



ISP RAS

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

Instructors:

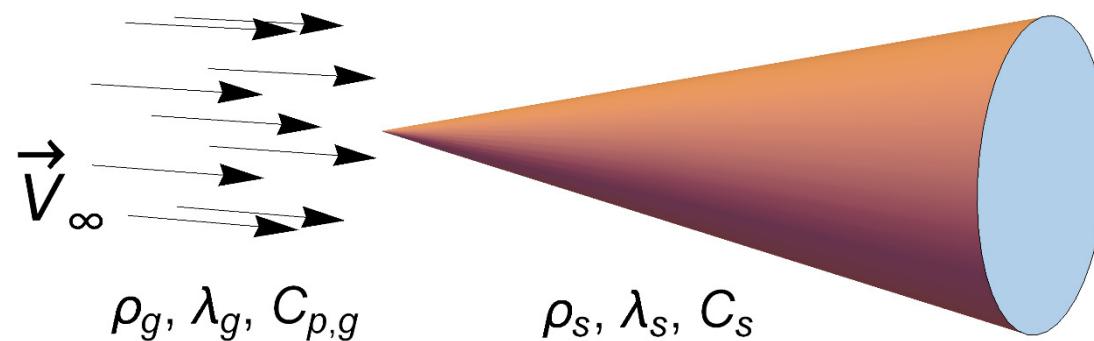
- 1) I. Marchevsky
- 2) M. Kravoshin

Contents

- Problem description
- Choice of the numerical method
- Implementation
- Test problems

Problem description

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



Governing equations

■ Perfect gas

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

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

■ Solid

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

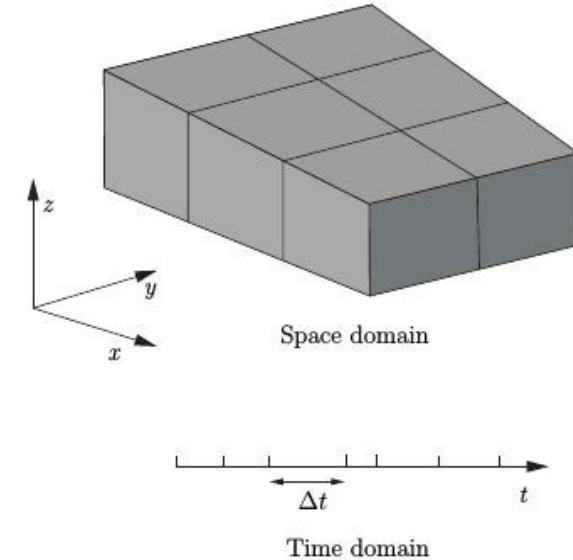
■ Ideal heat contact

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

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

Numerical model

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



- Numerical schemes
 - Mean theorem + Gauss theorem

$$\int_V \nabla \cdot \phi = \oint_{\partial V} \phi \cdot d\vec{S}$$

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

$$p = p^* + p'$$

$$\vec{U} = \vec{U}^* + \vec{U}'$$

$$\vec{U}' \sim -\nabla p'$$

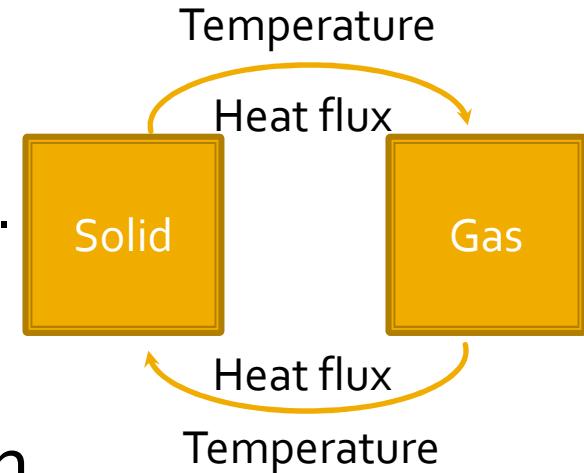
Models coupling

- 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 regions.
 - 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 ($\text{Ma} < 1$).



