Automatic case setup with pyFoamPrepareCase

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Outline I

Outline II

Outline

Outline

Purpose of this presentation

- Give an overview of `pyFoamPrepareCase.py`
  - A utility to help set up cases
    - Part of `pyFoam` for over 3 years
  - Not a GUI but something better: a flexible way to script cases

Intended audience

- People who have experience with OpenFOAM
  - Editing the dictionaries should not be a problem
- Worked a little with `pyFoam`
- Are lazy: Don't enjoy doing the same work over and over again
- Are not afraid of a little programming
  - But only a very little bit

History of the presentation

- This is the second version of this presentation
  - It was first held 2015 at the Workshop in Ann Arbor
- Surprisingly little had to be changed
  - All changes were about changes in OpenFOAM
  - None of them because of changes in `pyFoamPrepareCase.py`
- This is good
  - New versions of `PyFoam` don't break existing cases
- Goal with this utility is to only enhance it
  - ... without *breaking* it

Outline

Bernhard Gschaider

- Working with OpenFOAM™ since it was released
  - Still have to look up things in `Doxygen`
- I am not a core developer
  - But I don't consider myself to be an *Enthusiast*
- My involvement in the OpenFOAM™-community
  - Janitor of the `openfoamwiki.net`
  - Author of two additions for OpenFOAM™

    swak4foam Toolbox to avoid the need for C++-programming

    PyFoam Python-library to manipulate OpenFOAM™ cases and assist in executing them
  - In the admin-team of `foam-extend`
  - Organizing committee for the OpenFOAM™ *Workshop*
- The community-activies are not my main work but *collateral damage* from my real work at ...

Heinemann Fluid Dynamics Research GmbH

The company

- Subsidary company of *Heinemann Oil*
  - Reservoir Engineering
  - Reservoir management

Description

- Located in Leoben, Austria
- Works on
  - Fluid simulations
    - OpenFOAM™ and Closed Source
  - Software development for CFD
    - mainly OpenFOAM™
- Industries we worked for
  - Automotive
  - Processing
  - ...

Outline

Command line examples

- In the following presentation we will enter things on the command line. Short examples will be a single line (without output but a ">" to indicate *input*)

```
> ls $HOME
```

- Long examples will be a white box
  - Input will be prefixed with a > and blue
  - Long lines will be broken up
    - A pair of <brk> and <cont> indicates that this is still the same line in the input/output
  - «snip» in the middle means: "There is more. But it is boring"
    - Alternatively there are 3 dots

```
> this is an example for a very long command line that does not fit onto one line of the slide but we <brk>
      <cont>have to write it anyway
first line of output (short)
Second line of output which is too long for this slide but we got to read it in all its glory
```

How to follow this presentations

- All information to reproduce the results is on the slides
  - Assumes that you have an OpenFOAM v1712+ installation
    - Later we need a foam-extend 4.1 installation
- There is a file with the different stages on the Wiki
  - You can download and untar it in a convenient location

```
> cd work
> wget https://openfoamwiki.net/images/d/d6/PyFoamPrepare_Shanghai2018_Material.tar.gz
> tar xvzf PyFoamPrepare_Shanghai2018_Material.tar.gz
stage0_originalCase.tar.gz         stage5_coarseMesh.tar.gz
stage10_parameterVariation.tar.gz  stage6_meshCreate.tar.gz
stage1_addedCustomRegexp.tar.gz    stage7_initPotential.tar.gz
stage2_templateParameters.tar.gz   stage8_extendCoupled.tar.gz
stage3_rhoSimpleFoam.tar.gz        stage9_parallel.tar.gz
stage4_plotlines.tar.gz
```

Docker image with pre-installed PyFoam and swak4Foam

- Docker is a technology to run pre-packed containers based on Linux
  - Can be run on Linux, Windoze and Mac OS X
  - Saves the work of installing requirements and compiling software
    - Only docker is needed (see `https://www.docker.com/`)
    - Image downloads may be rather big
- There is a container maintained by the author
  - Based on the official ESI OpenFOAM v1712+ docker image
  - Most recent release of PyFoam
  - A development version of swak4Foam
- For installation instructions the README at `https://bitbucket.org/bgschaid/swak4foamandpyfoamdockerfile/src/default/`

Outline

Format of the cases

- OpenFOAM-cases are directories with files
  - "The filesystem is the database"
- Basic structure are key / value dictionaries
- Quite old
  - But the current plain-text formats in use (`XML`, `JSON`, `YAML`) have no functional advantage
    - Whether they are easier to read or edit is subjective (we can have an emotional discussion about this during the social part of the Workshop)
    - "The OpenFOAM file format was XML before XML was mainstream"
- Advantages of the format:
  - Human-readable (self-documenting)
  - Order is not important
    - Unused information is ignored
- Disadvantages:
  - Huge number of files in a case (problem of the sysadmin)
  - Special cases (`boundary`-file) and not always unambiguous

Enhancements of the format

During the years the format got a number of enhancements that

- increased readability
- decreased the amount of redundancy

Those were:

regular expressions Allows specifying similar keys only once
- Common use: boundary conditions

#include pull in another file
- Common use: Setting "standard" conditions

macro substitution with $ insert dictionary entries in different places
- Common use: `$internalField` in boundary conditions

Limitations of the data format

What the format can not do

- Conditions
  - "If we're using this solver use this setting. Otherwise the other one"
- Iterations
  - "Insert 20 STL-files into this `snappyHexMeshDict`"

But that is OK. It's a data format. Not a programming language

Current case setup (non-GUI)

- Manually calling the utilities
  - Tedious
  - Can lead to errors
- Scripts (for instance `Allrun`)
  - Parameter files are modified by `sed` or `awk` (if they are)
    - Not very flexible
    - Only textual replacements in the files

`pyFoamPrepareCase.py` tries to make this more flexible and robust

Outline

What is PyFoam

- PyFoam is a library for
  - Manipulating OpenFOAM-cases
  - Controlling OpenFOAM-runs
- It is written in Python
- Based upon that library there is a number of utilities
  - For case manipulation
  - Running simulations
  - Looking at the results
- All utilities start with pyFoam (so TAB-completion gives you an overview)
  - Each utility has an online help that is shown when using the -help-option
  - Additional information can be found
    - on openfoamwiki.net
    - in the two presentations mentioned above

Case setup

- Cloning an existing case

```
> pyFoamCloneCase.py $FOAM_TUTORIALS/incompressible/simpleFoam/pitzDaily test
```

- Decomposing the case

```
> blockMesh -case test
> pyFoamDecompose.py test 2
```

- Getting info about the case

```
> pyFoamCaseReport.py test --short-bc --decomposition | rst2pdf >test.pdf
```

- Clearing non-essential data

```
> pyFoamClearCase.py test --processors
```

- Pack the case into an archive (including the last time-step)

```
> pyFoamPackCase.py test --last
```

- List all the OpenFOAM-cases in a directory (with additional information)

```
> pyFoamListCases.py .
```

Running

- Straight running of a solver

```
> pyFoamRunner.py interFoam
```

- Clear the case beforehand and only show the time

```
> pyFoamRunner.py --clear --progress interFoam
```

- Show plots while simulating

```
> pyFoamPlotRunner.py --clear --progress interFoam
```

- Change `controlDict` to write all time-steps (afterwards change it back)

```
> pyFoamRunner.py --write-all interFoam
```

- Run a different OpenFOAM-Version than the default-one

```
> pyFoamRunner.py --foam=1.9-beta interFoam
```

- Run the debug-version of the current version

```
> pyFoamRunner.py --current --force-debug interFoam
```

Generated files

- Typically PyFoam generates several files during a run (the names of some of those depend on the case-name)

  case.foam Stub-file to open the case in ParaView

  PyFoamRunner.solver.logfile File with all the output that usually goes to the standard-output

  PyFoamRunner.solver.analyzed Directory with the results of the output analysis

    pickledPlots A special file that stores all the results of the analysis

  PyFoamHistory Log with all the PyFoam commands used on that case

Plotting

- Any logfile can be analyzed and plotted

```
> pyFoamPlotWatcher.py --progress someOldLogfile
```

- A number of things can be plotted
  - Residuals
  - Continuity error
  - Courant number
  - Time-step
- User-defined plots can be specified
  - Specified in a file `customRegexp`
  - Data is analyzed using regular expressions
  - We will see examples for this later
- The option `--hardcopy` generates pictures of the plots

What else can PyFoam do for me?

- Write and read dictionaries from the command line
- Display the `blockMeshDict`
- Generate plots of Surfaces and sample lines
- Interact with paraView
- Control OpenFOAM-runs over the net

Outline

The pitzDaily-tutorial

- One of the most popular tutorial cases in OpenFOAM
  - Used for a number of different solvers
- Backward-facing step
  - Described in a paper by *Pitz and Daily* with measurement data

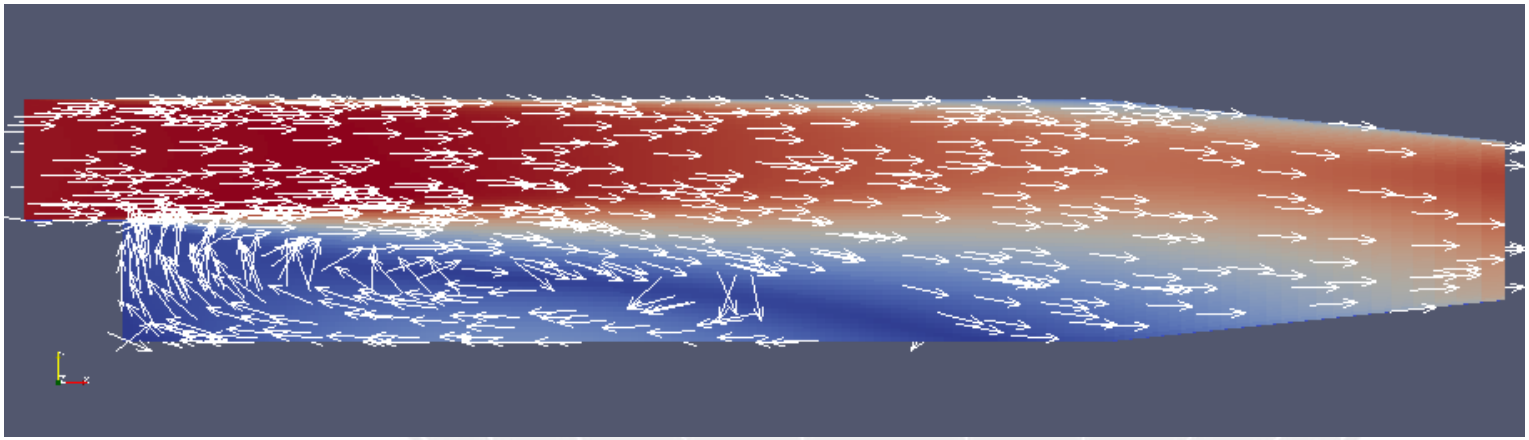


Figure: The pitzDaily-case

Measurement data on the case

From the original paper

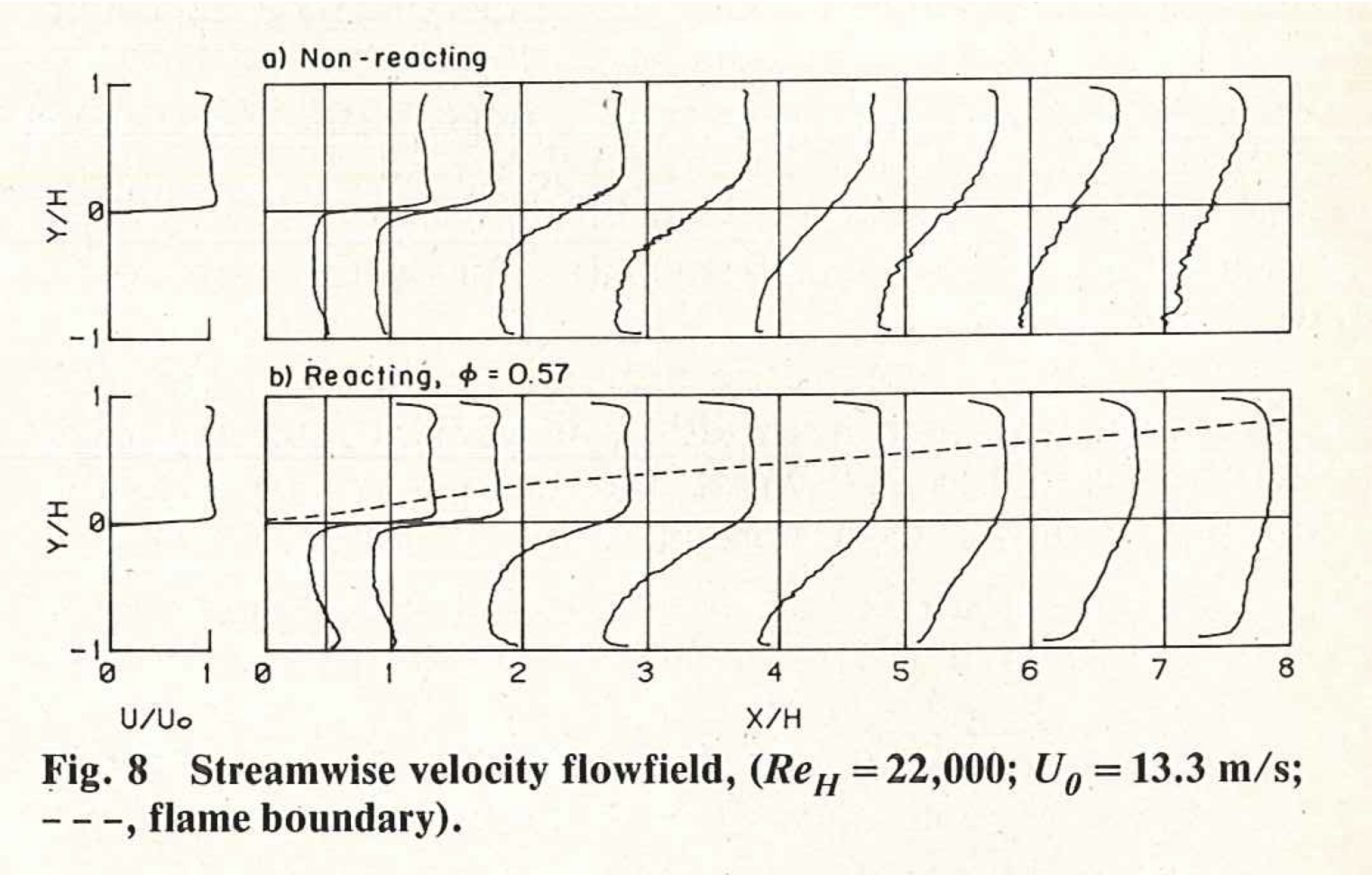


Fig. 8 Streamwise velocity flowfield, ($Re_H = 22{,}000$; $U_0 = 13.3$ m/s; – – –, flame boundary).

What we want to do with the case

- Modify the case so that we can compare
  - Different meshing strategies
  - Solvers
  - (Open)FOAM-versions
  - Influence of initial conditions
- In the end we want to be able to say "Set up the case with a coarse grid so that it runs with the coupled solver from `extend`. Go"
  - All from the same set of case-files

Outline

Outline

Getting the base case

- Make sure we use the same version

```
> . ~/OpenFOAM/OpenFOAM-v1712/etc/bashrc
```

- Go to a common place and create our own workspace

```
> cd $HOME
> mkdir pitzDailyWithMod
> cd pitzDailyWithMod
```

- Get the files from the original case

```
> cp -r $FOAM_TUTORIALS/incompressible/simpleFoam/pitzDaily/* .
```

Preparing it

- This is our first use of the utility
  - We didn't prepare the case for it

```
> pyFoamPrepareCase.py .
```

- A lot stuff is written to the terminal
  - Stuff about "looking for `template`-files"
    - Later we'll understand what this means
- `blockMesh` is automatically run
  - Because the utility found a `blockMeshDict`
    - The utility tries to be clever
    - ... but not too clever

