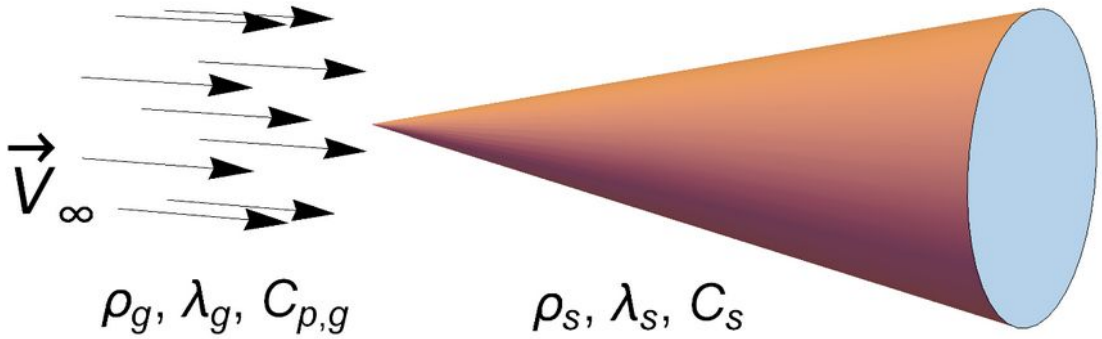
Implementation of the solver for coupled heat transfer in gas and solid

Instructors:
1) I. Marchevsky, Ph.D., Assoc.prof.
2) M. Kraposhin, Ph.D., Senior Researcher

Contents

Problem description

- Mach number – 0 < Ma < 5
- EoS – perfect gas
- Viscous flow of Newtonian media
- Transient heat transfer in solid (Fourier law)



Governing equations

- Perfect gas

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\vec{U}\rho) = 0, \quad \frac{\partial (\rho U)}{\partial t} + \nabla \cdot (\vec{U}\rho\vec{U}) = \nabla \cdot \hat{\Pi}, \quad \frac{\partial (\rho e)}{\partial t} + \nabla \cdot (\vec{U}\rho e) = -\nabla \cdot \vec{q} + \nabla \cdot (\hat{\Pi} \cdot \vec{U})$$

$$\hat{\Pi} = \mu\left(\nabla\vec{U} + \nabla\vec{U}^T\right) - \frac{2}{3}\hat{I}\mu\nabla \cdot \vec{U} - \hat{I}p, \qquad q = -\lambda\nabla T, \qquad p = \rho\frac{R}{M}T.$$

- Solid

$$\rho C\frac{\partial T}{\partial t} - \nabla \cdot (\lambda\nabla T) = 0.$$

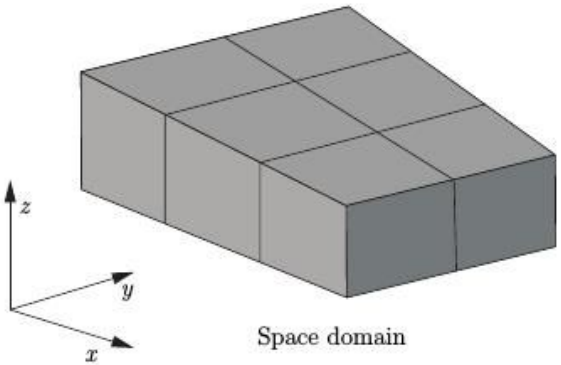
- Ideal heat contact

$$-(\lambda\nabla T)_{solid} \cdot n = -(\lambda\nabla T)_{fluid} \cdot n,$$

$$T_{solid} = T_{fluid}.$$

Numerical model

- Space & time discretization
  - Finite Volume Method – space and time divided on non-intersecting cells (intervals)



- Numerical schemes
  - Mean theorem + Gauss theorem

$$\int_V \nabla * \phi = \oint_{\partial V} \phi * dS$$

- Time integration algorithm
  - Operator-splitting methods like PISO or PIMPLE

$$\underset{\rightarrow}{p} = \underset{\rightarrow}{p}^* + \underset{\rightarrow}{p}'$$

$$\underset{\rightarrow}{U} = U^* + U'$$

$$U' \sim -\nabla p'$$

Models coupling

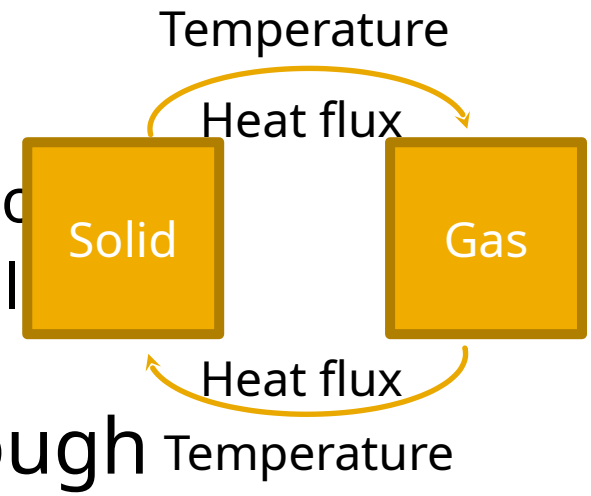
- Single matrix
  - Single equation of energy for both gas & solid.
  - Stable and robust, but hard to implement and use.

- Multiple domains, iterative coupling
  - Easy to work with complex geometries, performance degradation*).
  - Needs data interpolation on the interface.

*) Not very important when using operator splitting methods like PISO

Implementation in OpenFOAM

- Current implementation in OpenFOAM – **chtMultiRegionFoam**:
  - Iterative solution of energy balance between several solid and fluid regio
  - Uses outer **PIMPLE** loop and special B.C. for coupling between domains.