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 $p - \vec{U} - T$ coupling

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

$\overbrace{\frac{\rho^n \beta^n - \rho^o \beta^o}{\Delta t} + \frac{1}{V} \sum_f (\varphi_f^P + (1 - \kappa_f) \varphi_f^N) \beta_f^P + \frac{1}{V} \sum_f \kappa_f \varphi_f^N \beta_f^N =}$
 $= \frac{1}{V} \sum_f D_{\beta,f} \frac{\partial \beta}{\partial \vec{n}_f} |_{\vec{S}_f}$

«P» direction	«N» direction	
P ○	N ○	
X_j	$X_{j+1/2}$	X_{j+1}

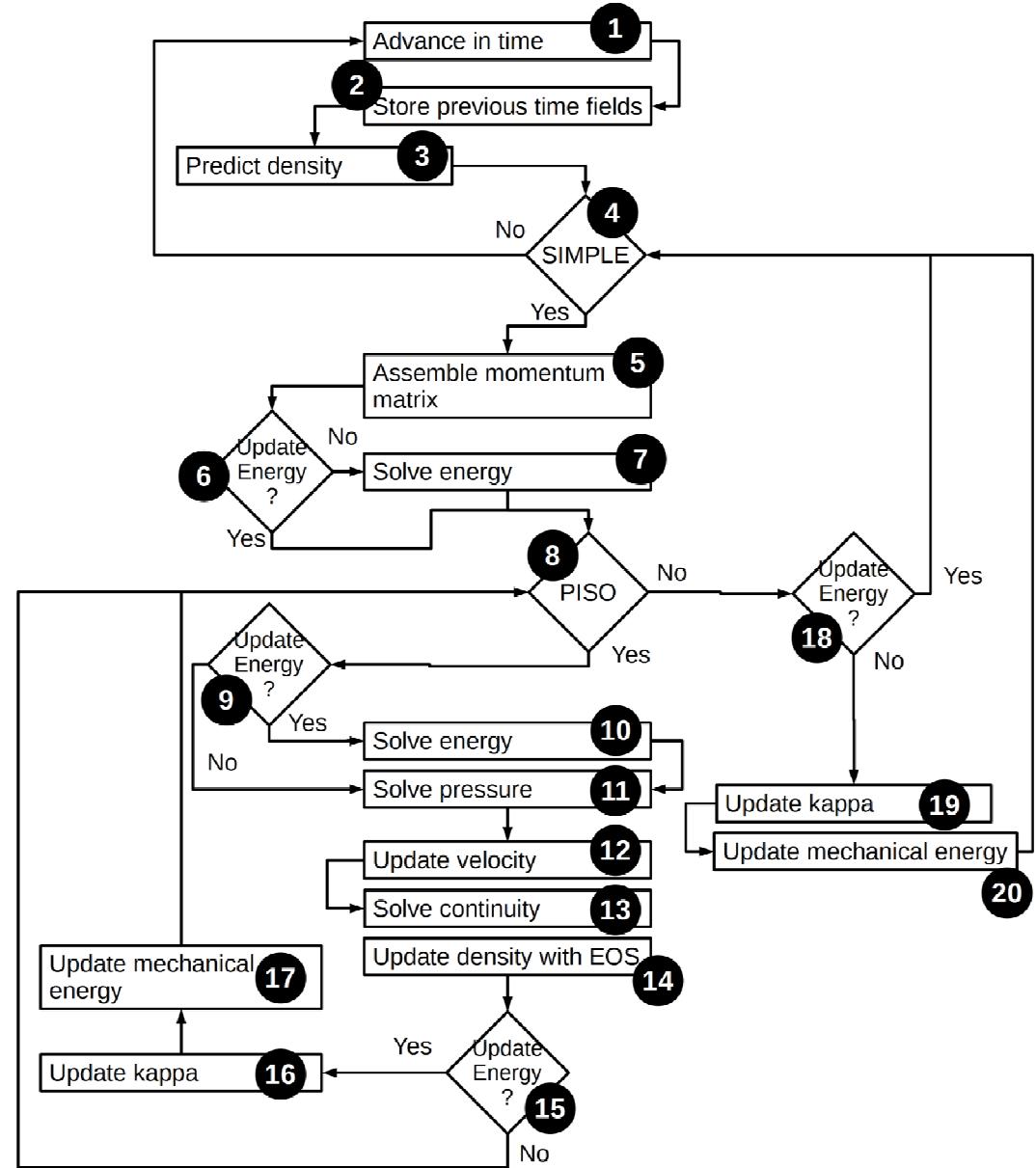
x

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 than 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

