AQUAgpusph - 1.5.03 .

Developers guide

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Contents

Chapter 1

Introduction

1.1 About AQUAgpusph

AQUAgpusph (Another QUAlity GPU-SPH) is a free CFD software licensed under GPLv3, and developed by J.L. Cercos-Pita as part of his PhD at CEHINAV-UPM group [1]. AQUAgpusph is based on Lagragian meshfree SPH (Smoothed Particles Hydrodynamics) method.

AQUAgpusph has been accelerated with OpenCL, that allows you to execute it over CPU based platforms, over GPUs based platforms, and eventually, over every platform developed in the future adapted to the OpenCL standard. For the moment the simultaneous use of several platforms in the same simulation is not supported.

The code has been widely validated, used and documented in several publications, for instance **?**] where boundary integrals are tested or **?**] where SPHERIC benchmark test case number 9 was simulated. Some examples provided within the package have been studied in these publications.

AQUAgpusph has been designed for UNIX like operative system, and tested on GNU/Debian Linux distributions. For the moment no ports has been developed for Windows or Mac operative systems. AQUAgpusph has been developed in C++ and OpenCL[2]. Also Python extensions has been developed.

1.2 License notes

AQUAgpusph is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

[1] Model Basin Research group, Technical University of Madrid (UPM), `http://canal.etsin.upm.es`

[2] OpenCL is so quite similar to C

1.3 Objectives of the present document

This document has been created aiming to provide a tool that allows the AQUAgpusph developers to know:

1. The structure of AQUAgpusph source code.
2. The location of the source codes and helper files.
3. The entry points to the main parts of AQUAgpusph

This document is trying to complement the Doxygen documentation. Such documentation can be get, either building it with CMake (see the user manual) or in the following web page (corresponding to the last stable AQUAgpusph package):

`http://canal.etsin.upm.es/aquagpusph/doc/doxygen/stable`

1.4 Required background

The background required for the developers depends on the section of the code to be read/modified:

1. The kernel of AQUAgpusph is written C++.
2. The computational tools are written in OpenCL.
3. The examples are built using XML files.
4. Also Python extension may be used in some examples.
5. The documentation (this document as well as the developers guide) is written in LaTeX.
6. The configuration and compilation is carried out with CMake.

Also, depending on the modifications to be done, some background in CFD, and more specifically in SPH, may be required.

Chapter 2

AQUAgpusph strcuture

2.1 General

AQUAgpusph package is divided in several parts:

1. AQUAgpusph kernel.
2. Computational tools.
3. Helper tools.
4. Examples.
5. Documentation.
6. CMake configuration and compiling files.

2.2 Kernel

The kernel on AQUAgpusph is basically the main program which will be executed in the CPU. When it is launched the following operations will be owned by the main program:

1. The input XML files loading.
2. The computational device setup.
3. The OpenCL kernels loading.
4. The OpenCL codes execution querying (this codes will be ran in the computational device).
5. The Python scripts loading and executing.

6. The output files writing.

The source code files are placed in both **src/** and **include/** package folders.

The kernel is divided in two main parts, widely denominated "host" and "server". Such division can be appreciated in figure 2.1. Developers interested in the "host" side, mainly responsible of the input and output, may start with the file **src/main.cpp**.

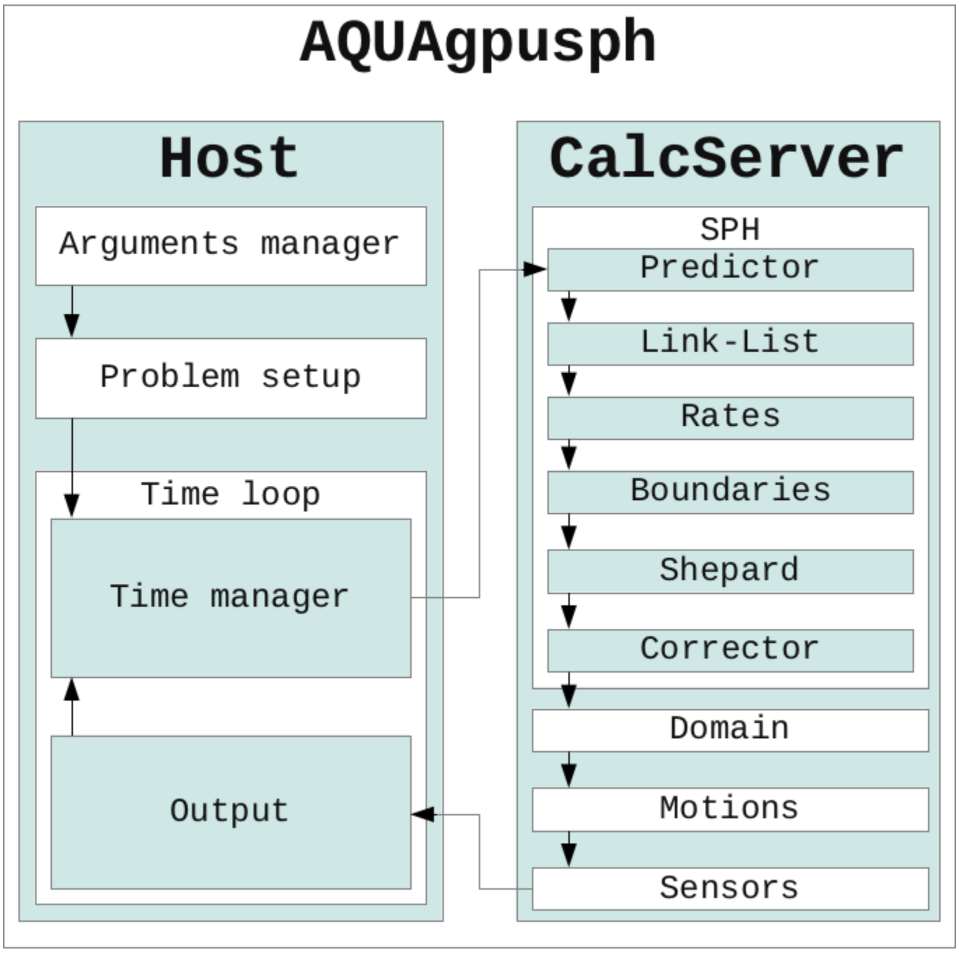

Figure 2.1: General AQUAgpusph flux diagram

Developers interested in the "server side", designed to control the simulation querying the OpenCL codes execution, may start with the class **CalcServer**.

You can learn more about the source code files location and objective in the Doxygen documentation:

`http://canal.etsin.upm.es/aquagpusph/doc/doxygen/stable/files.html`

2.3 Computational tools

The computational tools are OpenCL codes placed in **resources/OpenCL** folder. These codes are running in the computational device, and therefore are widely related with the kernel "server" side tools.

You can learn more about the OpenCL codes in the Doxygen documentation:

`http://canal.etsin.upm.es/aquagpusph/doc/doxygen/stable/files.html`

It should be mentioned that, being these codes the provided with AQUAgpusph package, they can be replaced by other ones for specific simulations just setting it in the input XML files.

2.4 Helper tools

With AQUAgpusph package several helper tools are provided. These tools are placed in the **tools/** folder.

Probably the most important tools are placed in **tools/aquagpusph_preprocessing**, being the particles generators. The generators are scripts that can read a mesh and generate the boundary particles in the mesh and the fluid ones inside it.