- List of domains managed through the **regionProperties** dictionary.
- Connection between regions established via boundary conditions for temperature.
- Main limitation – subsonic speeds of fluid (Ma<1).
- OpenFOAM version: 2112

Designing new solver

- **PISO**/**SIMPLE**/**PIMPLE** are known to be oscillatory at high speeds
  - we need different method for flows with Ma > 1.
- **rhoCentralFoam** was designed for flows with Ma > 1.
  - it is explicit , not efficient when Ma < 1.
- Solution – hybrid approach
  - Combine pimpleCentralFoam and chtMultiRegionFoam
- For the most general implementation, see

https://github.com/TonkomoLLC/hybridCentralSolvers

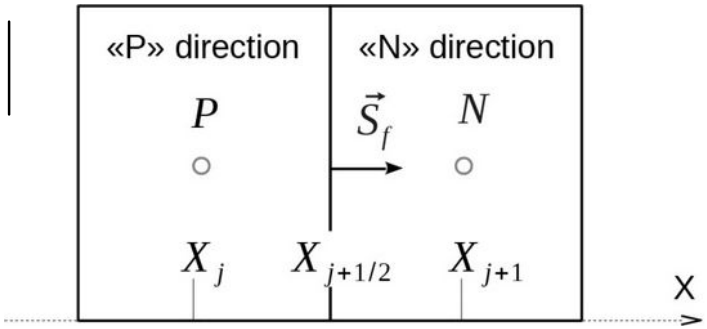
pimpleCentralFoam

- Implicit KT/KNP fluxes for advection
- PIMPLE algorithm for p - U - T coupling

$$\frac{\partial \rho\beta}{\partial t} + \nabla \cdot \left(\vec{U}\rho\beta\right) = \nabla \cdot D_\beta \nabla\beta$$

$$\frac{\rho^n\beta^n - \rho^o\beta^o}{\Delta t} + \frac{1}{V}\sum_f \left(\varphi_f^P + \left(1 - \kappa_f\right)\varphi_f^N\right)\beta_f^P + \frac{1}{V}\sum_f \kappa_f \varphi_f^N \beta_f^N =$$

$$= \frac{1}{V}\sum_f D_{\beta,f} \frac{\partial\beta}{\partial n_f}\left|\vec{S}_f\right|$$

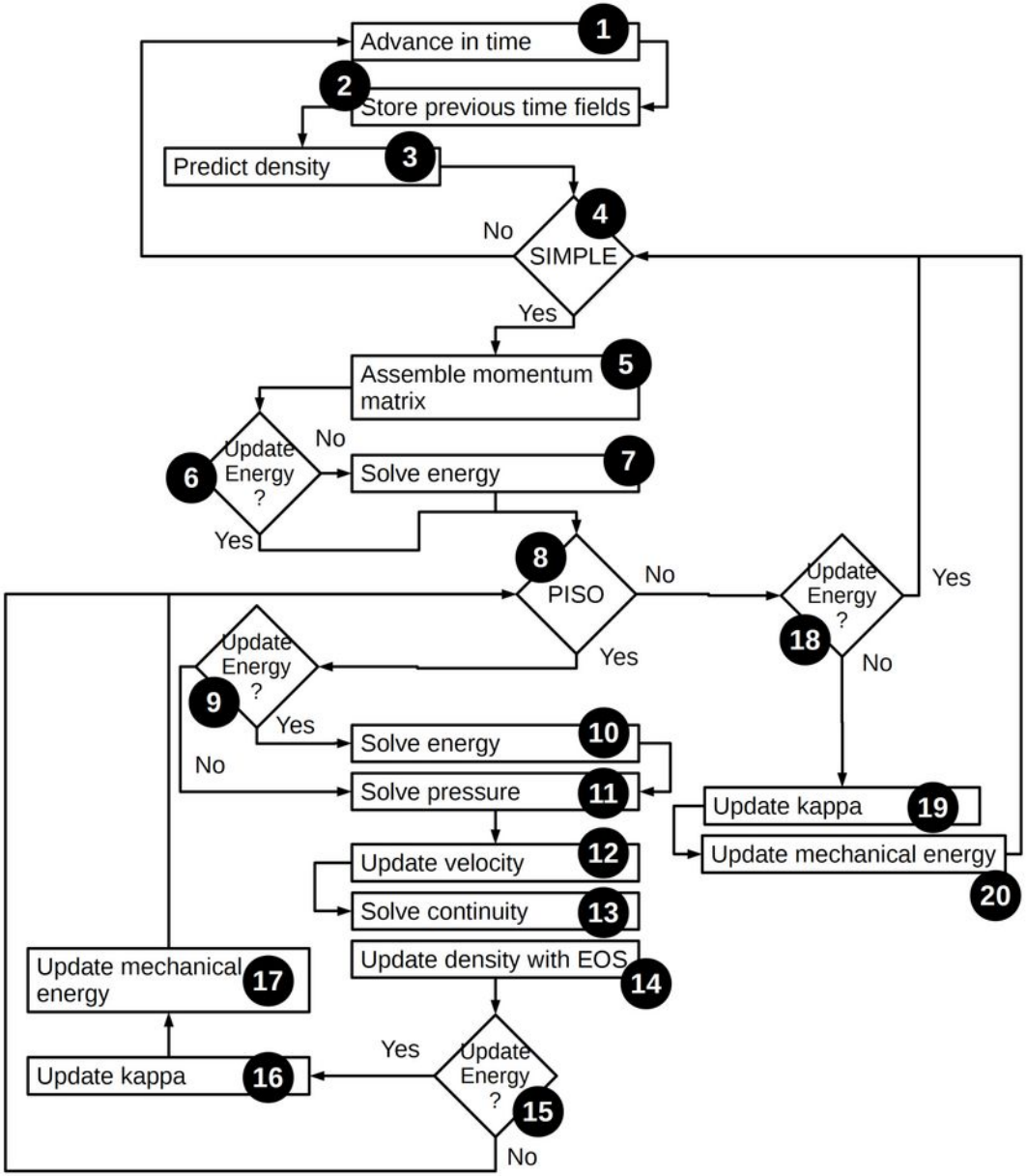


incompressible $\kappa_f = 0$

compressible $\kappa_f = 1$

Hybrid PIMPLE/KT algorithm

- Increase current time – **1**
- Solve explicit equation for density – **3**
- Start SIMPLE loop – **4**
- Assemble momentum matrix – **5**
- If only PISO iterations, solve for energy – **7**
- Start PISO loop – **8**
- If more then 1 SIMPLE iterations, solve for energy – **9**
- Solve continuity equation formulated for pressure, update velocity and density with EOS – **10-14**
- Update blending field “kappa” – **16**
- Update mechanical energy transport – **17**



