Application de la technologie ActivePapers pour la biologie computationnelle

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Retour d'expéRiences sur la Recherche Reproductible (R^4)
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What is ActivePapers?

- K. Hinsen - 2011: first paper mentioning the principles of ActivePaper. [1]
- Goal: computational science made reproducible and publishable
- ActivePaper solution:
  - a single file combining datasets and programs that works on it
  - Citable (DOI - unique and persistant identifiers)

[1] K. Hinsen. Procedia Computer Science 2011 (4) 579

Why ActivePapers?

Molecular Dynamics simulations specificities:

- Size of the data: several Gb

- Local storage in binary format (size optimization - efficient reading)

- Need to work on different computer (HPC, personal computer)

- MOSAIC - MOlecular SimulAtion Interchange Conventions [2]:

Detailed description of molecular simulation

Facilitate the exchange of data

[2] K. Hinsen. J. Chem Inf. Model. 2014 (54) 131

ActivePaper design

- HDF5 file + conventions
- HDF is supported by many commercial and non-commercial software platforms: Java, MATLAB, Scilab, Mathematica, Octave, IDL, Python, R …
- Can also be inspected using many generic HDF5 tools, in particular HDFView or HDF Compass

HDF5: Hierarchical Data Format (version 5).

- open-source format
- designed to store large amounts of data
- provide a hierarchical structure
- self-describing
- Maintained by the non-profit HDF Group (spin-off of the NCSA*)

* NCSA: National Center for Supercomputing Applications

A concrete example

THE JOURNAL OF CHEMICAL PHYSICS **139**, 154110 (2013)

Model-free simulation approach to molecular diffusion tensors

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(Received 5 July 2013; accepted 18 September 2013; published online 21 October 2013)

E. Availability of software and data

An ActivePaper[29] containing all the software, input datasets, and results from this study is available as the supplementary material.[30] The datasets can be inspected with any HDF5-compatible software, e.g., the free HDFView.[31] Running the programs on different input data requires the ActivePaper software.[32] These files also contain plots for all the components of all the correlation functions and mean-square displacements we have computed and of which we show only a selection in this article.

A concrete example - figshare

figshare.com/articles/Model_free_simulation_approach_to_molecular_diffusion_tensors_Water/808595

figshare

water_diffusion.ap download

Download

216 views

0 shares

cites coming soon

Published on **26 Sep 2013 - 14:59 (GMT)**

Filesize is **78.28 MB**

Share this: Share 0 Tweet 0 G+1 0 Embed*

Cite this: Chevrot, Guillaume; Hinsen, Konrad; Kneller, Gerald R. (2013): Model-free simulation approach to molecular diffusion tensors: Water. figshare. http://dx.doi.org/10.6084/m9.figshare.808595
Retrieved 17:31, Nov 27, 2015 (GMT)

*The embed functionality can only be used for non commercial purposes... more

Description

This file contains part 2 (water) of the supplementary material for the following publication:

Title: Model-free simulation approach to molecular diffusion tensors
Authors: Guillaume Chevrot, Konrad Hinsen, Gerald R. Kneller
Journal: Journal of Chemical Physics **139**, 154110 (2013)

It contains the software implementing the computations described in the article, the input datasets for water, the resulting output datasets, and the figures. A detailed list is given below.

The file water_diffusion.ap is a HDF5 file that can be read with any HDF5-compatible software, including the free HDFView package (http://www.hdfgroup.org/hdf-java-html/hdfview/). HDFView can be used to inspect the arrays and tables contained in this file. Reading the molecular structure for water requires software that understands the Mosaic data model (http://bitbucket.org/molsim/mosaic/).

Categories

- Condensed Matter Physics
- Computational Physics

Authors

Guillaume Chevrot
Konrad Hinsen
Gerald R. Kneller

Tags

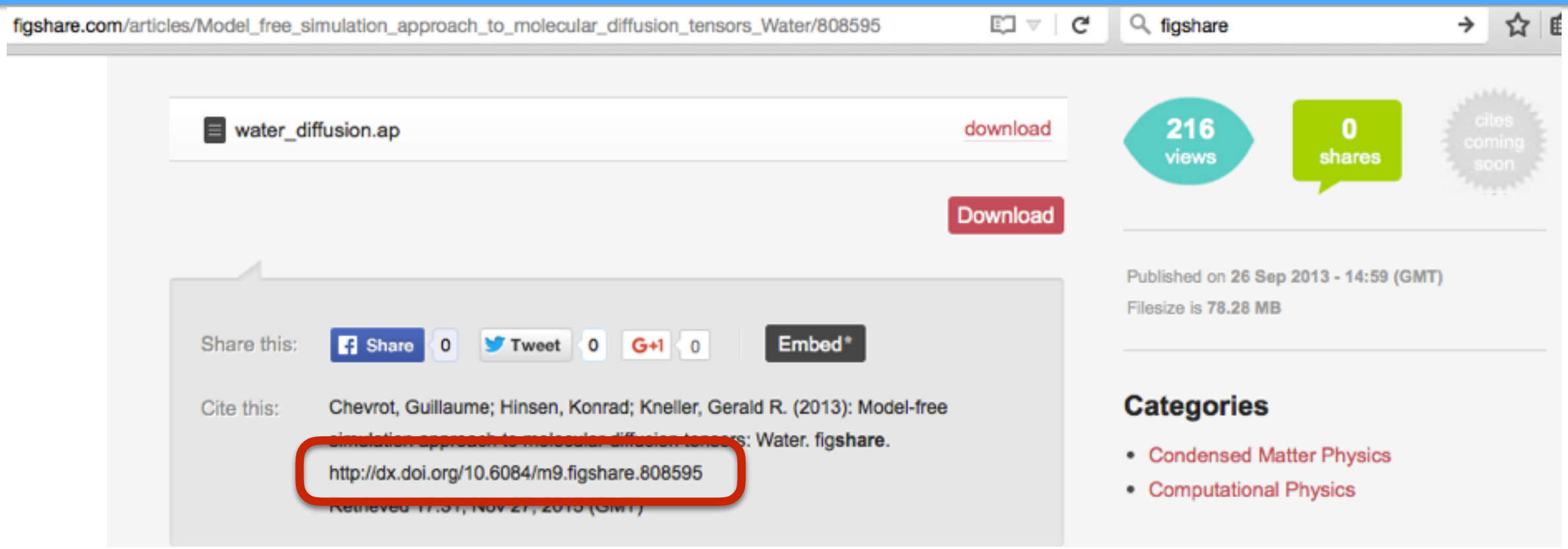
- Molecular Simulation
- ActivePapers
- diffusion tensor
- water