2.5 Examples

The examples are placed in the **examples/** folder. The examples available depends on whether the 2D or the 3D version of AQUAgpusph is built. In AQUAgpusph package each example has its files divided in 2 folders, namely:

1. **examples/*example_name***
2. **examples/cMake/*example_name***

where *example_name* is replaced by the example folder name. In the first folder the files which does not require any specific configuration are placed, while in the latter folder the files which require to be modified according to the cMake configuration are placed. When the examples are built, all the files (conveniently configured) are placed in the first folder.

In the built examples following files may be found:

1. Create.py: Python script to generate the particles input file.

2. Fluid.dat: Particles file generated by Create.py.

3. Main.xml: Main input XML file, it is just including other XML files.

4. Settings.xml: General program settings: `http://canal.etsin.upm.es/aquagpusph/doc/doxygen/stable/d8/dfe/structAqua_1_1InputOutput_1_1ProblemSetup_1_1sphSettings.html`

5. Time.xml: Simulation time flow options: `http://canal.etsin.upm.es/aquagpusph/doc/doxygen/stable/de/d49/structAqua_1_1InputOutput_1_1ProblemSetup_1_1sphTimingParameters.html`

6. SPH.xml: Physics simulation parameters: `http://canal.etsin.upm.es/aquagpusph/doc/doxygen/stable/d6/d08/structAqua_1_1InputOutput_1_1ProblemSetup_1_1sphSPHParameters.html`

7. GhostParticles.xml: Ghost particles boundaries (just when Ghost particles boundary condition is applied): `http://canal.etsin.upm.es/aquagpusph/doc/doxygen/stable/d5/d89/classAqua_1_1InputOutput_1_1ProblemSetup_1_1sphGhostParticles.html`

8. Fluids.xml: Fluids physics properties: `http://canal.etsin.upm.es/aquagpusph/doc/doxygen/stable/d7/da8/structAqua_1_1InputOutput_1_1ProblemSetup_1_1sphFluidParameters.html`

9. Movements.xml: Motions to be parsed: `http://canal.etsin.upm.es/aquagpusph/doc/doxygen/stable/dd/df7/classAqua_1_1InputOutput_1_1ProblemSetup_1_1sphMoveParameters.html`

10. Move/6DOF.xml: Specific motion type parameters.

11. Move/move.py: Python script which controls the solid motion (just in Python script controlled motions).

12. run.sh: Helper running script, type "./run.sh –help" in the example folder to learn more.

Some other files may be found, for instance, to plot the results in real time, or to load the prescribed solid motions.

Main.xml file is also including the shared XML file **resources/OpenCLMain.xml**, which is automatically setting all the computational tools discussed in the section 2.3.

2.6 Documentation

The documentation files, which include the user manual, the developers guide and the Doxygen documentation, are placed in the folder **doc/**.

In AQUAgpusph it is expected that the Doxygen documentation is built using cMake, so please do not try to build it manually.

Regarding the user manual and the developers guide, AQUAgpusph is providing already compiled version of them, however they can be edited and recompiled using the **buildPDF.sh** script provided with each one.

2.7 CMake

All the files called “`CMakeLists.txt`”, “`*.cmake`”, or included in a “cMake” folder are designed to let CMake to configure the package for the build and installation process. More specifically, the files called “`CMakeLists.txt`” are the ones where the instructions for CMake are written, while the other ones are templates that CMake is conveniently reading and editing.

Appendices

Appendix A

Directory tree

Following all the files provided with AQUAgpusph package, with its location, is shown. The files autogenerated during the configuration, build and install processes are not shown.

- aquagpusph-1.5
  - Releases notes
  - TODO
  - LICENSE
  - CMakeLists.txt
  - countLines.sh
  - Code styling
  - config.h.cmake
  - README.md
  - doc

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├── CMakeLists.txt
├── Doxygen Quick Reference.pdf
├── cMake
│   └── Doxyfile.in
├── devManual
│   ├── directory_tree.tex
│   ├── main.aux
│   ├── main.out
│   ├── structure.tex
│   ├── abstract.tex
│   ├── main.log
│   ├── buildPDF.sh
│   ├── main.toc
│   ├── main.tex
│   └── tree_py.tex
└── userManual
    ├── running.tex
    └── lateral_water_1x_ghost.tex
```

- warningMsg.tex
- elasticbounce.tex
- errorMsg.tex
- directory_tree.tex
- examples.tex
- asciiPartsInput.tex
- motionTypes.tex
- paraview.tex
- texput.log
- sensors.tex
- DeLeffe.tex
- infoMsg.tex
- ghostparticles.tex
- partsInput.tex
- aquagpusph.tex
- abstract.tex
- xmlPartsInput.tex
- lateral_water_1x_deleffe.tex
- buildPDF.sh

- bib.bib
- aquagpusph-usermanual.pdf
- physics.tex
- install.tex
- fixparticles.tex
- outputFiles.tex
- main.tex
- gidPartsInput.tex
- tree_py.tex
- xmlInput.tex
- motionControls.tex
- images
  - GhostParticlesCorner.svg
  - FixedParticles.png
  - DeLeffeCorner.svg
  - GhostParticles.svg
  - SPHInterpolation.png
  - FixedParticles.svg
  - ElasticBounce.svg

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├── LinkList.png
├── ElasticBounce.png
├── BC.png
├── CoalescenceRead.png
├── DeLeffe.svg
├── DeLeffeCorner.png
├── GhostParticlesCorner.png
├── BC.svg
├── SPHInterpolation.svg
├── LinkList.svg
├── DeLeffe.png
├── CC_88x31.png
├── Diagrams.odg
├── GeneralDiagram.png
└── lateral_water_1x_deleffe
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    ├── animation_freeslip.jpg
    └── particles.png
```

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  - paraviewcolormap.jpg
  - paraviewfilter.jpg
  - tank.png
  - sensors_noslip.png
  - particles.svg
  - paraviewfilteroptions.jpg
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- wendland
  - wendland2D.pdf
  - wendland2D.py
- tree
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  - Mimetypes-text-x-bibtex-icon.png

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Actions-edit-select-all-icon.png