pimpleCentralFoam source code

hybridCentralSolvers/OpenFOAM-v2112/

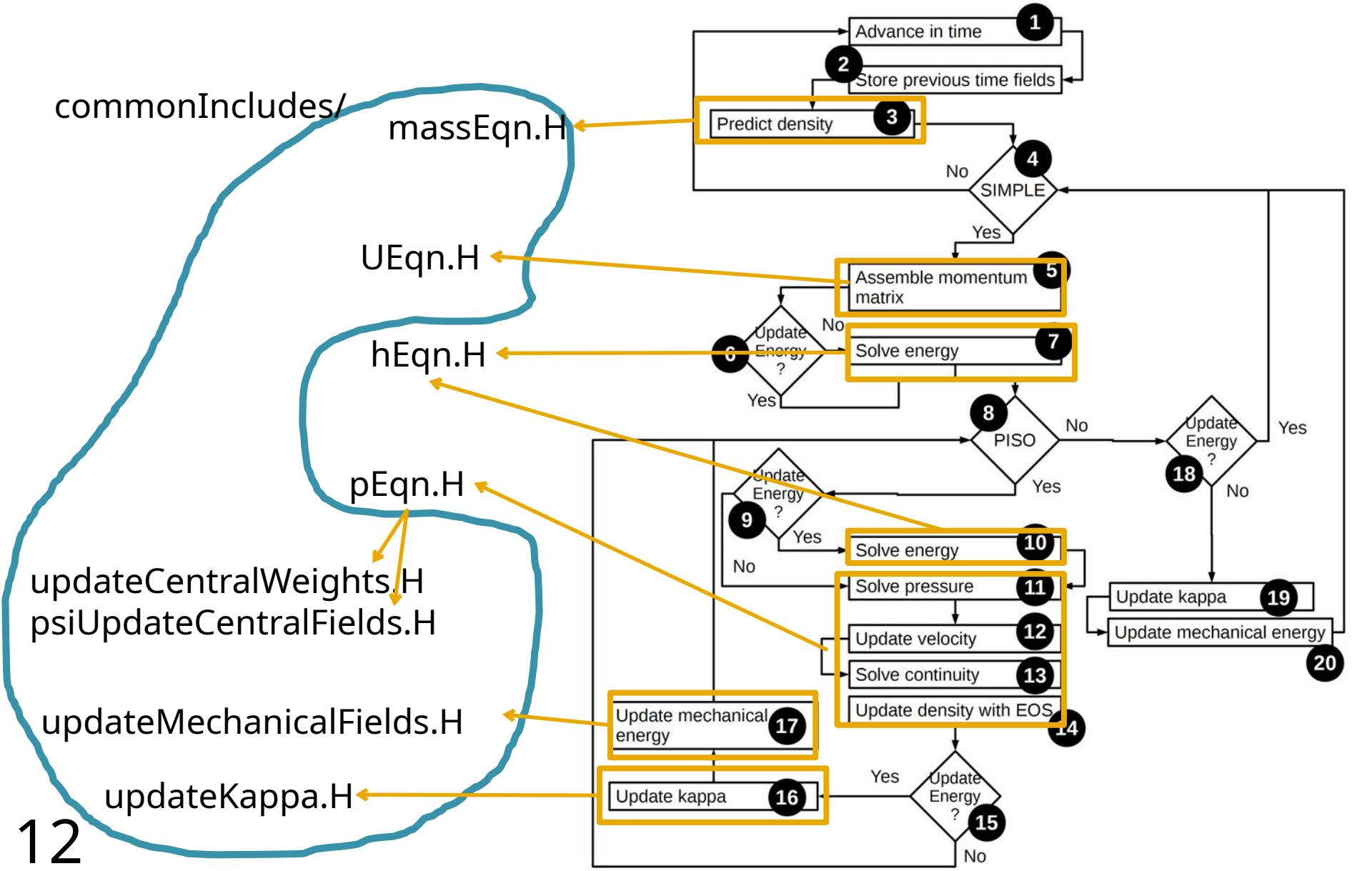
Library **libpimpleCentral.so** with common operations used **pimpleCentralFoam**

- pimpleCentral/
  - commonIncludes/
    - Eqns
    - createCommonCentralFields.H
    - updateKappa.H
  - kappaFunctions/

Source code for **pimpleCentralFoam** solver

- pimpleCentralFoam/
  - Make/
  - createFields.H
  - hEqn.H
  - pEqn.H
  - pimpleCentralFoam.C