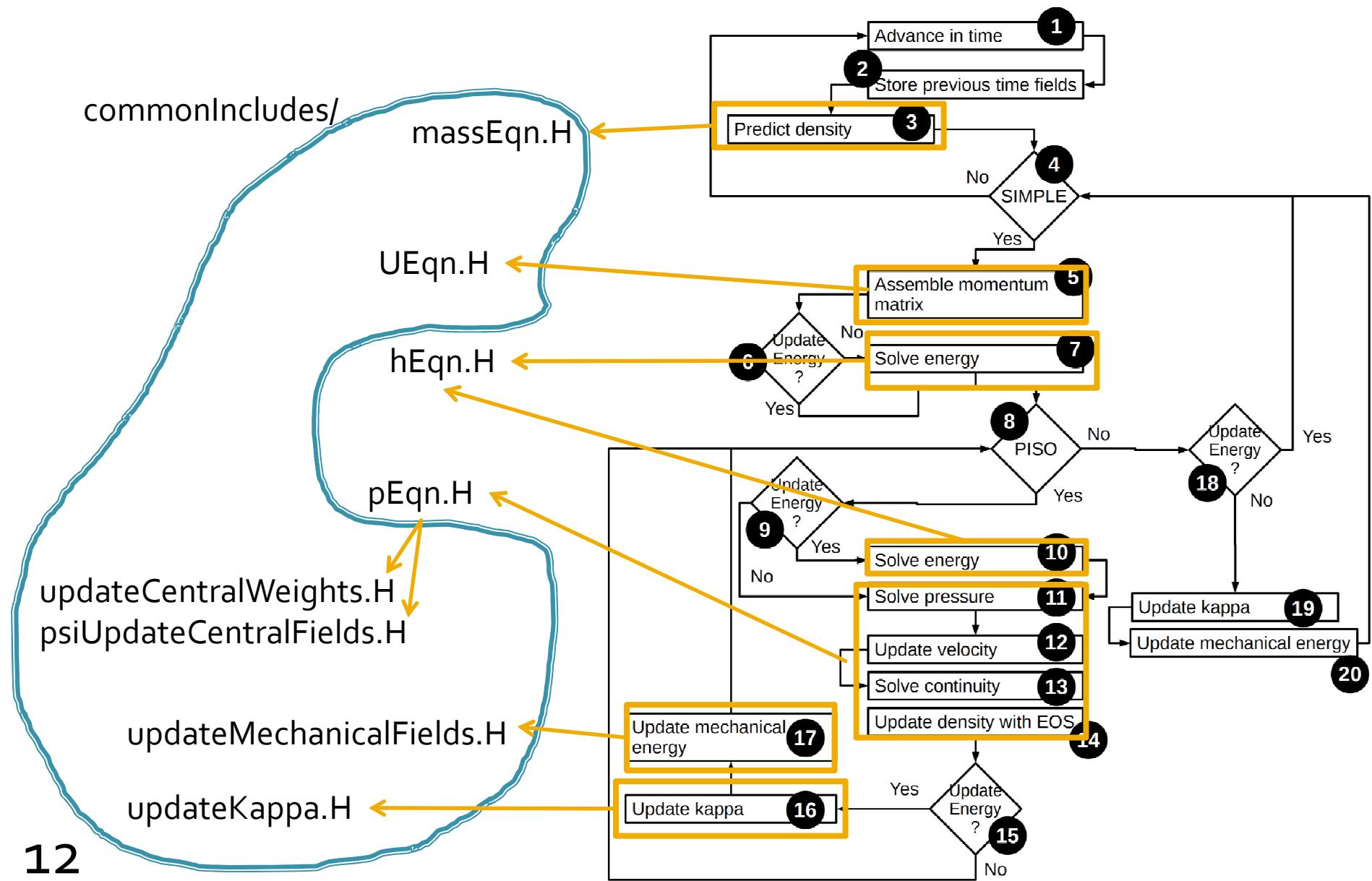
Library
libpisoCentral.so
with common
operations used
pimpleCentralFoam

Source code for
pimpleCentralFoam
solver

hybridCentralSolvers/OpenFOAM-4.1/

- pisoCentral/
 - commonIncludes/
 - Eqns
 - createCommonCentralFields.H
 - updateKappa.H
 - kappaFunctions/
- pimpleCentralFoam/
 - Make/
 - createFields.H
 - hEqn.H
 - pEqn.H
 - pimpleCentralFoam.C