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tree.py

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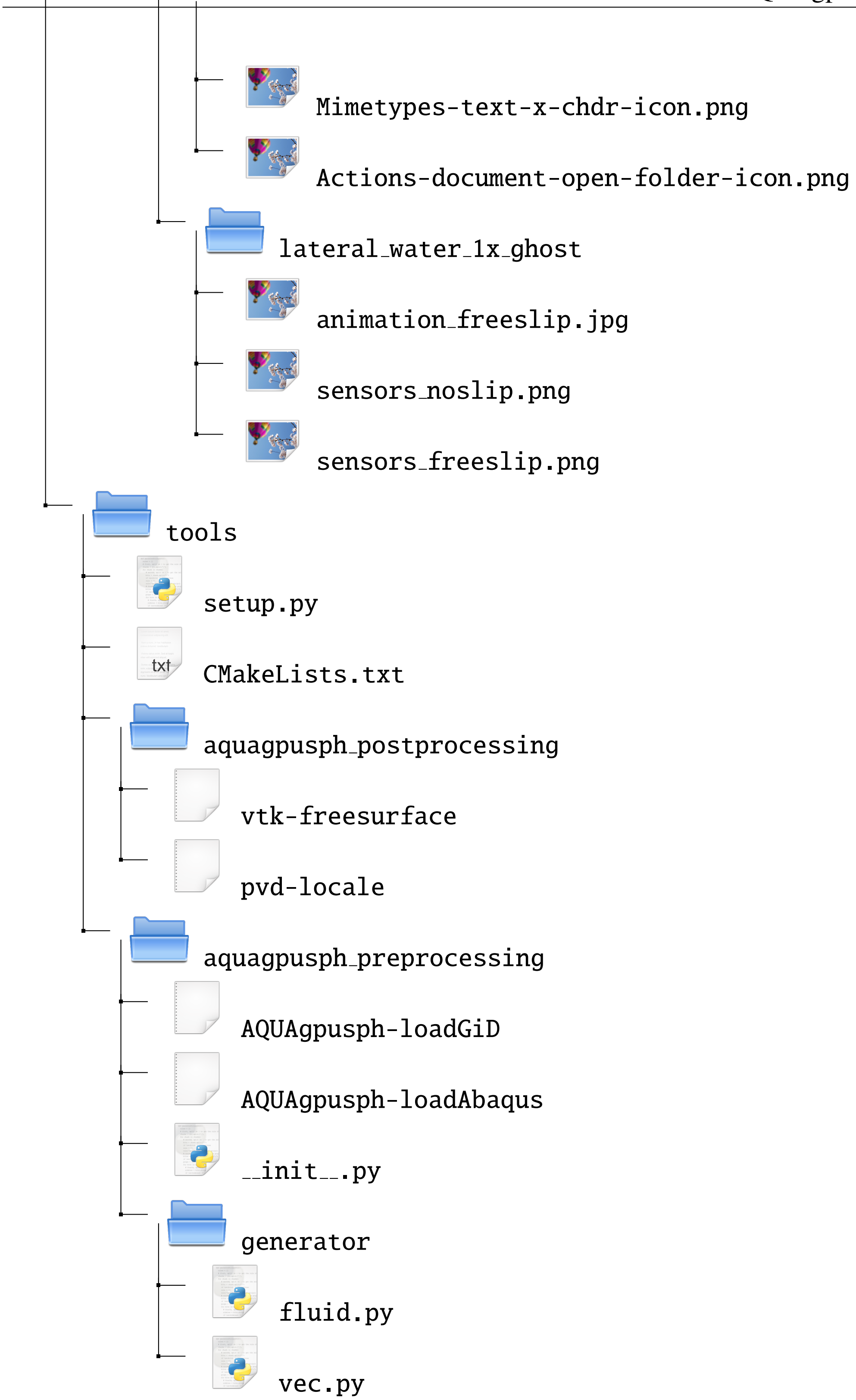
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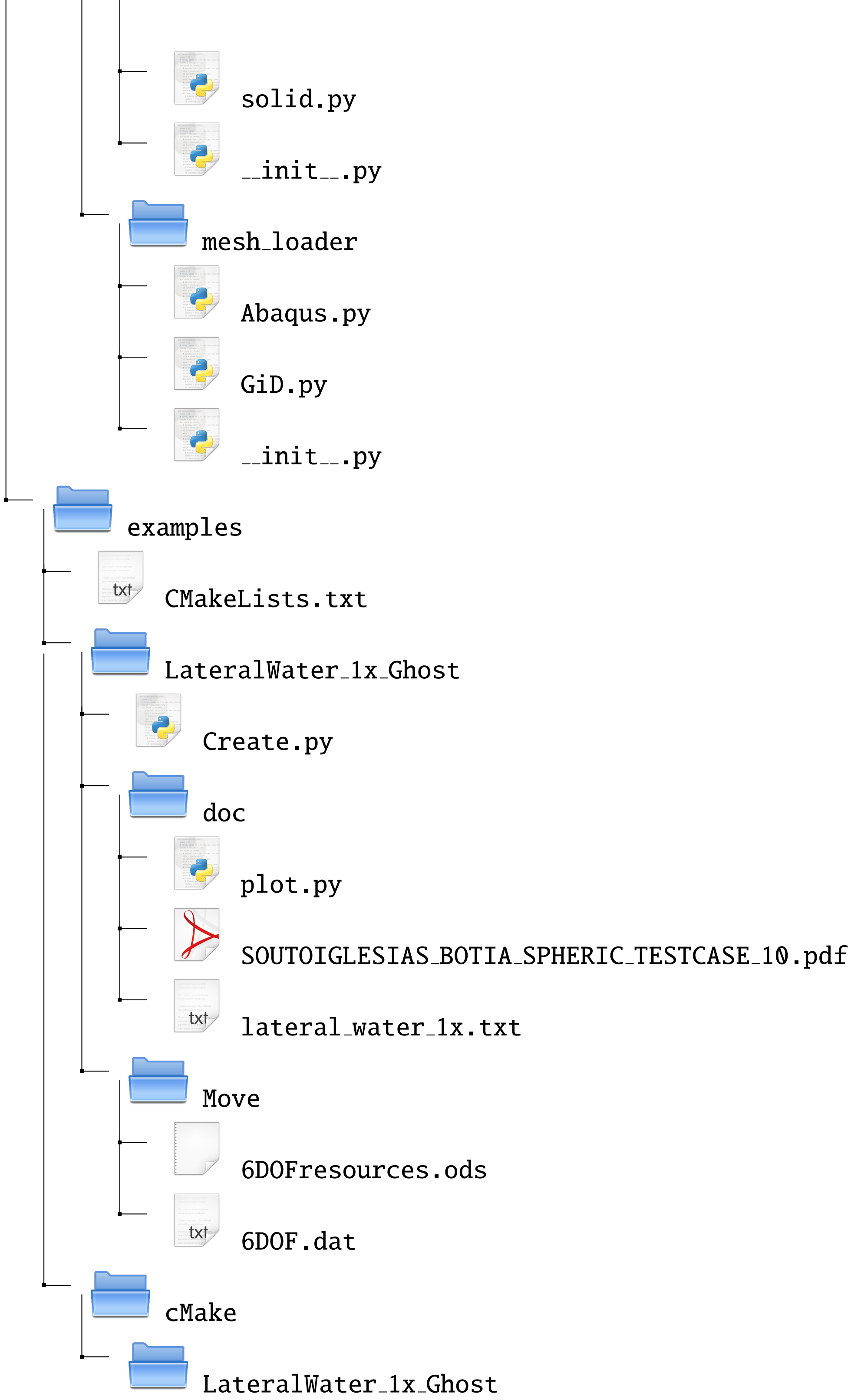
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Create.py
doc
plot.py
