Automatization with pyFoam

How Python helps us to avoid contact with OpenFOAM™

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5th OpenFOAM™-Workshop, Gothenburg
24.June 2010

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Overview

Aim of this presentation

This presentation shows how to use PyFoam to run a case automatically and evaluate the results

It does not give

- a full overview of Python
- an overview of all the capabilities of PyFoam

It assumes

- that you know your way around OpenFOAM™
- have programmed a little bit in **some** language (not necessarily Python)

What is PyFoam

PyFoam is

1. a Python library that
   - manipulates OpenFOAM™-cases
   - controls OpenFOAM™-runs
2. Utilities based on that library

What happened before

- Last year in Montreal a presentation PyFoam - Happy foaming with Python (URL below) was given
  - It is not necessary that you have read it
  - .... but helpful (Now it's to late. Read it later.)
- We were introduced to the CFD-engineer Ignaz Gartengschirrl
  - A specialist on calculating the `damBreak`-case
  - ... using PyFoam
- During the last year Ignaz extended
  - his professional range
  - his knowledge of PyFoam

`http://www.openfoamworkshop.org/2009/4th_Workshop/0_Feature_Presentations/OFW4_2009_Gschaider_PyFoam.pdf`

Conventions

Whenever Ignaz (and also you) writes something

- on the shell
- in an editor

it will be found in a coloured box. Sometimes there will be output, too

Ignaz writes on the shell

```
> date
Fri May 15 01:56:12 CEST 2009
```

Ignaz's Python-code

```
sum=0
for v in [7,13,42]:
    sum+=v
print "The sum is",sum
# this is a long line that will be <brk>
    <cont>continued in the next line
```

Ignaz edits a file

```
fooCoeffs {
  bar 23;
  lst ( inlet outlet );
}
```

Getting the git-archive with the data

- The data and programs needed are in a `tar`-file on the stick
  - If you haven't booted from the stick the paths may be different for you
- First we copy it to your home and create a working directory:

Preparing for work

```
> cd $HOME
> mkdir pyFoamAdvanced
> cd pyFoamAdvanced
> tar xzf /cdrom/OFW5/Advanced_Training/pyFoamAdvanced.git.tgz
```

- Now there should be a directory `pyFoamAdvanced.git`

Getting to a specific step

- What we extracted is a GIT-archive
- There are several branches for different phases
  - So if you couldn't follow you can catch up

Going to a specific step

```
> cd $HOME/pyFoamAdvanced
> git clone pyFoamAdvanced.git -b step1manualStarting step1
```

- Now there should be a directory `step1`

What is Python

PYTHON

- Is a scripting language
  - No compilation required
- Is object-oriented
- Comes *batteries included*: has a large standard-library for many common tasks
  - Non essential parts (like regular expressions) were moved to the library
- Widely used
  - Pre-installed on most LINUX-systems because many system tools (installers for instance) use it
  - Becomes *scripting language of choice* for a number of programs (amongst others the post-processors PARAVIEW and VISIT and the pre-processor SALOME)

3 things you have to know about Python

... to understand the programming examples

1. Indentation does the same thing `{` and `}` do for C++
2. `[]` signifies a list (which is an array)
3. `{}` is a dictionary (whose elements are accessed with `[key]`)
4. `self` is the same as `this` in C++ (The object itself)

Aeh. The 4 things to know about PYTHON *are ....*

The Python Shell

- PYTHON-files usually end with the extension `.py`

Running a Python-file

```
> python test.py
```

- But you can also use it interactively

Using the Python-shell

```
> python
Python 2.6.5 (r265:79063, May 18 2010, 10:54:45)
[GCC 4.2.1 (Apple Inc. build 5659)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> 1+1
2
>>> import sys
>>> print sys.platform
darwin
>>>
```

exit with `Ctrl+D`

Basic constructs - lists and dictionaries

Basic usage of lists and dictionaries

```
>>> lst=[2,"interFoam",1.3]
>>> lst[0]
2
>>> lst+=["nothing"]
>>> print lst
[2, 'interFoam', 1.3, 'nothing']
>>> order={'interFoam':1,'blockMesh':0,'paraFoam':2}
>>> order['interFoam']
1
>>> 'paraFoam' in order
True
>>> order['setFields']=0.5
>>> print order
{'blockMesh': 0, 'interFoam': 1, 'setFields': 0.5, 'paraFoam': 2}
```

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Basic constructs - loops

Two kinds of loops

```
>>> vals=[2,3,5,7,11,13,17,19]
>>> for v in vals:
...     print v*v,
...
4 9 25 49 121 169 289 361
>>> i=0
>>> while i<len(vals):
...     vals[i]="no"
...     i+=2
...
>>> print vals
['no', 3, 'no', 7, 'no', 13, 'no', 19]
```

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Basic constructs - branches

One kind of branch is sufficient

```
>>> for i in range(-3,3):
...     if i==0:
...         print "zero",
...     elif (i%2)==0:
...         print "even",
...     else:
...         print "odd",
...
odd even odd zero odd even
```

Basic constructs - classes

Ignaz tells us all he knows

```
>>> class Ignaz:
...     def __init__(self,val):
...         self.val = val
...     def __str__(self):
...         return "Ignaz says "+str(self.val)
...     def forget(self):
...         self.val = None
...
>>> ig=Ignaz(1+1)
>>> print ig
Ignaz says 2
>>> ig.forget()
>>> print ig
Ignaz says None
```

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Basic constructs - importing libraries

Standing on the shoulders of ... other programmers

```
>>> from time import time
>>> time()
1275658314.7988529
>>> import sys
>>> dir(sys)
['__displayhook__', '__doc__', '__egginsert', '__excepthook__', '__name__', '<brk>
    <cont>__package__', '__plen', '__stderr__', '__stdin__', '__stdout__', '<brk>
    <cont>_clear_type_cache', '_current_frames', '_getframe', 'api_version', '<brk>
    <cont>argv', 'builtin_module_names', 'byteorder', 'call_tracing', '<brk>
    <cont>callstats', 'copyright', 'displayhook', 'dont_write_bytecode', '<brk>
    <cont>exc_clear', 'exc_info', 'exc_type', 'excepthook', 'exec_prefix', '<brk>
    <cont>executable', 'exit', 'flags', 'float_info', 'getcheckinterval', '<brk>
    <cont>getdefaultencoding', 'getdlopenflags', 'getfilesystemencoding', '<brk>
    <cont>getprofile', 'getrecursionlimit', 'getrefcount', 'getsizeof', '<brk>
    <cont>gettrace', 'hexversion', 'last_type', 'last_value', 'maxint', '<brk>
    <cont>maxsize', 'maxunicode', 'meta_path', 'modules', 'path', 'path_hooks',<brk>
    <cont> 'path_importer_cache', 'platform', 'prefix', 'ps1', 'ps2', '<brk>
    <cont>py3kwarning', 'setappdefaultencoding', 'setcheckinterval', '<brk>
    <cont>setdlopenflags', 'setprofile', 'setrecursionlimit', 'settrace', '<brk>
    <cont>stderr', 'stdin', 'stdout', 'subversion', 'version', 'version_info', <brk>
    <cont>'warnoptions']
>>> print sys.version
2.6.5 (r265:79063, May 18 2010, 10:54:45)
[GCC 4.2.1 (Apple Inc. build 5659)]
```

How to get help - On the shell

What is that ParsedParameterFile anyway

```
>>> from PyFoam.RunDictionary.ParsedParameterFile import <brk>
    <cont>ParsedParameterFile
>>> print ParsedParameterFile.getCaseDir.__doc__
Return the path to the case of this file (if any valid case is found).
        Else return None
>>> help(ParsedParameterFile
Help on class ParsedParameterFile in module PyFoam.RunDictionary.<brk>
    <cont>ParsedParameterFile:

class ParsedParameterFile(PyFoam.RunDictionary.FileBasis.FileBasisBackup)
 |  Parameterfile whose complete representation is read into
 |  memory, can be manipulated and afterwards written to disk
 |
 |  Method resolution order:
...
```

- All these texts were extracted from the source:
  - PYTHON comes with an included DOXYGEN