Hybrid PIMPLE/KT algorithm sources

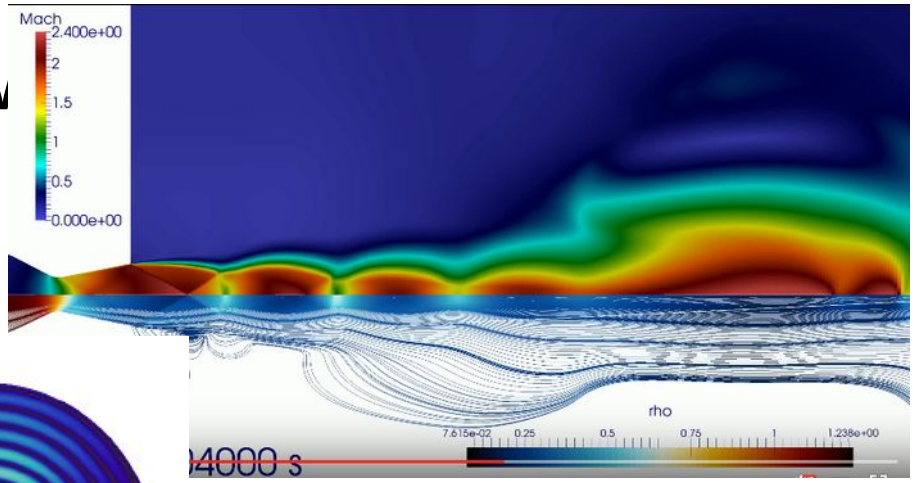


Other hybrid PIMPLE/KT solvers

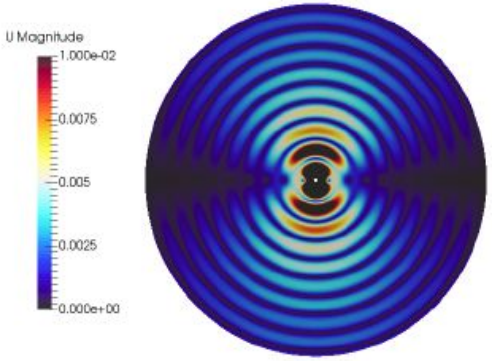
- **pimpleCentralDyMFoam** – solver with mesh motion
- **rhoPimpleCentralFoam** – solver for gases with equations of state, different to perfect gas
- **reactingPimpleCentralFoam** – solver for multicomponent mixtures flow with chemical reactions
- **twoPhaseMixingCentralFoam** – solver for two phase homogeneous liquids flows (water & air, for example)
- **chtMultiRegionCentralFoam** – this Track solver

Examples of pimpleCentralFoam solver

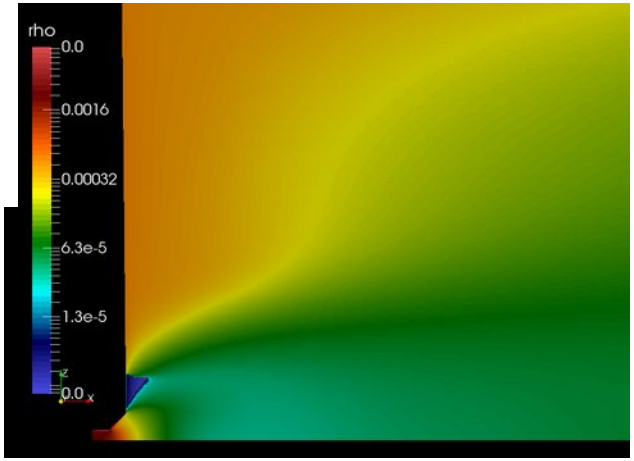
- Supersonic jet flow



- Acoustics



- Plasma flows



Boundary conditions

- Inlet (for subsonic and supersonic flows)
- Outlet – mixed subsonic/supersonic (**subsonicSupersonicPressureOutlet**, **libcompressibleTools**, can be downloaded from github.com)
- Walls – adiabatic, coupled to solids

Steps to develop supersonic coupled with heat transfer solver

- Step 1. Create new solver and link with **regionProperties** to allow multiple domains in single case.
- Step 2. Move fluid domain from default location to user-specified.
- Step 3. Create source code to solve for heat transfer in several (solid) bodies.
- Step 4. Link created code with new solver. Compile the solver.

Resulting source codes of each step stored in separate folders of training track materials in the folder src/

https://github.com/unicfdlab/TrainingTracks/tree/master/OpenFOAM/gasThermoCoupled-OFv2112

Simplifications

Single domain for fluid, multiple domains for solids

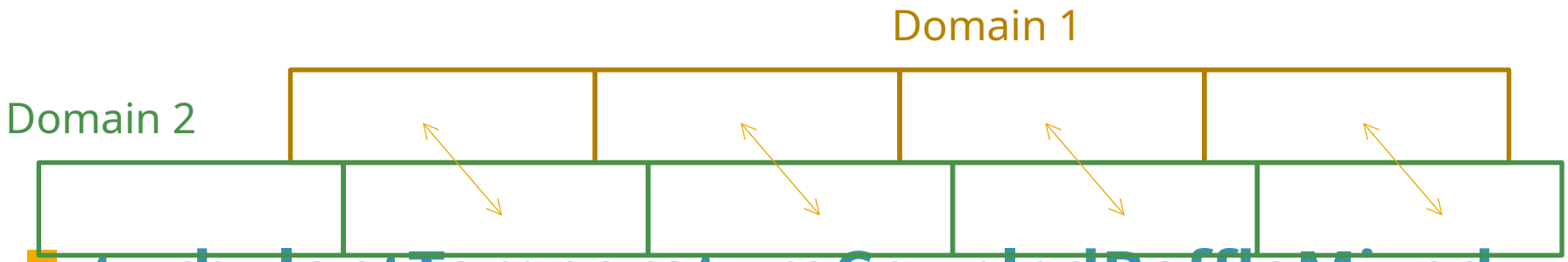
Application: flow over several bodies, or structure composed of several materials

Benefits: No need to rewrite most of the code for gas dynamics

More general case – ToncomoLLC github page
https://github.com/TonkomoLLC/hybridCentralSolvers

Simplifications - 2

- Nearest cell interpolation — for meshes with relatively uniform and equal grid distribution on external boundaries



- **turbulentTemperatureCoupledBaffleMixed** uses approximated expressions for heat fluxes to satisfy ideal heat contact condition

Initialization steps

1. Download hybridCentralSolvers
   https://github.com/unicfdlab/hybridCentralSolvers
2. Build library and solvers: ./Allwmake
3. Download libcompressibleTools
   https://github.com/unicfdlab/libcompressibleTools
4. Build library ./makeLib.sh

Step 1

- Make a copy of pimpleCentralFoam solver, rename it to myChtPimpleCentralFoam and update its wmake settings:

```
mv pimpleCentralFoam.C myChtPimpleCentralFoam.C
```

- Update Make/files

```
myChtPimpleCentralFoam.C
EXE = $(FOAM_USER_APPBIN)/myChtPimpleCentralFoam
```

- Update Make/options

```
HCS_SRC=/path/to/library/source/pimpleCentral
EXE_INC = \
 -I$(HCS_SRC)/lnInclude \
...
-I$(LIB_SRC)/regionModels/regionModel/lnInclude
...
EXE_LIBS = \
...
-lregionModels
```

Include path and library of classes for handling multi-domain cases

Step 1 results

- After this step we have new solver "**myChtPimpleCentralFoam**" which can work potentially with multiple domains (meshes) simultaneously.