SOUTOIGLESIAS_BOTIA_SPHERIC_TESTCASE_10.pdf
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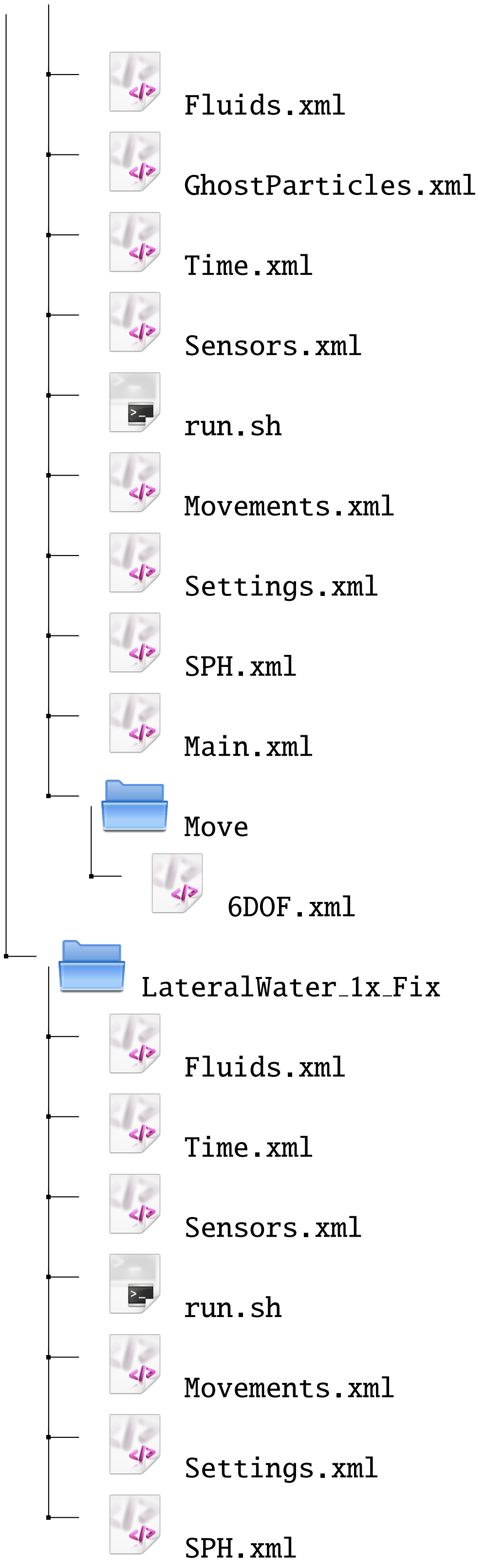
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Time.xml
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Settings.xml
SPH.xml
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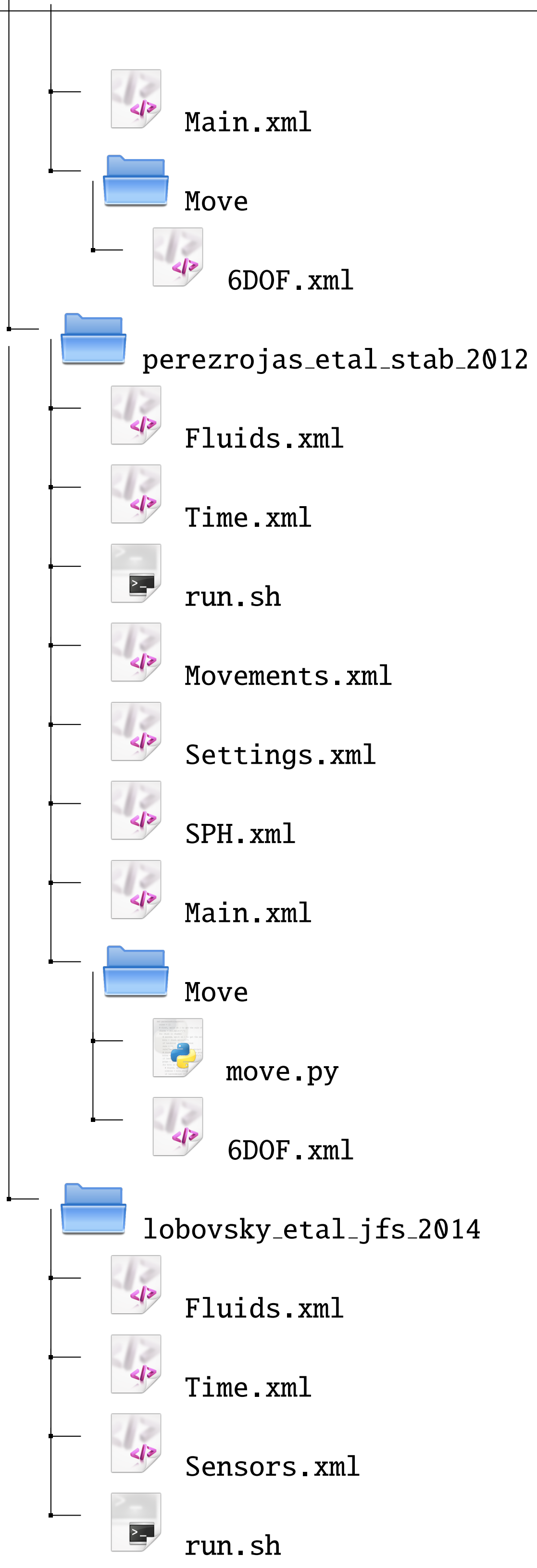