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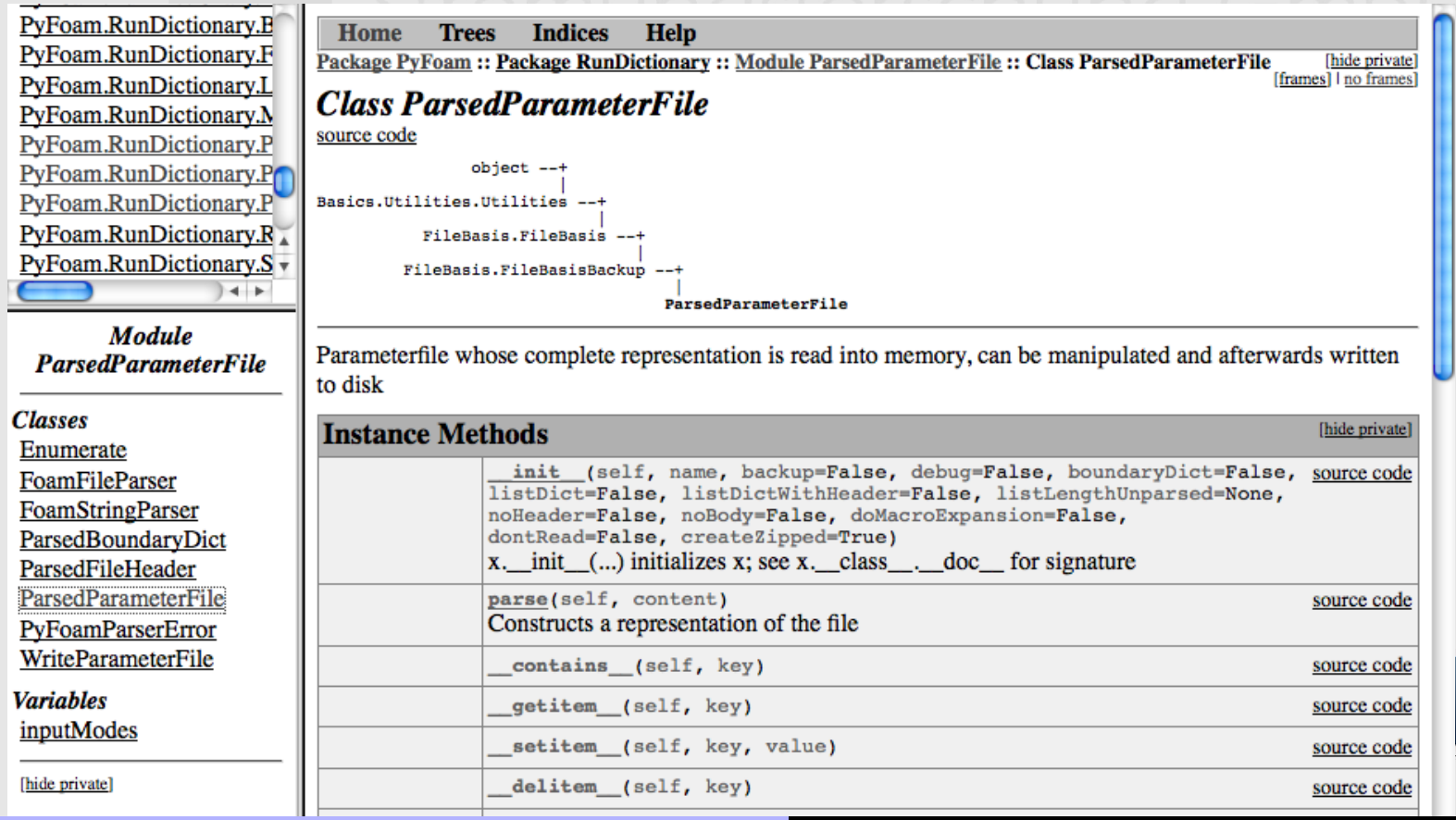
Help on PyFoam

- With the help of a program called epydoc a more user friendly HTML-documentation can be produced
  - This documentation is included in the normal distribution



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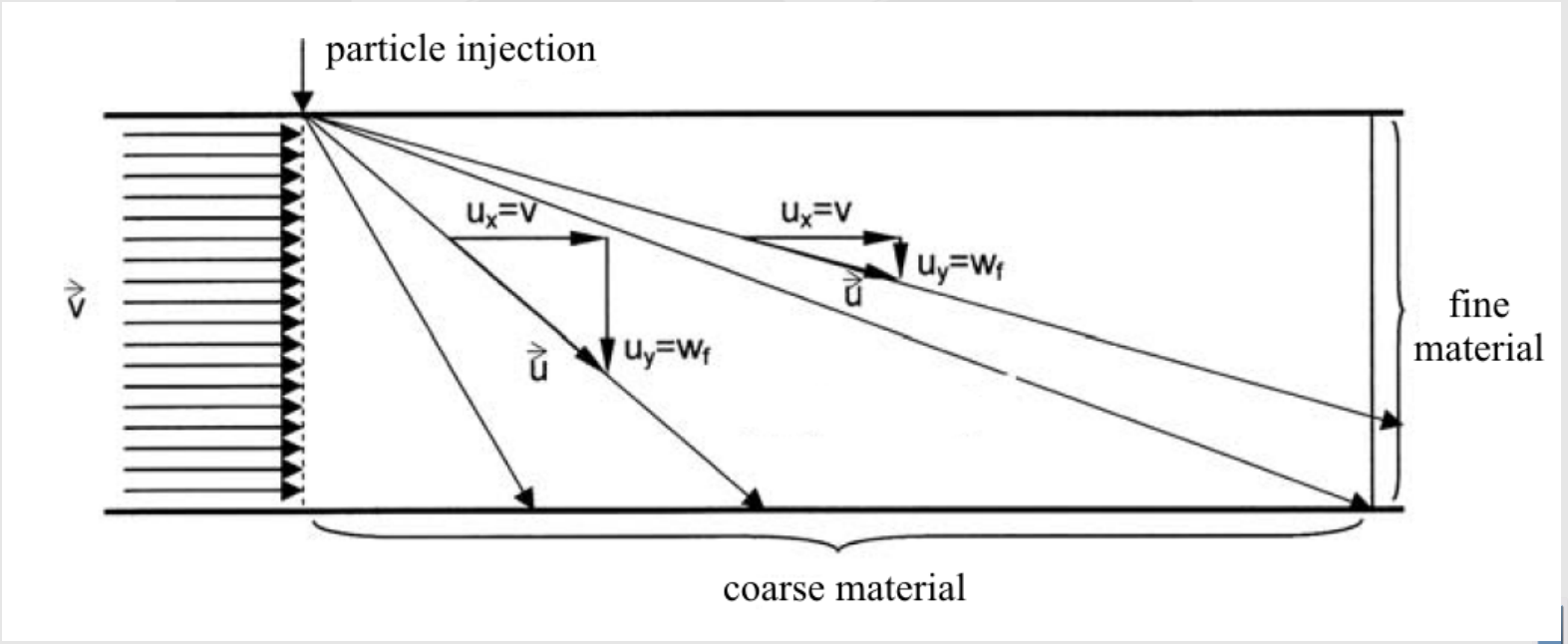
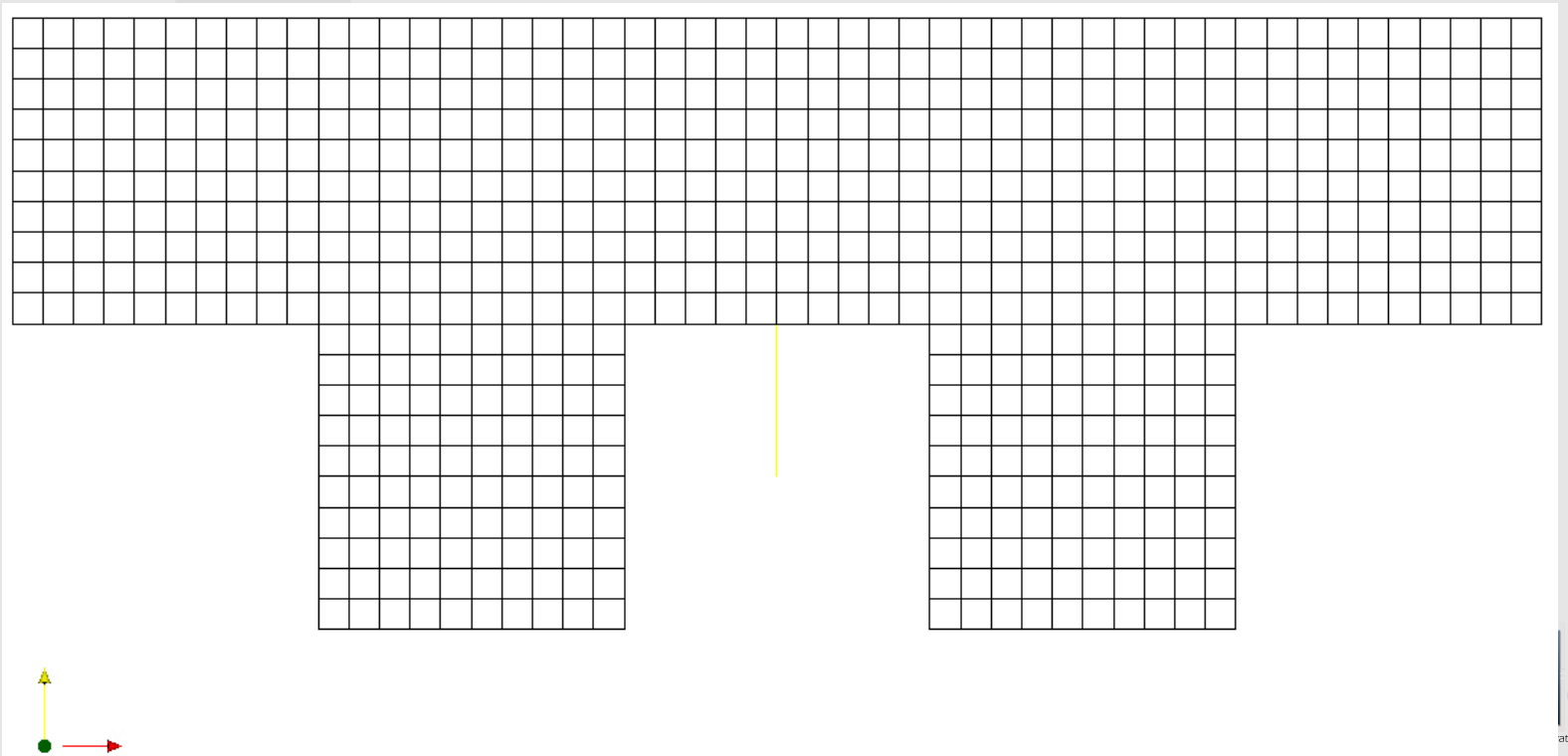
Separating particles of different size