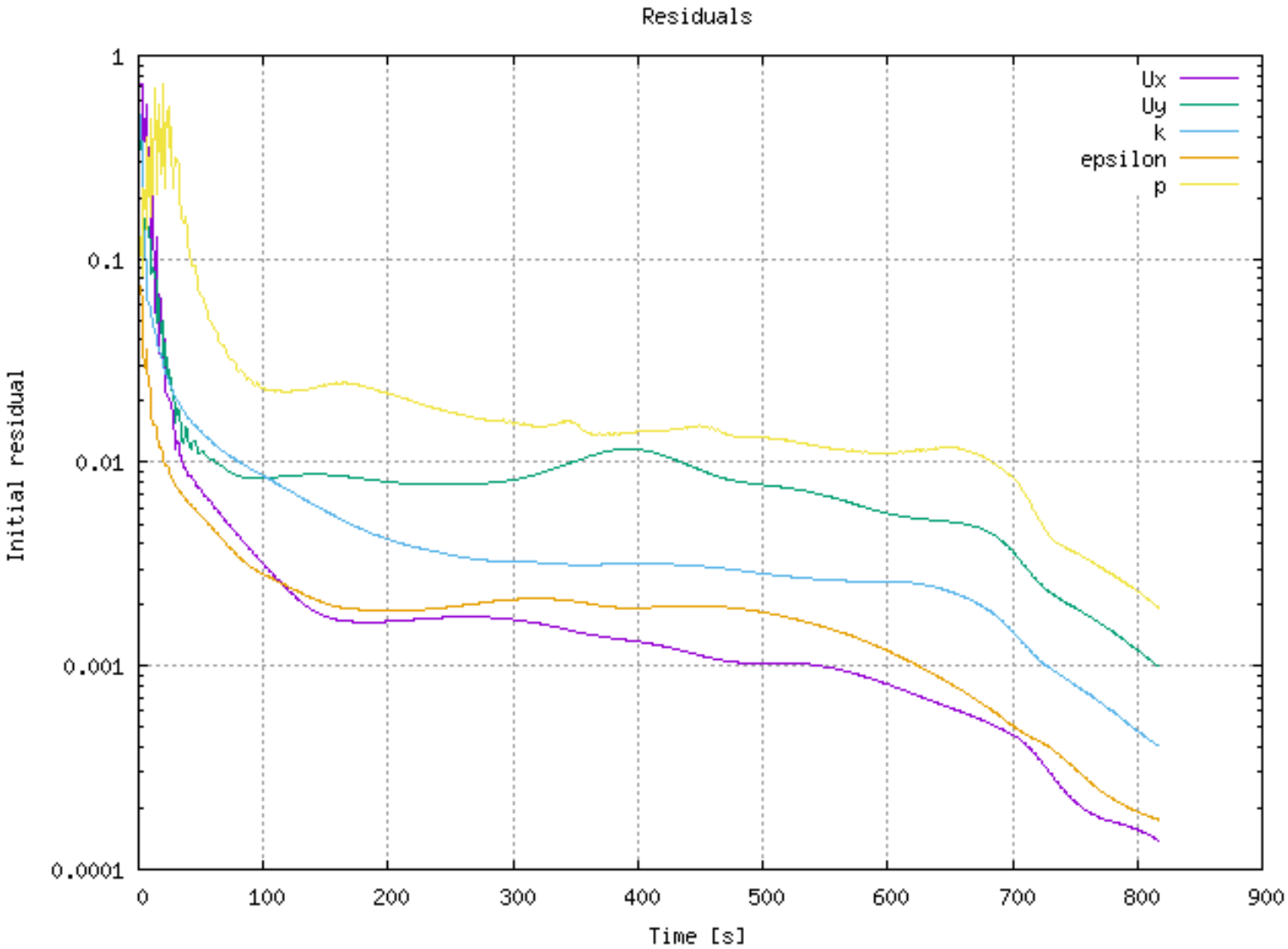
Running

- The case is now ready to run
  - So we'll run it

```
> pyFoamPlotRunner.py --clear --progress --hardcopy --prefix=baseline simpleFoam
Clearing out old timesteps ....
Duration of pickling 0.04135417938232422 too long. Extending frequency from 1.0 to <brk>
      <cont>2.067708969116211
 t =        817
  29.02s user 1.53s system 91% cpu 33.505 total
```

- This pops up some windows with residuals etc
  - We generated hardcopies for later reference

Residuals


Residuals
Initial residual
Time [s]
Ux
Uy
k
epsilon
p
1
0.1
0.01
0.001
0.0001
0
100
200
300
400
500
600
700
800
900

Spawn point

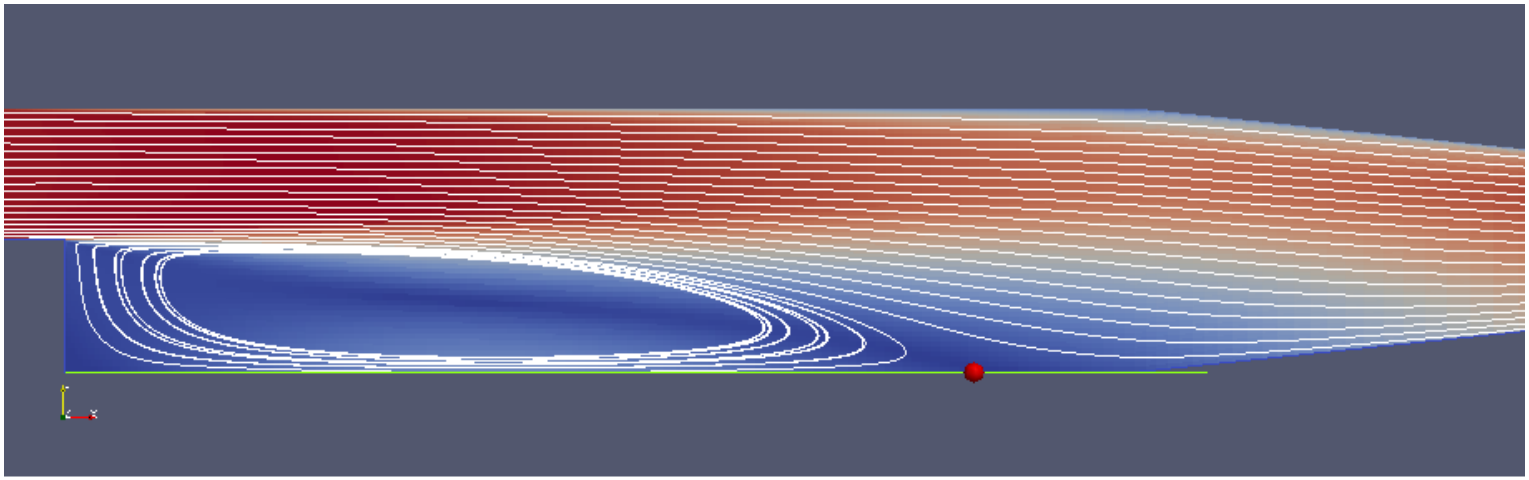
To get to the current state use `stage0_originalCase.tar.gz`

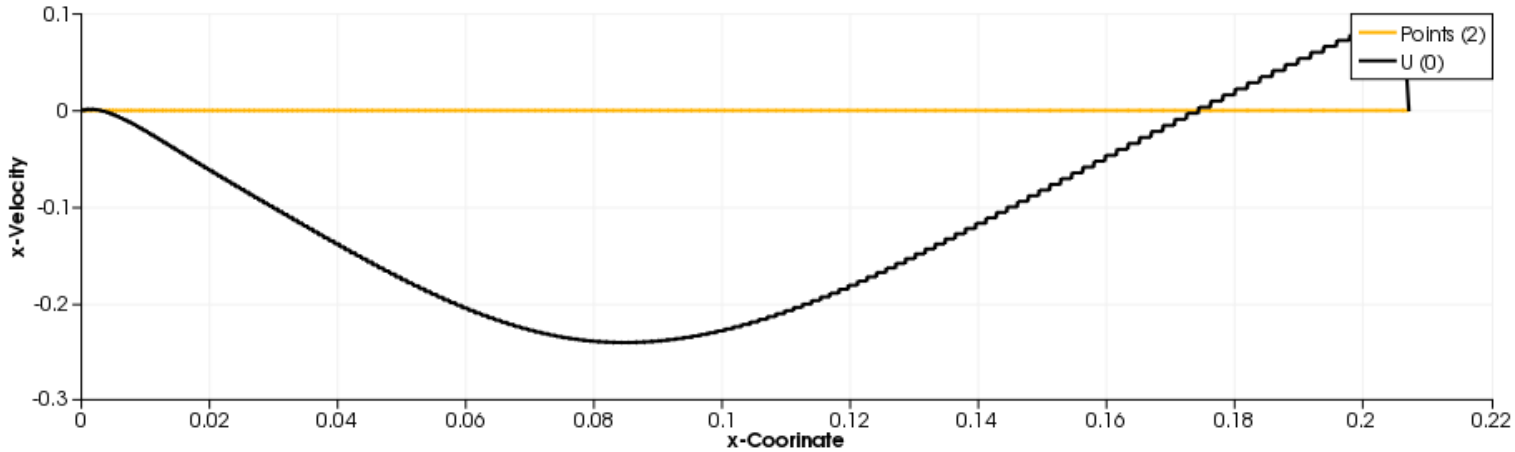
Adding a little

- Numerical convergence is not everything
  - Especially as the convergence criteria we use are quite low
    - But they were set that way in the tutorial
- To check how well converged the case is we add two evaluations
  1. Pressure difference between inlet and outlet
  2. The detachment point of the vortex behind the step
- We'll use `swak4Foam` to calculate these during the calculation

The detachment point

Definition: "Where the velocity over the lower wall becomes positive"





Adding swak-functionObjects

- Adding a few libraries to have the swak4Foam-functionality

controlDict

From now on a box (like this one) means "Add these files to the controlDict)

```
libs (
    "libsimpleSwakFunctionObjects.so"
    "libswakFunctionObjects.so"
    "libsampling.so"
);
```

Pressure difference

- Calculated by subtracting the average of the pressure on the two patches

controlDict in functions dictionary

```
pressureDiff {
    type patchExpression;
    patches (
        inlet
    );
    variables (
        "pOut{patch'outlet}=sum(p*area())/sum(area());"
    );
    accumulations (
        average
    );
    expression "p-pOut";
    verbose true;
}
```

Errata: this is the way it is done in the provided files. Probably using `weightedAverage` instead of `average` is more accurate

Find the detachment point

- On every face:
  - If the velocity is negative use the current position
  - Otherwise use a value "south" of the patch (-0.1)
- Get the maximum of all face-values (no pun intended)
  - This is the position of the detachment point
    - To be exact: half a face left of it ... but good enough

controlDict in functions

```
findPoint {
    type swakExpression;
    verbose true;
    valueType patch;
    patchName lowerWall;
    expression "internalField(U).x<0 ? pos().x : -0.1";
    accumulations (
        max
    );
}
```

Making PyFoam pick up the values

- swak4Foam writes the files to the console
  - We've got to tell PyFoam how to find them

customRegexp

```
deltaP {
        theTitle "Pressure difference";
        expr "Expression pressureDiff on inlet:  average=(%f%)";
        titles (avg);
        progress "dp: $0";
}
detatch {
        expr "Expression findPoint :  max=(%f%)";
        theTitle "Location of the detachment point";
        titles ( x );
        progress "detach: $0";
}
```

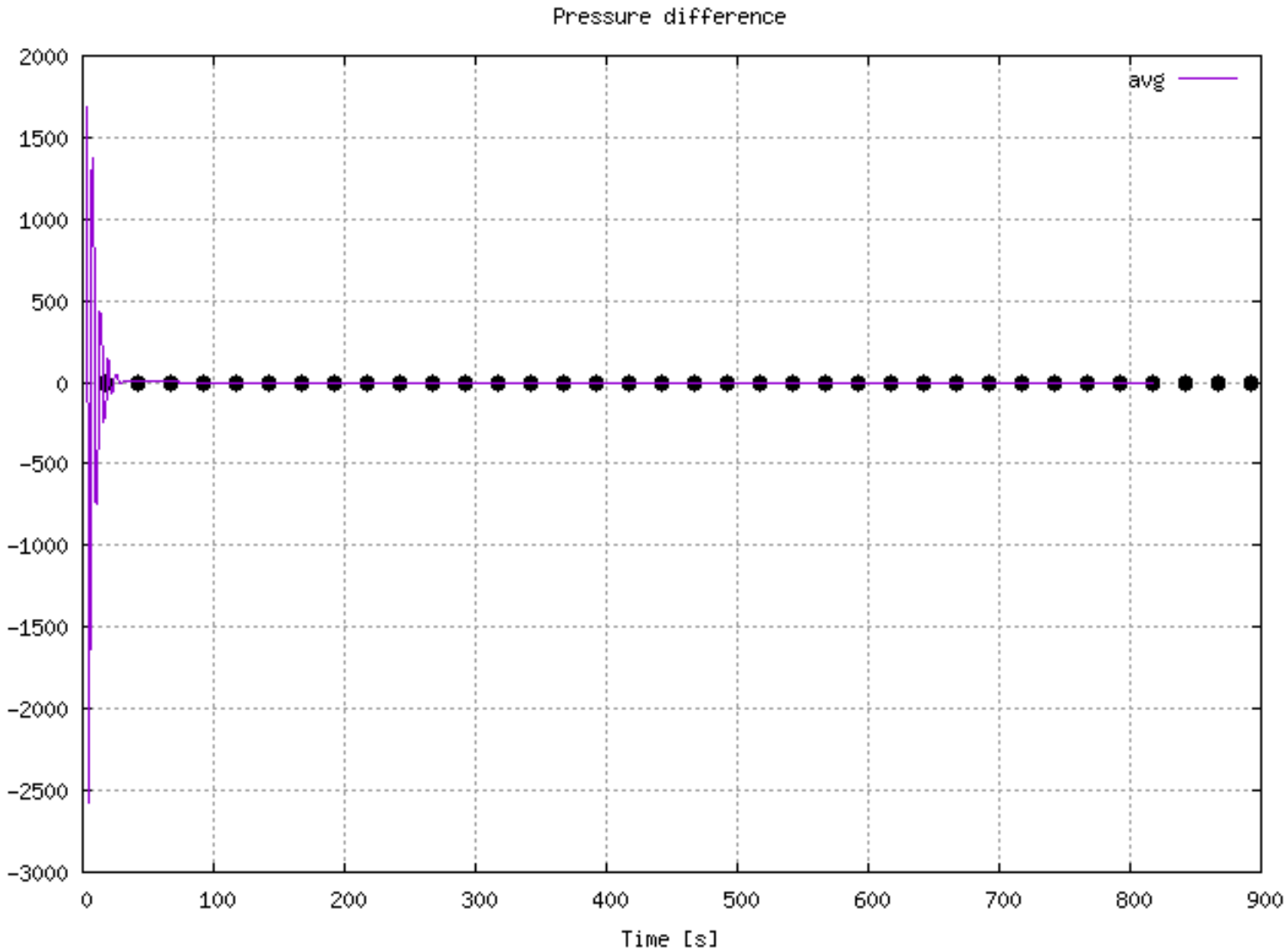
Re-running

- Now we re-run the case

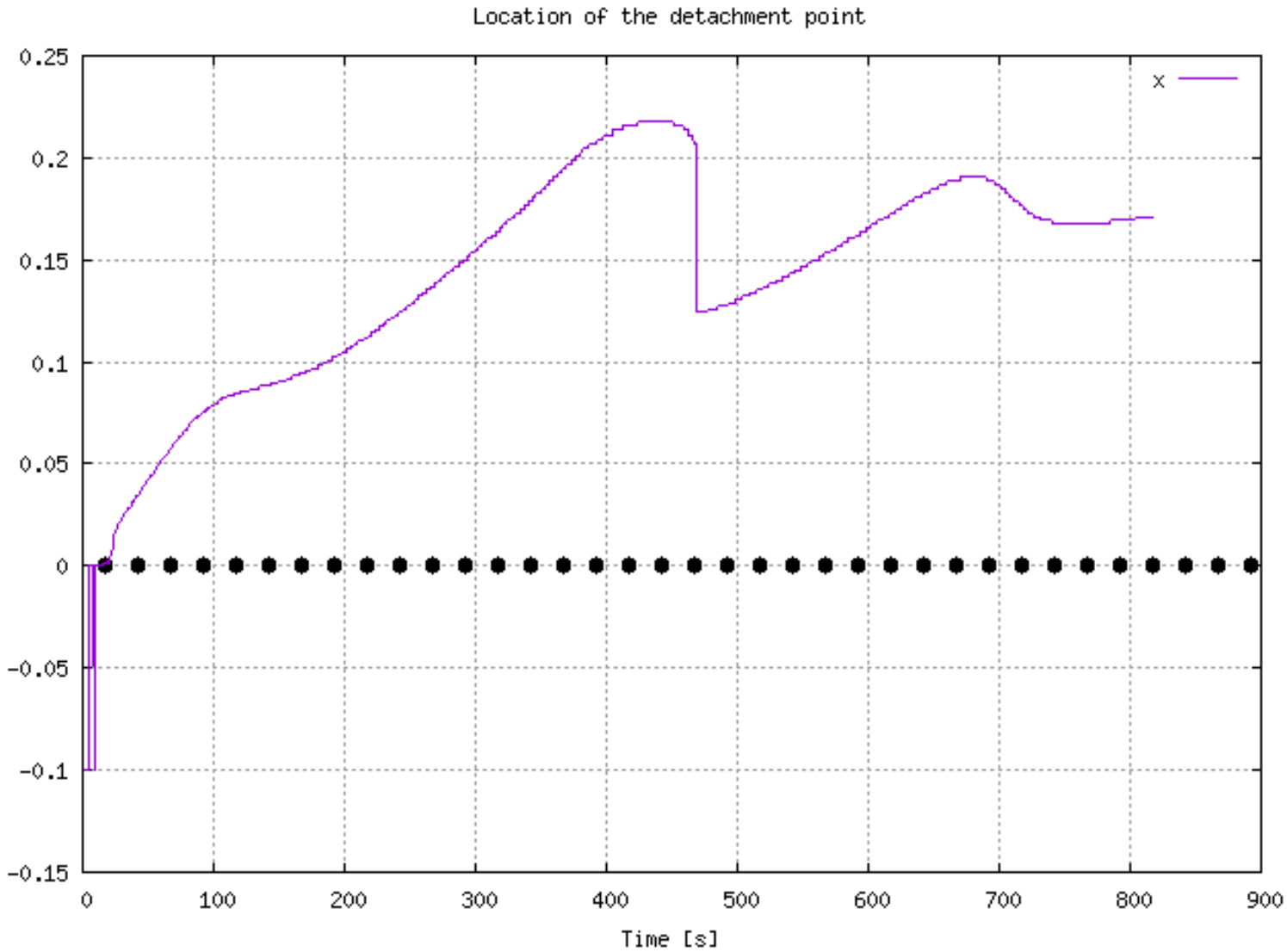
```
> pyFoamPlotRunner.py --clear --progress --hardcopy --prefix=baseline simpleFoam
 Reading regular expressions from /Volumes/Foam/Workshop2015/pitzDailyWorkshopStages/<brk>
       <cont>customRegexp
Clearing out old timesteps ....
 t =         817 dp: -4.63389 detach: 0.17127
```

- Needs the same amount of iterations
- Position and pressure difference are printed to the console
- We get nice plots of the evolution of these values