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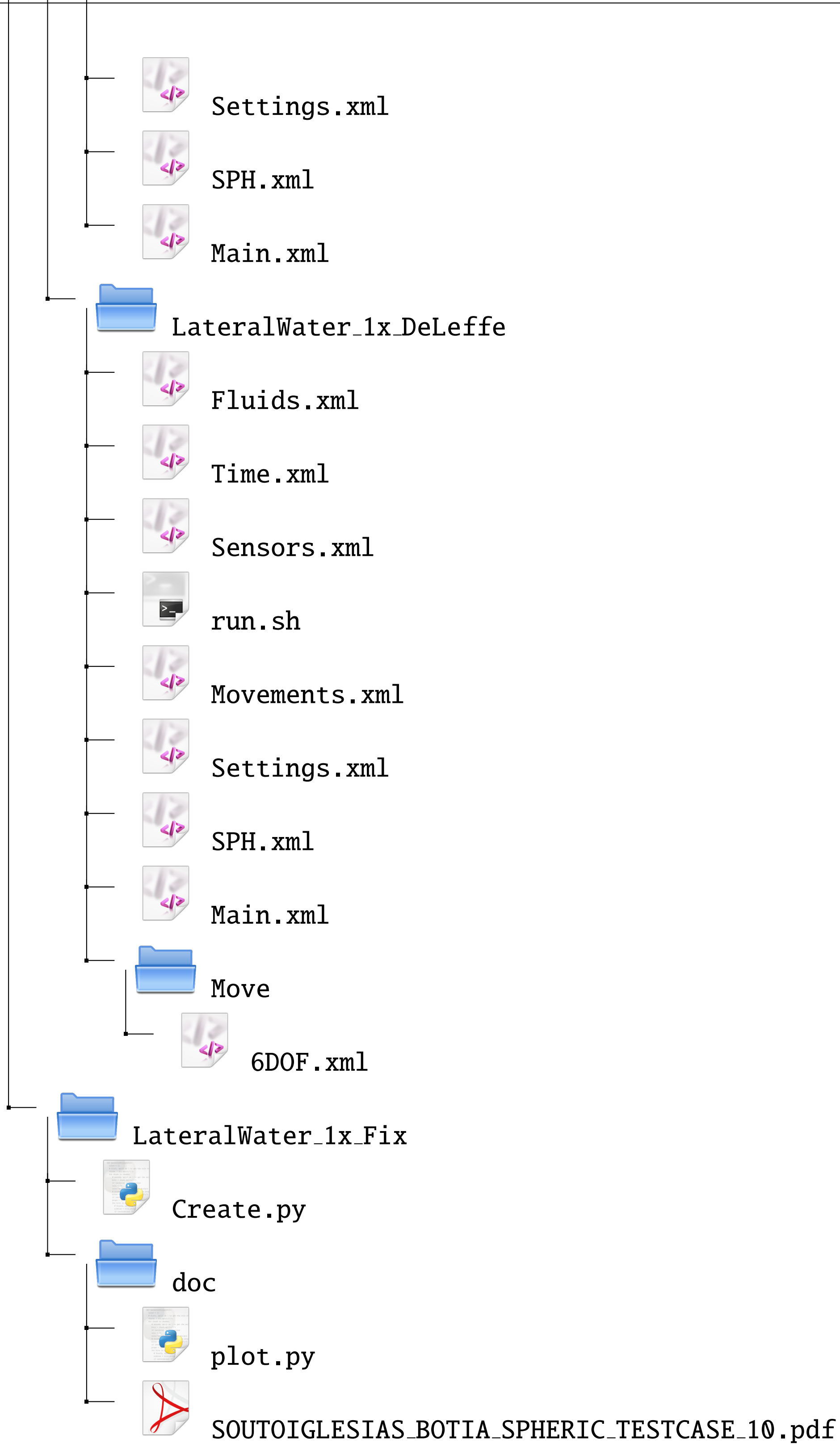
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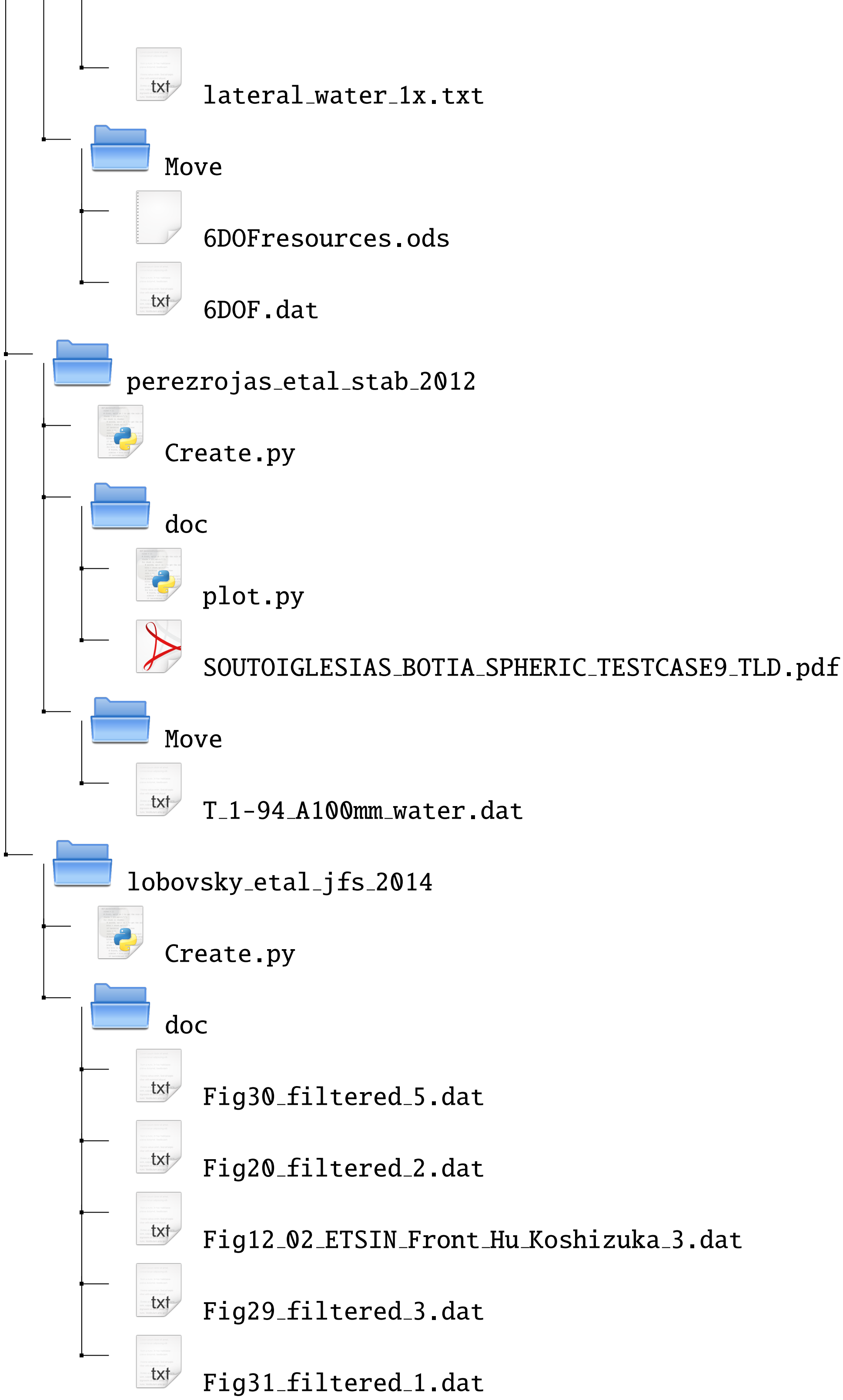
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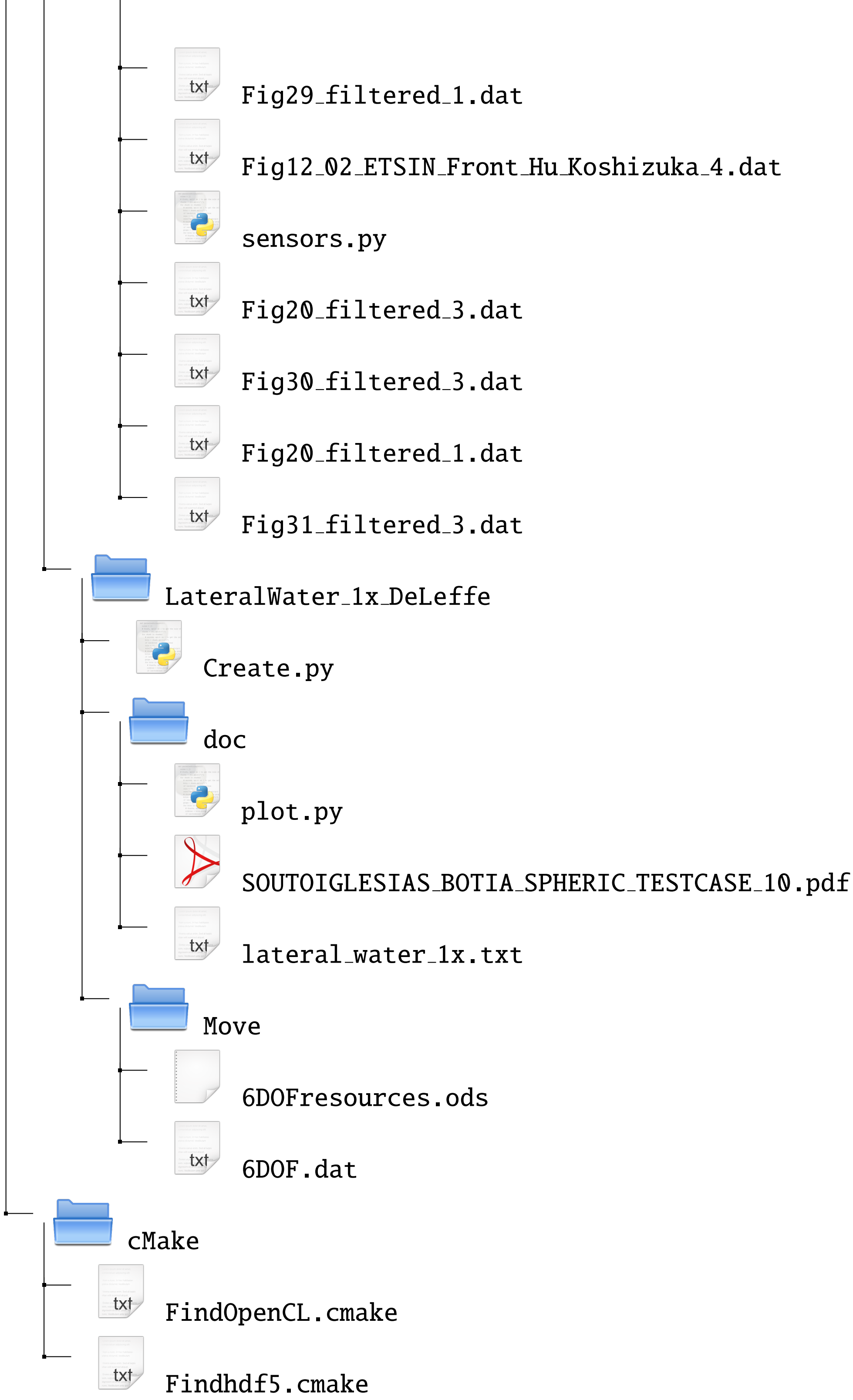