- Ignaz is asked to design a particle separator
- He knows the physics: Drag-force vs. gravity



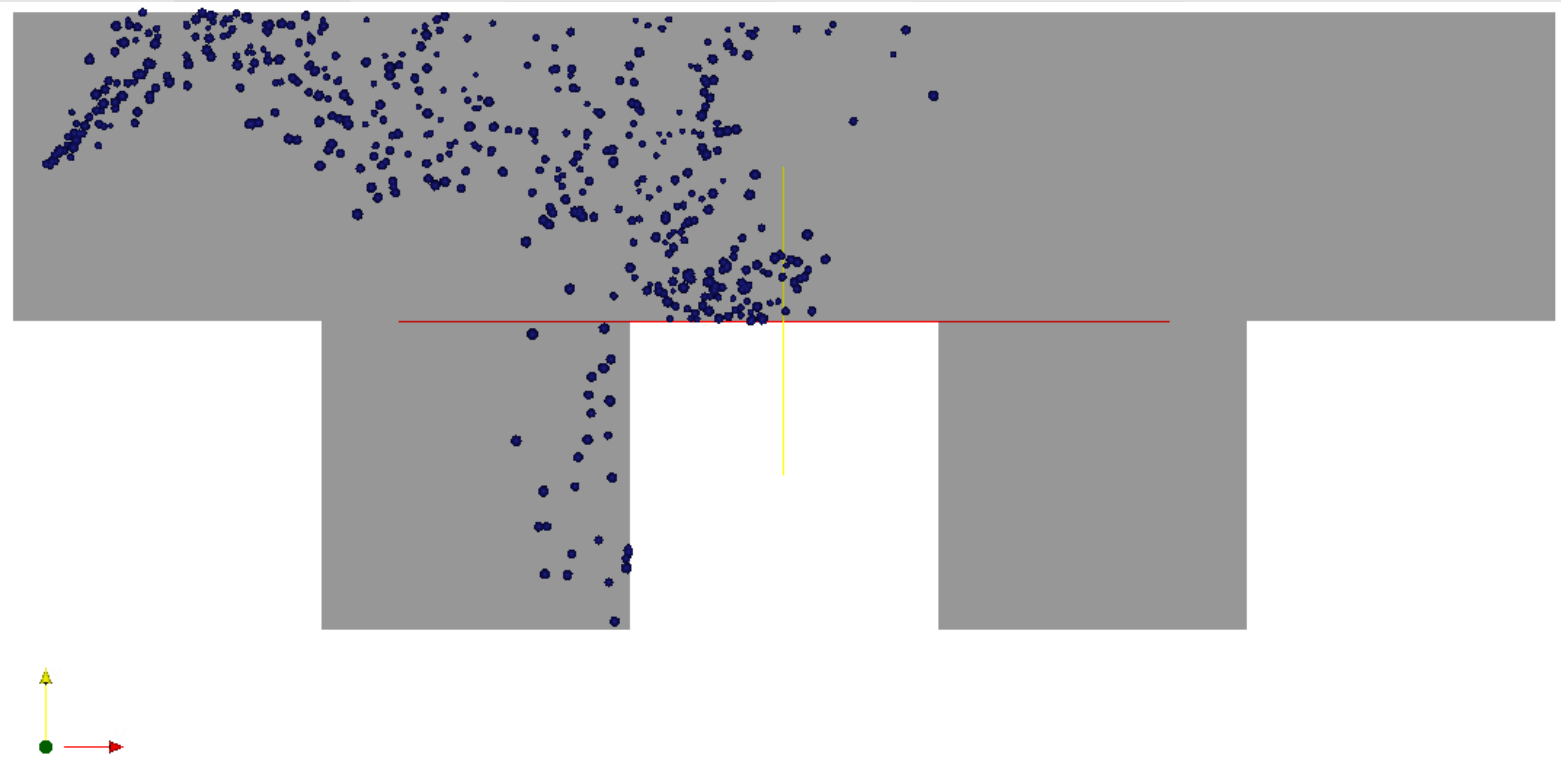
The simplified particle separator

- After 2 weeks the CAD-engineer came up with this complex design
  - Inlet and particle injector at the left



What a solution looks like

- The goal is: Change the inlet velocity of the channel in such a way that
  - The number of particles in the second bin maximizes
  - No (or as few as possible) particles leave through the oultet



Basis: rhoPisoTwinParcelFoam

- Our solver is based on `rhoPisoTwinParcelFoam` which can be found in the tutorials. It is
  - transient
  - compressible
  - turbulent
  - has two different populations of particles
- Changes in `rhoPisoAbscheidParcelFoam` are
  - Only one particle population
  - New particle class

Where do the particles go

- The whole solver had to be written for this method:

In basicAbscheideParcel.C

```
1  void Foam::basicAbscheideParcel::hitPatch
   (
3      const polyPatch& p,trackData& td
   )
5  {
       Pout << "Abgeschieden at " << p.name() << " with m: " << mass()
7           << " N: " << nParticle() << " = total: "
           << mass()*nParticle() <<  endl;
9      KinematicParcel<basicAbscheideParcel>::hitPatch(p,td);
   }
```

- When a particle hits a patch (not a wall), this is the output:

Output on the terminal

```
Abgeschieden at outlet with m: 3.605329877e-10 N: 41386.01459 = total: 1.492102349e-05
```

- We notice that Ignaz never bothered to look up the English word for abscheiden in his dictionary

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Building the solver

1. Get the first stage (if we haven't already done so)

Getting it with Git

```
> cd $HOME/pyFoamAdvanced
> git clone pyFoamAdvanced.git -b step1manualStarting step1
> cd step1
```

2. Compiling the solver (we only have to do this once)

Making sure we use the right OpenFOAM™-version

```
> pyFoamExecute.py --foam=1.5-dev wmake solver/rhoPisoAbscheidParcelFoam15
 PyFoam WARNING on line 152 of file /software/PyFoam/FoamInformation.py : 1.5-dev is <brk>
      <cont>already being used
```

Compiling it for debugging

```
> pyFoamExecute.py --foam=1.5-dev --force-debug wmake solver/rhoPisoAbscheidParcelFoam15
```