Hybrid PIMPLE/KT algorithm sources

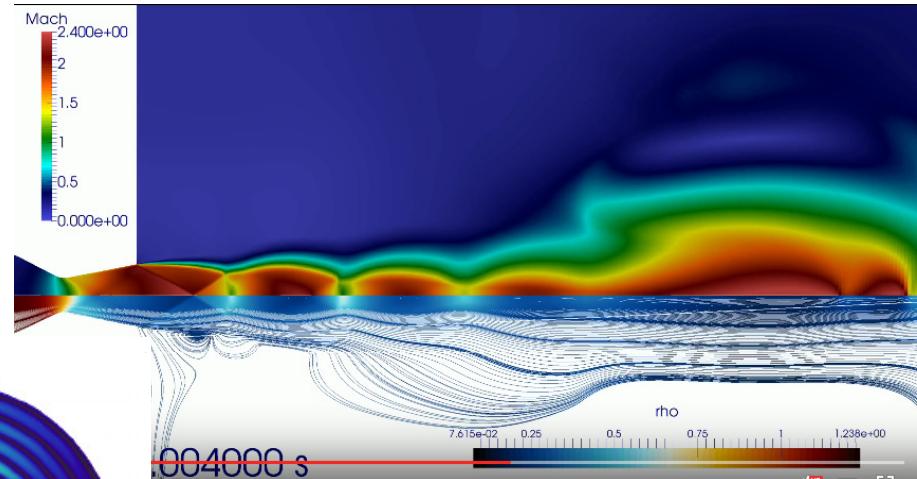


Other hybrid PIMPLE/KT solvers

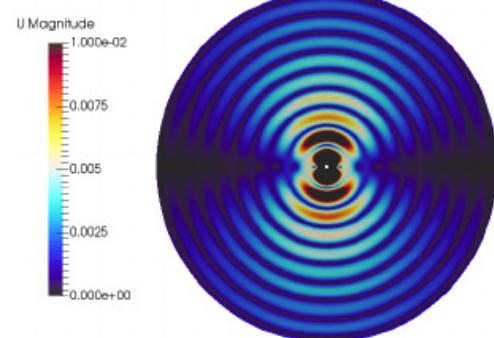
- **pimpleCentralDyMFoam** – solver with mesh motion
- **rhoPimpleCentralFoam** – solver for gases with equations of state, different to perfect gas
- **reactingPimpleCentralFoam** – solver for multicomponent mixtures flow with chemical reactions
- **twoPhaseMixingCentralFoam** – solver for two phase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

Examples of pimpleCentralFoam solver

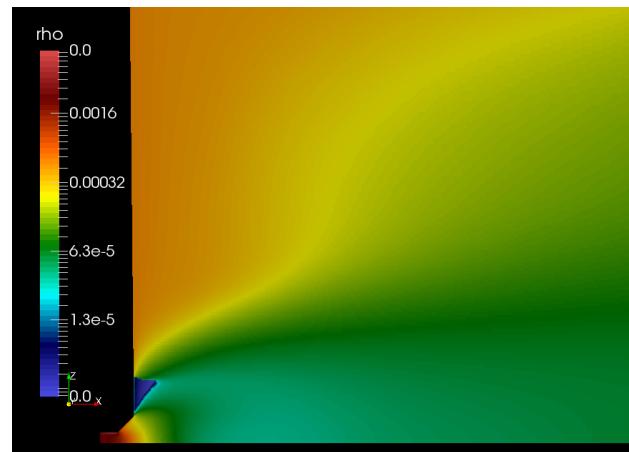
- Supersonic jet flows



- 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-OF4.1>

Simplifications

Single domain for fluid, multiple domains for solids



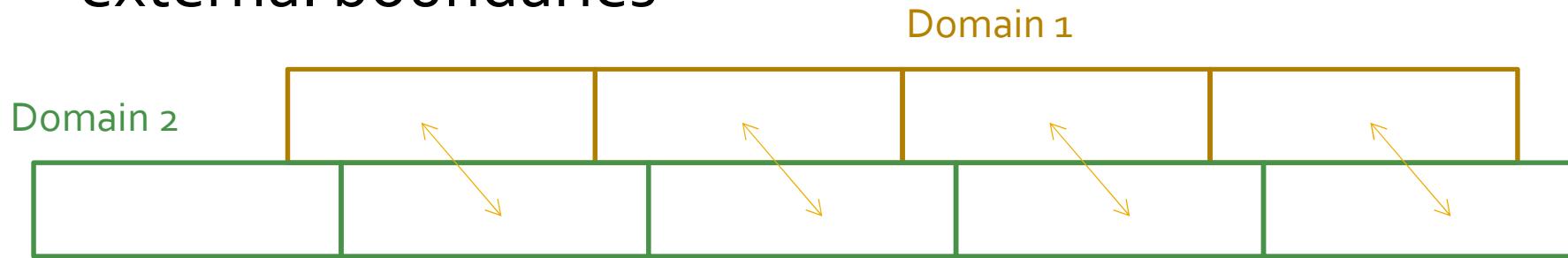
Application: flow over several bodies, or structure composed of several materials

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

More general case – TonkomoLLC 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

```
hybridCentralSolvers=/path/to/library/source
```

```
EXE_INC = \
```

```
  -I$(hybridCentralSolvers)/pisoCentral/lnInclude \
```

```
...
```

```
-I$(LIB_SRC)/regionModels/regionModel/lnInclude
```

```
...
```

```
EXE_LIBS = \
```

```
...
```

```
-lregionModels
```

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

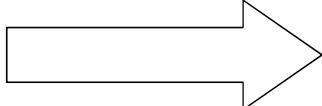
Step 1 results

- 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"
```

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

- Update **createFields.H**:

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

- 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
            ...
        )
    );
}
```