Step 2

- Change space discretization storage for gas from «**defaultRegion**» to «**fluid**» region

```
0/
constant/
    polyMesh/
system/
```

```
0/
constant/
    fluid/
        polyMesh/
system/
    fluid/
```

- Goal of this step is to separate mesh storage for fluid (gas) and solids. Each mesh is stored in the unique folder on HDD (and object in memory)

```
regionProperties rp(runTime);
```

To manage several domains **regionProperties** object must be created in the program before executing all other mesh operations

General settings

- Create file **createMeshes.H**:

```
regionProperties rp(runTime);
#include "createFluidMeshes.H"
```

- Update **createFields.H**:

```
#include "createFluidFields.H"
```

Operations to create mesh and fields for fluid are now stored in new files

- Update **Make/options**:

```
EXE_INC = \
…
-I./fluid
```

Fluid model files are stored in folder «fluid»
which is known to compiler to lookup for includes

Remove LTS

- Update **main** procedure in **myChtPimpleCentralFoam.C** — remove LTS *)
- Start of the time step will look like:

```
....
while (pimple.loop())
{
    #include "readAdditionalPimpleControl.H"
    #include "acousticCourantNo.H"
    #include "centralCompressibleCourantNo.H"
    #include "readTimeControls.H"
    #include "setDeltaT.H"
```

```
if (LTS)
{
…
}
```

- Add include for **regionProperties** class:

```
#include «regionProperties.H»
```

*) LTS – Local Time Stepping

Create fluid mesh & fields

- Put fluid-associated operations in separate files:

```
mkdir fluid; cd fluid/
mv ../hEqn.H ./
mv ../pEqn.H ./
mv ../createFields.H createFluidFields.H
touch createFluidMeshes.H
```

Fluid fields are now created in **createFluidFields.H**

- Create mesh for gas domain - **createFluidMeshes.H**:

```
const wordList fluidNames(rp["fluid"]);
autoPtr<fvMesh> fluidMeshPtr;
fluidMeshPtr.reset(
    new fvMesh(
        IOobject(
            fluidNames[0],
            runTime.timeName(),
            runTime,
            IOobject::MUST_READ
        )
    )
);
```

Pointer to gas mesh

Specify location for gas mesh

Create reference to fluid (gas) mesh

```
fvMesh& fluidMesh =
fluidMeshPtr();
fvMesh& mesh = fluidMesh;
```

Update createFluidFields.H

- Move initialization operations related to fluid (gas) domain from **myChtPimpleCentralFoam.C** to **createFluidFields.H**:

```
#include "readAdditionalPimpleControl.H"
#include "createCommonCentralFields.H",
autoPtr<compressible::turbulenceModel> turbulence
(compressible::turbulenceModel::New(rho,U,phi,thermo));
#include "createFvOptions.H"
#include "createMRF.H"
#include "initContinuityErrs.H"
#include "readCourantType.H"
#include "markBadQualityCells.H"
#include "psiUpdateCentralFields.H"
#include "updateKappa.H"
#include "updateCentralWeights.H"
#include "createCentralCourantNo.H"
```

Step 2 results

- At this step gas domain relocated from standard folder to location specified by user in the **regionProperties** dictionary.
- Source code of gas dynamics equations approximation is now stored in separate folder “**fluid/**”.

Step 3

- Create source code to solve for heat transfer equations in solids and link necessary libraries to executable.

```
mkdir solid
```

← Folder to store sources for solid body heat transfer model

- Examples of the source code can be retrieved from chtMultiRegionPimpleFoam sources.
- Add “includes” to main procedure (**myChtPimpleCentralFoam.C**):

```
#include "coordinateSystem.H"
#include "solidThermo.H"
```

- Update wmake settings (**Make/options**):

```
-I$(LIB_SRC)/thermophysicalModels/
  solidThermo/lnInclude \
```

- Resulting source code structure will become:

myChtPimpleCentralFoam/

fluid/ **solid/** **Make/**

General solution procedure for solids

- Create meshes for solids.
- Create fields describing heat exchange process in solids.
- Create approximations of energy balance equations in solids (matrices).
- Solve matrices (equations) for energy balances for all solids.

Create solid domains

- Unlike gas, for solids we have several computational domains and thus we have to store several meshes, several temperature fields, several thermal conductivity coefficients and so on.
- Create **createSolidMeshes.H**:

```
const wordList solidsNames(rp["solid"]);
PtrList<fvMesh> solidRegions(solidsNames.size());
forAll(solidsNames, i)
{
    solidRegions.set
    (
        i,
        new fvMesh
        (
            IOobject
            (
                solidsNames[i],
                runTime.timeName(),
                runTime,
                IOobject::MUST_READ
            ...
```

Names for solid domains

Number of solid domains

Loop over all solid domains

For solid No. i, create mesh

For complete example see **createSolidMeshes.H** from training materials

Create solid fields and objects

- Place initialization operations in **createSolidFields.H** file.
- For each solid we must create:
  - Coordinate system transformation tensor (for anisotropic conductivity)

```
PtrList<coordinateSystem> coordinates(solidRegions.size());
```

  - Thermodynamic library

```
PtrList<solidThermo> thermos(solidRegions.size());
```

  - Volumetric heat sources (fvOptions objects)

```
PtrList<fv::options> solidHeatSources(solidRegions.size());
```

  - Porosity field

```
PtrList<volScalarField> betavSolid(solidRegions.size());
```

  - Field of anisotropic thermal diffusivity coefficient

```
PtrList<volSymmTensorField> aniAlphas(solidRegions.size());
```