A clean slate

- Ignaz likes to start with a new case

Making a copy

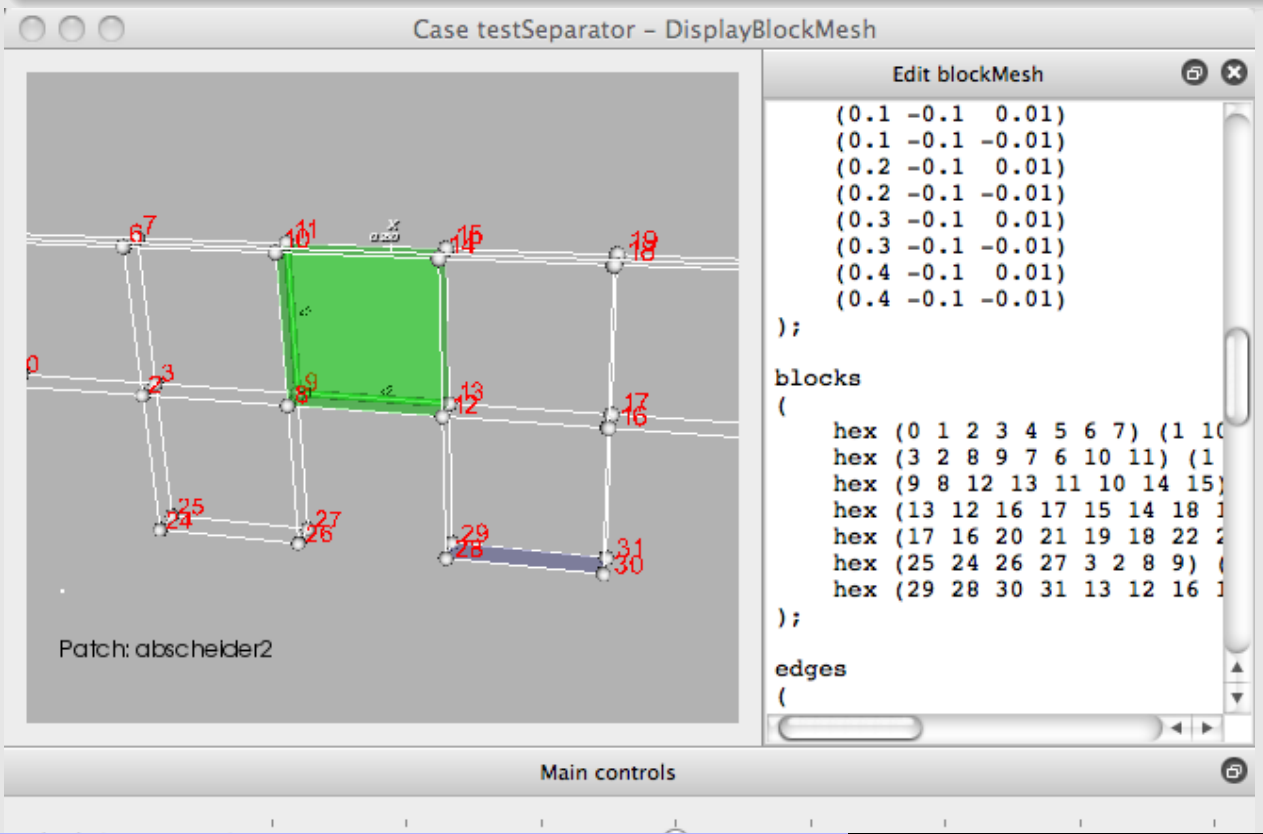
```
> pyFoamCloneCase.py --add=default.pvsm cases/twoCavityChannel <brk>
    <cont>testSeparator
PyFoam WARNING on line 85 of file /Users/bgschaid/private_python/PyFoam/<brk>
    <cont>Applications/CloneCase.py : Directory  does not exist. Creating
> cd testSeparator
```

- Now he can modify the case any way he likes

Editing the blockMesh

Making `blockMesh` less painful

```
1 > pyFoamDisplayBlockMesh.py constant/polyMesh/blockMeshDict
```



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Checking the boundary conditions

All boundary conditions at once

```
> pyFoamCaseReport.py --short-bc .

Table of boundary conditions for t = 0

          | abscheider1  | abscheider2  | bottom       | defaultFaces | inlet        | outlet       | top
-------------------------------------------------------------------------------------------------------------
Patch Type | patch        | patch        | wall         | empty        | patch        | patch        | wall
Length     | 10           | 10           | 70           | 1400         | 10           | 10           | 50
-------------------------------------------------------------------------------------------------------------
T          | inletOutlet  | inletOutlet  | zeroGradient | empty        | fixedValue   | zeroGradient | zeroGradient
U          | fixedValue   | fixedValue   | fixedValue   | empty        | fixedValue   | inletOutlet  | fixedValue
epsilon    | inletOutlet  | inletOutlet  | zeroGradient | empty        | fixedValue   | inletOutlet  | zeroGradient
k          | inletOutlet  | inletOutlet  | zeroGradient | empty        | fixedValue   | inletOutlet  | zeroGradient
p          | zeroGradient | zeroGradient | zeroGradient | empty        | zeroGradient | fixedValue   | zeroGradient
```

Other things the tool can report

```
> pyFoamCaseReport.py --help
```

Preparing for parallel runs

2 CPUs is all we have

```
> pyFoamDecompose.py . 2
...
> pyFoamCaseReport.py --decomposition .
Case is decomposed for 2 processors
              |      0      1
------------------------------
      Points  |    814    770
       Faces  |   1486   1404
       Cells  |    360    340
------------------------------
 abscheider1  |     10      0
 abscheider2  |      0     10
      bottom  |     36     34
defaultFaces  |    720    680
       inlet  |     10      0
      outlet  |      0     10
         top  |     26     24
```

Hey! Ho! Let's go!

At last Ignaz is eager to see some numbers ...

Removing old data and starting the run

```
> pyFoamRunner.py --progress --proc=2 --clear rhoPisoAbscheidParcelFoam
 Reading regular expressions from /Volumes/Rest/StickTest/Shared/AdvanzedWork/step1/<brk>
      <cont>testSeparator/customRegexp
Clearing out old timesteps ....
 t =  0.0736599

...

> less PyFoamRunner.rhoPisoAbscheidParcelFoam.logfile
/*---------------------------------------------------------------------------*\
| =========                 |                                                 |
| \\      /  F ield         | OpenFOAM: The Open Source CFD Toolbox           |
|  \\    /   O peration     | Version:  1.5-dev                               |
|   \\  /    A nd           | Revision: exported                              |
|    \\/     M anipulation  | Web:      http://www.OpenFOAM.org               |
\*---------------------------------------------------------------------------*/
Exec   : rhoPisoAbscheidParcelFoam
...
```

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Regular expressions in 3 minutes

- Regular expressions are essential for `customRegexp` (therefor the name)
- Usually a letter is matched by itself
  - `.` matches any letter
- Patterns are enclosed by `(` and `)`
  - Patterns are numbered by the order in which they appear in the expression
- `+` means "repeat the previous pattern at least once"
- `%f%` is PyFoam-shorthand for a regular expression that matches any floating-point number

Parcels in the system

Ignaz wants a plot of the parcels in the system

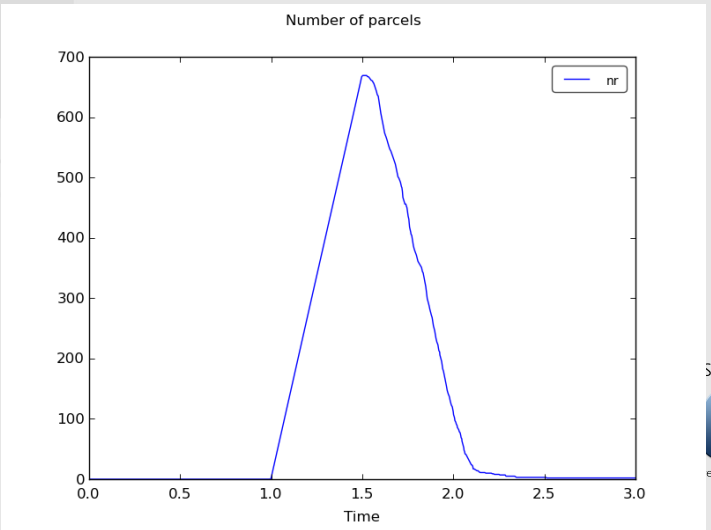
expr The regular expression that should be matched

theTitle Title of the plot

name List of annotations

Simple plot

```
parcels
{
        theTitle "Number of parcels";
        expr "Current number of <brk>
             <cont>parcels        =  (%f <brk>
             <cont>%)";
        titles ( nr );
}
```



Mass leaving the system

List of exits is not previously known. `type dynamic` allows to dynamically build it