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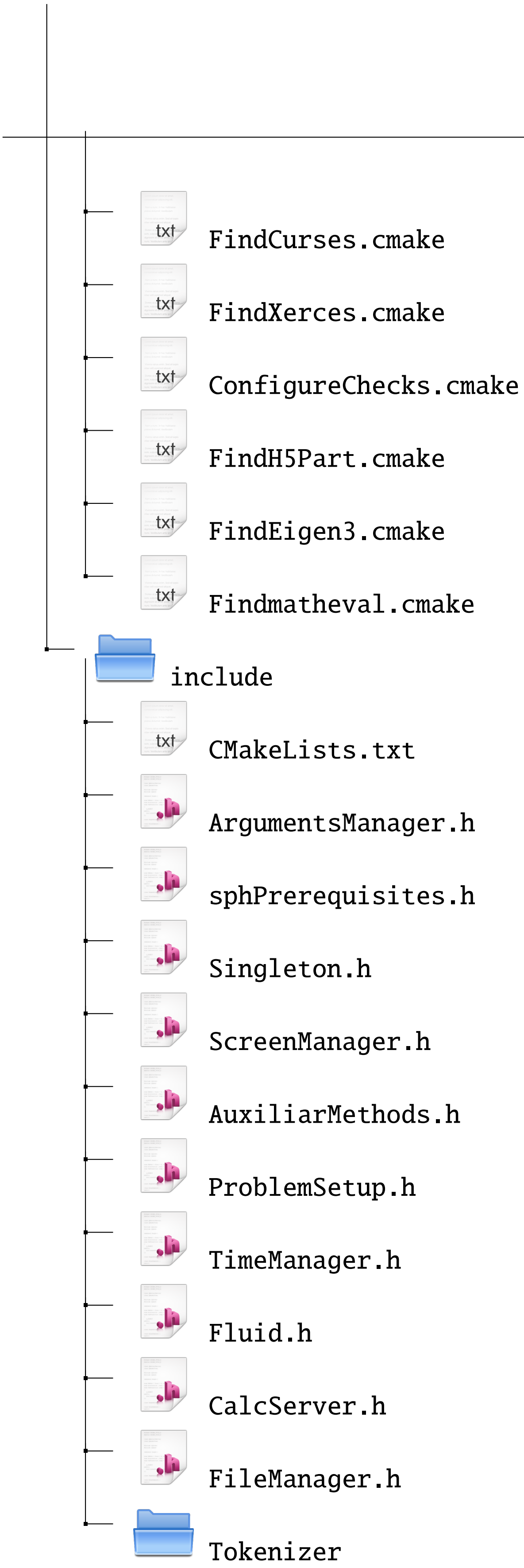
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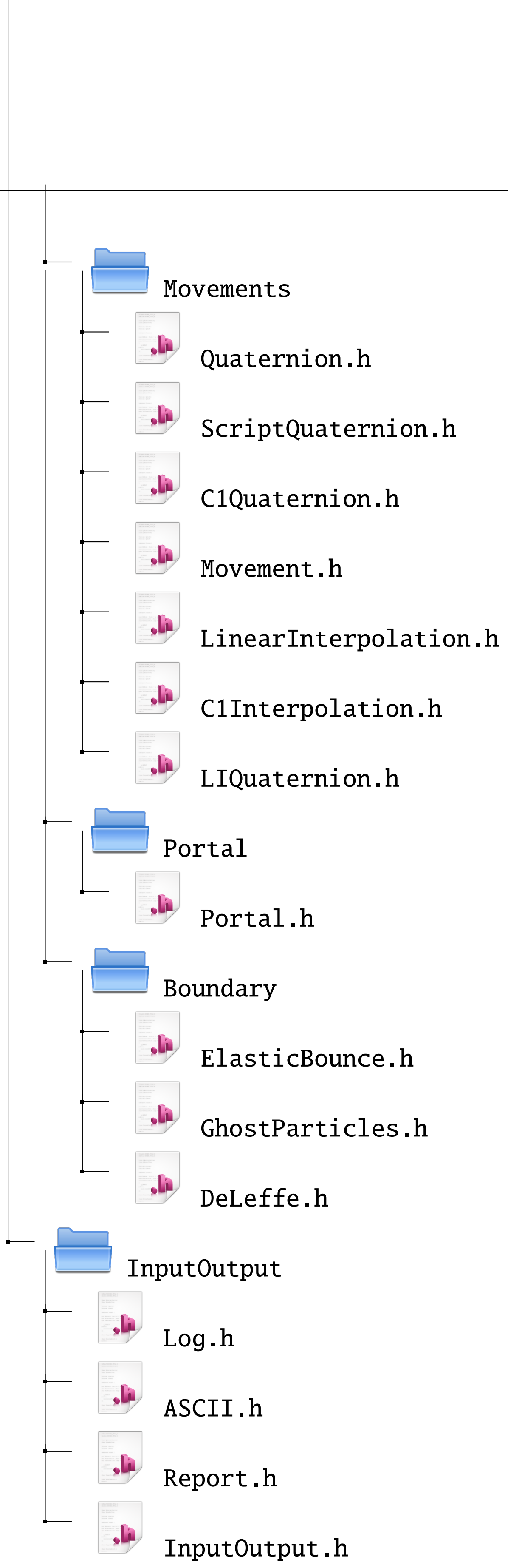
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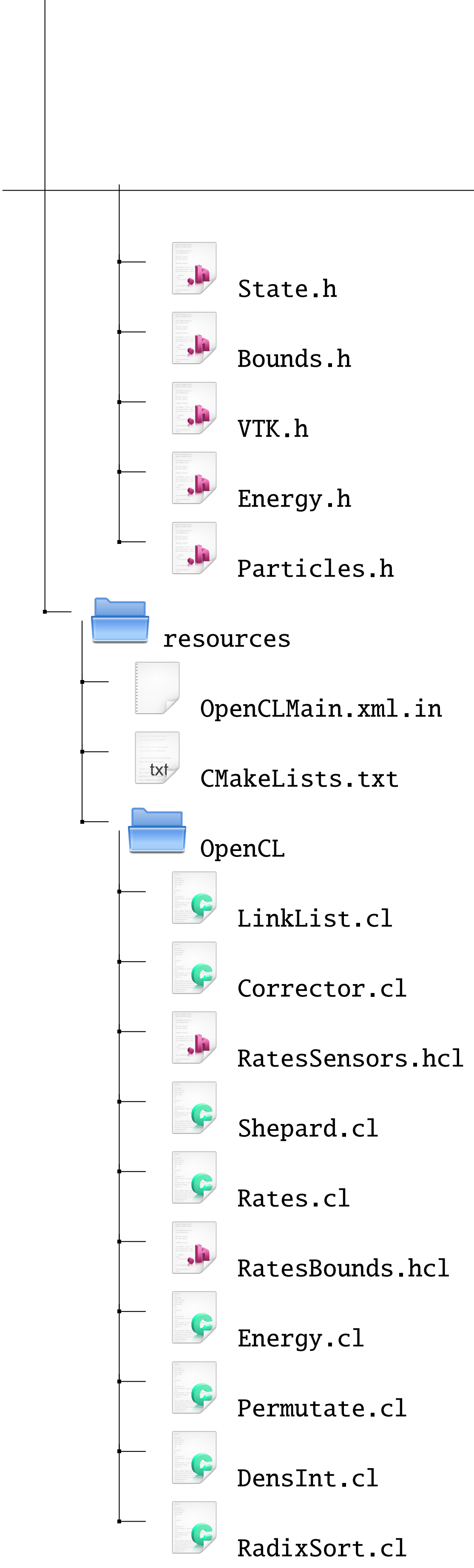
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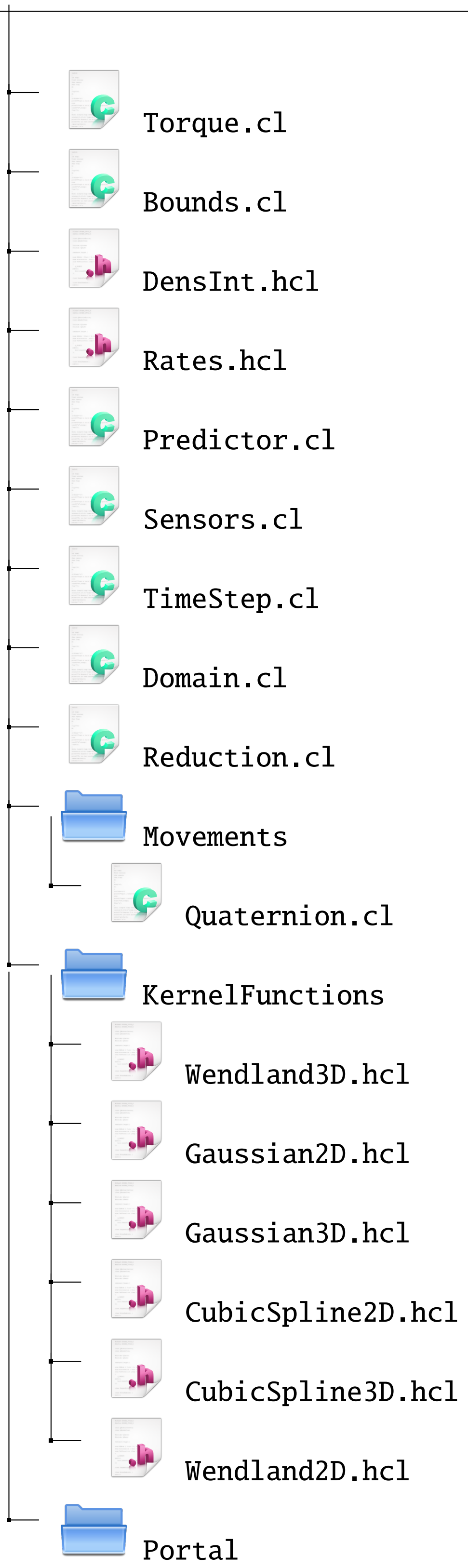
