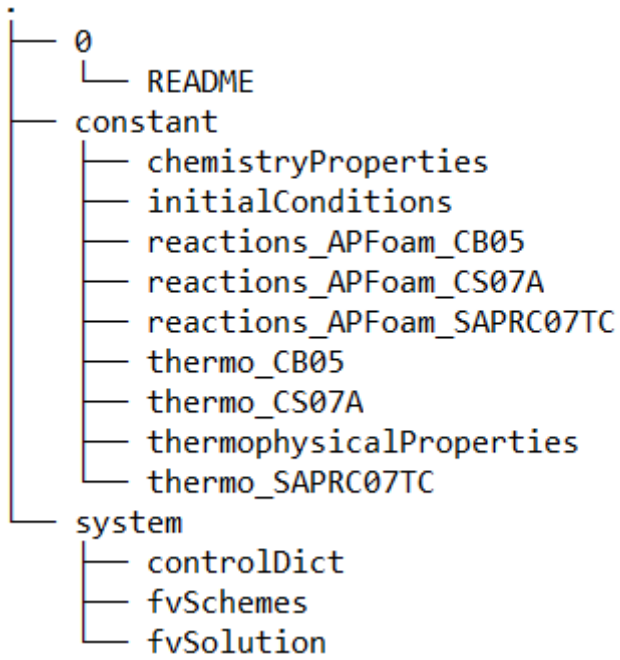
APFoam Tutorial

1. Introduction

This tutorial maninly focus on introducing the usage of APFoam. The aim of the tutorial is to understands how to setup and run a simple case with APChemFoam and APreacingFoam (consistent with APonlyChemReactingFoam and APSteadyReactingFoam). Since the APFoam is based on the OpenFOAM, the process of setting up a simulation case is similar to OpenFOAM settting. If the problems or setups are not mentioned in this tutorial, users can further check the OpenFOAM user guide to find the detailed descriptions and solutions.

2. APChemFoam

APChemFoam is a solver only concerns the chemical concentration and reaction heat variation during simulation, and calculations are started from initial conditions within a single cell mesh.
The files included in a typical case are as follows:
(see the APFoam/APFoam_tutorials/APChemFoam/)



2.1 Setting up the chemistry properties:

chemistryProperties: chemistry solver option
initialConditions: the initial concentration of species
thermophysicalProperties: the thermoType of the chemistry

The chemistry mechanism is set in *thermophysicalProperties*:

```
chemistryReader foamChemistryReader;
foamChemistryFile "$FOAM_CASE/constant/reactions_APFoam_CB05";
foamChemistryThermoFile "$FOAM_CASE/constant/thermo_CB05";
```

These two files is the chemistry mechanism files setting in *thermophysicalProperties*. If the user want to change the mechanism, please change these file paths. All the mechanism files are placed in the *constant/* folder in the simulation case folder.

2.2 Setting up the numerical properties:

controlDict: suimulation time setting (including time step, start time, end time, output interval time, etc.)

fvSchemes: discretisation schemes used in the solution may be selected at run-time

fvSolution: the equation solvers, tolerances and other algorithm controls are set for the run