Loop over all solid domains

Names for solid domains

Number of 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 references 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

```
fvScalarMatrix hEqn
(
    fvm::ddt(solidBetav, solidRho, solidH)
    -
```

- Heat flux

```
    fvm::laplacian
    (
        solidBetav*solidThermo.alpha(),
        solidH,
        "laplacian(alpha,h)"
    )
```

- Volumetric energy sources

```
    ==
    solidFvOptions(solidRho, solidH)
);
```

Step 3 results

- Source code for simulation of heat transfer in solids using single solver was created
- 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**:

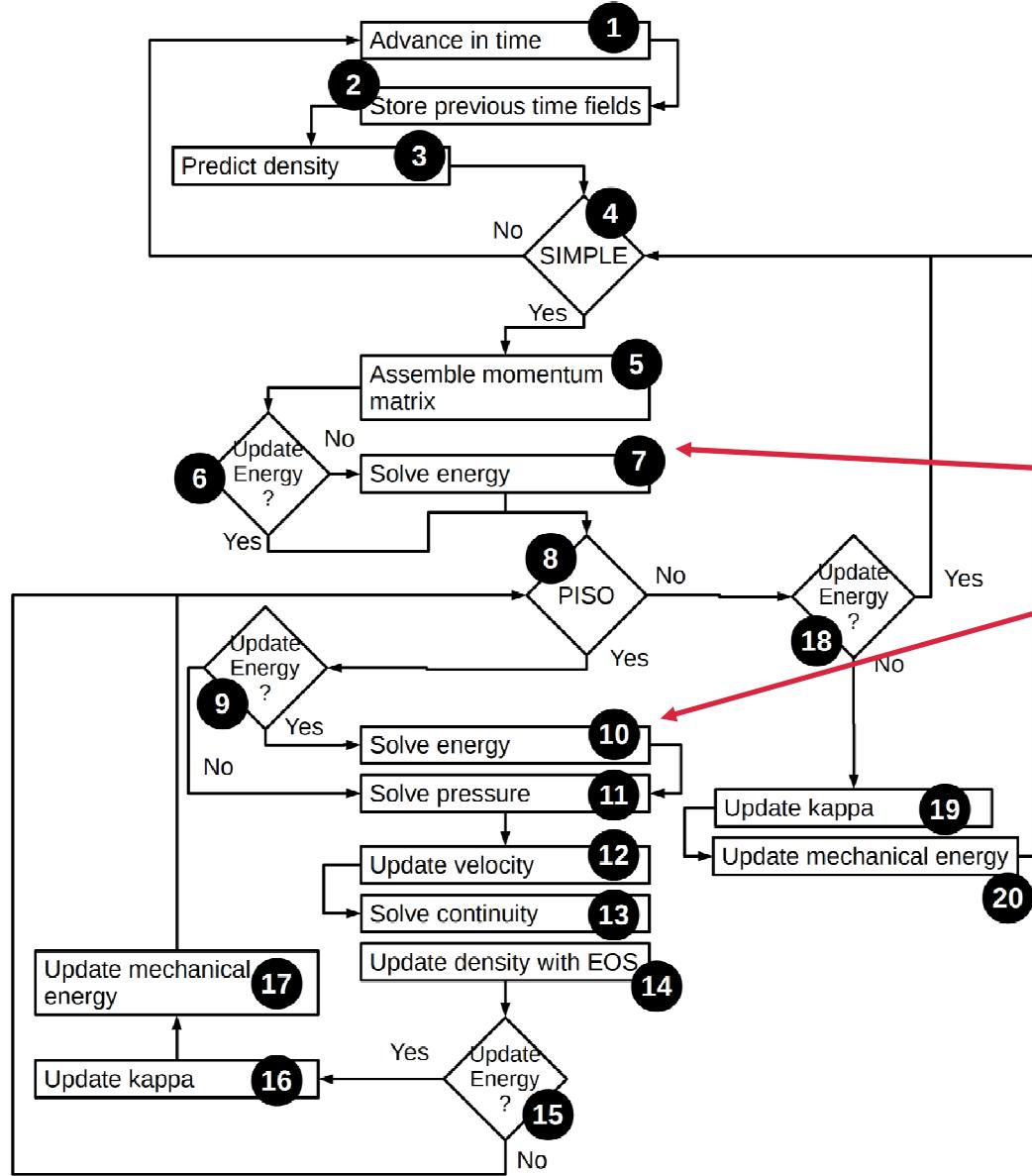
```
#include "createFluidFields.H"  
#include "createSolidFields.H"
```