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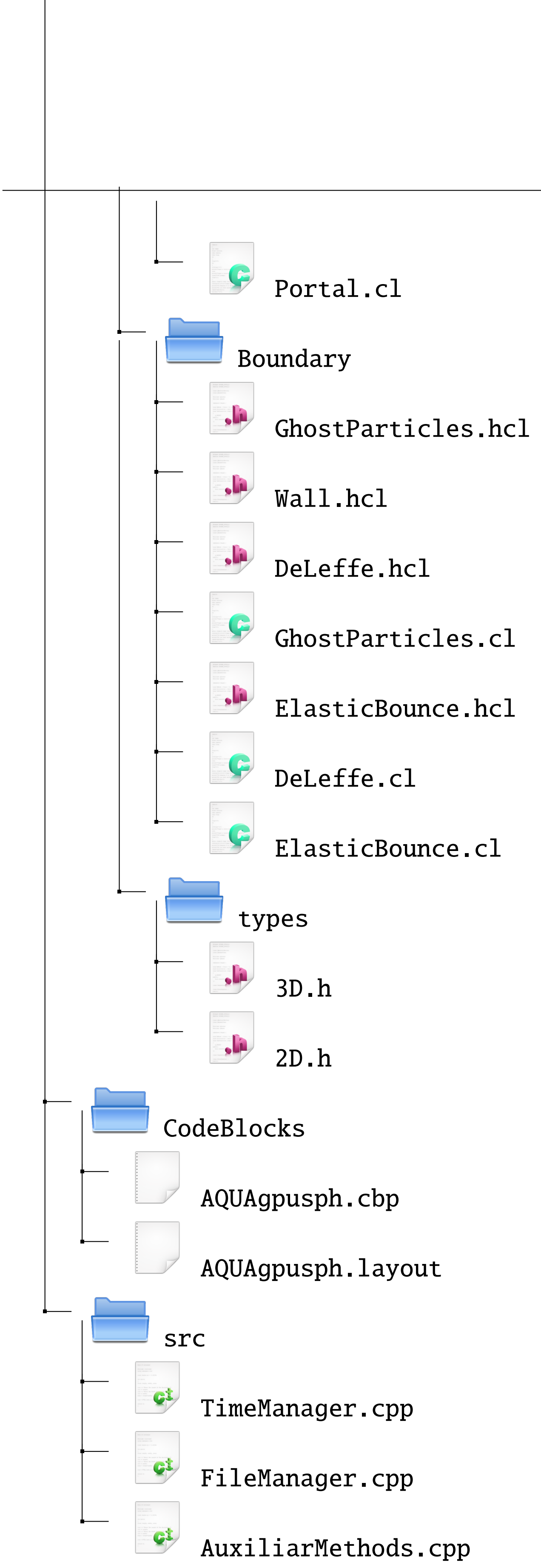
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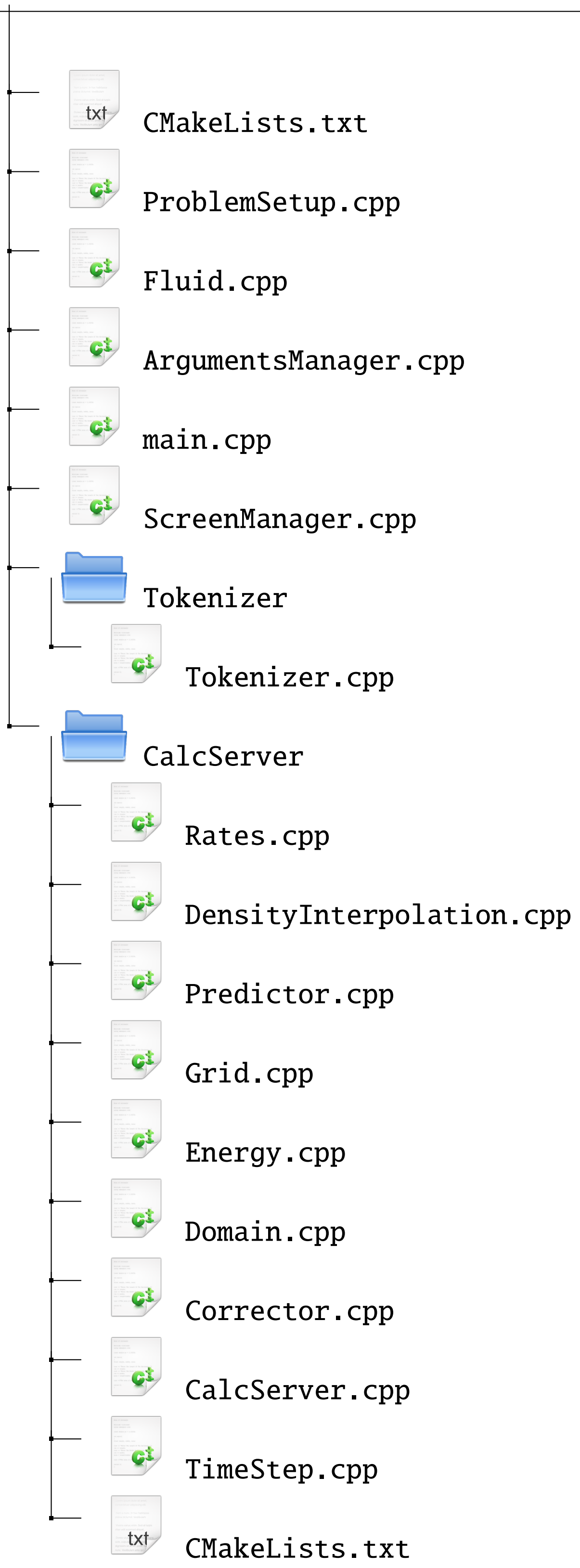
AuxiliarMethods.cpp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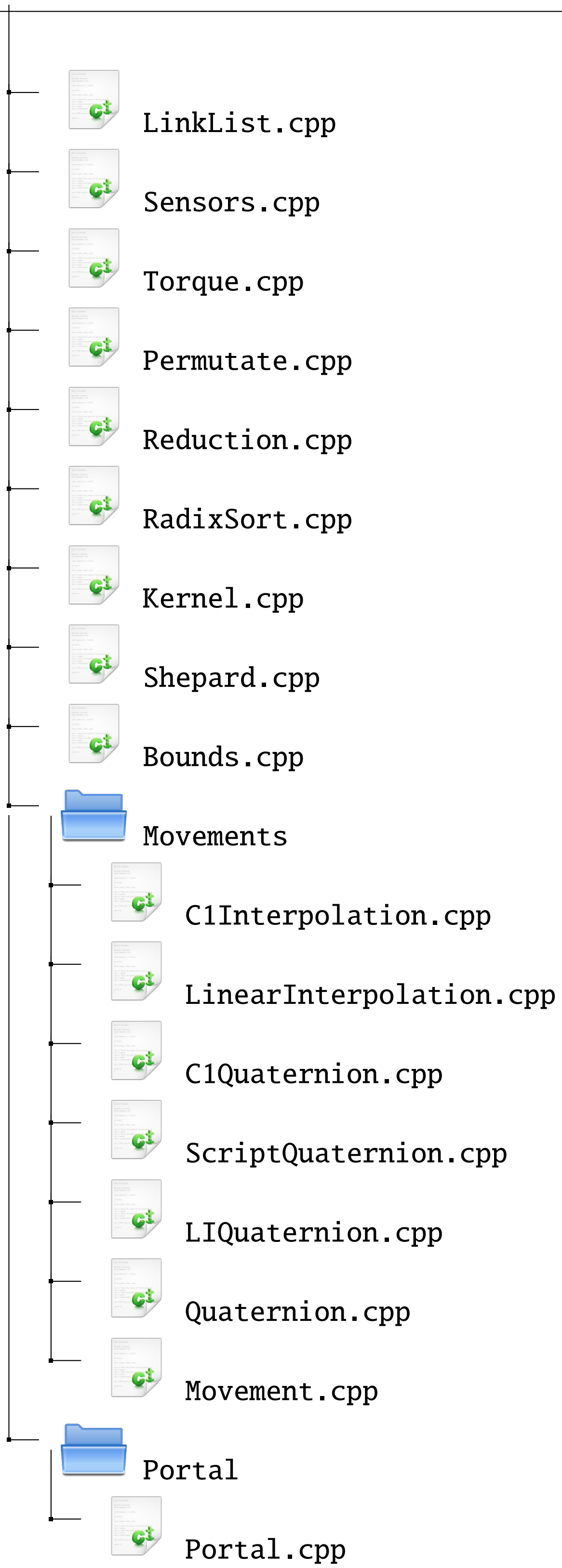