Initialization of solid fields and objects

- After declaration, objects are initialized (see **createSolidFields.H** for example) in cycle:

```
forAll(solidRegions, i)
{
    ...
    thermos.set(i, solidThermo::New(solidRegions[i]));
    ...
    solidHeatSources.set
    (i,new fv::options(solidRegions[i]));
    ...
    coordinates.set
    (i,coordinateSystem::New(solidRegions[i],thermos[i]));
    ...
    aniAlphas.set(i,new volSymmTensorField...
    ...
    betavSolid.set(i, new volScalarField...
    ...
}
```

Solution process for heat transfer in multiple solid bodies

- Loop over all solids (**solveSolidRegions.H**)

```
forAll(solidRegions, i)
{
```

- Create refernces for fields, coefficients and mesh for region No. i

```
#include "setRegionSolidFields.H"
```

- Solve for energy balance for solid No. I

```
#include "solveSolid.H"
```

Energy equation in solid

- In case of isotropic material properties, energy balance in solid (in terms of enthalpy) reads:

$$\frac{\partial \beta_v \rho h}{\partial t} - \nabla \cdot \left(\beta_v \frac{\lambda}{C} \nabla h \right) = S$$

- Change of energy in volume
- Heat flux
- Volumetric energy sources

```
fvScalarMatrix hEqn
(
    fvm::ddt(solidBetav,solidRho,solidH)
    -
    fvm::laplacian
    (
        solidBetav*solidThermo.alpha(),
        solidH,
        "laplacian(alpha,h)"
    )
  ==
    solidFvOptions(solidRho, solidH)
);
```

Step 3 results

- Source code for simulation of heat transfer in solids using single solver was create
- Simulation process includes:
  - Initialization of meshes and fields for each solid: **createSolidMeshes.H** and **createSolidFields.H**
  - Energy balance equation discretization and solution: files **solveSolidRegions.H**, **setRegionSolidFields.H** and **solveSolid.H**
- Source code of heat transfer approximation for solid bodies stored in separate folder "**solid/**"
- Though sources created, they are not linked to the **main** program

Step 4

- Put solid equations solution block in PIMPLE algorithm for coupled simulation:
  - Update **createMeshes.H**:

```
#include "createFluidMeshes.H"
#include "createSolidMeshes.H"
```

  - Update **createFields.H**:

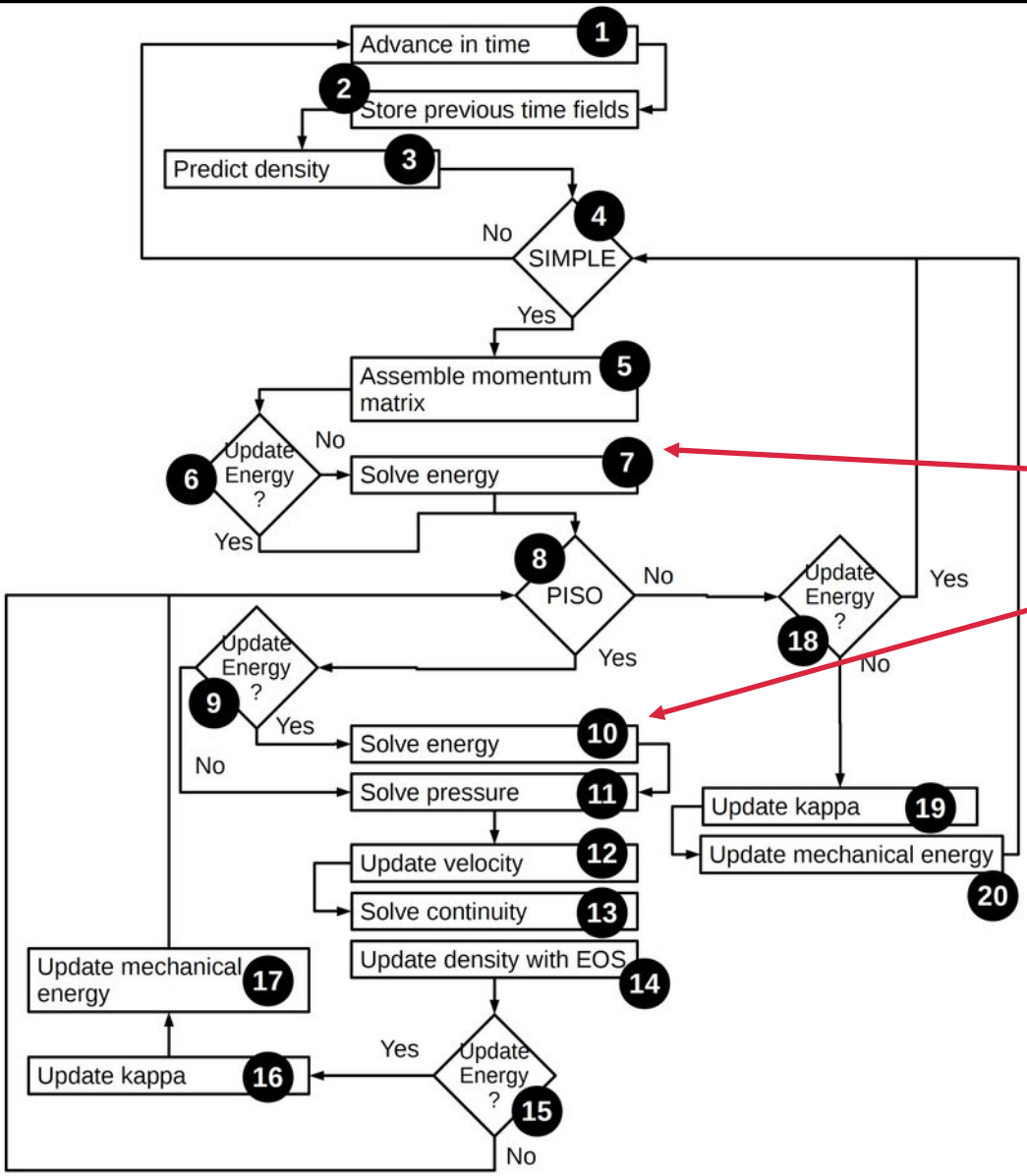
```
#include "createFluidFields.H"
#include "createSolidFields.H"
```