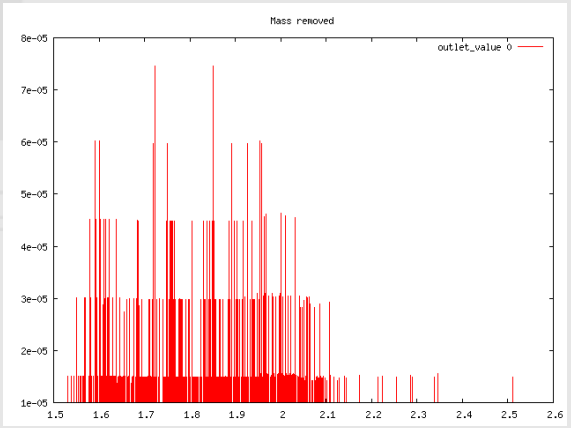
idNr The pattern number of the ID (name)

accumulation `sum` means that several occurences of a pattern in a time-step will be added (usually only the first is used)

with How the data should be plotted (see `with` in GnuPlot)

Simple plot

```
amount
{
        theTitle "Mass removed";
        expr "Abgeschieden at (.+) <brk>
              <cont>with .+total: (%f%) <brk>
              <cont>";
        type dynamic;
        idNr 1;
        with impulses;
        accumulation sum;
}
```



Using it to plot

Displaying from a logfile

```
1 > pyFoamPlotWatcher.py PyFoamRunner.rhoPisoAbscheidParcelFoam.logfile
```

Saving pictures afterwards

```
1 > pyFoamPlotWatcher.py --progress PyFoamRunner.rhoPisoAbscheidParcelFoam.logfile --<brk>
      <cont>hardcopy
```

Using matplotlib

```
1 > pyFoamPlotWatcher.py --progress PyFoamRunner.rhoPisoAbscheidParcelFoam.logfile --<brk>
      <cont>hardcopy --implementation=matplotlib
```

Or using stuff stored by the pyFoamPlotRunner

```
1 > pyFoamRedoPlot.py --pickle PyFoamRunner.rhoPisoAbscheidParcelFoam.analyzed/<brk>
      <cont>pickledPlots
```

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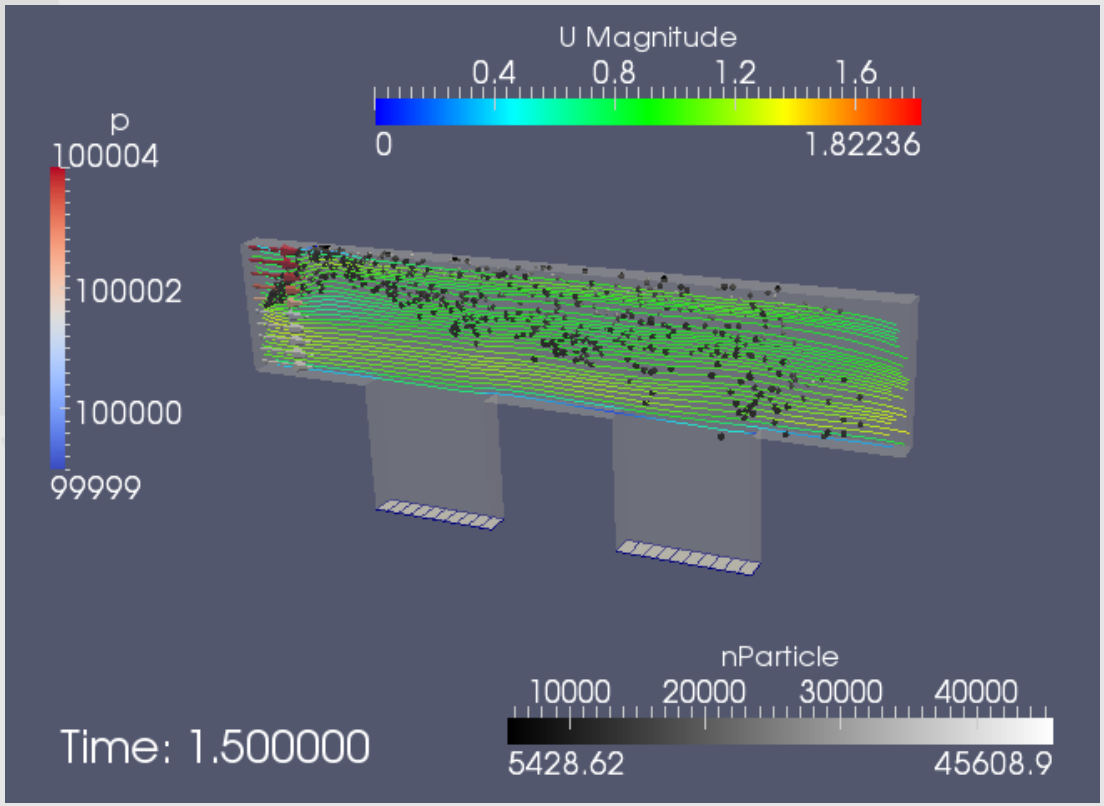
Ignaz prepared a complex visualization

He saved a ParaView-statefile named `default.pvsm`

```
1 > pyFoamPVSnapshot.py --time=1.5 .
```



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Other things to do with state-files

If you haven't cloned `default.pvsm`

```
> pyFoamPVSnapshot.py --time=1.5 . --state=../cases/twoCavityChannel/<brk>
    <cont>default.pvsm
```

Plotting more than one time ... for a poster

```
> pyFoamPVSnapshot.py --time=2 --time=1.5 . --maginfication=3
```

Starting ParaView with that state

```
> pyFoamPVLoadState.py . --state=../cases/twoCavityChannel/default.pvsm
```

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Exercise - What did I do?

- Have a look at the `PyFoamHistory`-file in the case
- What does it tell you?
- Who has the fewest lines?
- Who has the most?

Preparing for a new take

1. Get the second stage

Getting it with Git

```
> cd $HOME/pyFoamAdvanced
> git clone pyFoamAdvanced.git -b step2template step2
> cd step2
```

2. A clean copy

Cloning again

```
> pyFoamCloneCase.py --add=default.pvsm cases/twoCavityChannel <brk>
    <cont>testSeparator
 PyFoam WARNING on line 85 of file /Users/bgschaid/private_python/PyFoam/<brk>
      <cont>Applications/CloneCase.py : Directory  does not exist. Creating
> cd testSeparator
```

Getting to the heart of PyFoam

- Now Ignaz wants to prepare his case for automatic setup
  - Changing the inlet velocity
  - Changing the geometry
- Before testing a script we try it with commands

Changing the velocity

This is the part of `0/U` that Ignaz does not want to touch with his text editor

```
dimensions      [0 1 -1 0 0 0 0];

internalField   uniform (0 0 0);

boundaryField
{
    inlet
    {
        type            fixedValue;
        value           uniform (1 0 0);
    }
...
```

Reading a dictionary

This abstract example shows how a dictionary-file is "seen" inside a PYTHON-program

The dictionary testDict

```
model theModel;

patches ( inlet
          outlet );

theModelCoeffs {
        alpha 0.3;
        beta 2 inlet ;
}
```

The Python-code

```
from PyFoam.RunDictionary.ParsedParameterFile import ParsedParameterFile

file=ParsedParameterFile("testDict")

# none of these should fail
assert file["model"]=="theModel"
assert len(file["patches"])==2
assert file["patches"][0]=="inlet"
assert file["theModelCoeffs"]["beta"][1]=="inlet"

# manipulation is possible
file["theModelCoeffs"]["alpha"]+=1
file["newCoeffs"]={"a":1,"b":[2,3,4]}

print file
```

Trying half the original velocity

Not the most elegant way to set the velocity

```
> pyFoamWriteDictionary.py 0/U "boundaryField['inlet']['value']" "uniform <brk>
    <cont>(0.5 0 0)" --strip-quotes-from-value
```

Ignaz checks what has changed

```
1  > pyFoamCompareDictionary.py 0/U ../cases/twoCavityChannel
   PyFoam WARNING on line 90 of file /software/PyFoam/Applications/<brk>
        <cont>CompareDictionary.py : Found /data/step2/cases/twoCavityChannel<brk>
        <cont>/0/U and using this
3  >>>< Field U[boundaryField][inlet][value] : Differs
   >>Source:
5  uniform (0.5 0 0)
   <<Destination:
7  uniform (1 0 0)
```