2.3 Running the APChemFoam

After well preparing the files and setting, enter

APChemFoam

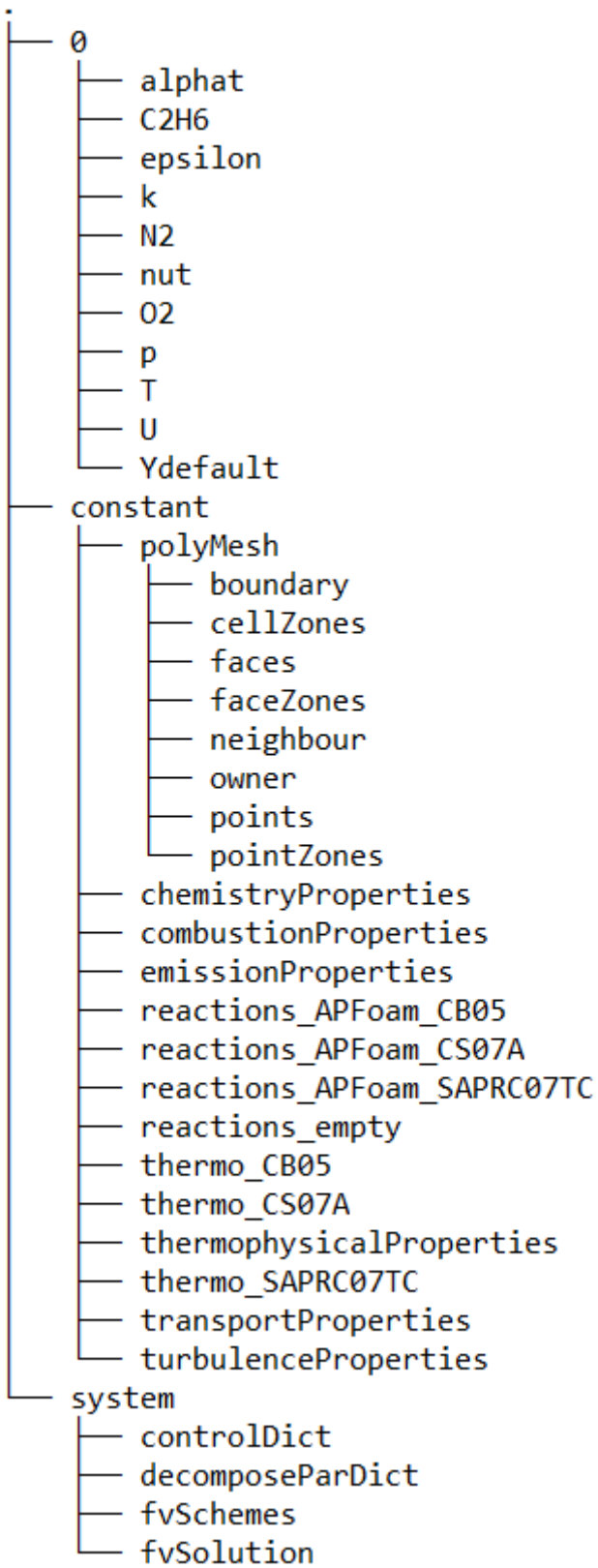
in the command line to run the simulation. The results will be saved in the "Time" folders. The name of these "Time" folders are the output interval time which is set in the *controlDict*.

3. APreactingFoam

APreactingFoam is a solver that solving the flow field, chemical reaction and pollutant dispersion simultaneously in the same time step in 2D or 3D simulation case.

The files included in a typical case are as follows:

(see the APFoam/APFoam_tutorials/APReactingFoam/)



3.1 Setting up the Mesh:

In the simulation case folder, the mesh is saved in the *constant/polyMesh*. The mesh files can be generated use the *blockMesh* tool in OpenFOAM which can be referred in the OpenFOAM user

guide. Additionally, The mesh files can be generated from *.msh format by *fluent3DMeshToFoam*. This tool can conver the mesh made by Fluent, Gambit, etc to the OpenFOAM format.

3.2 Setting up the initial and boundary condition:

In the 2D or 3D simulation, the initial and boundary condition including turbenlence parameter and species concentration is set in the "0" folder. Typeically, each parameter should have a corresponding file. *Ydefaults* is the file that declares the concentration of species when there is no corresponding file in the "0" folder.

3.3 Setting up the emission properties:

In *emissionProperties*, the number of emission source region, the coordinate and emission quantity (in the unit of kg/s) for each species can set in this file. The region or species which are not declared is set as 0.

3.4 Setting up the chemistry and turbulence properties:

chemistryProperties: chemistry solver option
thermophysicalProperties: the thermoType of the chemistry
transportProperties: specifying the algorithm of kinematic viscosity
turbulenceProperties: specifying the turbulence model in the simulation

3.5 Setting up the numerical properties:

controlDict: suimulation time setting (including time step, start time, end time, output interval time, etc.)
fvSchemes: discretisation schemes used in the solution may be selected at run-time
fvSolution: the equation solvers, tolerances and other algorithm controls are set for the run
decomposeParDict: the decomposition setting for the parallel run.

3.6 Running the APReactingFoam in single core

After well preparing the files and setting, enter
APreactingFoam
in the command line to run the simulation. The results will be saved in the "Time" folders. The name of these "Time" folders are the output interval time which is set in the *controlDict*.

3.7 Running the APReactingFoam in parallel

After well preparing the files and setting, enter

decomposePar	(decompose the mesh and fields)
APreactingFoam -parallel	(run the solver in parallel)
reconstructPar	(reconstruct the mesh and fields)

in the command line to run the simulation. After typing *reconstructPar*, the results will be saved in the “Time” folders. The name of these “Time” folders are the output interval time which is set in the *controlDict*.