Pressure difference evolution



Evolution of the detachment point



Good enough

- Critique of the results
  - Pressure difference gets quite a kick in the beginning
    - This is typical for "unphysical" intial conditions
  - Detachment point still "searching for his destination" (this means: not converged)
  - Also: the numerical criteria (10^{-3}) are ... liberal
- But this is not the topic of this presentation
  - If you don't like the results: increase accuracy in `fvSolution` and rerun the examples

Spawn point

To get to the current state use `stage1_addedCustomRegexp.tar.gz`

Outline

Phases of pyFoamPrepareCase.py

pyFoamPrepareCase does these things (in this order):

1. Clear old data from the case
2. Look for template-files and create real files from them
3. Create a mesh
4. Copy *original* files
5. Expand postTemplate-files
6. Execute a script for setting up initial conditions
7. Finally expand finalTemplate-files

We'll talk about all these things. But not in that order

- New versions of PyFoam allow executing *decomposition scripts* after mesh generation and field setups
  - Because different mesh workflows need different decomposition strategies

Original files

- If `pyFoamPrepareCase.py` finds a file or directory with the extension `.org` it assumes that it should replace the extension-less file/directory with this
- We move the first time-step "out of the way"

```
> mv 0 0.org
```

- This makes sure that things we edit are not overwritten by OpenFOAM-utilities

Template files

- Files with the extension `.template` are handled by the Template engine built into PyFoam
  - Based on 3rd Party software (see below)
- Definition of *Template engine* in Wikipedia:
  - "A template processor (also known as a template engine or template parser) is a piece of software or a software component that is designed to combine one or more templates with a data model to produce one or more result documents."
  - In our context:

    piece of software PyFoam (concrete: the class `TemplateFile`)

    templates the `.template` files

    result documents the case files
- For testing the template engine we can use the `pyFoamFromTemplate.py`-utility
  - Will be used on the next slides

First evaluation

- Strings beween |- and -| are evaluated by Python
  - The string representation of the result is inserted into the *result document*
- Available functions:
  - The regular `builtin`-functions of Python
  - All functions from the `math` module

testfile.template

```
Sin(1) = |-sin(1)-|
```

Shell

```
> pyFoamFromTemplate.py --template-file=testfile.template --values-string="{}" --stdout
Sin(1) = 0.8414709848078965
```

Variables

- Variables are regular Python-variables
  - Primitive types: strings, number, booleans
  - Complex types: lists, dictionaries or objects
- Variables are usually set at the beginning
  - Can be used like regular global variables
- If a variable is used but has not been set the template evaluation fails
  - This can be changed: see online documentation for `--tolerant-expression-evaluation`
    - Usually not recommended

Adding a variable

- Now a variable `t` is used
- Variables can be passed to the utility (also `pyFoamPrepareCase.py`) with `--values-string`)
  - This string is in Python-syntax
    - Not the OpenFOAM-syntax like everything else
    - The `pyFoamPrepareCase.py` utility will accept OpenFOAM-syntax

testfile.template

```
Sin(|-t-|) = |-sin(t)-|
```

Shell

```
> pyFoamFromTemplate.py --template-file=testfile.template --values-string="{'t':1}" --<brk>
      <cont>stdout
Sin(1) = 0.8414709848078965
```

Local variables

- These variables are local to a template file
- Allow breaking up of complex evaluations
  - Remove redundancy if an expression is needed more than once in the file
- Declaration of variable is in a line that starts with $$
  - This line will be completely removed from the *result document*
- The variable can be used from the line at which it was declared till the end of the template

Storing an intermediate Result

testfile.template

```
$$ x=sin(t)
Sin(|-t-|) = |-x-| or |-sin(t)-|
```

Shell

```
> pyFoamFromTemplate.py --template-file=testfile.template --values-string="{'t':1}" --<brk>
      <cont>stdout
Sin(1) = 0.8414709848078965 or 0.8414709848078965
```

Assignments only

- In the usual syntax after `$$` only lines of the form `<value> = <expression>` are allowed
  - Other valid Python-lines (like `import os`) do not work
- A more general syntax can be switched on with `--allow-exec-instead-of-assignment`
  - This can also be switched on for a case in the `LocalConfigPyFoam`-file
- The reason why this is not switched on by default is for security concerns: Allowing general execution allows the template to do anything

Allowing execution

testfile.template

```
$$ import os
I am |-os.environ["USER"]-|

The machine: |-os.uname()-|
```

Shell

```
> pyFoamFromTemplate.py --template-file=testfile.template --values-string="{'t':1}" --stdout
 Error in /Users/bgschaid/Development/OpenFOAM/Python/PyFoam/bin/pyFoamFromTemplate.py : FatalError in<brk>
       <cont> PyFoam: 'PyFoam FATAL ERROR on line 130 of file /Users/bgschaid/private_python/PyFoam/<brk>
       <cont>Basics/TemplateFile.py: Each definition must be of the form: <name>=<value> The string $$ <brk>
       <cont>import os is not. Try running the utility with the option --allow-exec-instead-of-<brk>
       <cont>assignment'
> pyFoamFromTemplate.py --template-file=testfile.template --values-string="{'t':1}" --stdout --allow-<brk>
      <cont>exec
I am bgschaid

The machine: posix.uname_result(sysname='Darwin', nodename='bgs-cool-greybook', release='14.3.0', <brk>
      <cont>version='Darwin Kernel Version 14.3.0: Mon Mar 23 11:59:05 PDT 2015; root:xnu-2782.20.48~5/<brk>
      <cont>RELEASE_X86_64', machine='x86_64')
```

What can be done between pipes

- Between |- and -| almost any regular Python-expression can be used
  - This includes *list comprehension* and *string formatting*
  - You can check on the Python-shell whether things work the way you think they should
- |- / -| can be inside a string of the template file
  - Will be replaced
  - No need to escape the " if the Python-expression needs a string
    - Hint: " and ' can be used interchangeably in Python. So there is almost never a need to escape strings (see above uses of `--values-string`)

Roles of " and '

- In

```
--values-string="{'t':1}"
```

the roles are

" " This is for the shell: "I'm only one argument. And don't try to interpret the {}"

' ' This is for Python: "I am a string"

- How the string is interpreted can be always checked in Python:

Python-shell

```
> python
Python 3.4.3 (default, May 25 2015, 18:48:21)
[GCC 4.2.1 Compatible Apple LLVM 6.0 (clang-600.0.56)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> {'t':1}
{'t': 1}
>>>
```

Nice Python-tricks

testfile.template

```
$$ import os
The machine reformatted: |-",␣".join(os.uname())-|
Sum of squares: |-sum([i*i for i in range(100)])-|
Formatted: |-"%015.7E" % pi-|
$$ from os import path
Build path: |-path.join("theCase","system","controlDict")-|
```

Shell

```
> pyFoamFromTemplate.py --template-file=testfile.template --values-string="{'t':1}" --<brk>
      <cont>stdout --allow-exec
The machine reformatted: Darwin, bgs-cool-greybook, 14.3.0, Darwin Kernel Version 14.3.0: <brk>
      <cont>Mon Mar 23 11:59:05 PDT 2015; root:xnu-2782.20.48~5/RELEASE_X86_64, x86_64
Sum of squares: 328350
Formatted: 003.1415927E+00
Build path: theCase/system/controlDict
```

The .template-files

This is waht pyFoamPrepareCase.py does with them

- The case is searched recursively for .template-files
  - Each found file is evaluated as a template
  - The *result document* is saved under the same filename without the extension
    - If a file of that name was present it is overwritten
- The same set of variables is used for all templates

Setting the velocity

We now want to select the inlet velocity

1. Make the original velocity file a template

```
> mv 0.org/U 0.org/U.template
```

1. Replace 10 with a template expression

0.org/U.template

```
boundaryField
{
    inlet
    {
        type            fixedValue;
        value           uniform (|-UIn-| 0 0);
    }
```

Preparing the case

The output of pyFoamPrepareCase.py starts with list of the used variables

```
> pyFoamPrepareCase.py . --value="{'UIn':10}"
Looking for template values .
Updating values {'UIn':10}
 Warning in /Users/bgschaid/Development/OpenFOAM/Python/PyFoam/bin/pyFoamPrepareCase.py : <brk>
       <cont>Values for which no default was specified: UIn

Used values

              Name - Value
-----------------------------------------
               UIn - 10
          caseName - "pitzDailyWorkshopStages"
          casePath - "/Volumes/Foam/Workshop2015/pitzDailyWorkshopStages"
          foamFork - openfoam
       foamVersion - 2.4.x
numberOfProcessors - 1

No script ./derivedParameters.py for derived values
Clearing .
Writing parameters to ./PyFoamPrepareCaseParameters
...
```

Python-format is "old school"

- Old versions of `pyFoamPrepareCase.py` only supported Python-format for `--value`

```
pyFoamPrepareCase.py . --value="{'UIn':10}"
```

- Current versions support a more "foamy" format
  - Looks like an excerpt from a dictionary
    - The semicolon is important

```
pyFoamPrepareCase.py . --value="UIn 10;"
```

- The utility will try both formats
  - Use the one that works

Pre-defined values

Some variables are automatically defined:

casePath full file-system path to the current case

caseName name of the case. Last component of `casePath`

foamVersion version of the currently used (Open)FOAM installation

- a Python-tuple

foamFork which fork of FOAM this is (usually `openfoam` or `extend`)

numberOfProcessors On how many processors the case is going to be run

- Can be set with the `--number-of-processors`-option

Parameter files

- With many parameters using only `--values-string` would be tedious
- Variable values can be collected in parameter files
  - The syntax of these files is: regular OpenFOAM-dictionaries
    - No header necessary
    - Alert: Not Python-syntax like `--values-string`. This sometimes confuses people
- Multiple parameter files can be read
  - If there are multiple values for a variable: the last one wins
  - Values from `--values-string` overrule all

Default parameters

- If a file `default.parameters` is found in the case it is used first
  - Sets the default values for all parameters
- With the following file this is sufficient:

```
> pyFoamPrepareCase.py .
```

`default.parameters`

```
UIn 10;
```

Structured `default.parameters`

- `default.parameters` is special as it allows structuring the variables
  - This structuring is only for documentation purposes. It has no effect during replacement
- If a dictionary with the entries `description` and `values` is found it is assumed that this is a group of variables
  - Groups can be nested
- A dictionary with the entries `description` and `default` is assumed to be a verbose variable declaration
- Other dictionaries are assumed to be "real" dictionaries

Adding documentation

We now rewrite `default.parameters` with documentation on the variable

- Completely equivalent to the previous form
  - But more informative

`default.parameters`

```
boundary {
    description "Boundary conditions";
    values {
        UIn {
            description "Inlet velocity";
            default 10;
        }
    }
}
```

Slow inlet

pyFoamPrepareCase.py reports if a value was changed from the default value:

```
>  pyFoamPrepareCase.py . --value="UIn 5;"
Using default values from /Volumes/Foam/Workshop2015/pitzDailyWorkshopStages/default.<brk>
      <cont>parameters
Looking for template values .
Updating values {'UIn':5}

Used values

              Name - Value
-----------------------------------------
               UIn - 5
          caseName - "pitzDailyWorkshopStages"
          casePath - "/Volumes/Foam/Workshop2015/pitzDailyWorkshopStages"
          foamFork - openfoam
       foamVersion - 2.4.x
numberOfProcessors - 1

No script ./derivedParameters.py for derived values
Clearing .
Writing parameters to ./PyFoamPrepareCaseParameters
Writing report to ./PyFoamPrepareCaseParameters.rst
Found 0.org. Clearing 0
...
```

Reporting the used parameters

- The used variable values are reported in two files
  PyFoamPrepareCaseParameters a OpenFOAM-dictionary with all the values
  PyFoamPrepareCaseParameters.rst A *ReStructured Text*-file
  - This is a markup-language
- The *ReST*-file can be converted to more readable form with utilities like

```
> rst2pdf PyFoamPrepareCaseParameters.rst
```

(HTML-export also possible)

A printed report

Contents

1 Overwritten parameters

These parameters were set from the command line

Uln

5

2 Parameters with defaults

2.1 Boundary conditions

Short name: `boundary`

	default	description	Value
Uln	10	Inlet velocity	**5**

Figure: Part of the generated PDF

Regular parameter files

- Variables can be collected in parameter-files
  - These files are read with the `--parameter-file`-option

`slow.parameters`

```
UIn 5;
```

Using the file

```
> pyFoamPrepareCase.py . --parameter-file=slow.parameters
Using default values from /Volumes/Foam/Workshop2015/pitzDailyWorkshopStages/default.<brk>
      <cont>parameters
Looking for template values .
Reading values from slow.parameters
```

Spawn point

To get to the current state use `stage2_templateParameters.tar.gz`

Outline

Why control structures?

- Currently templates are only a glorified sed (the stream editor. Old people know it)
  - Values can be inserted, but ...
  - No decisions can be made
  - If we want to repeat something we've got to put it into the template multiple times
    - And we can't change the number
- Control structures enable programming languages to
  - Take decisions
  - Repeat things
- We need some of those

Changing the solver

- We want to select the incompressible and the compressible variant of `simpleFoam`
  - We add a parameter for this

`default.parameters`

```
solver {
    description "Used solver";
    default simpleFoam;
    options (
        simpleFoam
        rhoSimpleFoam
    );
}
```

But what is this `options`-entry for?

options for parameters

- options allows us to specify parameters that only have a finite list of choices
  - The value of options is a list with these choices
- If the user specifies a value for that parameter that is not in the list pyFoamPrepareCase.py fails with an error message
  - In our case the user can't specify interFoam as the solver

Variables derived from parameters

- Sometimes you want parameters that depend on the parameters you set
  - Here we need to distinguish between compressible and incompressible solvers
    - This is important if we're going to support more than 2 solvers
- If present the Python-file `derivedParameters.py` will be executed after all the parameters are read
- Python-variables that are created here will be available in all the templates

`derivedParameters.py`

```
if solver in ["rhoSimpleFoam"]:
    compressible=True
else:
    compressible=False
```

Testing the values

- Before really setting up the case we want to check if the values are set correctly
  - `--only-variables` reads the parameters and prints them
  - Then stops

```
> pyFoamPrepareCase.py . --only-variables
Using default values from /Volumes/Foam/Workshop2015/pitzDailyWorkshopStages/default.parameters
Looking for template values .

Used values

              Name - Value
----------------------------------------
               UIn - 10
          caseName - "pitzDailyWorkshopStages"
          casePath - "/Volumes/Foam/Workshop2015/pitzDailyWorkshopStages"
          foamFork - openfoam
       foamVersion - 2.4.x
numberOfProcessors - 1
            solver - simpleFoam

Deriving variables in script ./derivedParameters.py
Added values: compressible
```

Kinematic vs Dynamic

- One problem people usually have with the incompressible FOAM-solvers is that the density has been "canceled out"
  - Also known as the "why is my pressure drop 40% wrong"-problem (answer: because your density is 1.4)
- This means for incompressible:
  1. We use the *kinematic viscosity* $\nu = \frac{\mu}{\rho}$ instead of the *dynamic* μ
  2. Pressure dimensions are different (divided by $\frac{kg}{m^3}$
- to adapt the files we use the `compressible`-parameter

Preparing for compressible solvers

- We copy some additional files from a compressible tutorial case
  - And make them templates
- We modify files that are affected by the different dimensions to be templates

```
> cp $FOAM_TUTORIALS/compressible/rhoPimpleFoam/les/pitzDaily/constant/<brk>
    <cont>thermophysicalProperties constant/thermophysicalProperties.template
> cp $FOAM_TUTORIALS/compressible/rhoPimpleFoam/les/pitzDaily/0/T 0.org/T.template
> mv 0.org/p 0.org/p.template
> mv 0.org/k 0.org/k.template
> mv 0.org/epsilon 0.org/epsilon.template
> mv constant/transportProperties constant/transportProperties.template
```

Properties of air

Adding material properties as parameters

default.parameters

```
air {
    description "Properties of air";
    values {
        dynVisc {
            description "Dynamic viscosity";
            default 1.8e-5;
        }
        molarWeight {
            description "Molar weight of air";
            default 28.9;
        }
        TAir {
            description "Temperature of the air";
            default 293;
        }
        pAir {
            description "Pressure of the air on the outlet";
            default 1e5;
        }
    }
}
```

Setting the new nu

- Instead of the previous value we now calculate the *kinematic viscosity*
  - From the dynamic viscosity (a parameter `dynVisc`)
  - From the density `rhoAir`
    - Which is calculated from other parameters (`TAir`, `molarWeight`) by the *perfect gas* equation

`constant/transportProperties.template`

```
$$ rhoAir=pAir/(TAir*8.1415e3/molarWeight)

// With rho=|-rhoAir-|
nu              nu [ 0 2 -1 0 0 0 0 ] |-dynVisc/rhoAir-|;
```

Setting compressible properties

- The material properties are directly inserted here

constant/thermophysicalProperties.template

```
mixture
{
    specie
    {
        nMoles          1;
        molWeight       |-molarWeight-|;
    }
    thermodynamics
    {
        Cv              712;
        Hf              0;
    }
    transport
    {
        mu              |-dynVisc-|;
        Pr              0.7;
    }
}
```

`if` in templates

- All control structures in our templates are enclosed in `<!--(` and `)-->`
  - This syntax has its origins in HTML (comments)
- Apart from that the syntax (and behavior) is similar to the `if` in Python
  - First keyword `if`. Then a condtion
- The `if`-block is ended with a `<!--(end)-->`
  - The `<` has to be in the same column as the `<` of the starting `if`
- The text between `if` and `end` is only inserted if the condition is `True`
- It is also possible to have an `<!--(else)-->`-branch
  - Inserted if the condition is false
  - Or cascading with `<!--(elif ..)-->`

Trivial if-example

- Selecting text and setting a variable depending on an expression

testfile.template

```
<!--(if 1>2)-->
$$ val=True
Falsch
<!--(else)-->
$$ val=False
Richtig
<!--(end)-->
val: |-val-|
```