- 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

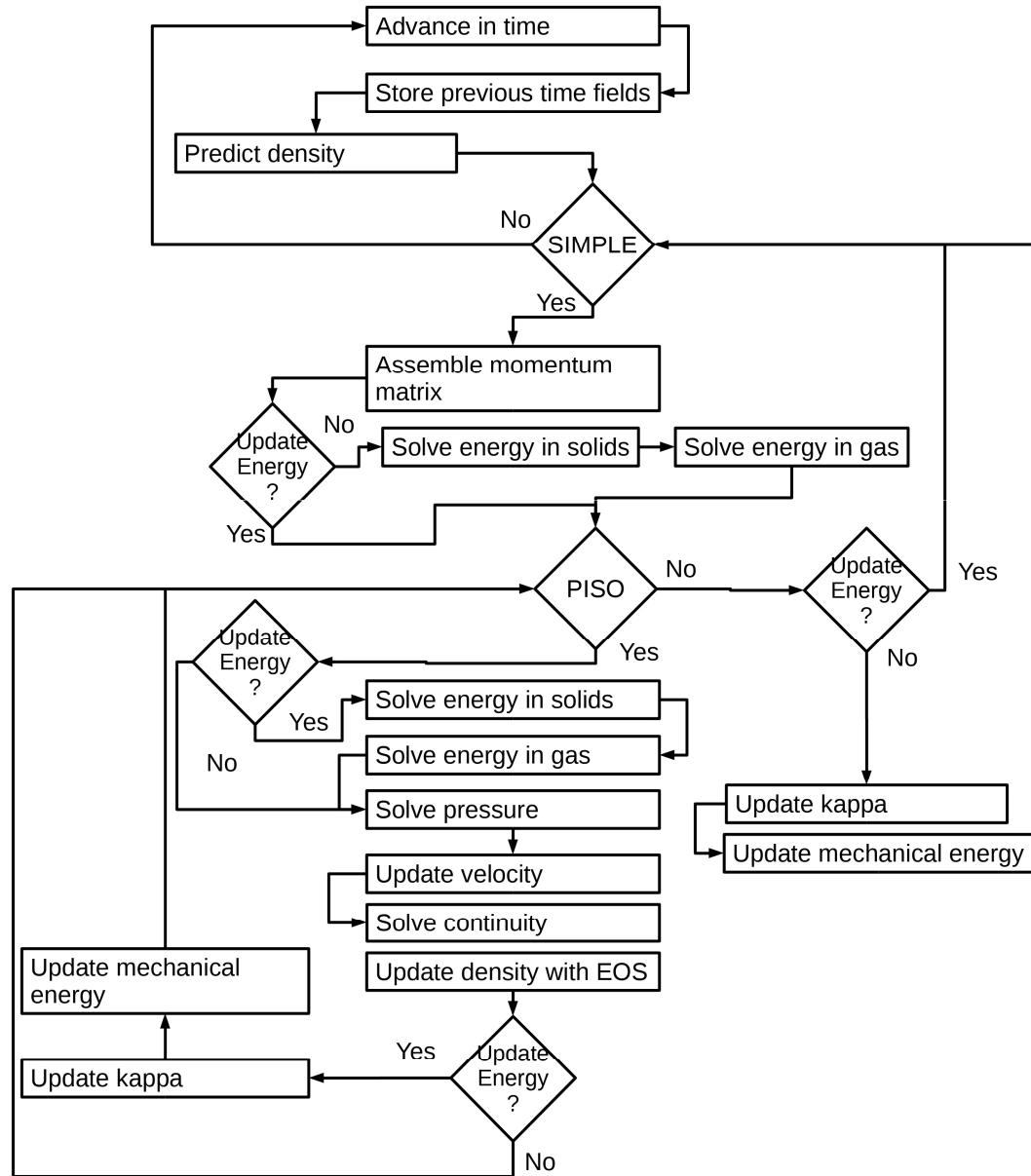


Add steps to solve for energy balance in solids before solving energy balance in fluid