  - Update **Make/options**:

```
EXE_INC = \
… \
-I./solid
```

  - Update **myChtPimpleCentralFoam.C** — insert solution for heat transfer in solids in the PIMPLE algorithm

Where to place solid body heat transfer block

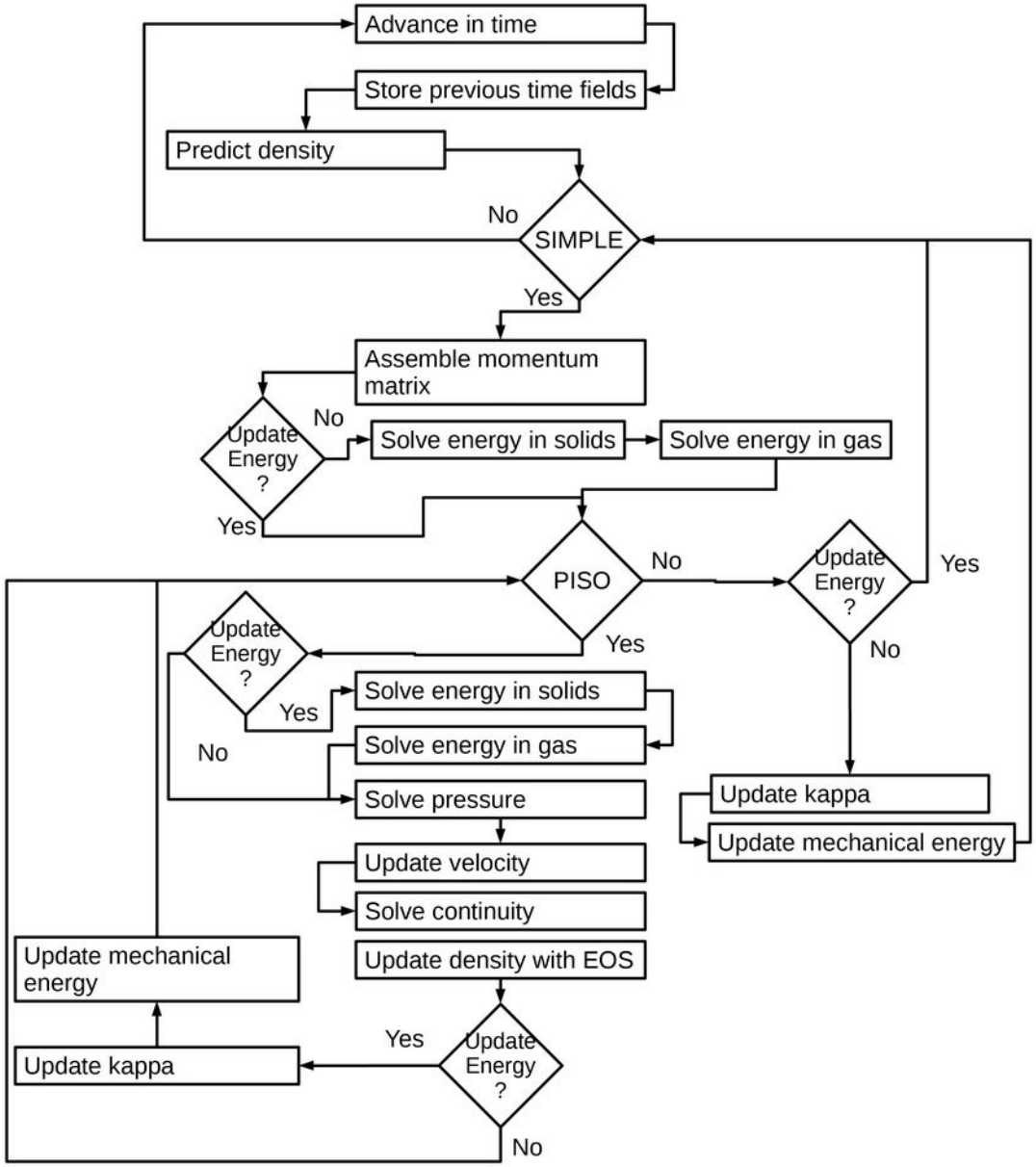


Add steps to solve for energy balance in solids
before solving energy balance in fluid

solveSolidRegions.H

solveSolidRegions.H

Final PIMPLE algorithm



Compile solver

- To compile solver, type

```
wmake
```

- Screenshot

mc [openfoam@cluster.fsc]:~/OF2017/TrainingTracks/OpenFOAM/gasThermoCoupled-OF4.1/src/Step-4/myChtPimpleCentralFoam