Shell

```
> pyFoamFromTemplate.py --template-file=testfile.template_ --stdout
Richtig
val: False
```

Different pressure dimensions

- Distinguish between compressible and incompressible solvers

0.org/p.template

```
<!--(if compressible)-->
dimensions      [1 -1 -2 0 0 0 0];
internalField   uniform |-pAir-|;
<!--(else)-->
dimensions      [0 2 -2 0 0 0 0];
internalField   uniform 0;
<!--(end)-->

boundaryField
{
    outlet
    {
        type            fixedValue;
        value           $internalField;
    }
```

Attention: the `$internalField` is important (used to be 0)

Single line `if`

- Wall functions have a prefix `compressible::` in their compressible form
- The "single line" `if` allows a very compact code
  - But like the C++ conditional `a ? b : c` it shouldn't be overused as it tends to make things unreadable

0.org/k.template

```
$$ prefix="compressible::" if compressible else ""

boundaryField
{
    upperWall
    {
        type            |-prefix-|kqRWallFunction;
        value           uniform 0.375;
    }
    lowerWall
    {
        type            |-prefix-|kqRWallFunction;
        value           uniform 0.375;
    }
```

Same Problem for epsilon

0.org/epsilon.template

```
$$ prefix="compressible::" if compressible else ""

boundaryField
{
    upperWall
    {
        type            |-prefix-|epsilonWallFunction;
        value           uniform 14.855;
    }
    lowerWall
    {
        type            |-prefix-|epsilonWallFunction;
        value           uniform 14.855;
    }
```

T means 'trivial'

- The only thing we do here is add the `TAir` we used to calculate the density

0.org/T.template

```
internalField   uniform |-TAir-|;

boundaryField
{
    inlet
    {
        type            fixedValue;
        value           $internalField;
    }

    outlet
    {
        type            inletOutlet;
        inletValue      $internalField;
        value           $internalField;
    }
```

Adding discretization schemes

- rhoSimpleFoam needs a few additional schemes

system/fvSchemes

```
divSchemes
{
    default          none;
    div(phi,U)       bounded Gauss upwind;
    div(phi,k)       bounded Gauss upwind;
    div(phi,epsilon) bounded Gauss upwind;
    div(phi,R)       bounded Gauss upwind;
    div(R)           Gauss linear;
    div(phi,nuTilda) bounded Gauss upwind;
    div((nuEff*dev(T(grad(U))))) Gauss linear;

    // Added for rhoSimpleFoam
    div((muEff*dev2(T(grad(U))))) Gauss linear;
    div(phi,e)       bounded Gauss upwind;
    div(phi,Ekp)       bounded Gauss upwind;
}
```

Adding support for energy equation e

system/fvSolution

```
    "(U|k|epsilon|R|nuTilda|e)"
    {
        solver          smoothSolver;
        smoother        symGaussSeidel;
        tolerance       1e-05;
        relTol          0.1;
    }
}
SIMPLE
{
    nNonOrthogonalCorrectors 0;
    rhoMin          rhoMin [ 1 -3 0 0 0 ] 0.5;
    rhoMax          rhoMax [ 1 -3 0 0 0 ] 1.5;

    residualControl
    {
        p               1e-2;
        U               1e-3;
        e               1e-3;
        "(k|epsilon|omega)" 1e-3;
    }
}
```

Running Compressible

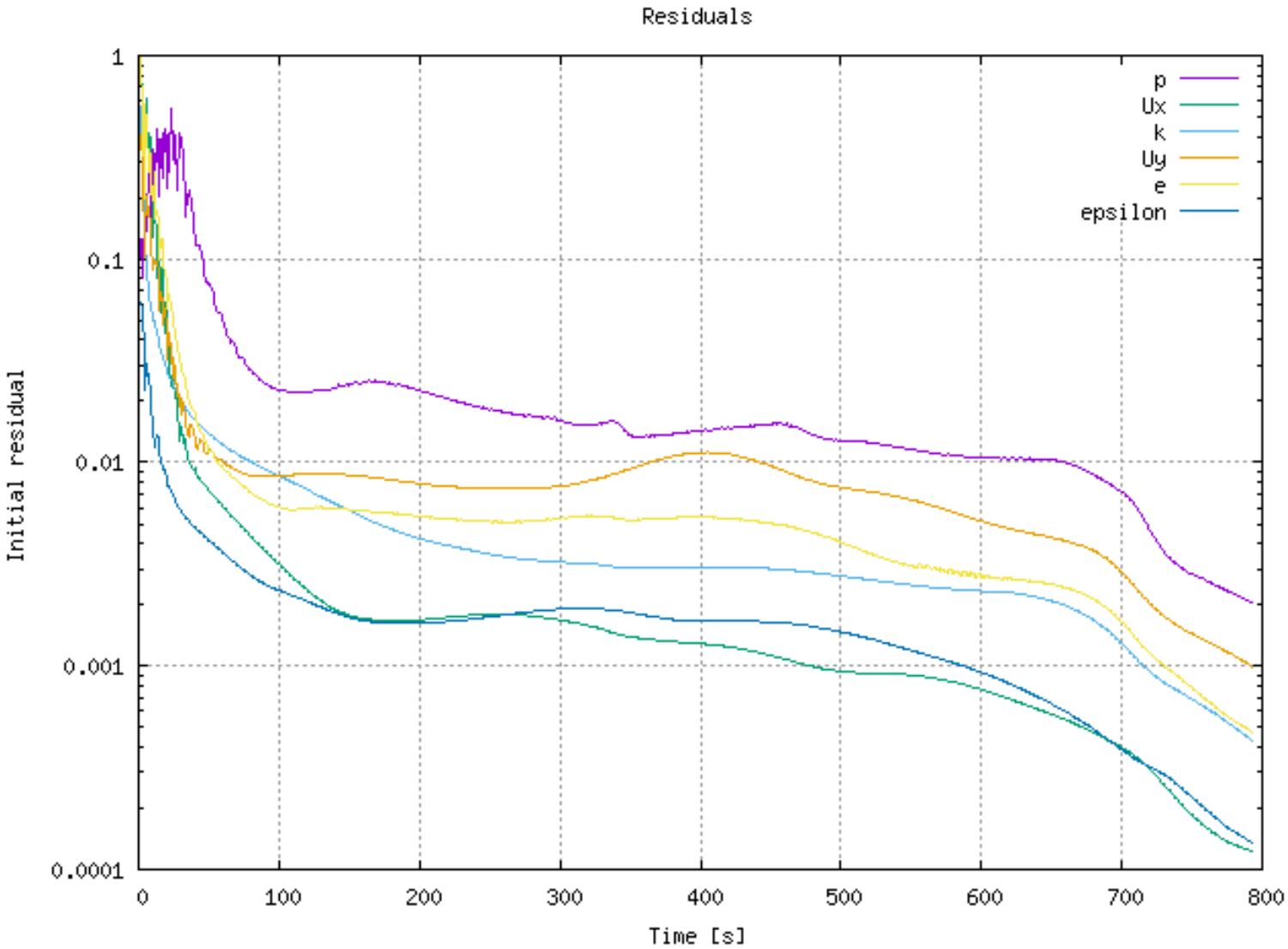
- We prepare and run for/with `rhoSimpleFoam`

```
> pyFoamPrepareCase.py . --values="solver rhoSimpleFoam;"
...
> pyFoamPlotRunner.py --clear --progress rhoSimpleFoam
 Reading regular expressions from /Volumes/Foam/Workshop2015/pitzDailyWorkshopStages/<brk>
       <cont>customRegexp
Clearing out old timesteps ....
 t =        793 dp: -4.3575 detach: 0.169432
```

- The values for `simpleFoam` now have changed (because `nu` changed from 10^{-5} to $1.48 \cdot 10^{-5}$

```
> pyFoamPrepareCase.py . --values="solver simpleFoam;"
...
> pyFoamPlotRunner.py --clear --progress simpleFoam
 t =        796 dp: -3.83197 detach: 0.169432
```

Compressible residuals



Exercise: Pressure difference

- Pressure differences are different
  - Reason: Factor ρ (≈ 1.2) is missing in the incompressible case
- Your mission: make sure that in the incompressible case the "real" pressure is used
  1. Turn `controlDict` into a template
  2. Multiply the `expression` in `pressureDiff` with ρ
     - But only if not `compressible`
     - Use formula for ρ from `transportProperties.template`

Spawn point

To get to the current state use `stage3_rhoSimpleFoam.tar.gz`

Repetitive tasks

- Computers are good at doing the same over and over again
  - Humans are not
    - And they make mistakes
- The `for`-loop is similar to the Python `for` (except for the `<!--( )-->` around it)
  1. Keyword `for`
  2. Name of the (running) variable
  3. Keyword `in`
  4. A list
     - Frequently: `range(5)` for numbers from 0 to 4

The for-loop

Printing square numbers and summing them

testfile.template

```
$$ total=0
<!--(for i in range(5))-->
$$ sq=i*i
$$ total+=sq
|-i-|*|-i-| = |-sq-|
<!--(end)-->
Total: |-total-|
```

Shell

```
0*0 = 0
1*1 = 1
2*2 = 4
3*3 = 9
4*4 = 16
Total: 30
```

Adding multiple sample lines

- We want to sample pressure and velocity on multiple lines in our geometry
- All the lines should be vertical
- Instead of specifying them by hand we make `controlDict` a template:

```
> mv system/controlDict system/controlDict.template
```

Specifying x-values to sample

- The locations of the lines are specified in a parameter
  - This way the number can be easily modified

`default.parameters`

```
postproc {
    description "Postprocessing stuff";
    values {
        xProfiles {
            description "List of locations of the profiles in mm";
            default ( -10 0 50 100 150 200 250 );
        }
    }
}
```

- In `controlDict` the sets are generated by a loop over `xProfiles`
  - Names of the sets are generated from the values

Adding the lines

sytem/controlDict.template

```
functions
{
    profiles {
        type sets;
        fields (
            p  U
        );
        outputControl   outputTime;
        interpolationScheme cell;
        setFormat raw;
        sets (
<!--(for x in xProfiles)-->
$$ xVal=1e-3*x
            x|-"%04.0f"%x-|
            {
                type midPoint;
                axis y;
                start ( |-xVal-|  -0.0255  0);
                end   ( |-xVal-|   0.0255  0);
            }
<!--(end)-->
        );
    }
```

Preparing and running

- This gives the same results as before
  - Except for the added profiles

```
> pyFoamPrepareCase.py . --values="solver simpleFoam;"
...
> pyFoamPlotRunner.py --clear --progress simpleFoam
 t =        796 dp: -3.83197 detach: 0.169432
> ls postProcessing/profiles/
100/ 150/ 200/ 250/ 300/ 350/ 400/ 450/ 50/  500/ 550/ 600/ 650/ 700/ 750/ 796/
```

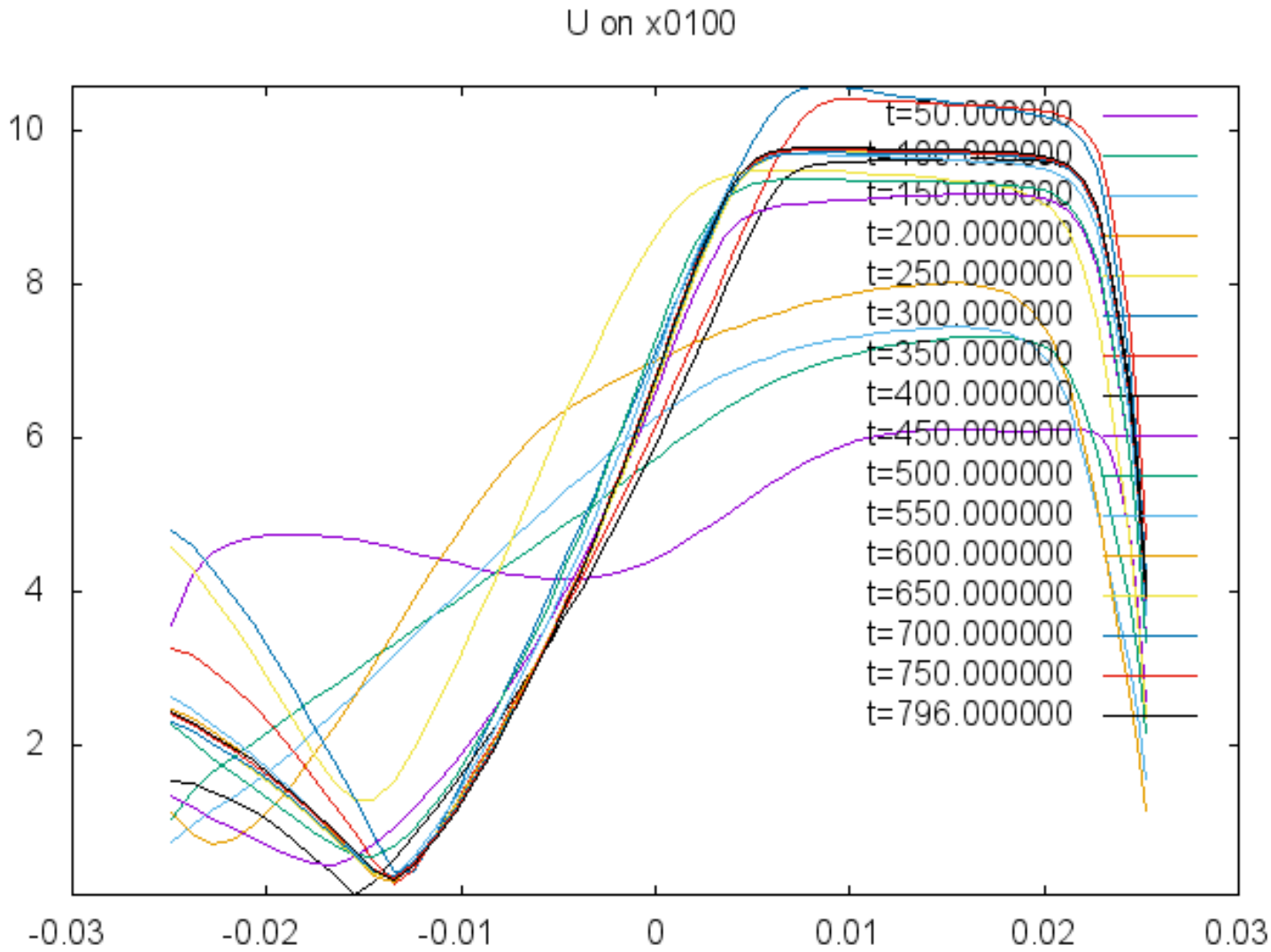
- Plotting 7 profiles can be quite . . . confusing
  - But PyFoam offers a utility for that

Plotting the sample data

- The `pyFoamSamplePlot.py` knows how to handle profile data
  - It can give information about the data present
  - Generate Gnuplot-commands to plot the data
    - Just pipe into GnuPlot
  - Collect the data and write into an Excel-file
- With all these things it is flexible about missing fields

```
> pyFoamSamplePlot.py . --dir=postProcessing/profiles --info
Times :  ['50', '100', '150', '200', '250', '300', '350', '400', '450', '500', '550', <brk>
      <cont>'600', '650', '700', '750', '796']
Lines :  ['x-010', 'x0000', 'x0050', 'x0100', 'x0150', 'x0200', 'x0250']
Fields:  ['U', 'p']
> pyFoamSamplePlot.py . --dir=postProcessing/profiles --line=x0100 --mode=timesInOne | <brk>
      <cont>gnuplot
> ls *.png
postProcessing_profiles_x0100_U.png
> pyFoamSamplePlot.py . --dir=postProcessing/profiles --line=x0100 --mode=timesInOne --<brk>
      <cont>excel-file=simpleFoam_Line0100.xls
```

Velocity at different times



Further info on templates

- As the base of the template engine an independent library was "borrowed":
  `http://www.simple-is-better.org/template/pyratemp.html`
  - The reason for the `<!---`syntax is that this library was intended for web-development
- The library is included with the sources of PyFoam
  - Therefor there is no need to install an external dependency
    - This is also the main reasons why this and not a more popular templating engine like `Jinja2` is used

Nesting of controls

- If control structures are nested then it is important that the inner structures are indented
  - <-- opening and closing the structure must be aligned
- In the following example there is branch inside a loop

testing.template

```
<!--(for p in ["in","out","topWall","wallBottom"])-->
  <!--(if p.lower().find("wall")>=0)-->
|-p-| is a wall
  <!--(end)-->
<!--(end)-->
```