How templates work

- The template file is called the same as the file it will produce
  - Just with `.template` appended
- Lines that start with $$ are variable declarations
  - They don't appear in the final output
- Strings between $ and $ are treated as PYTHON-expressions and evaluated
  - Previously declared variables are used
- Everything else is copied to the output

Declaring helper variables

In constant/polyMeshDict.template

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * <brk>
     <cont>* //

$$ x1=preLen
$$ x2=preLen+cavityWidth
$$ x3=preLen+cavityWidth+interLen
$$ x4=preLen+2*cavityWidth+interLen
$$ x5=2*preLen+2*cavityWidth+interLen
$$ y1=channelHeight
$$ y2=-cavityDepth

convertToMeters 1.0;

...
```

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The actual points

Later in constant/polyMeshDict.template

```
...
vertices
(
    (0     0    -0.01)
    (0     0     0.01)
    ($x1$  0     0.01)
    ($x1$  0    -0.01)
    (0     $y1$ -0.01)
    (0     $y1$ 0.01)
    ($x1$  $y1$ 0.01)
    ($x1$  $y1$ -0.01)
    ($x2$   0     0.01)
    ($x2$   0    -0.01)
...
```

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The blocks

Further down in constant/polyMeshDict.template

```
....
blocks
(
    hex (0 1 2 3 4 5 6 7) (1 $int(ceil(preLen/dx))$ $int(ceil(channelHeight<brk>
        <cont>/dx))$) simpleGrading (1 1 1)
    hex (3 2 8 9 7 6 10 11) (1 $int(ceil(cavityWidth/dx))$ $int(ceil(<brk>
        <cont>channelHeight/dx))$) simpleGrading (1 1 1)
    hex (9 8 12 13 11 10 14 15) (1 $int(ceil(interLen/dx))$ $int(ceil(<brk>
        <cont>channelHeight/dx))$) simpleGrading (1 1 1)
    hex (13 12 16 17 15 14 18 19) (1 $int(ceil(cavityWidth/dx))$ $int(ceil(<brk>
        <cont>channelHeight/dx))$) simpleGrading (1 1 1)
    hex (17 16 20 21 19 18 22 23) (1 $int(ceil(preLen/dx))$ $int(ceil(<brk>
        <cont>channelHeight/dx))$) simpleGrading (1 1 1)
    hex (25 24 26 27 3 2 8 9) (1 $int(ceil(cavityWidth/dx))$ $int(ceil(<brk>
        <cont>cavityDepth/dx))$) simpleGrading (1 1 1)
    hex (29 28 30 31 13 12 16 17) (1 $int(ceil(cavityWidth/dx))$ $int(ceil(<brk>
        <cont>cavityDepth/dx))$) simpleGrading (1 1 1)
);
....
```

Converting the template

The secret is to get a complete Python-dictionary into a string

```
> pyFoamFromTemplate.py constant/polyMesh/blockMeshDict "{'preLen':0.2,'<brk>
    <cont>cavityWidth':0.15,'channelHeight':0.1,'interLen':0.05,'<brk>
    <cont>cavityDepth':0.02,'dx':0.005}"
```

Produces a constant/polyMesh/blockMeshDict with lines like

```
blocks
(
    hex (0 1 2 3 4 5 6 7) (1 40 20) simpleGrading (1 1 1)
    hex (3 2 8 9 7 6 10 11) (1 30 20) simpleGrading (1 1 1)
    hex (9 8 12 13 11 10 14 15) (1 10 20) simpleGrading (1 1 1)
    hex (13 12 16 17 15 14 18 19) (1 30 20) simpleGrading (1 1 1)
    hex (17 16 20 21 19 18 22 23) (1 40 20) simpleGrading (1 1 1)
    hex (25 24 26 27 3 2 8 9) (1 30 4) simpleGrading (1 1 1)
    hex (29 28 30 31 13 12 16 17) (1 30 4) simpleGrading (1 1 1)
);
```

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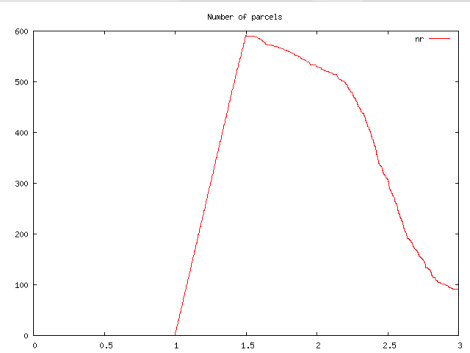
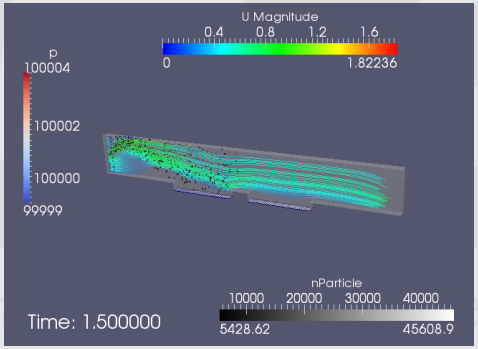
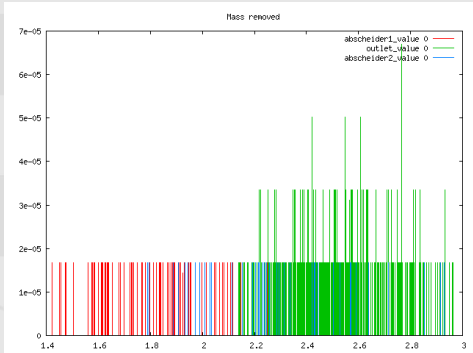
Isidor wants to see the results

Running it

```
> blockMesh
> pyFoamPlotRunner.py --hardcopy --progress --clear <brk>
    <cont>rhoPisoAbscheidParcelFoam
> pyFoamPVSnapshot.py --time=1.5 .
```







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Cloning again

1. Get the third stage

Getting it with `Git`

```
> cd $HOME/pyFoamAdvanced
> git clone pyFoamAdvanced.git -b step3shellScript step3
> cd step3
```

2. This time no `pyFoamCloneCase.py`

One script to bind them all

- Ignaz knows the commands by heart
- .. but doesn't want to execute them every time by hand
- So he copies them into a script
- .. and adds some *shell sugar*

The shell script

The file scripts/prepareRun.sh

```
1  #! /bin/sh
3  TEMPLATE=$1
   TARGET=$2
5  VELOCITY=$3
   DX=$4
7
   GEOMETRY="{'preLen':0.2,'cavityWidth':0.15,'channelHeight':0.1,'interLen':0.05,'cavityDepth<brk>
        <cont>':0.02,'dx':$DX}"
9
   echo "Creating case $TARGET"
11
   pyFoamCloneCase.py $TEMPLATE $TARGET
13 pyFoamFromTemplate.py $TARGET/constant/polyMesh/blockMeshDict $GEOMETRY
   pyFoamWriteDictionary.py $TARGET/0/U "boundaryField['inlet']['value']" "uniform ($VELOCITY 0 0)"<brk>
        <cont> --strip-quotes-from-value
15
   echo "Calling blockMesh and decompose"
17
   pyFoamRunner.py --clear --progress blockMesh -case $TARGET
19 pyFoamDecompose.py --progress $TARGET 2
21 pyFoamCaseReport.py --decomposition $TARGET
23 echo "Running"
25 pyFoamRunner.py --progress --proc=2  --foam=1.5-dev rhoPisoAbscheidParcelFoam -case $TARGET
```

Executing it

... is easy

```
> ./scripts/prepareRun.sh cases/twoCaviyChannel testSeparator 0.7 0.01
Creating case testSeparator
...
```

That's all you hear about shell-scripts here

There's more to `git` than clone

... but we don't use it

The only `git` command you see in this presentation

```
> cd $HOME/pyFoamAdvanced
> git clone pyFoamAdvanced.git -b step4pythonScript step4
> cd step4
```

Script reloaded

- Now Ignaz becomes ambitious
- He wants to do it better ... in pure PYTHON
- The end result is longer
- ... but will be much easier to modify

Reading the parameters

No PyFoam here - Start of scripts/prepareRun.py

```
1  #! /usr/bin/env python

3  import sys
   from os import path
5
   if len(sys.argv)<4:
7      print "Need␣<template>␣<target>␣<velocity>␣[<dx>]"
       sys.exit(-1)
9
   template=sys.argv[1]
11 target=sys.argv[2]
   velocity=float(sys.argv[3])
13
   dx=0.01
15 if len(sys.argv)>4:
       dx=float(sys.argv[4])
```

- sys.argv is the list of command-line parameters

Cloning the directory

First time we use the library - scripts/prepareRun.py