File Edit View Search Terminal Help

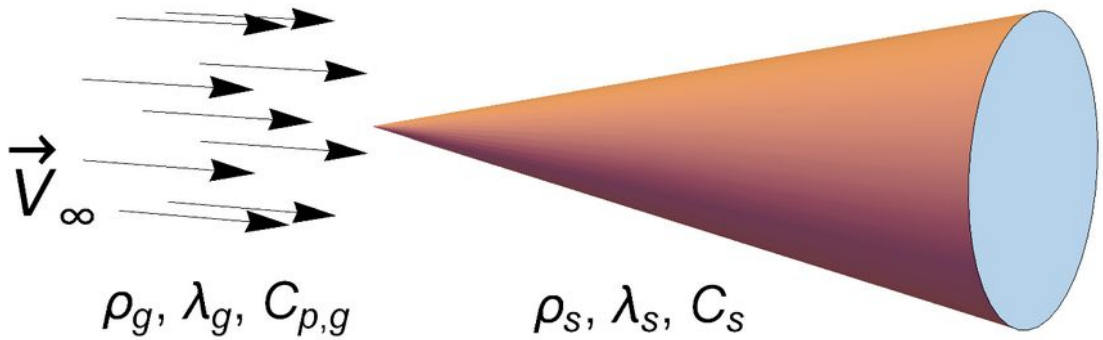
```
IlnInclude -I. -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/OpenFOAM/lnInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.
x/src/OSspecific/POSIX/lnInclude   -fPIC -c myChtPimpleCentralFoam.C -o Make/linux64IccDPInt32Opt/myChtPimpleCentr
alFoam.o
icpc -std=c++0x -fp-trap=common -fp-model precise -Dlinux64 -DWM_ARCH_OPTION=64 -DWM_DP -DWM_LABEL_SIZE=32 -Wall -
Wextra -Wnon-virtual-dtor -Wno-unused-parameter -Wno-invalid-offsetof -diag-disable 654,1125,2304 -O3  -DNoReposit
ory -I/home/openfoam/OF2017/hybrid/pisoCentral/lnInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/finiteVolume/l
nInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/transportModels/compressible/lnInclude -I/home/openfoam/OpenFO
AM/OpenFOAM-4.x/src/thermophysicalModels/basic/lnInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/thermophysical
Models/specie/lnInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/TurbulenceModels/turbulenceModels/lnInclude -I/
home/openfoam/OpenFOAM/OpenFOAM-4.x/src/TurbulenceModels/compressible/lnInclude -I/home/openfoam/OpenFOAM/OpenFOAM
-4.x/src/dynamicMesh/lnInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/meshTools/lnInclude -I/home/openfoam/Ope
nFOAM/OpenFOAM-4.x/src/fvOptions/lnInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/regionModels/regionModel/lnI
nclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/thermophysicalModels/solidThermo/lnInclude -I./fluid -I./solid -
IlnInclude -I. -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/OpenFOAM/lnInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.
x/src/OSspecific/POSIX/lnInclude   -fPIC -Xlinker --add-needed -Xlinker --no-as-needed Make/linux64IccDPInt32Opt/m
yChtPimpleCentralFoam.o -L/home/openfoam/OpenFOAM/OpenFOAM-4.x/platforms/linux64IccDPInt32Opt/lib \
            -L/home/openfoam/OpenFOAM/openfoam-4.x/platforms/linux64IccDPInt32Opt/lib -lpisoCentral -lfiniteVolume
 -lfluidThermophysicalModels -lspecie -lturbulenceModels -lcompressibleTransportModels -lcompressibleTurbulenceMod
els -lmeshTools -lfvOptions -lregionModels -lOpenFOAM -ldl  \
             -L/lib -lm -o /home/openfoam/OpenFOAM/openfoam-4.x/platforms/linux64IccDPInt32Opt/bin/myChtPimpleCent
ralFoam
[openfoam@cluster myChtPimpleCentralFoam]$
[openfoam@cluster myChtPimpleCentralFoam]$ wmake
make: `/home/openfoam/OpenFOAM/openfoam-4.x/platforms/linux64IccDPInt32Opt/bin/myChtPimpleCentralFoam' is up to da
te.
[openfoam@cluster myChtPimpleCentralFoam]$
```

Step 4 results

- Source code for simulation of heat transfer in solid bodies added to **main** program.
- Energy balance equations for solids are solved in **PIMPLE** algorithm before solving for energy balance of gas.
- New solver **myChtPimpleCentralFoam** was compiled.

Test cases

- Laminar flow
- Turbulent flow



$V_{g,\infty} = 750 \text{ m/s}$

$p_{g,\infty} = 26500 \text{ Pa}$

$T_{g,\infty} = 223 \text{ K}$

$C_{p,g} = 1005 \text{ J/(kg} \cdot \text{K)}$

Viscosity model - Sutherland

$\rho = 4500 \text{ kg/m}^3$

$\lambda = 20 \text{ W/(m} \cdot \text{K)}$

$T_{s,0} = 293 \text{ K}$

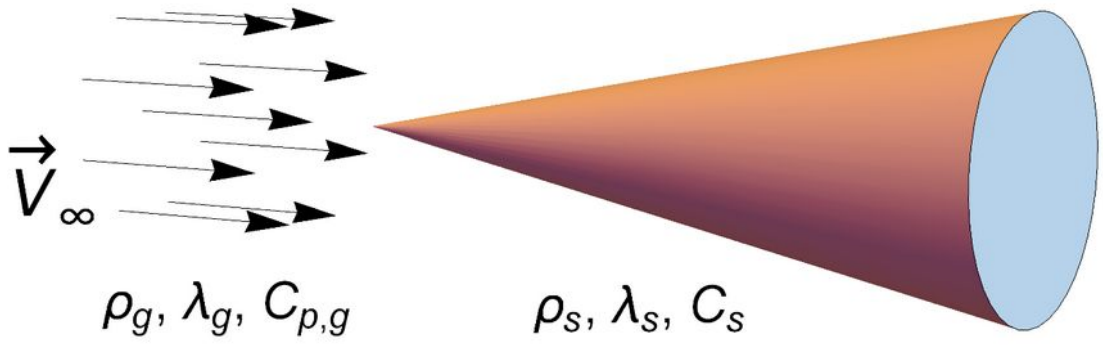
$C_{p,g} = 600 \text{ J/(kg} \cdot \text{K)}$

RAS simulation – k-w SST turbulence model

https://github.com/unicfdlab/TrainingTracks/tree/master/OpenFOAM/gasThermoCoupled-OFv2112/cases

Run test cases

- Laminar flow
- Turbulent flow



- Decompose regions
  - **decomposePar -region solid**
  - **decomposePar -region fluid**
- Run cases
  - **mpirun -np 4 myChtPimpleCentralFoam -parallel**
- Reconstruct solution (if necessary)
  - **reconstructPar**

wallHeatFlux postprocessor

- Source code is copied to **/src**
- **/Make/options** is changed

  ($FOAM_APPBIN → $FOAM_USER_APPBIN)
- To compile: **wmake libso**
- Run:

  mpirun -np 4 wallHeatFlux -parallel -region solid

  or

  wallHeatFlux -region solid

  Computed heat flux (wedge angle 5 deg.)

- for laminar case: ~ 100 W
- for turbulent case: ~ 1150 W

Thank you for your attention!

All the source codes and numerical examples are available online

https://github.com/unicfdlab/