Shell

```
topWall is a wall
wallBottom is a wall
```

Spawn point

To get to the current state use `stage4_plotlines.tar.gz`

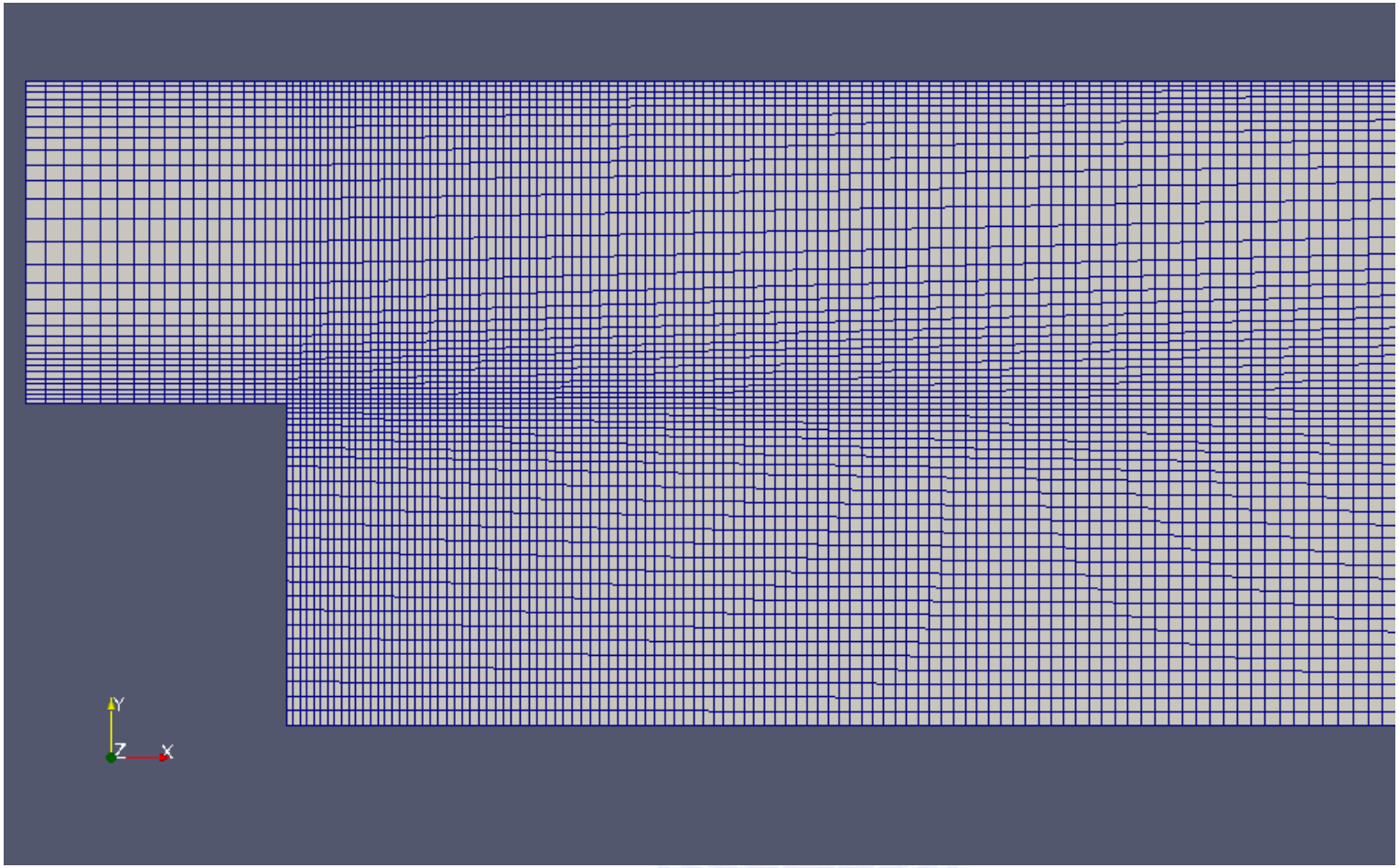
Outline

Outline

Automatic mesh creation

- Until now we didn't have to do anything to create a mesh
  - The mesh was just there
- Reason is that if `pyFoamPrepareCase.py` has no information about the mesh creation it assumes `blockMesh`
- *Information about mesh creation* means
  - A script `meshCreate.sh` exists!
- `meshCreate.sh` is executed instead of `blockMesh`
  - That is not a big improvement over `Allrun`
  - but
  - `meshCreate.sh` can be a `.template`
    - Those are expanded before the mesh creation phase
- We're now going to write a `meshCreate.sh.template`
  - But first we'll just modify `blockMeshDict`

The original mesh



Preparing blockmeshDict.template

- The original mesh is
  - Graded
  - Fine
- We want to check the influence of
  - Grading
  - The fineness

```
> mv constant/polyMesh/blockMeshDict constant/polyMesh/blockMeshDict.template
```

Adding parameters for blockMesh

- Adding two parameters
  - One to multiply the number of cells in each block with
  - One to switch off grading
- Defaults are to reproduce the original mesh

default.parameters

```
meshing {
    description "Meshing parameters";
    values {
        resFactor {
            description "Resolution compared to the original";
            default 1.;
        }
        graded {
            description "Whether mesh grading should be used";
            default true;
        }
    }
}
```

Calculating mesh number

- Add a few variables
  - One for each number of cells in the blocks
- Simply multiply with the factor
  - `ceil` rounds up (avoids zero cell blocks)
  - Result is a `float`. `int` 'casts' back to what Foam expects

blockMeshDict.template

```
$$ nrX1=int(ceil(18*resFactor))
$$ nrX2=int(ceil(180*resFactor))
$$ nrX3=int(ceil(25*resFactor))
$$ nrY1=int(ceil(30*resFactor))
$$ nrY2=int(ceil(27*resFactor))
```

Defining the blocks

- Use the mesh number variables from above
- Using an inline `if` to switch off grading

blockMeshDict.template

```
$$ posYRStr="$posYR"

blocks
(
    hex (0 3 4 1 11 14 15 12)
    (|-nrX1-| |-nrY1-| 1)
    simpleGrading |-"(0.5 "+posYStr+" 1)" if graded else "(1 1 1)"-|

    hex (2 5 6 3 13 16 17 14)
    (|-nrX2-| |-nrY2-| 1)
    |-"edgeGrading (4 4 4 4 "+negYStr+" 1 1 "+negYStr+" 1 1 1 1)" if graded else "simpleGrading (1 1 1)"-|

    hex (3 6 7 4 14 17 18 15)
    (|-nrX2-| |-nrY1-| 1)
    |-"edgeGrading (4 4 4 4 "+posYStr+" "+posYRStr+" "+posYRStr+" "+posYStr+" 1 1 1 1)" if graded else "simpleGrading (1 1 1)"-|

    hex (5 8 9 6 16 19 20 17)
    (|-nrX3-| |-nrY2-| 1)
    simpleGrading |-"(2.5 1 1)" if graded else "(1 1 1)"-|

    hex (6 9 10 7 17 20 21 18)
    (|-nrX3-| |-nrY1-| 1)
    simpleGrading |-"(2.5 "+posYRStr+" 1)" if graded else "(1 1 1)"-|
);
```

Setting an running a coarser mesh

- Time for our first serious parameter file
  - Parameter files can have any name
    - But PyFoam recognizes `.parameters` during cloning
  - Format of the file is: FOAM-dictionary without header
- Collect settings that belong together in one file
  - Use with `--parameter-file`
    - Can be specified more than once

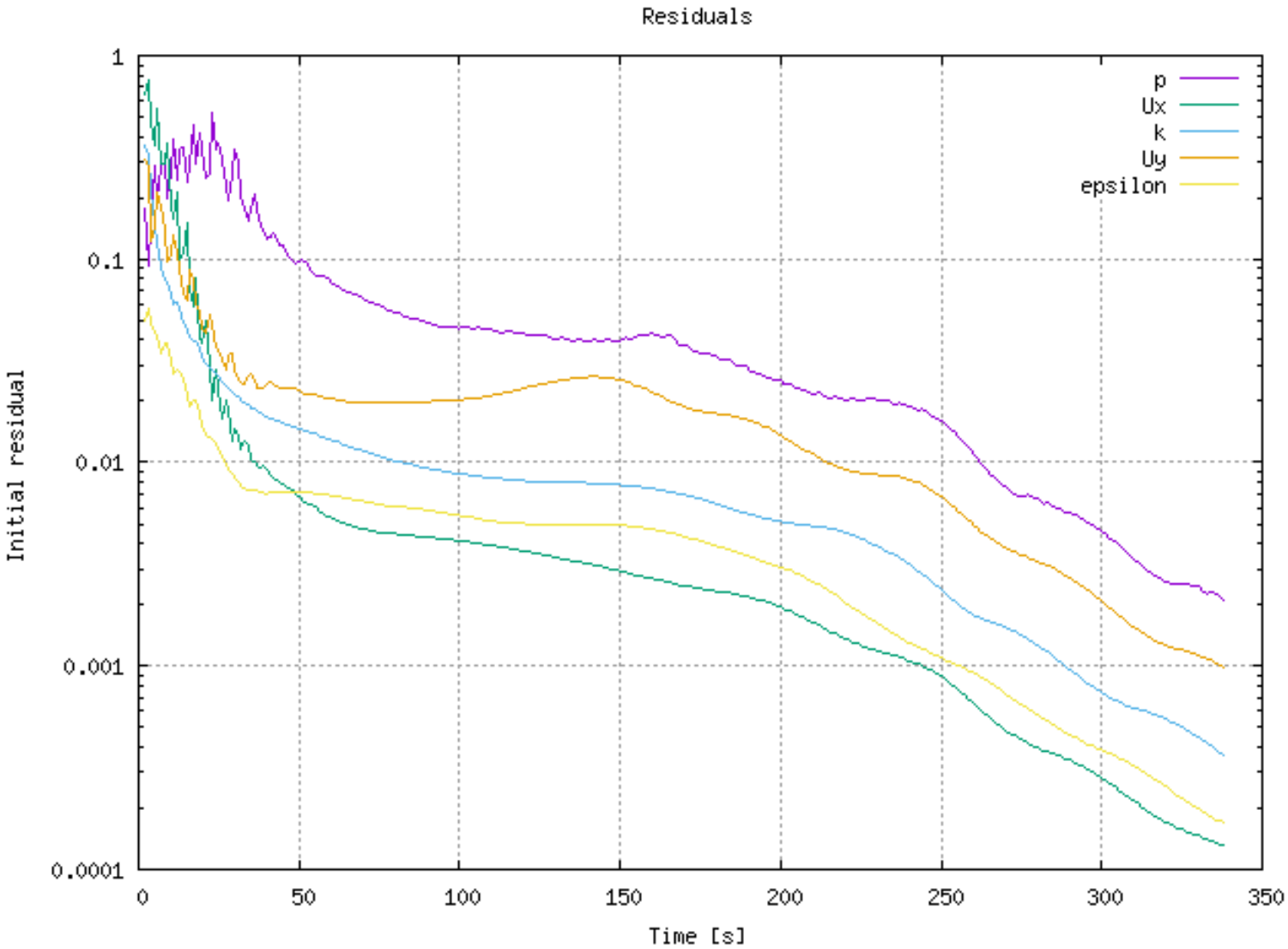
`coarseMesh.parameters`

```
resFactor 0.5;
graded no;
```

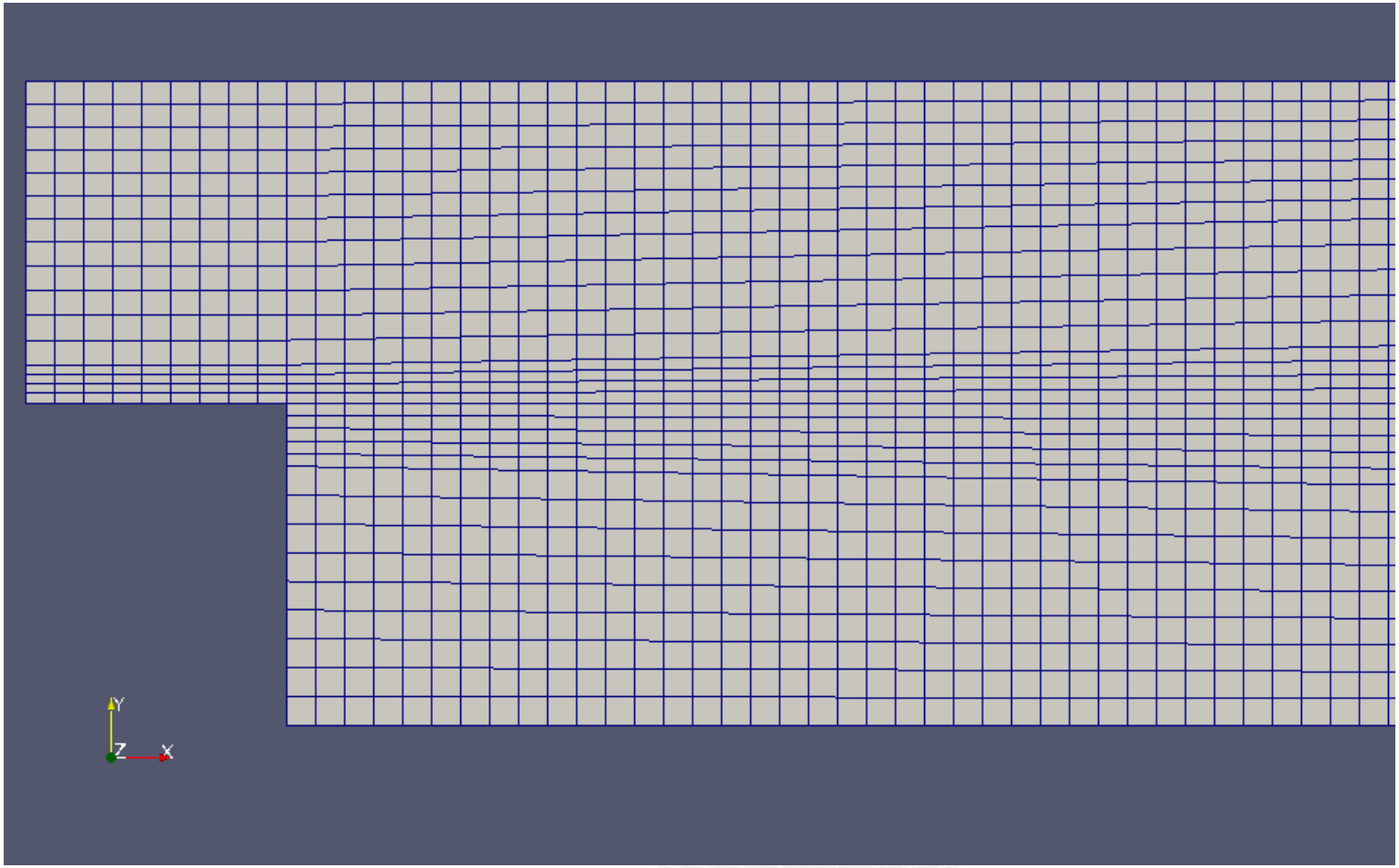
Running

```
> pyFoamPrepareCase.py . --parameter=coarseMesh.parameters
...
> pyFoamPlotRunner.py --clear --progress simpleFoam
 t =        338 dp: -5.75093 detach: 0.172811
```

Residuals for the coarse mesh



The coarse ungraded mesh



Spawn point

To get to the current state use `stage5_coarseMesh.tar.gz`

Adding a boundary layer

- The question:
  - "Is an ungraded mesh with a boundary layer as good as a graded mesh?"
    - Will not be answered in this presentations
    - But we will implement the tools to answer it
- User can specify the number of boundary layers
  - Each boundary layer is created by splitting the boundary cells exactly in half
    - Modifying this ratio is left as an exercise to the reader
  - A number of 0 keeps the original mesh

```
mv meshCrate.sh meshCreate.sh.template
```

The parameter

- Adding one more parameter to the `meshing` group

defaultParameters

```
meshing {
    description "Meshing parameters";
    values {
        nrBoundaryLayers {
            description "Number of boundary layers";
            default 0;
        }
        resFactor {
            description "Resolution compared to the original";
            default 1.;
        }
        graded {
            description "Whether mesh grading should be used";
            default true;
        }
    }
}
```

Setting up the mesh

- Template generates a script to
  - First call `blockMesh`
  - Then call `refineWallLayer` for the wall-patches

`meshCreate.sh.template`

```
#! /bin/bash

blockMesh

<!--(for i in range(nrBoundaryLayers))-->
refineWallLayer -overwrite "(upperWall lowerWall)" 0.5
<!--(end)-->
```

It would have also been possible to have a loop in the bash-language. I just happen to not like the syntax of shell scripts

Reusing coarse parameters with #include

- Copy/Pasting parameter sets is not always the best idea
  - The meaning of 'coarse' changes and you'll have to change in all files
- Recommendation:
  - Collect settings for *a coarse mesh* in one file
  - Reuse it with `#include`

`coarseMeshLayers.parameters`

```
#include "coarseMesh.parameters"

nrBoundaryLayers 2;
```

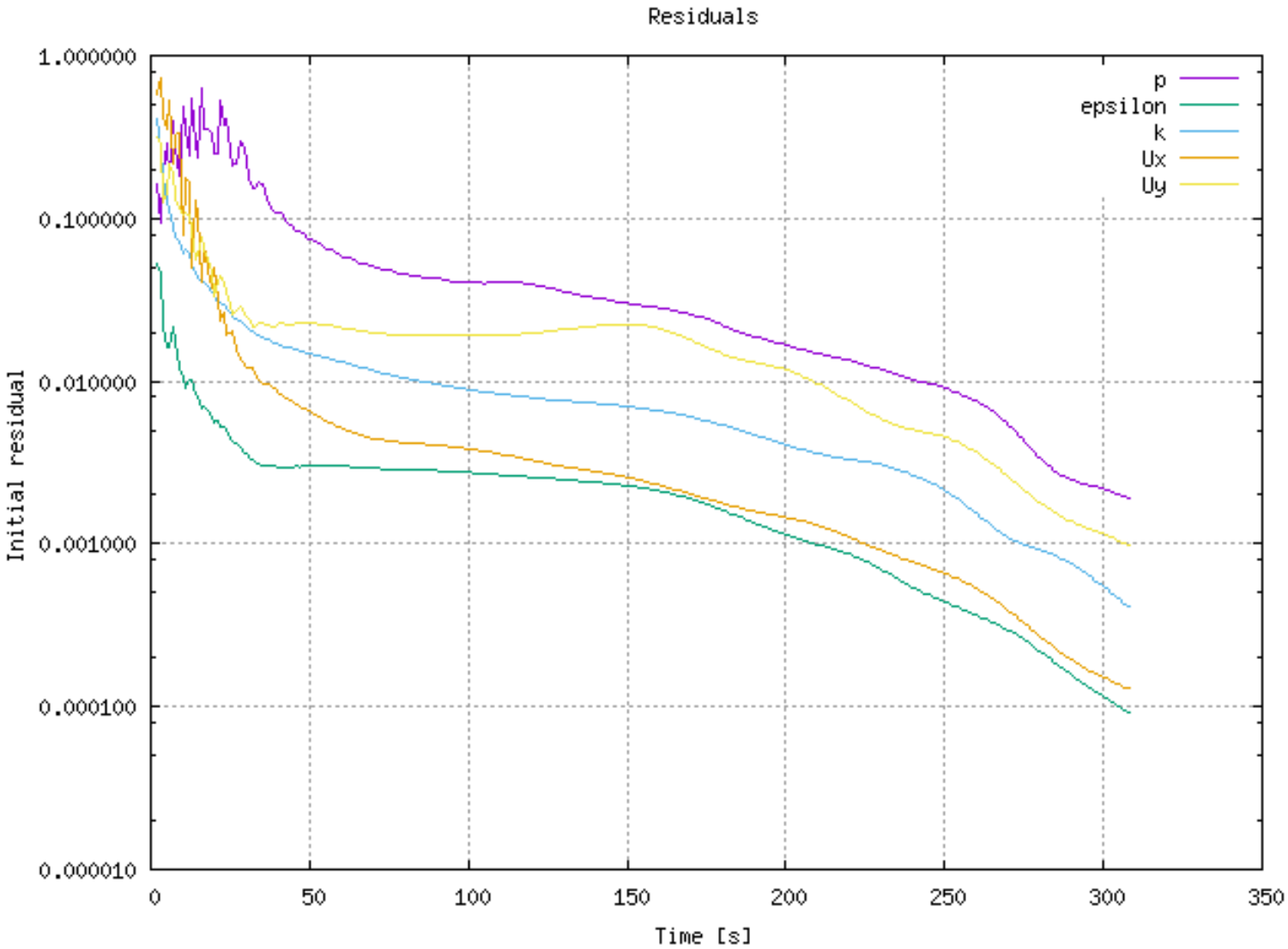
Testing layers

- We run the layered mesh
- Observations:
  - Number of iterations decrease
  - Both results also change significantly
    - Whether this is to the better: no idea