`solveSolidRegions.H`

`solveSolidRegions.H`

Final PIMPLE algorithm

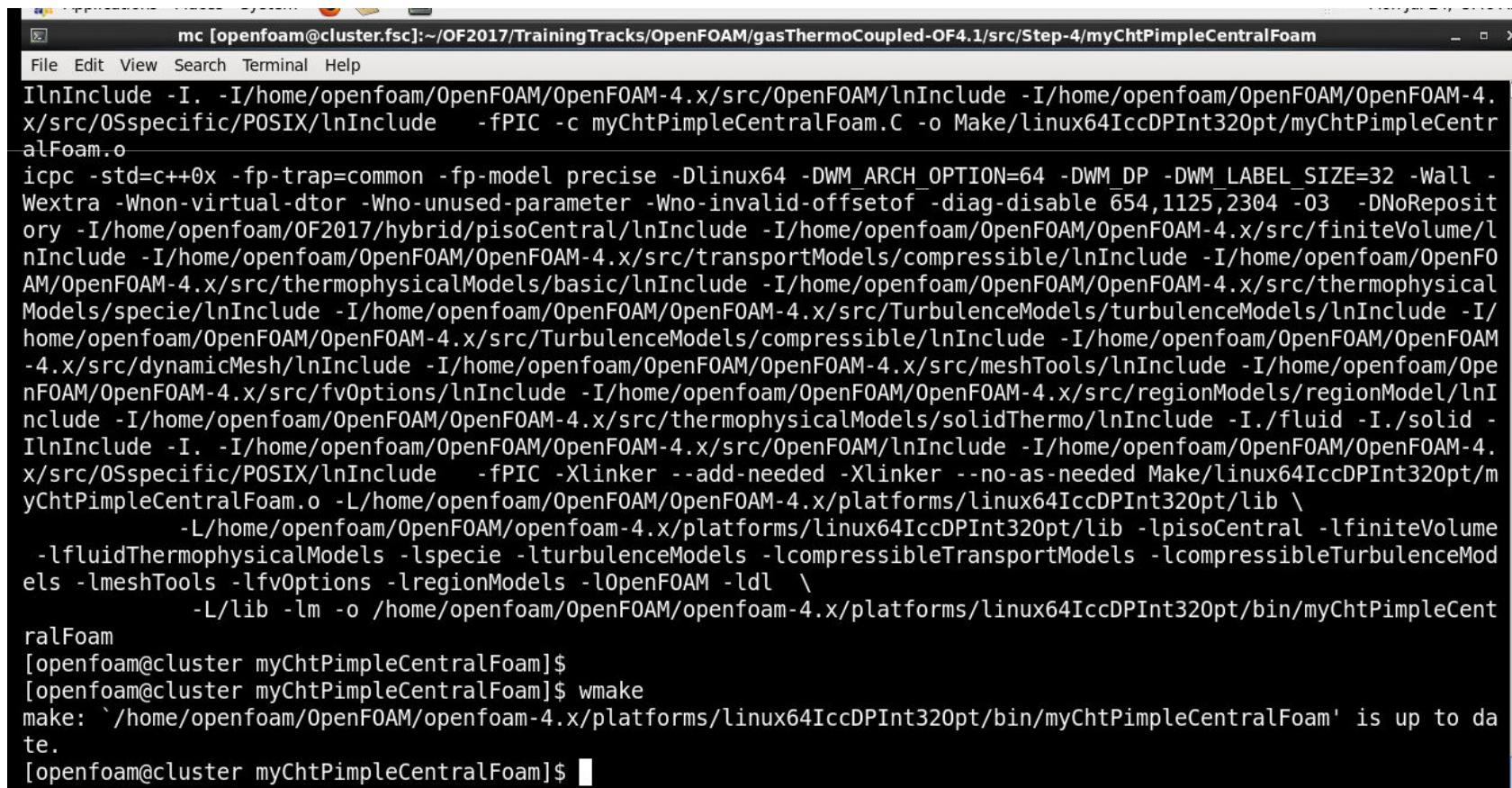


Compile solver

- To compile solver, type

wmake

- Screenshot



The screenshot shows a terminal window titled "mc [openfoam@cluster.fsc]:~/OF2017/TrainingTracks/OpenFOAM/gasThermoCoupled-OF4.1/src/Step-4/myChtPimpleCentralFoam". The terminal displays the command "wmake" being run, which triggers a complex compilation process. The output shows numerous compiler flags (e.g., -I, -D, -fPIC, -c) and linker options (-L, -l, -o) for linking against various OpenFOAM libraries and models. The compilation is successful, as indicated by the message "make: `/home/openfoam/OpenFOAM/openfoam-4.x/platforms/linux64IccDPInt320pt/bin/myChtPimpleCentralFoam' is up to date." at the end.

```
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-4.x/src/OpenFOAM/lInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/OSspecific/POSIX/lInclude -fPIC -c myChtPimpleCentralFoam.C -o Make/linux64IccDPInt320pt/myChtPimpleCentralFoam.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 -DNoRepository -I/home/openfoam/OF2017/hybrid/pisoCentral/lInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/finiteVolume/lInclude -I/home/openfoam/OpenFOAM-4.x/src/transportModels/compressible/lInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/thermophysicalModels/basic/lInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/thermophysicalModels/specie/lInclude -I/home/openfoam/OpenFOAM-4.x/src/TurbulenceModels/turbulenceModels/lInclude -I/home/openfoam/OpenFOAM-4.x/src/TurbulenceModels/compressible/lInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/dynamicMesh/lInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/meshTools/lInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/fvOptions/lInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/regionModels/regionModel/lInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/thermophysicalModels/solidThermo/lInclude -I./fluid -I./solid -IlnInclude -I. -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/OpenFOAM/lInclude -I/home/openfoam/OpenFOAM/OpenFOAM-4.x/src/OSspecific/POSIX/lInclude -fPIC -Xlinker --add-needed -Xlinker --no-as-needed Make/linux64IccDPInt320pt/myChtPimpleCentralFoam.o -L/home/openfoam/OpenFOAM/OpenFOAM-4.x/platforms/linux64IccDPInt320pt/lib \
-L/home/openfoam/OpenFOAM/openfoam-4.x/platforms/linux64IccDPInt320pt/lib -lpisoCentral -lfiniteVolume \
-lfluidThermophysicalModels -lspecie -lturbulenceModels -lcompressibleTransportModels -lcompressibleTurbulenceModels -lmeshTools -lfvOptions -lregionModels -lOpenFOAM -ldl \
-L/lib -lm -o /home/openfoam/OpenFOAM/openfoam-4.x/platforms/linux64IccDPInt320pt/bin/myChtPimpleCentralFoam
[openfoam@cluster myChtPimpleCentralFoam]$
[openfoam@cluster myChtPimpleCentralFoam]$ wmake
make: `/home/openfoam/OpenFOAM/openfoam-4.x/platforms/linux64IccDPInt320pt/bin/myChtPimpleCentralFoam' is up to date.
[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

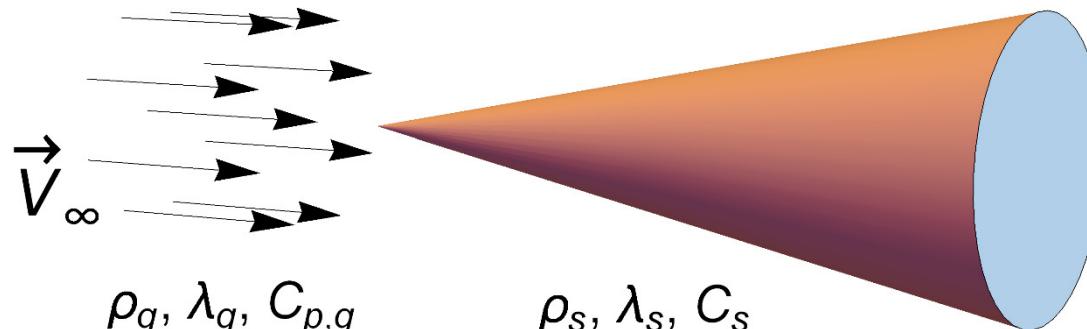
$$V_{g,\infty} = 750 \text{ m/s}$$

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

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

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

Viscosity model - Sutherland



$$\rho_g, \lambda_g, C_{p,g}$$

$$\rho_s, \lambda_s, C_s$$

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

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

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

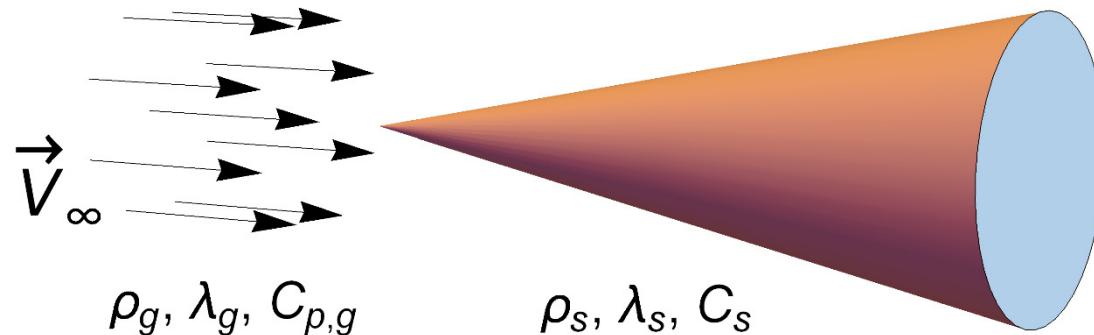
$$C_{p,g} = 600 \text{ J/(kg} \cdot \text{K)}$$

RAS simulation – k-w SST turbulence model

<https://github.com/unicfdlab/TrainingTracks/tree/master/OpenFOAM/gasThermoCoupled-OF4.1/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
 $\text{\$FOAM_APPBIN} \longrightarrow \text{\$FOAM_USER_APPBIN}$
- 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: ~ 35 W
- for turbulent case: ~ 1000 W