    }
    lowerInlet
    {
        type            fixedValue;
        value uniform 0.0;
    }

    outlet
    {
        type            zeroGradient;
    }

    upperWall
    {
        type            zeroGradient;
    }
```

We are now ready to run:

```
reactingFoamLES > log
```

Use another mechanism

One might want to simulate different fuels or use a more detailed mechanism

```
cp ../reactingFoamLES/tutFiles/WD2steps.inp constant/chemkin/
```

```
ELEMENTS
C H O N
END
SPECIE
CH4 O2 CO H2O CO2 N2
END
REACTIONS
 CH4  +  1.5O2  =>  CO + 2H2O          2.80E+09       0.0     48400.
    FORD /CH4 -0.3/
    FORD /O2 1.3/
 CO2 => CO + 0.5O2                     5.00E+08       0.0     40000.
    FORD /CO2 1.0 /
 CO + H2O + 0.5O2 => CO2 + H2O         3.98E+14       0.0     40000.
    FORD /CO  1.0 /
    FORD /H2O 0.5 /
    FORD /O2  0.25/
END
```

```
cp 0/C7H16 0/CH4
```

Accordingly the *constant*/*thermophysicalProperties* file should be updated:

```
/* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * */
thermoType hMixtureThermo<reactingMixture>;

//CHEMKINFile                  "chemkin/chem.inp";
CHEMKINFile                  "chemkin/WD2steps.inp";
CHEMKINThermoFile            "chemkin/therm.dat";
```