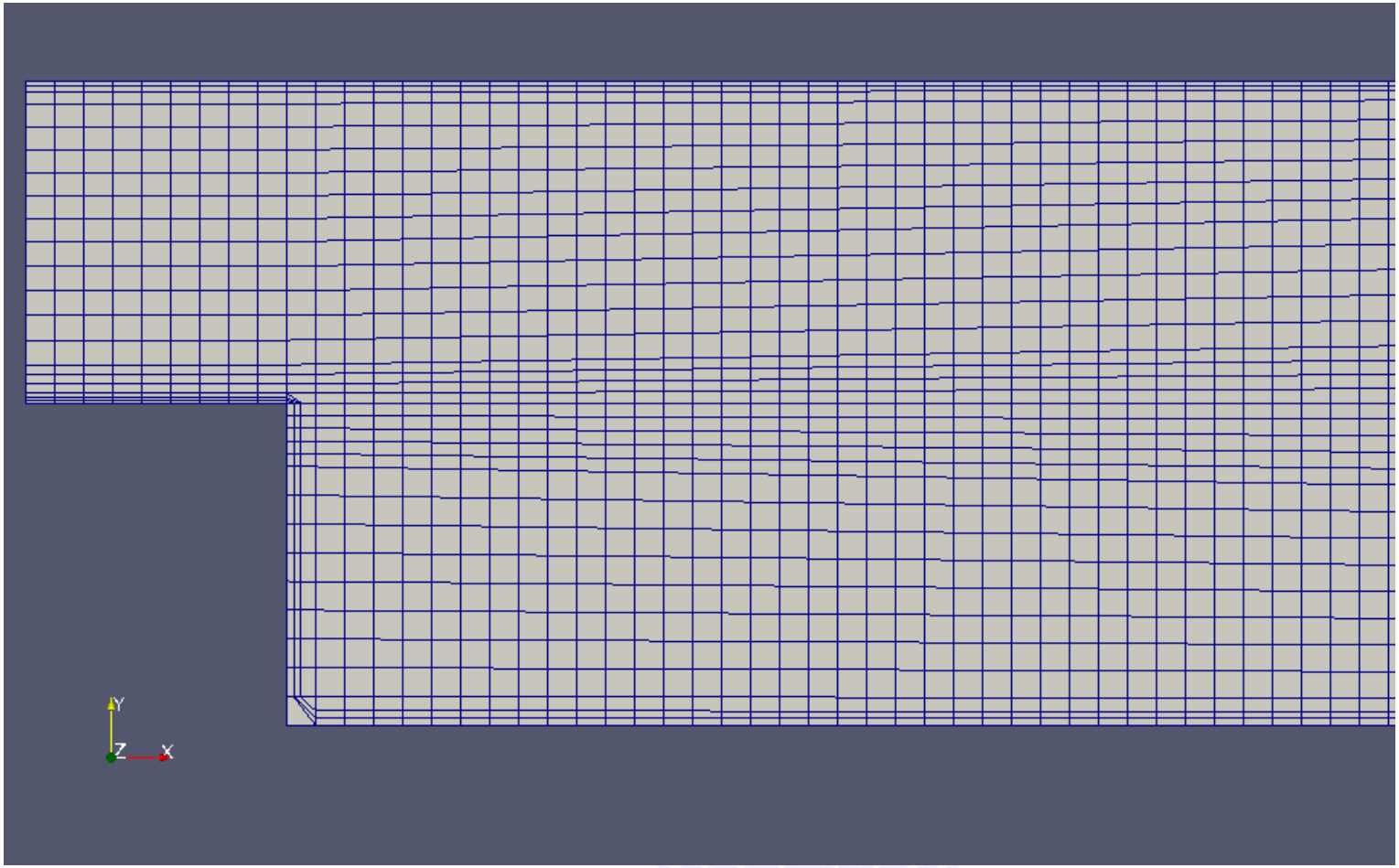
Shell

```
> pyFoamPrepareCase.py . --parameter=coarseMeshLayers.parameters
...
> pyFoamPlotRunner.py --clear --progress simpleFoam
 t =         308 dp: -3.0063 detach: 0.168234
```

Better convergence with layers



Mesh with layers



Logfiles for the scripts

- The output of `meshCreate.sh` can be very long
  - for instance if one of the tools used in the script is `snappyHexMesh`
- ... and interesting
  - for instance `snappyHexMesh`
- Therefor the full output goes to a file `meshCreate.sh.log`
  - And to the terminal as well
- The `caseSetup.sh`-phase (see below) also has a logfile

Spawn point

To get to the current state use `stage6_meshCreate.tar.gz`

Outline

Scripting initial conditions

- Sometimes life is more complicated than `uniform 0`
- Then you need to call some utilities to set the initial conditions
  - `setFields`
  - `funkySetFields`
- To do this `pyFoamPrepareCase.py` calls a script `caseSetup.sh`
  - This script can also be generated from a template
- In our case we want to initialize the velocity field with `potentialFoam`
  - Check if this leads to faster convergence

Different templates for different stages

- Some utilities need different versions of the same file
  - `controlDict` for instance
    - Some utilities choke on the `functions`
    - Some need different timesteps (`foamyHexFoam`)
- Sometimes a template needs results that are only available after the meshing phase
  - Names of the patches for instance
- So in addition to `.template` two other templates are available

  .postTemplate expanded after meshing but before case setup
  .finalTemplate expanded after case setup

Adaptions necessary for potentialFoam

To use potential foam some things have to be done

- Add a switch
- A setup-script
- Special pressure field
- Numerical settings
  - in `fvSchemes` and `fvSolution`

New parameter

Default is to not use potentialFoam

default.parameters

```
initial {
    description "Initial conditions";
    values {
        potentialFlow {
            description "Initialize with potentialFoam";
            default false;
        }
    }
}
```

The setup script

- Does two things:
  - Call `potentialFoam`
  - Remove `phi` as the dimensions don't fit the compressible solver

`caseSetup.sh.postTemplate`

```
#! /bin/sh

<!--(if potentialFlow)-->
potentialFoam

  <!--(if compressible)-->
rm 0/phi*
  <!--(end)-->
<!--(end)-->
```

This could also have been a normal `.template`

Special pressure file

- `potentialFoam` needs an 'incompressible' pressure
  - Also: an initial pressure of 10^5 causes numerical problems
- Copy so that our 'old' pressure template will be used for the flow solver

```
> cp 0.org/p.template 0.org/p.finalTemplate
```

- Edit the pressure for `potentialFoam`

0.org/p.template

```
dimensions      [0 2 -2 0 0 0 0];

internalField   uniform 0;

boundaryField
{
    outlet
    {
        type            fixedValue;
        value           $internalField;
    }
```

Numerical stuff

system/fvSolution

```
    Phi
    {
        $p;
    }
}
potentialFlow
{
    $SIMPLE;
    nNonOrthogonalCorrectors 3;
}
```

system/fvSchemes

```
fluxRequired
{
    default           no;
    p                 ;
    Phi               ;
}
```

This run has potential

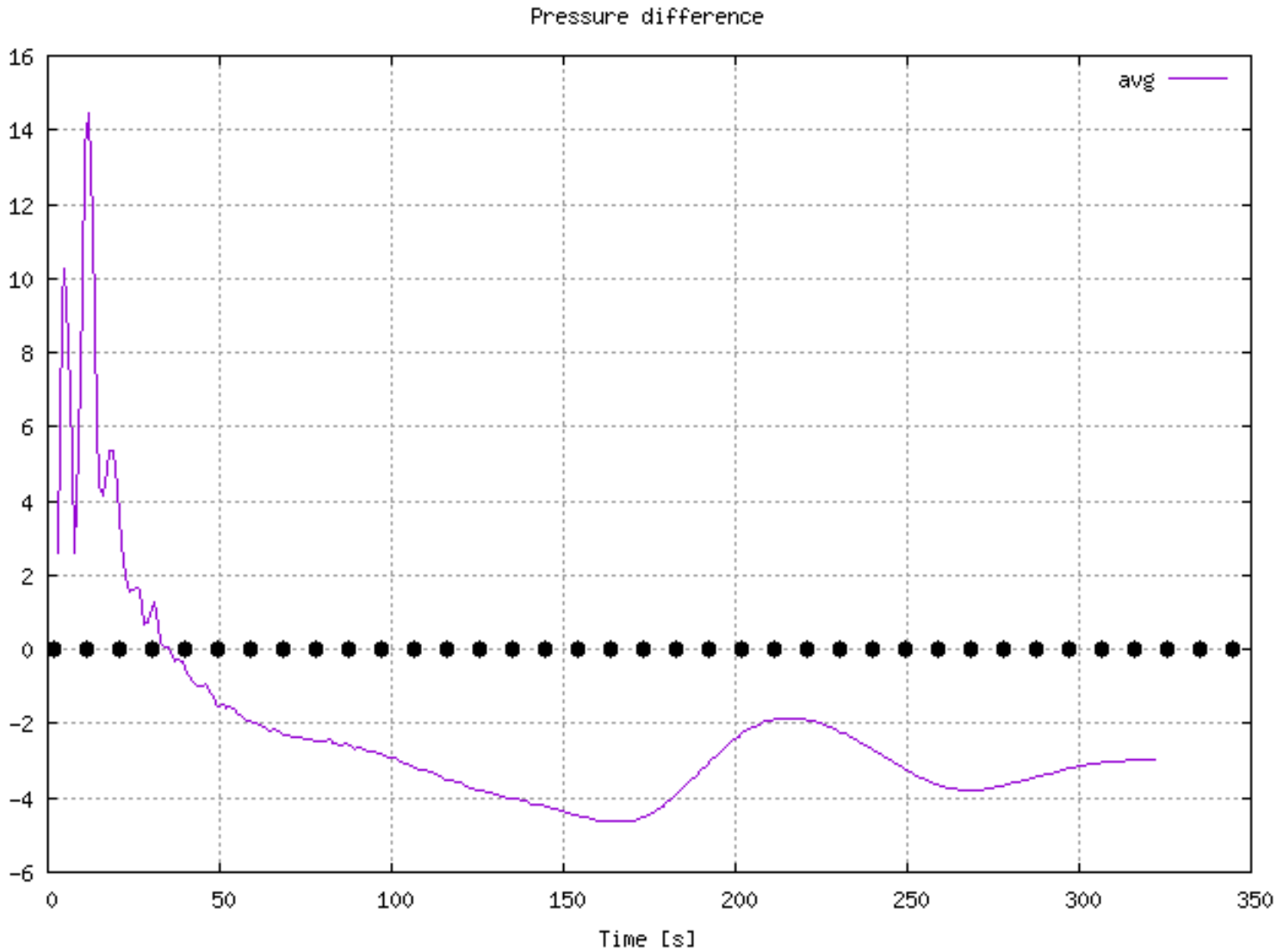
Again: our two utilities

Shell

```
> pyFoamPrepareCase.py . --parameter=coarseMeshLayers.parameters --value="potentialFlow yes<brk>
      <cont>;"
...
> pyFoamPlotRunner.py --clear --progress --hardcopy --prefix=potential simpleFoam
 t =         322 dp: -2.97042 detach: 0.168234
```

- More iterations than before, but improvement on the pressure

Initial pressure spike: almost gone



Spawn point

To get to the current state use `stage7_initPotential.tar.gz`

Outline

Outline

foam-extend and the pUCoupledFoam-solver

- Until now we've been working with `OpenFOAM v1712+`
  - OF 5.0 should also work
- But there is also `foam-extend 4.1`
  - Which has slightly different formats for files
  - But also a very interesting additional solver: `pUCoupledFoam`
    - Steady state, incompressible
    - Pressure and momentum equation are solved simultaneously
- We'd like to compare the fully coupled solver with the others
  - And also whether `simpleFoam` between the two forks differs

Adding the solver

First we add a third solver to the list

default.parameters

```
solver {
    description "Used solver";
    default simpleFoam;
    options (
        simpleFoam
        rhoSimpleFoam
        pUCoupledFoam
    );
}
```

Different usage for old refineWallLayer

- In foam-extend it can only handle one patch at a time
  - This was the default behavior for OpenFOAM before 2.3.1
- Using the automatically defined foamFork and foamVersion parameters we can select the right behavior

meshCreate.sh.template

```
#! /bin/bash

blockMesh

<!--(for i in range(nrBoundaryLayers))-->
  <!--(if foamFork!="extend" and foamVersion>(2,3,1))-->
refineWallLayer -overwrite "(upperWall␣lowerWall)" 0.5
  <!--(else)-->
refineWallLayer -overwrite lowerWall 0.5
refineWallLayer -overwrite upperWall 0.5
  <!--(end)-->
<!--(end)-->
```

Missing function object in extend

- foam-extend has no streamLine function object
  - Not a big deal, because we didn't use it in our evaluations

system/controlDict.template

```
functions {

<snip>

<!--(if foamFork!="extend")-->
    streamLines
    {
        type            streamLine;

<snip>

    }
<!--(end)-->
}
```

No bounded in extend

- Problem: `foam-extend` has no bounded for `div`-schemes
- Make `fvSchemes` a template

```
> mv system/fvSchemes system/fvSchemes.template
```

- and only use bounded when available

fvSchemes.template

```
<!--(if foamFork!="extend")-->
$$ bounded="bounded"
<!--(else)-->
$$ bounded=""
<!--(end)-->

divSchemes
{
    default          none;
    div(phi,U)       |-bounded-| Gauss upwind;
    div(phi,k)       |-bounded-| Gauss upwind;
```

Proposal for an exercise

- Add a configuration parameter to switch off bounded in FOAM-versions that support it
  - See how it affects convergence

Additional schemes

- The coupled solver also needs an additional `div`-scheme

fvSchemes.template

```
...

    // differences in foam-extend
    div((muEff*dev2(grad(U).T()))) Gauss linear;
    div(U,p) Gauss upwind phi;
    div(phi,h)      |-bounded-| Gauss linear;
    div((nuEff*dev(grad(U).T()))) Gauss linear;

<!--(if solver=="pUCoupledFoam")-->
    div(U)          Gauss linear;
<!--(end)-->
}
```

Coupled solver

- The coupled solver needs a special linear solver
- Also: energy is a different field: `e` vs `h`

```
> mv system/fvSolution system/fvSolution.template
```

fvSolution.template

```
solvers
{
<!--(if solver=="pUCoupledFoam")-->
    Up
    {
        solver BiCGStab;
        preconditioner Cholesky;

        tolerance 1e-09;
        relTol  0.0;

        minIter 1;
        maxIter 500;
    }
<!--(end)-->
...
    "(U|k|epsilon|R|nuTilda|e|h)"
    {
        solver          smoothSolver;
...
```

Convergence criterion

- foam-extend sets one convergence criterion for all fields
  - Instead of the "per-field" crtiterion of OpenFOAM

fvSolution.template

```
SIMPLE
{
...
<!--(if foamFork=="extend")-->
    convergence 1e-3;
<!--(end)-->
}
```

Settings for pUCoupledFoam

- Coupled solver needs additional settings

fvSolution.template

```
<!--(if solver=="pUCoupledFoam")-->
blockSolver
{
    $SIMPLE;
}

fieldBounds
{
    U       500;
    p       -5e4 5e4;
}
<!--(end)-->
```

Different relaxation

- Also: relaxation is specified in a slightly different way
  - And the coupled solver allows higher relaxation

fvSolution.template

```
relaxationFactors
{
...
<!--(if foamFork=="extend")-->
  <!--(if solver=="pUCoupledFoam")-->
    U               0.99;
  <!--(else)-->
    U               0.7;
  <!--(end)-->
    p               0.3;
    rho             0.05;
    k               0.9;
    epsilon         0.9;
    h               0.9;
<!--(end)-->
}
```

Old thermophysics format

- The format of `thermoType` is still in the old-school 'Fortrany' style

thermophysicalProperties.template

```
<!--(if foamFork=="extend")-->
thermoType      hPsiThermo<pureMixture<constTransport<specieThermo<hConstThermo<perfectGas<brk>
      <cont>>>>>>;
mixture         air 1 |-molarWeight-| 1000 0 |-dynVisc-| 0.7;
<!--(else)-->
thermoType
{
    type            hePsiThermo;
...
}
<!--(end)-->
```