```
from PyFoam.RunDictionary.SolutionDirectory import SolutionDirectory

orig=SolutionDirectory(template,
                       archive=None,
                       paraviewLink=False)
work=orig.cloneCase(target)
```

- SolutionDirectory represents an OpenFOAM™-case
  - Including time-steps etc
- cloneCase returns another SolutionDirectory

Using the template

The dictionary now looks more natural - scripts/prepareRun.py

```
from PyFoam.Basics.TemplateFile import TemplateFile

bmName=path.join(work.polyMeshDir(),"blockMeshDict")

template=TemplateFile(bmName+".template")
template.writeToFile(bmName,{'preLen':0.2,
                             'cavityWidth':0.15,
                             'channelHeight':0.1,
                             'interLen':0.05,
                             'cavityDepth':0.02,
                             'dx':dx})
```

- os.path is a convenient way to keep pathnames portable
  - This line should need no change on Windows (never tested it though)

Modifying the velocity

Dictionary modification is trivial - scripts/prepareRun.py

```
1  from PyFoam.RunDictionary.ParsedParameterFile import ParsedParameterFile
   from PyFoam.Basics.DataStructures import Vector
3
   velFile=ParsedParameterFile(path.join(work.initialDir(),"U"))
5  velFile["boundaryField"]["inlet"]["value"].setUniform(Vector(velocity,0,0))
   velFile.writeFile()
```

- ParsedParameterFile is the workhorse of PyFoam
- Mastering it is easy:
  1. Create it. The file is read
  2. Manipulate it like a regular Python-dictionary
  3. Write it back

Administrative stuff

Make sure we use the right version - scripts/prepareRun.py

```
from PyFoam.FoamInformation import changeFoamVersion
changeFoamVersion("1.5-dev")

from PyFoam.Error import error
```

- changeFoamVersion makes sure that the *right* OpenFOAM™-version is used
- error prints an error message and aborts the program

Running `blockMesh`

Running and checking - `scripts/prepareRun.py`

```
from PyFoam.Execution.BasicRunner import BasicRunner
blockRun=BasicRunner(argv=["blockMesh",
                           "-case",work.name],
                     silent=True,
                     server=False,
                     logname="Blocky")
print "Running blockMesh"
blockRun.start()
if not blockRun.runOK():
    error("There was a problem with blockMesh")
```

- BasicRunner runs any OpenFOAM™-command
  - **argv** Command-line passed to OpenFOAM™
  - **silent** No output to the terminal
  - **server** No server-process that controls the execution
  - **logname** Name of the logfile

Decomposing

Using the functionality of a command line-tool - scripts/prepareRun.py

```
from PyFoam.Applications.Decomposer import Decomposer
print "Decomposing"
Decomposer(args=["--progress",
                 work.name,
                 2])

from PyFoam.Applications.CaseReport import CaseReport
CaseReport(args=["--decomposition",
                 work.name])
```

- Most utilities are implemented by a class
  - Found in the PyFoam.Applications-sublibrary
  - Name is usually the utility-name without pyFoam and .py
- The parameter args is the command line we would use on the shell
- The command is executed immediately at construction

Setting up for a parallel run

Still using only 2 CPUs - scripts/prepareRun.py

```
1  from PyFoam.Execution.ParallelExecution import LAMMachine
   machine=LAMMachine(nr=2)
```

- LAMMachine is used to interface with MPI
  - It is named like that for historic reasons
- Also works with machine-files

Setting up the run

Ignaz only wants a progress indicator - scripts/prepareRun.py

```
from PyFoam.Execution.AnalyzedRunner import AnalyzedRunner
from PyFoam.LogAnalysis.FoamLogAnalyzer import FoamLogAnalyzer
from PyFoam.LogAnalysis.TimeLineAnalyzer import TimeLineAnalyzer
analyzer=FoamLogAnalyzer()
analyzer.time=0. # fix around a bug
analyzer.addAnalyzer("time",TimeLineAnalyzer(progress=True))
```

- xxxLineAnalyzers look at one line of output at a time
  - The TimeLineAnalyzer searches for an expression Time = x.xx and updates it's parents
  - The parameter progress makes sure that only the time is printed to the standard-output
- FoamLogAnalyzer takes care of one or more LineAnalyzers and feeds them the log-lines

Starting the actual run

Finally the run is started - scripts/prepareRun.py

```
print "Running"
theRun=AnalyzedRunner(analyzer,
                      argv=["rhoPisoAbscheidParcelFoam",
                        "-case",work.name],
                      silent=True,
                      lam=machine)
theRun.start()
```

- AnalyzedRunner is a sub-class of BasicRunner
  - Any LogAnalyzer can be added and will be handed the output for analysis
- The lam-parameter starts the run in parallel

Running it

Ignaz tries the script

```
> ./scripts/prepareRun.py cases/twoCavityChannel testSeparator 0.7 0.01
 PyFoam WARNING on line 152 of file /software/PyFoam/FoamInformation.py : <brk>
      <cont>1.5-dev is already being used
Running blockMesh
Decomposing
Case is decomposed for 2 processors
              |      0      1
-----------------------------
      Points |    906    918
       Faces |   1658   1682
       Cells |    402    408
-----------------------------
 abscheider1 |      0     15
 abscheider2 |     15      0
      bottom |     27     26
defaultFaces |    804    816
       inlet |      0     10
      outlet |     10      0
         top |     37     38
Running
 t =  0.02567
```

Last `git` of the day

... we'll miss it

Once more with feeling

```
> cd $HOME/pyFoamAdvanced
> git clone pyFoamAdvanced.git -b step5parameterVariation step5
> cd step5
```

Aiming for world domination

- Now Ignaz wants it all:
  - Run a parameter variation unattended
  - Have the data analyzed
    - And written to a file he can open with a spreadsheet-program
  - Get pictures of every run

The class that stares at goats

- First we write a class that inherits from `LogLineAnalyzer`
- The purpose of this class is to look at every line of the OpenFOAM™ output and
  - See what it can learn from it
  - Store that data
  - Give it back if asked to
- In this concrete case this means: every time a particle leaves through a patch its mass will be added
  - to the total mass
  - to the data entry of the patch

Setting up the class

Constructor - scripts/AbscheideAnalyzer.py

```
1  import re

3  from PyFoam.LogAnalysis.LogLineAnalyzer import LogLineAnalyzer

5  class AbscheideAnalyzer(LogLineAnalyzer):
       def __init__(self):
7          LogLineAnalyzer.__init__(self)

9          self.massLeft=0
           self.removed={}
11
           self.removedExpr=re.compile("Abgeschieden at (.+) with m: (.+) N: <brk>
               <cont> (.+) = total: (.+)")
13         self.massExpr=re.compile("Current mass in system                    = (.+)")
```

- Making it a sub-class of LogLineAnalyzer
- The module re is PYTHONs module for parsing regular expressions

Analyzing a line

These two methods are necessary - scripts/AbscheideAnalyzer.py

```
1     def doAnalysis(self,line):
          self.analyzeLine(line)
3
      def analyzeLine(self,line):
5         m=self.removedExpr.match(line)
          if m!=None:
7             name=m.groups()[0]
              mass=float(m.groups()[1])
9             nr=float(m.groups()[2])
              total=float(m.groups()[3])
11
              try:
13                self.removed[name]+=<brk>
                      <cont>total
              except KeyError:
15                self.removed[name] =<brk>
                      <cont>total

17        m=self.massExpr.match(line)
          if m!=None:
19            self.massLeft=float(m.<brk>
                  <cont>groups()[0])
```

- analyzeLine
  - Checks whether one of the regular expressions was matched
  - Updates the data according to the matches
- The try/except-construct makes sure that only field entries that are needed are added

Reporting

These two methods are Ignazs idea - scripts/AbscheideAnalyzer.py

```
1       def doReport(self):
            summe=self.massLeft
3           print "Mass left in system:",<brk>
                <cont>self.massLeft
            for k,v in self.removed.<brk>
                <cont>iteritems():
5               print "Removed by",k,":",v
                summe+=v
7           print "Total mass accounted <brk>
                <cont>for:",summe

9       def addCSVLine(self,csv):
            csv["mass left in system"]=<brk>
                <cont>self.massLeft
11          for k,v in self.removed.<brk>
                <cont>iteritems():
                csv[k]=v
13
        def addTimeListener(self,other):
15          pass
```

doReport Prints the summarized information

addCSVLine Add data to a CSVCollector (a convenience-class for generating a consistent csv-file

addTimeListener Desgin relict. Forget it

An analyzer

A class to call the LineAnalyzer - scripts/AbscheideAnalyzer.py

