Combustion Modeling

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Outline of the presentation

Basic shell commands

command name	action
pwd	show the current directory
ls	show the files in the current directory
cd *<a1>*	change directory to the specified one
mkdir *<a1>*	make a new directory
cp *<a1>* *<a2>*	copy the file *<a1>* and paste it as *<a2>**
mv *<a1>* *<a2>*	cut the file *<a1>* and paste it as *<a2>**
rm *<a1>*	delete *<a1>* *
cat *<a1>*	show the content of *<a1>*
grep *<a1>*<a2>	check if *<a1>* is in file *<a2>*

Unix bashrc

- The .bashrc file is a script file that's executed when a user logs in. In such file some configurations are prescribed.
- Environment variables defines addresses to directories of interest
- Aliases are shortcut for long commands.

Let's now load the OpenFoam Environment using the "source" command.

```
source /path/etc/bashrc
```

Unix

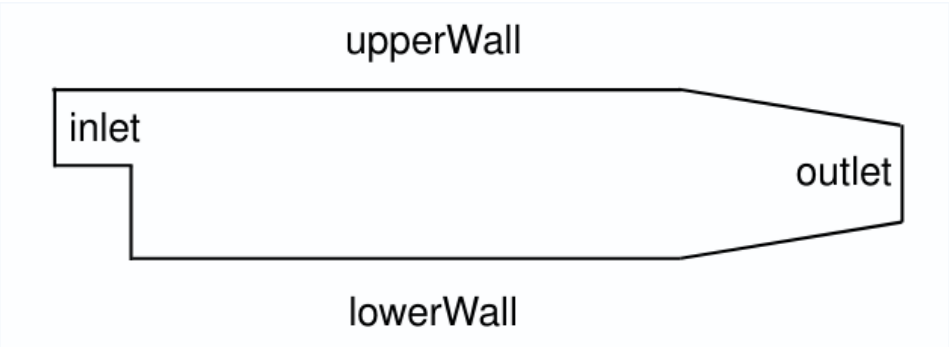
Any Questions?

Pitz - Daily Test case

- Copy the directory to your workspace
- Visit the new directory
- Take a look to what is inside

```
cp $FOAM_TUTORIALS/incompressible/simpleFoam/pitzDaily .
cd pitzDaily
ls
```

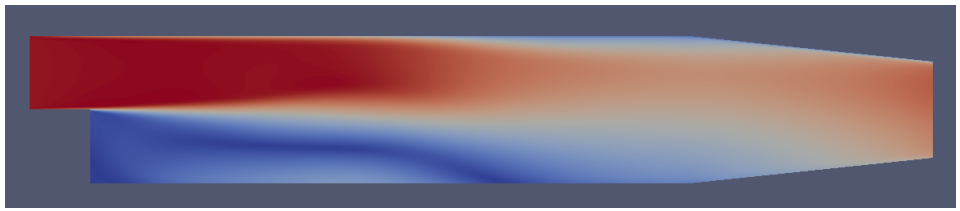
- **0** Initial and boundary conditions
- **constant** Physical properties.
- **system** Numerical settings



Pitz - Daily Test case

- Create the domain mesh
- Run the simulation
- Check the results using ParaView

```
blockMesh
simpleFoam
paraFoam -builtin
```



Pitz - Daily Test case

Any Questions?

chemFoam

- Solver for chemistry problems, designed for use on single cell cases
- Test Cases
  - Simple gas phase reaction
  - H_2 combustion

Single gas Phase reaction

chem.inp

- The reactions occurring in our single cell model are:

$$A \xrightarrow{k_1} B$$

$$2A \xrightarrow{k_2} C$$

- Reaction rates are first and second order:

$$r_1 = k_1[A]$$

$$r_2 = k_2[A]^2$$

- Reaction rates are given in the by:

$$k_i = A_i T^{\beta_i} e^{-\left(\frac{E_i}{RT}\right)}$$

Single gas Phase reaction

therm.dat

- Temperature dependant physical properties must be provided:

$$C^o_{p,k}/R = \sum_{i=1}^{N=5} a_{i,k} T_k^{i-1}$$

$$H^o_k/RT_k = a_{1,k} + \frac{a_{2,k}}{2} T_k + \frac{a_{3,k}}{3} T_k^3 + \frac{a_{4,k}}{4} T_k^3 + \frac{a_{5,k}}{5} T_k^4 + \frac{a_{6,k}}{T_k}$$

$$S^o_k/R = a_{1,k} ln\left(T_k\right) + \frac{a_{2,k}}{2} T_k + \frac{a_{3,k}}{3} T_k^3 + \frac{a_{4,k}}{4} T_k^3 + \frac{a_{5,k}}{5} T_k^4 + a_{7,k}$$

Single gas Phase reaction

Simulations settings

- Initial Conditions are specified in terms of reactants mole fractions, pressure and temperature.

$$A = 1; \qquad B = 0; \qquad C = 0; \qquad N_2 = 3.76;$$

$$p = 202650 \quad [Pa]$$

$$T = 630 \quad [K]$$

- Simulations settings such as the physical time simulated and numerical time-steps are given in the *controlDict* file.

$$t_{end} = 2 \cdot 10^{-3} \quad [s]; \qquad dt = 2 \cdot 10^{-5}$$

Single gas Phase reaction

Run - Results observation

- Run the simulation

```
./Allrun
```

- Temperature evolution available in *chemFoam.out*
- Some other quantities are available in the 0* directories
- Plot some results!

H_2 Combustion

Marinov et al.

- The detailed combustion mechanism follows the Marinov et al. findings

```
// H2-O2 chain reactions
   OH+H2=H+H2O              2.14E+08  1.52  3449.0
   O+OH=O2+H                2.02E+14  -0.4     0.0
   O+H2=OH+H                5.06E+04  2.67  6290.0
// Formation and consumption of HO2
   H+O2(+M)=HO2(+M)         4.52E+13  0.0      0.0
   H+O2(+N2)=HO2(+N2)       4.52E+13  0.0      0.0
   H+O2(+H2)=HO2(+H2)       4.52E+13  0.0      0.0
   LOW / 1.52E+19  -1.133    0.0 /
   H+O2(+H2O)=HO2(+H2O)     4.52E+13  0.0      0.0
   LOW / 2.10E+23  -2.437    0.0 /
   OH+HO2=H2O+O2            2.13E+28 -4.827 3500.0
   OH+HO2=H2O+O2            9.10E+14  0.0   10964.0
```

```
// Formation and consumption of H2O2
   HO2+HO2=H2O2+O2          4.20E+14  0.0 11982.0
   HO2+HO2=H2O2+O2          1.30E+11  0.0 -1629.0
   OH+OH(+M)=H2O2(+M)       1.24E+14 -0.37    0.0
   H2O2+H=HO2+H2            1.98E+06  2.0  2435.0
   H2O2+H=OH+H2O            3.07E+13  0.0  4217.0
   H2O2+O=OH+HO2            9.55E+06  2.0  3970.0
   H2O2+OH=H2O+HO2          2.40E+00 4.042 -2162.0
// H2-O2 dissociation/Recombination reactions
   H+HO2=H2+O2              8.45E+11  0.65 1241.0
   O+HO2=O2+OH              3.25E+13  0.0     0.0
   H+H+M=H2+M               1.00E+18 -1.0     0.0
   H+H+H2=H2+H2             9.20E+16 -0.6     0.0
   H+H+H2O=H2+H2O           6.00E+19 -1.25    0.0
```

- Study the evolution of such system by varying some initial conditions (temperature and pressure).