Running on foam-extend

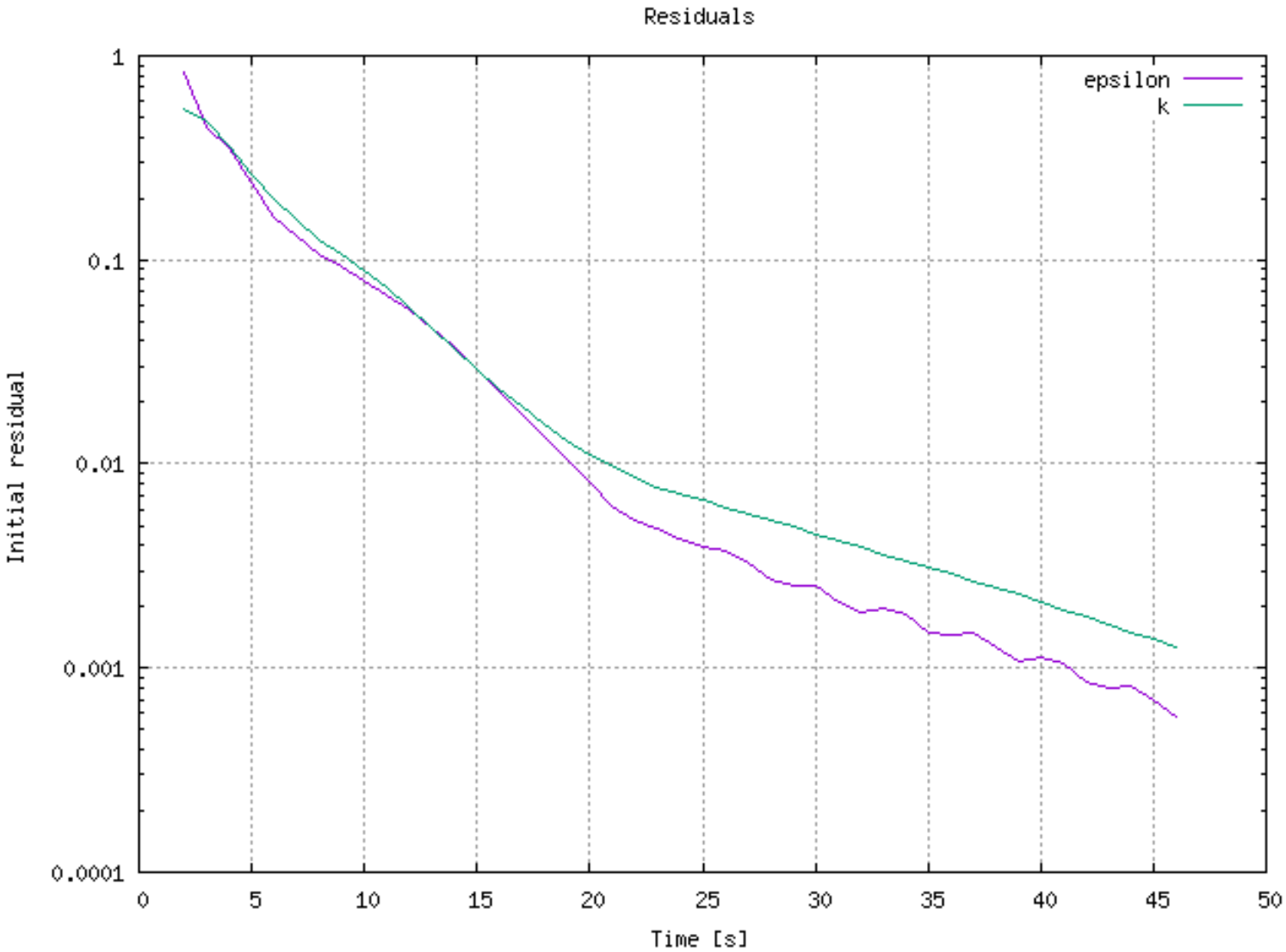
- Now we switch the shell to foam-extend and try different solvers

Shell

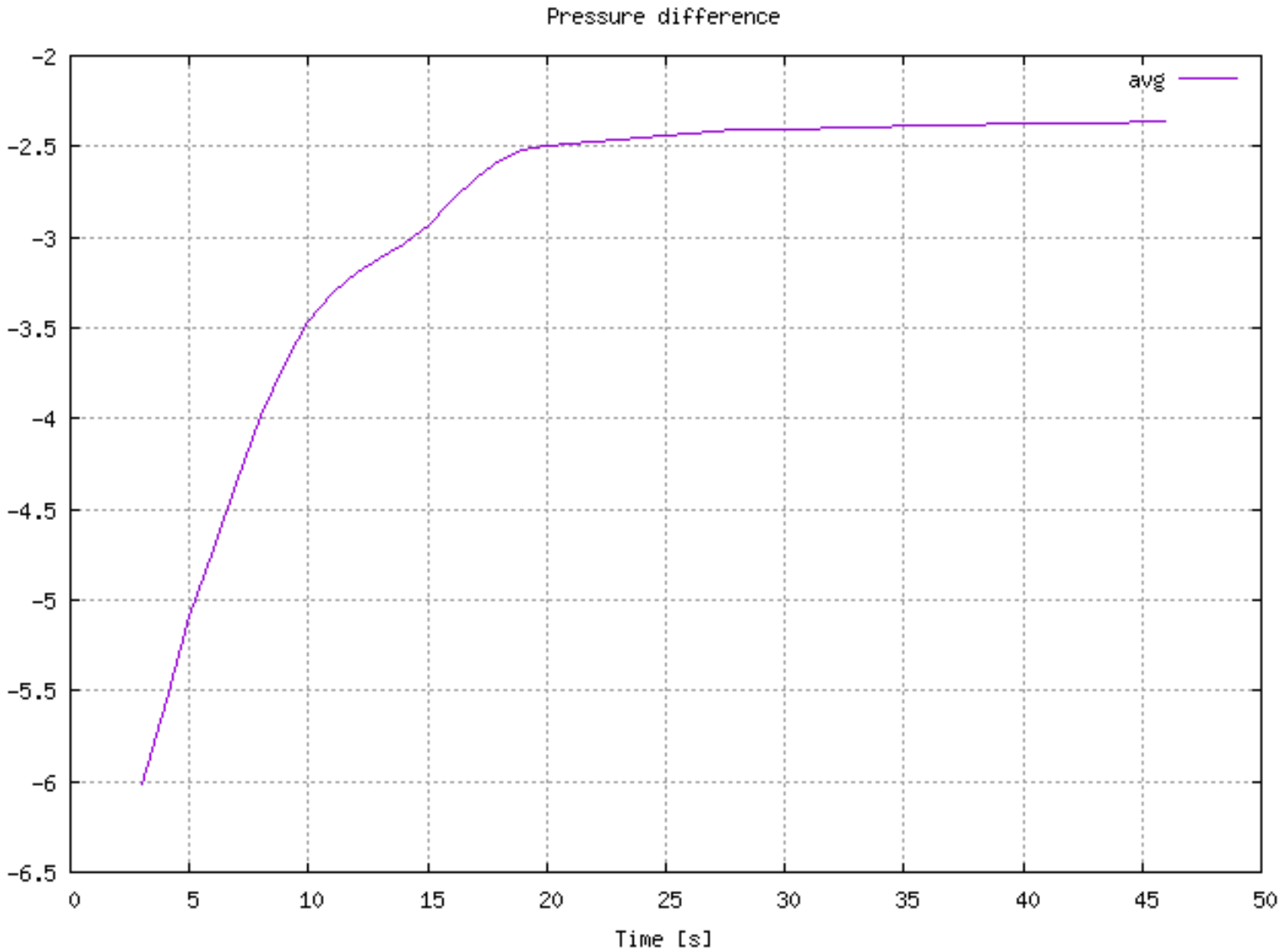
```
> . ~/foam/foam-extend-4.1/etc/zshrc
> pyFoamPrepareCase.py . --parameter=coarseMeshLayers.parameters --value="potentialFlow yes;"
...
> pyFoamPlotRunner.py --clear  --progress simpleFoam
 t =         267 dp: -2.78484 detach: 0.168234
> pyFoamPrepareCase.py . --parameter=coarseMeshLayers.parameters --value="potentialFlow yes; solver pUCoupledFoam;"
...
> pyFoamPlotRunner.py --clear  --progress pUCoupledFoam
 t =          43 dp: -2.35515 detach: 0.165944
> pyFoamPrepareCase.py . --parameter=coarseMeshLayers.parameters --value="solver pUCoupledFoam;"
...
> pyFoamPlotRunner.py --clear  --progress pUCoupledFoam
 t =          46 dp: -2.36399 detach: 0.168234
```

- Number of iterations for simpleFoam slightly different
- Coupled solver has drastically less iterations

Coupled solver residuals



Pressure difference with coupled



Spawn point

To get to the current state use `stage8_extendCoupled.tar.gz`

Outline

Working around decomposePar

- Obviously we want our tests to run in parallel too
- But there are some problems:
  - `decomposePar` doesn't like `.template` files when it finds them in `0`
    - Thinks their format is incorrect and dies
- `pyFoamPrepareCase.py` does not automatically support parallelization
  - Because it differs too much between work-flows what can be done in parallel
    - There is no "one size fits all"
- But it offers some help
  - Command line option that sets the number of processors
  - Some "regular PyFoam" features

Decomposing

- Using `pyFoamDecompose.py` for decomposition
- Moving template files to where `decomposePar` won't find them
  - And move them back again

`meshCreate.sh.template`

```
<!--(if numberOfProcessors>1)-->
cp -r 0.org 0
rm 0/*.template

mkdir 0.tmp
mv 0/*.finalTemplate 0.tmp

pyFoamDecompose.py . |-numberOfProcessors-|

  <!--(for p in range(numberOfProcessors))-->
cp 0.tmp/* processor|-p-|/0/
  <!--(end)-->

rm -r 0.tmp
<!--(end)-->
```

--autosense-parallel

- pyFoamRunner.py has an option -autosense-parallel
  - This say:
    - If you find processor-directories then run the program in parallel
    - ... otherwise: single processor
- Prefixing utilities after the decomposition with this saves us from having a if parallel for every on of them

caseSetup.sh.postTemplate

```
#! /bin/sh

<!--(if potentialFlow)-->
pyFoamRunner.py --auto potentialFoam
  <!--(if compressible)-->
rm -f 0/phi* processor*/0/phi*
  <!--(end)-->
<!--(end)-->
```

Files have to be removed from the processor directories as well

Making sure it runs in parallel

- Because `.finalTemplate` has not been decomposed we have to make sure manually that it works
  - Add `procBoundary`-files to `p`

`0.org/p.finalTemplate`

```
boundaryField
{
...
    "procBoundary.*"
    {
        type            processor;
        value           $internalField;
    }
}
```

Running

For running the solver we use `--autosense-parallel` for the `pyFoamRunner.py` as well

Shell

```
> . ~/OpenFOAM/OpenFOAM-v1712/etc/bashrc
> pyFoamPrepareCase.py . --parameter=coarseMeshLayers.parameters --value="potentialFlow yes<brk>
      <cont>;" --number-of-processors=2
...
> pyFoamPlotRunner.py --clear  --progress --auto simpleFoam
 t =        323 dp: -2.97127 detach: 0.168234
```

Recent developments

- New versions of `PyFoam` look for scripts for decomposing in different phases

  decomposeMesh.sh runs after `meshCreate.sh`
  decomposeFields.sh runs after `0.org` has been copied to `0`
  decomposeCase.sh runs after `caseSetup.sh`
- Usually not all of them are used
  - Depends on the way the mesh was generated
  - But it gives us flexibility

Spawn point

To get to the current state use `stage9_parallel.tar.gz`

Outline

Parameter variations

- The utility `pyFoamRunParameterVariation.py` is based on the functionality of `pyFoamPrepareCase.py`
  - Idea: set up and run as usual.
    - Just change some parameters systematically
- Specification of the variation in a dictionary
- `values` is a dictionary with parameters and their variations
  - Either a list of simple values
  - Or a list of dictionaries
    - This is for cases where only specific sets of parameters make sense
    - Needs a `defaults`-entry if values are missing from the set

The variation file

- Compare solvers and mesh resolutions

meshResolution.variation

```
defaults {
    nrBoundaryLayers 0;
    graded true;
}

values {
    solver (
        simpleFoam
        pUCoupledFoam
    );
    resFactor (
        0.5 1 1.5 2
    );
    sets (
        {
            nrBoundaryLayers 1;
            graded false;
        }
        { }
    );
 }
```

Explanation

solver	Compare two solvers ■ This entry is always required (even if only one entry)
resFactor	try 4 resolution factors
sets	Compare grading/no layers with ungraded/layers ■ but no graded/layers and ungraded/no layers

Total of $4 \times 2 = 16$ variations

Preparing

- The utility has to be executed outside our case

```
cd ..
```

- Will create a clone of our case for every variation specified
  - This behavior can be changed
    - Do variations in the original case
    - Create only one clone and do all variations there
  - But we'll go for the extra copies
    - That way we can afterwards check the full results
    - Not only the summaries

Listing the variations

- Every variation has a number
  - We want to see which one sets which values

Shell

```
> pyFoamRunParameterVariation.py ../pitzDailyWorkshopStages ../pitzDailyWorkshopStages/meshResolution.variation  --<brk>
      <cont>list-variations

================================
16 variations with 3 parameters
================================


==================
Listing variations
==================

Variation 0 : {'solver': 'simpleFoam', 'resFactor': 0.5, 'nrBoundaryLayers': 1, 'graded': false}
Variation 1 : {'solver': 'pUCoupledFoam', 'resFactor': 0.5, 'nrBoundaryLayers': 1, 'graded': false}
Variation 2 : {'solver': 'simpleFoam', 'resFactor': 1, 'nrBoundaryLayers': 1, 'graded': false}
Variation 3 : {'solver': 'pUCoupledFoam', 'resFactor': 1, 'nrBoundaryLayers': 1, 'graded': false}
Variation 4 : {'solver': 'simpleFoam', 'resFactor': 1.5, 'nrBoundaryLayers': 1, 'graded': false}
Variation 5 : {'solver': 'pUCoupledFoam', 'resFactor': 1.5, 'nrBoundaryLayers': 1, 'graded': false}
Variation 6 : {'solver': 'simpleFoam', 'resFactor': 2, 'nrBoundaryLayers': 1, 'graded': false}
Variation 7 : {'solver': 'pUCoupledFoam', 'resFactor': 2, 'nrBoundaryLayers': 1, 'graded': false}
Variation 8 : {'solver': 'simpleFoam', 'resFactor': 0.5, 'nrBoundaryLayers': 0, 'graded': true}
Variation 9 : {'solver': 'pUCoupledFoam', 'resFactor': 0.5, 'nrBoundaryLayers': 0, 'graded': true}
Variation 10 : {'solver': 'simpleFoam', 'resFactor': 1, 'nrBoundaryLayers': 0, 'graded': true}
Variation 11 : {'solver': 'pUCoupledFoam', 'resFactor': 1, 'nrBoundaryLayers': 0, 'graded': true}
Variation 12 : {'solver': 'simpleFoam', 'resFactor': 1.5, 'nrBoundaryLayers': 0, 'graded': true}
Variation 13 : {'solver': 'pUCoupledFoam', 'resFactor': 1.5, 'nrBoundaryLayers': 0, 'graded': true}
Variation 14 : {'solver': 'simpleFoam', 'resFactor': 2, 'nrBoundaryLayers': 0, 'graded': true}
Variation 15 : {'solver': 'pUCoupledFoam', 'resFactor': 2, 'nrBoundaryLayers': 0, 'graded': true}
```

Running the variation

- We run the actual variation
  - Specify the variation file
  - and the original case
- This takes some time
  - And creates 16 new directories

Shell

```
> pyFoamRunParameterVariation.py pitzDailyWorkshopStages pitzDailyWorkshopStages/<brk>
      <cont>meshResolution.variation  --every-variant-one-case-execution --auto-create-<brk>
      <cont>database --quiet
...
> ls
meshResolution.variation_00000_pitzDailyWorkshopStages/
meshResolution.variation_00001_pitzDailyWorkshopStages/
meshResolution.variation_00002_pitzDailyWorkshopStages/
```

List the cases

We want to get an overview of the created case directories

Shell

```
> pyFoamListCases.py
                  mtime |     hostname | first - last (nrSteps)   nowTime s    state | solver | name
-------------------------------------------------------------------------------------------------------------
Sat Jun 13 02:36:19 2018 | bgs-greybook |     0 -  279 (      7)     279.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00000_pitzDailyWorkshopStages
Sat Jun 13 02:36:34 2018 | bgs-greybook |     0 -   43 (      2)      43.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00001_pitzDailyWorkshopStages
Sat Jun 13 02:37:12 2018 | bgs-greybook |     0 -  664 (     15)     664.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00002_pitzDailyWorkshopStages
Sat Jun 13 02:38:38 2018 | bgs-greybook |     0 -   75 (      3)      75.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00003_pitzDailyWorkshopStages
Sat Jun 13 02:41:00 2018 | bgs-greybook |     0 - 1168 (     25)    1168.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00004_pitzDailyWorkshopStages
Sat Jun 13 02:46:04 2018 | bgs-greybook |     0 -   95 (      3)      95.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00005_pitzDailyWorkshopStages
Sat Jun 13 02:50:32 2018 | bgs-greybook |     0 - 1325 (     28)    1325.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00006_pitzDailyWorkshopStages
Sat Jun 13 02:59:12 2018 | bgs-greybook |     0 -   86 (      3)      86.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00007_pitzDailyWorkshopStages
Sat Jun 13 02:59:26 2018 | bgs-greybook |     0 -  313 (      8)     313.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00008_pitzDailyWorkshopStages
Sat Jun 13 02:59:33 2018 | bgs-greybook |     0 -   46 (      2)      46.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00009_pitzDailyWorkshopStages
Sat Jun 13 03:00:09 2018 | bgs-greybook |     0 -  833 (     18)     833.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00010_pitzDailyWorkshopStages
Sat Jun 13 03:01:04 2018 | bgs-greybook |     0 -   60 (      3)      60.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00011_pitzDailyWorkshopStages
Sat Jun 13 03:03:51 2018 | bgs-greybook |     0 - 1477 (     31)    1477.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00012_pitzDailyWorkshopStages
Sat Jun 13 03:08:16 2018 | bgs-greybook |     0 -   97 (      3)      97.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00013_pitzDailyWorkshopStages
Sat Jun 13 03:14:15 2018 | bgs-greybook |     0 - 1910 (     40)    1910.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00014_pitzDailyWorkshopStages
Sat Jun 13 03:23:10 2018 | bgs-greybook |     0 -   91 (      3)      91.0 s Finished |   None | ./meshResolution.<brk>
      <cont>variation_00015_pitzDailyWorkshopStages
```