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- Sensors.cpp
- Torque.cpp
- Permutate.cpp
- Reduction.cpp
- RadixSort.cpp
- Kernel.cpp
- Shepard.cpp
- Bounds.cpp
- Movements
  - C1Interpolation.cpp
  - LinearInterpolation.cpp
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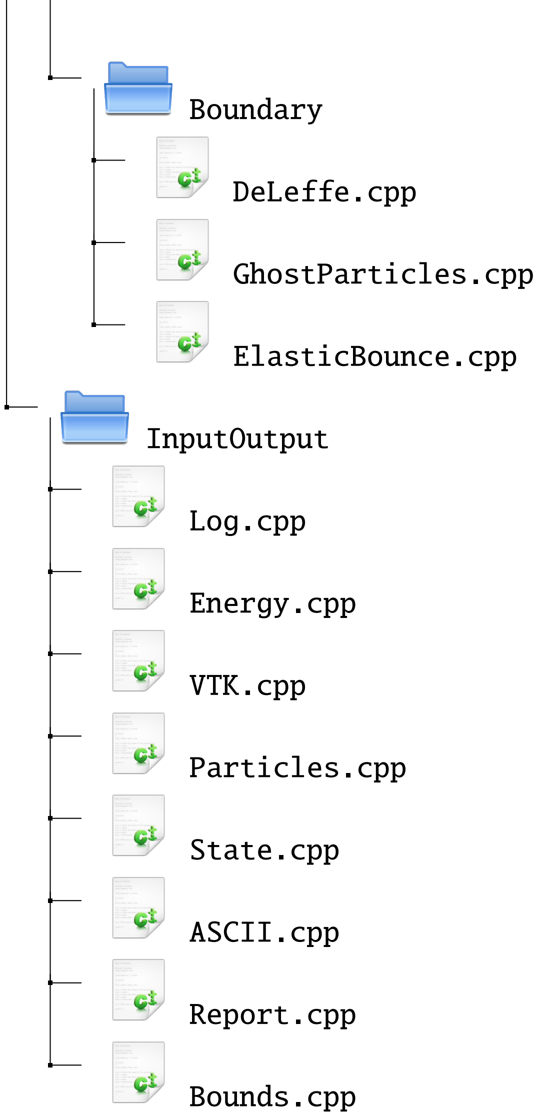
- Portal
  - Portal.cpp



All the files called “`CMakeLists.txt`”, “`*.cmake`”, or included in a “cMake” folder are designed to let cmake to configure the package for the build and installation process. More specifically, the files called “`CMakeLists.txt`” are the ones where the instructions for cmake are written, while the other ones are templates that cmake is conveniently reading and editing.

A CodeBlocks project is provided for the developers in the file “CodeBlocks/AQUAgpusph.cbp”. However, it is strongly recommended to use cmake to perform compilations.