```
1  from PyFoam.LogAnalysis.FoamLogAnalyzer import FoamLogAnalyzer

3  class AbscheideLogAnalyzer(FoamLogAnalyzer):
       def __init__(self):
5          super(AbscheideLogAnalyzer,self).__init__()
           self.addAnalyzer("abscheid",AbscheideAnalyzer())
7
       def doReport(self):
9          self.getAnalyzer("abscheid").doReport()
```

- A wrapper for the AbscheideAnalyzer
- Only needed for the testing-code

Some code to test the class

Usually not used - scripts/AbscheideAnalyzer.py

```
1  import sys
   if __name__=='__main__':
3      log=sys.argv[1]

5      abscheid=AbscheideLogAnalyzer()
       from PyFoam.LogAnalysis.LogAnalyzerApplication import <brk>
           <cont>LogAnalyzerApplication
7      analyze=LogAnalyzerApplication(abscheid)
       analyze.run(log)
9
       abscheid.doReport()
```

Using the script

```
> ./scripts/AbscheideAnalyzer.py ../step1/testSeparator/PyFoamRunner.<brk>
      <cont>rhoPisoAbscheidParcelFoam.logfile
2  Mass left in system: 2.920114636e-05
   Removed by outlet : 0.00997079885178
4  Total mass accounted for: 0.00999999999814
```

Testing the waters

Ignaz creates two simple scripts:

prepareTheCase.py A lobotomized version of the script in the last chapter:

- Creates the case
- Does not run the solver

This script has to be run also to prepare a case for the parameter variation

runSolverAndAnalyze.py Runs the solver and prints the report from the analyzer

Using the two scripts

```
> ./scripts/prepareTheCase.py cases/twoCavityChannel testCase 0.01
Running blockMesh
> ./scripts/runSolverAndAnalyze.py testCase
Mass left in system: 0.01
Total mass accounted for: 0.01
```

Setting up stuff

Start of scripts/inletVelocityVariation.py

```
1  import re,sys
   from os import path
3
   sys.path.append(path.dirname(path.abspath(sys.argv[0])))
5
   from AbscheideAnalyzer import AbscheideAnalyzer
7
   from PyFoam.Execution.AnalyzedRunner import AnalyzedRunner
9  from PyFoam.Applications.ClearCase import ClearCase
   from PyFoam.RunDictionary.ParsedParameterFile import ParsedParameterFile
11 from PyFoam.Basics.CSVCollection import CSVCollection
   from PyFoam.Applications.PVSnapshot import PVSnapshot
13
   from PyFoam.FoamInformation import changeFoamVersion
15 changeFoamVersion("1.5-dev")

17 case=sys.argv[1]
   csv=CSVCollection(sys.argv[2]+".csv")
```

- Nothing new here

The actual variation

Second part and end of scripts/inletVelocityVariation.py

```
for v in [0.1, 0.5, 1, 1.5, 2, 3]:
    print "Velocity set to",v
    ClearCase(args=[case])
    uInit=ParsedParameterFile(path.join(case,"0","U"))
    uInit["boundaryField"]["inlet"]["value"].setUniform([v,0,0])
    uInit.writeFile()

    abscheid=AbscheideAnalyzer()

    run=AnalyzedRunner(abscheid,
                       argv=["rhoPisoAbscheidParcelFoam","-case",case],
                       silent=True)
    run.start()

    csv["Velocity"]=v
    abscheid.addCSVLine(csv)
    csv.write()

    abscheid.doReport()

    PVSnapshot(args=[case,
                     "--time=1",
                     "--time=1.5",
                     "--time=2",
                     "--time=3",
                     "--file-prefix=velocity=%g" % v])
```

- The only new thing is the loop

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Running the variation

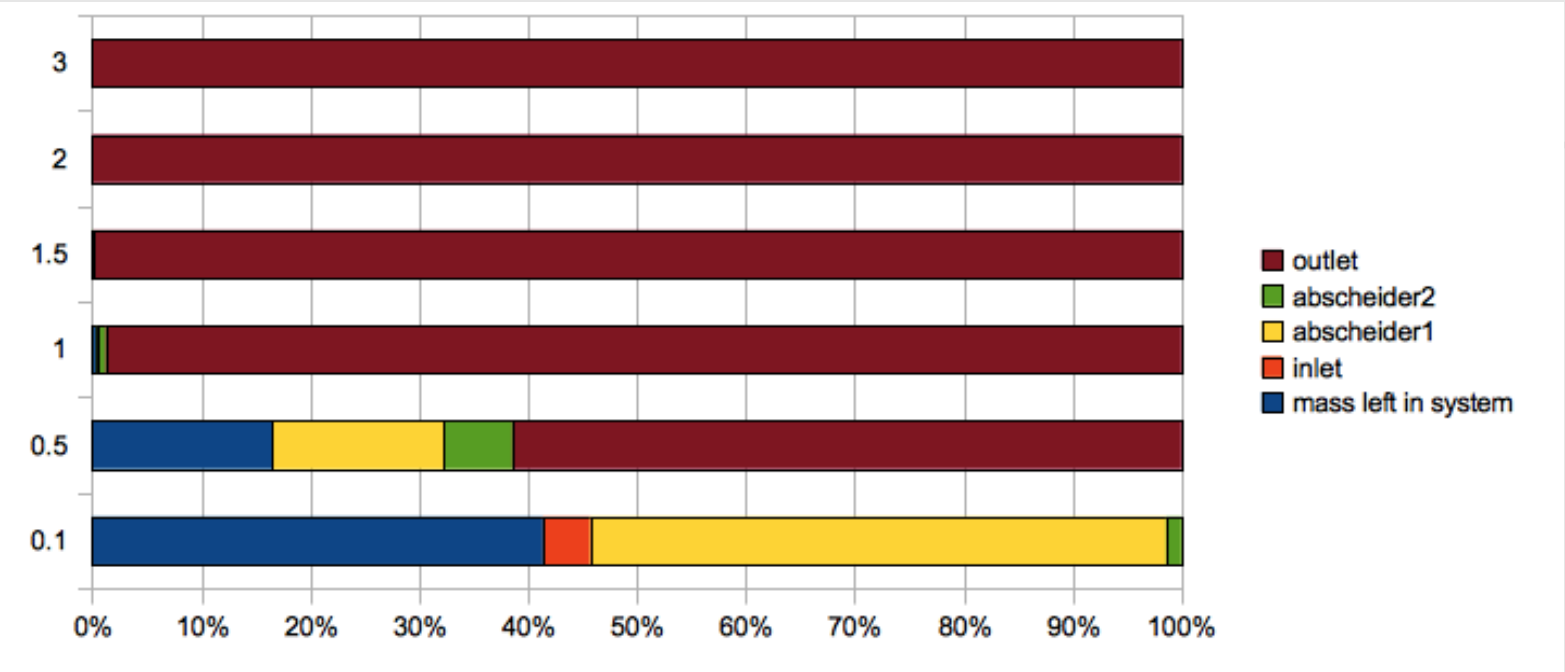
One command. 6 runs. One result file. 24 Pictures

```
> ./scripts/prepareTheCase.py cases/twoCavityChannel testVariation 0.005
Running blockMesh
> ./scripts/inletVelocityVariation.py testVariation variationData
```

- While this is running you can have a look at the data this will produce in `exampleResults/velTest.csv`
- Another remark: due to a bug in ParaView or `PVSnapshot` each iteration of the loop will produce multiple copies of the same pictures

The end result

The data from the CSV-file in one picture:



- Most variations were inefficient (no particles separated)
- Too slow is bad, too
- For low velocities the simulation time is too short (still mass in system)

Suggested exercises

- Try to find the optimum velocity (where the most mass comes to `abscheider2`)
  - Obviously extend the simulation time. But not too long. Suggestion: set it dependent on the inlet-velocity
- For the optimal velocity try varying the direction of the injector
- Check whether the cavities are to shallow
  - For this the mesh preparation would have to be pulled into the loop
- Try varying the upper channel wall
  - uniform (just the height)
  - making it narrower or wider in the middle

Acknowledgments

Thanks to

Holger Marschall for the idea for this tutorial

Astrid Mahrla for some pictures

Suggestions/Questions

Thanks for listening

- Questions?
- Suggestions for the library?

Bug reports at `http://sourceforge.net/apps/mantisbt/openfoam-extend/view_all_bug_page.php`