Data of one run

- Data from each run is stored in a *pickled file*.
- Can be dumped with a utility
  - Read from any Python-script with the `pickled` module

Shell

```
> pyFoamEchoPickledApplicationData.py --print-data --pickled-file=meshResolution.variation_00000_pitzDailyWorkshopStages/<brk>
      <cont>meshResolution.variation_simpleFoam.analyzed/pickledData
{'OK': True,
 'analyzed': {'Continuity': {'Cumulative': 0.356656, 'Global': -6.27369e-05},
              'Custom': {'deltaP': {'avg': -4.60039},
                         'detatch': {'x': 0.168234}},
              'Custom01_deltaP': {'avg': -4.60039},
              'Custom02_detatch': {'x': 0.168234},
              'Execution': {'clock': 0.0, 'cpu': 0.010000000000000231},
...
 'parameters': {'TAir': 293,
                'UIn': 10,
                'caseName': '"meshResolution.variation_00000_pitzDailyWorkshopStages"',
                'casePath': '"/Volumes/Foam/Workshop2018/meshResolution.variation_00000_pitzDailyWorkshopStages"',
                'compressible': 'False',
                'dynVisc': 1.8e-05,
                'foamFork': 'extend',
                'foamVersion': [4, 1],
                'graded': false,
                'molarWeight': 28.9,
                'nrBoundaryLayers': 1,
                'numberOfProcessors': 1,
                'pAir': 100000.0,
                'potentialFlow': 'false',
                'resFactor': 0.5,
                'solver': 'simpleFoam',
                'xProfiles': '"[-10, 0, 50, 100, 150, 200, 250]"'},
...
```

Reading the database information

- Data of the variations is stored in a `SQlite`-database
- There is also a utility to dump this to (for instance) Excel
  - But can also be processed in Python

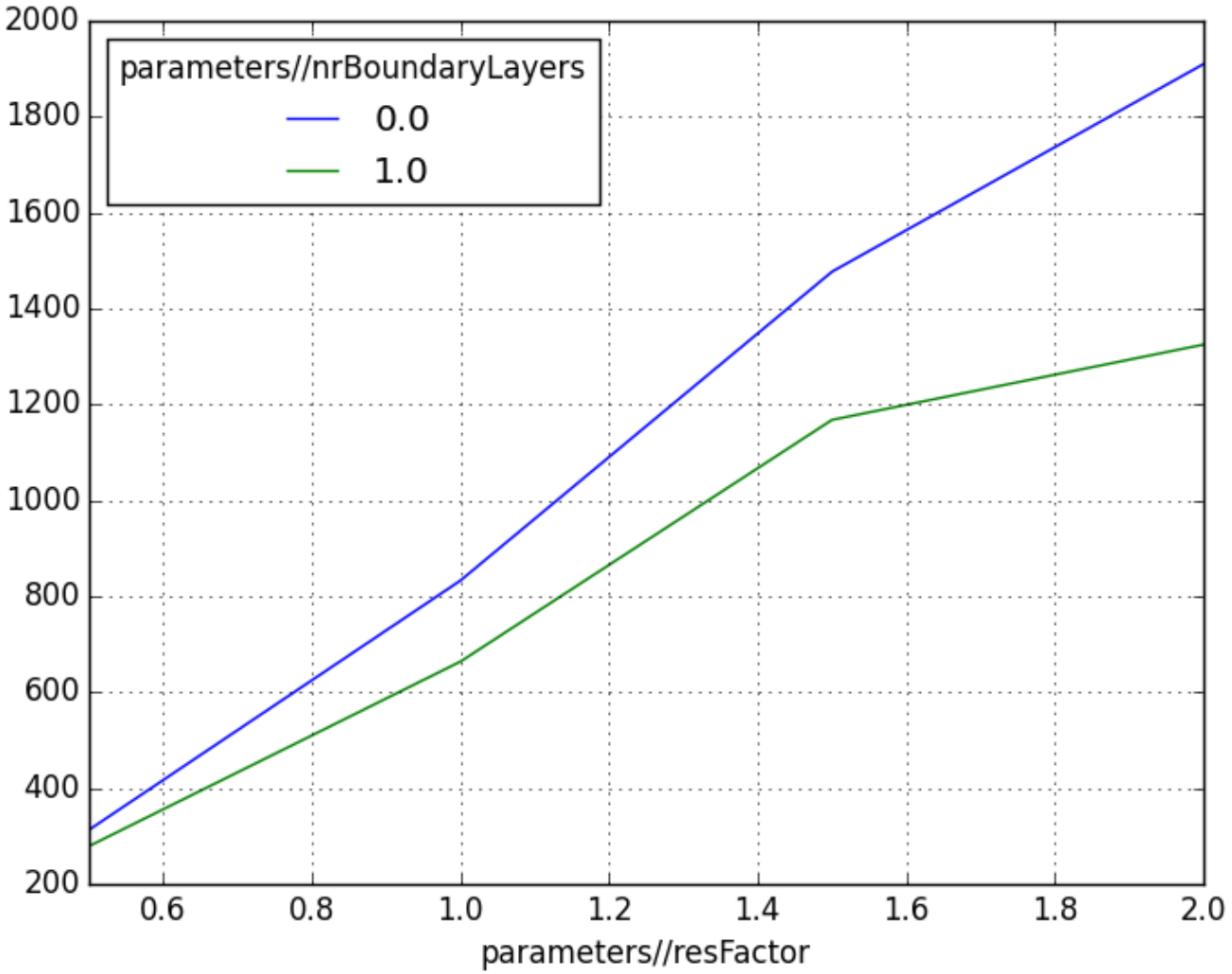
Shell

```
> pyFoamDumpRunDatabaseToCSV.py meshResolution.variation.database pitzDaily.xls --interactive-after --excel

Dropping to interactive shell ... found IPython ...up-to-date IPython

Python 3.4.3 (default, May 25 2015, 18:48:21)

In [1]: %matplotlib
Using matplotlib backend: Qt4Agg
In [2]: dump=self.getData()["dump"]
In [3]: dump.keys()
Out[3]:
Index(['analyzed//Continuity//Cumulative', 'analyzed//Continuity//Global',
       'analyzed//Custom//deltaP//avg', 'analyzed//Custom//detatch//x',
       'analyzed//Custom01_deltaP//avg', 'analyzed//Custom02_detatch//x',
       'analyzed//Execution//clock', 'analyzed//Execution//cpu',
...
In [4]: pivot=dump[dump["parameters//solver"]=="simpleFoam"].pivot("parameters//resFactor","parameters//nrBoundaryLayers")
In [5]: pivot2=dump[dump["parameters//solver"]=="pUCoupledFoam"].pivot("parameters//resFactor","parameters//nrBoundaryLayers")
In [6]: pivot2["runInfo//time"]
Out[6]:
parameters//nrBoundaryLayers   0   1
parameters//resFactor
0.5                           46  43
1.0                           60  75
1.5                           97  95
2.0                           91  86
In [7]: pivot2["runInfo//time"].plot()
Out[7]: <matplotlib.axes._subplots.AxesSubplot at 0x115434438>
In [8]: pivot["runInfo//time"]/pivot2["runInfo//time"]
Out[8]:
parameters//nrBoundaryLayers          0          1
parameters//resFactor
0.5                            6.804348   6.488372
1.0                           13.883333   8.853333
1.5                           15.226804  12.294737
2.0                           20.989011  15.406977
```

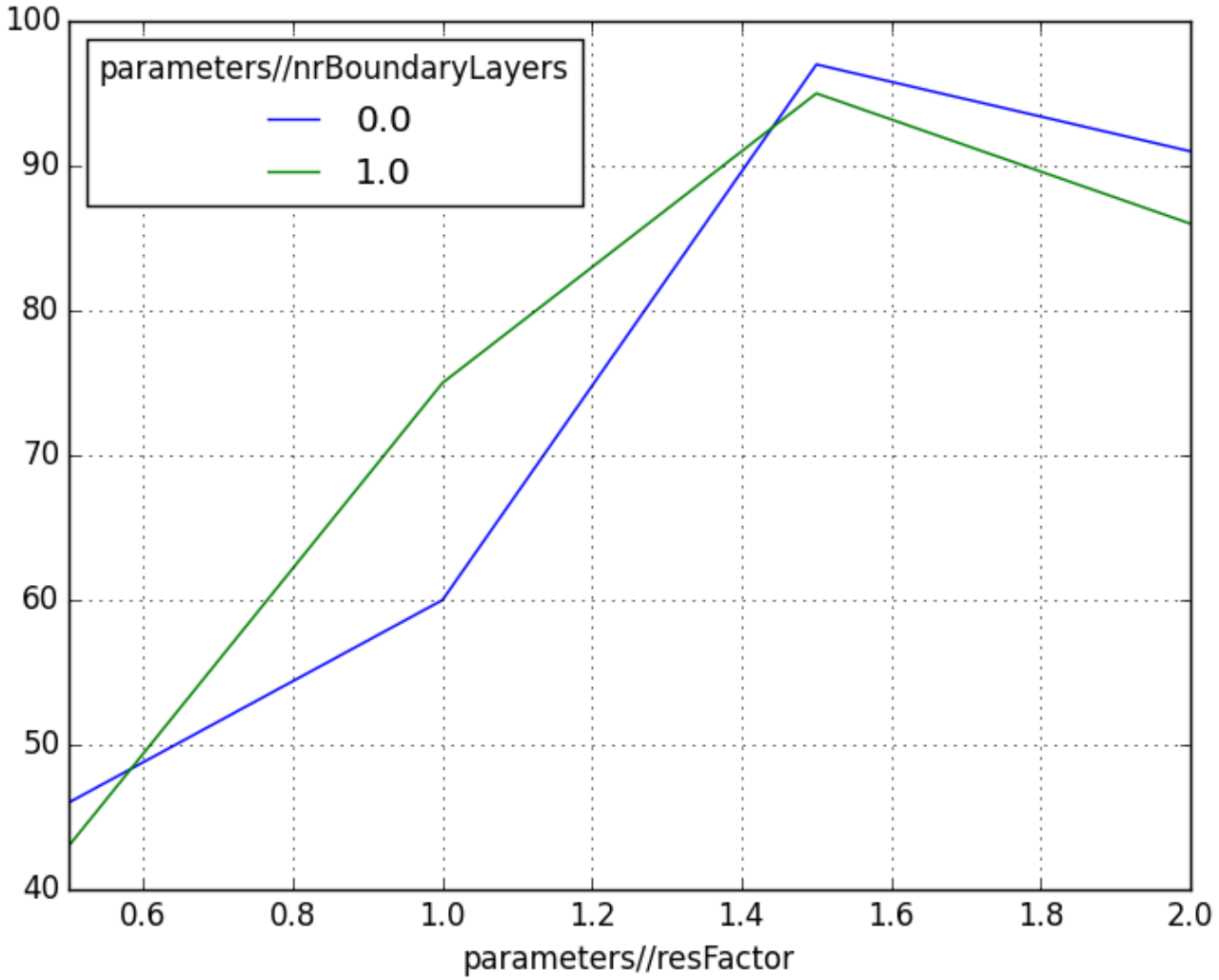
Analyzing the variation data

- This only gives a glimpse of what is possible
  - Wouldn't draw any conclusion on this concrete case
- Data is stored in formats that require no additional Python-modules
  - *Pickled* files
  - `SQlite` databases
- So it should be easy to write your own solution
- For analyzing use the toolset you're most comfortable with
  - `pandas`
  - Excel ...

Iterations of simpleFoam

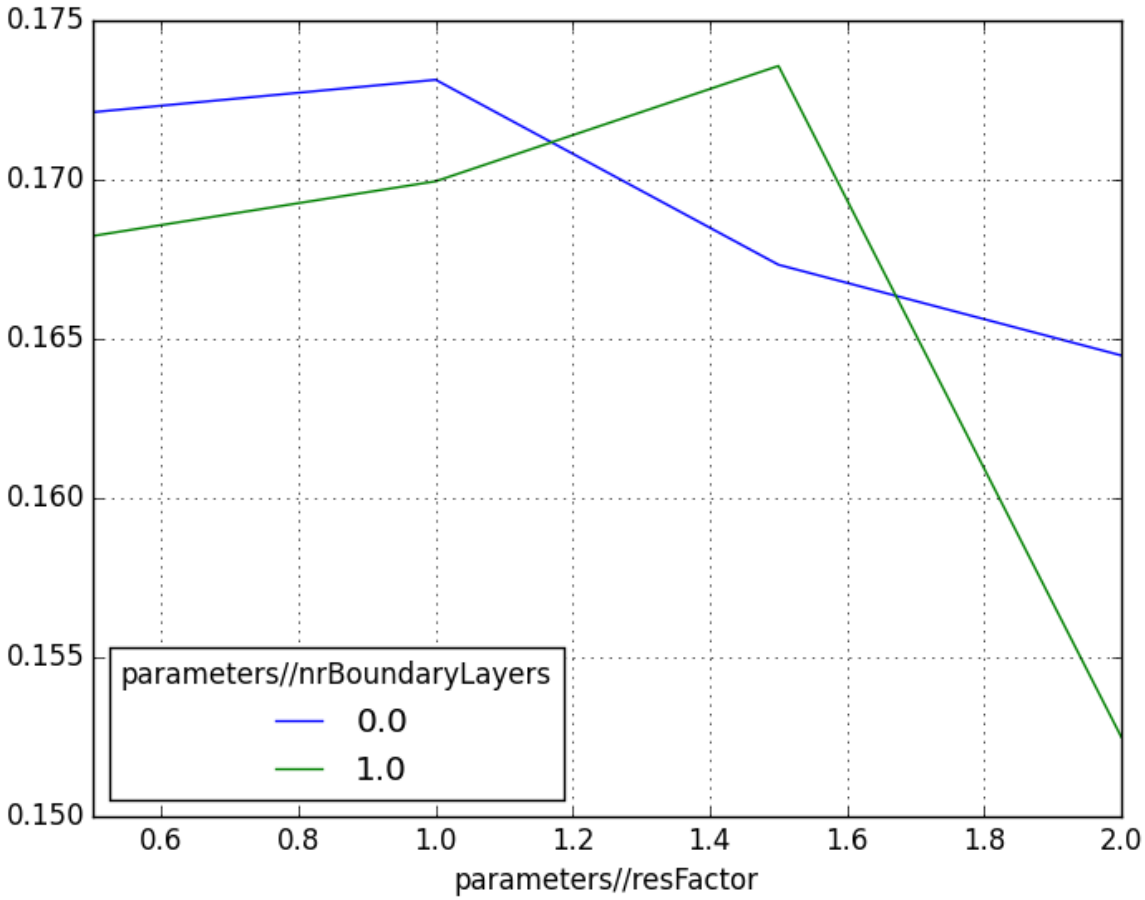


Iterations of pUCoupledFoam



Not yet converged

```
pivot["analyzed//Custom//detatch//x"].plot()
```



End of game

To get to the current state use `stage10_parameterVariation.tar.gz`

Outline

Switching off phases

- There is a number of switches that switches off certain phases
- Most used: `--no-meshing`
  - Exampled: Meshing is a big `snappyHexMesh`
    - You don't want to wait hours just because you set up new boundary conditions

Version control systems

- Setting up a case for `pyFoamPrepareCase.py` is a bit like programming
- When programming it is good to use a *version control system*
  - Mercurial
  - Git
  - ...
- Only put the files you actually edit under version control
- Benefits:
  - Documentation on "when was this set and why"
  - Branching allows trying things

Cluster scripts

- The class `PrepareCaseJob` in the module `PyFoam.Infrastructure.ClusterJob` uses `pyFoamPrepareCase.py` to set up the case
  - and run the case afterwards
    - Also takes care of case decomposition and reconstruction
- Currently this supports the *Sun Grid Engine*
  - But other queueing systems are possible

Outline

What we learned

- "Programming" a case to be set up with `pyFoamPrepareCase.py`
  - Disadvantage:
    - Needs a bit of work and thought
  - Advantages:
    - Once done it is a two-step to set up a case and run it
    - Harder to make mistakes while setting it up
- We only showed a little example case, but this utility has been successfully used for big, complex cases
  - Automatically adding large numbers of STLs, snapping them. Calculating initial conditions depending on the conditions of the STLs

Recommended Execises

- Set up `fvSchemes` to try different discretization schemes
- Adapt so that transient solvers can be used as well
- Modify to use a `snappyHexMesh`-geometry
- Find the "real" detachment point

Goodbye to you

Thanks for listening

Questions?

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Bernhard F.W. Gschaider original author and responsible for the strange English grammar. Contact him for a copy of the sources if you want to extend/improve/use this presentation