License (what's this?)

CC-BY

Export

A concrete example - DOI



DOI
Digital Object Identifier

DOI: Digital Object Identifier

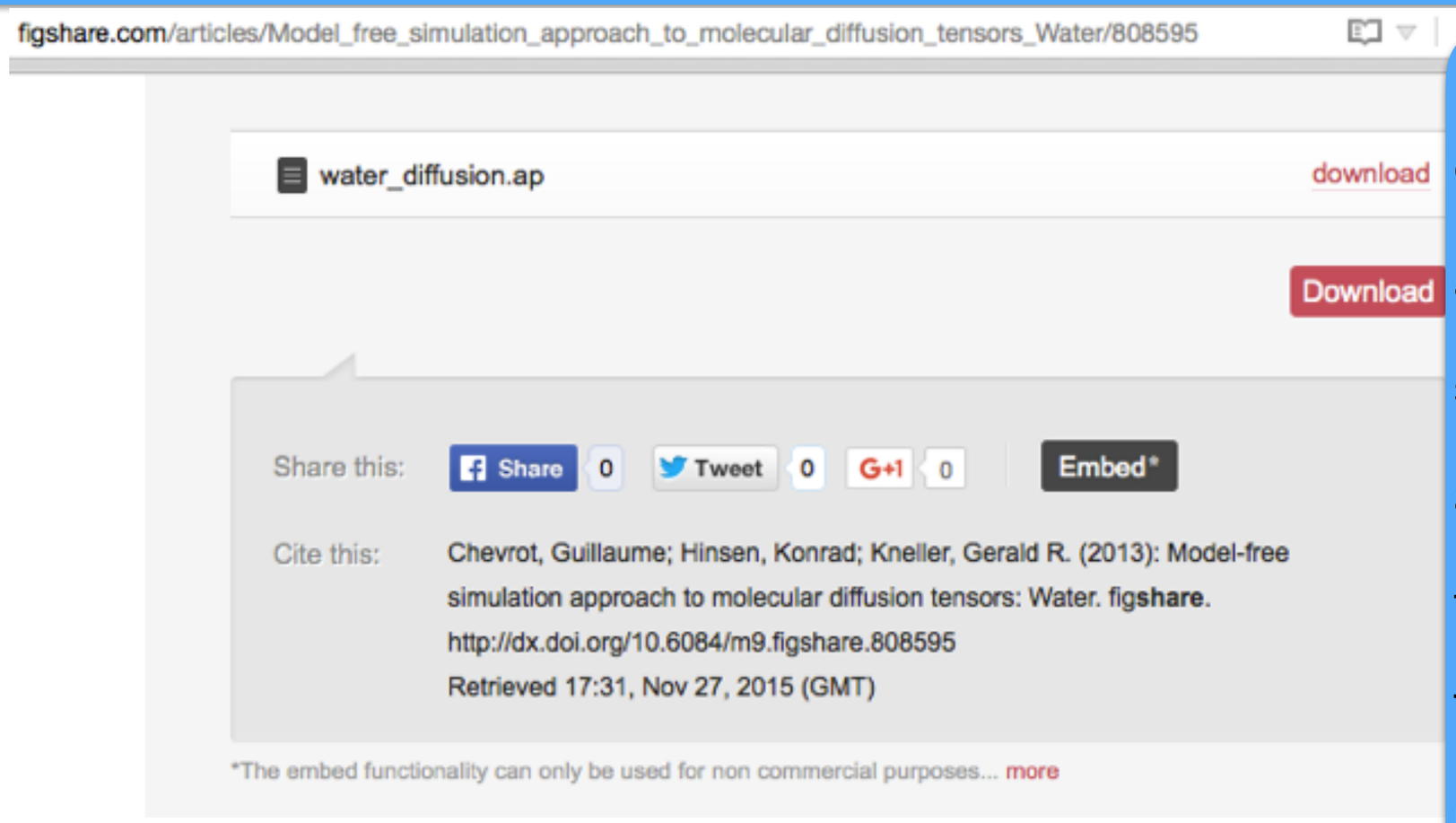
It provides unique and persistent identifiers

for electronic documents on the internet.

The uniqueness of the identifiers is

guaranteed by a central registry.

A concrete example - License



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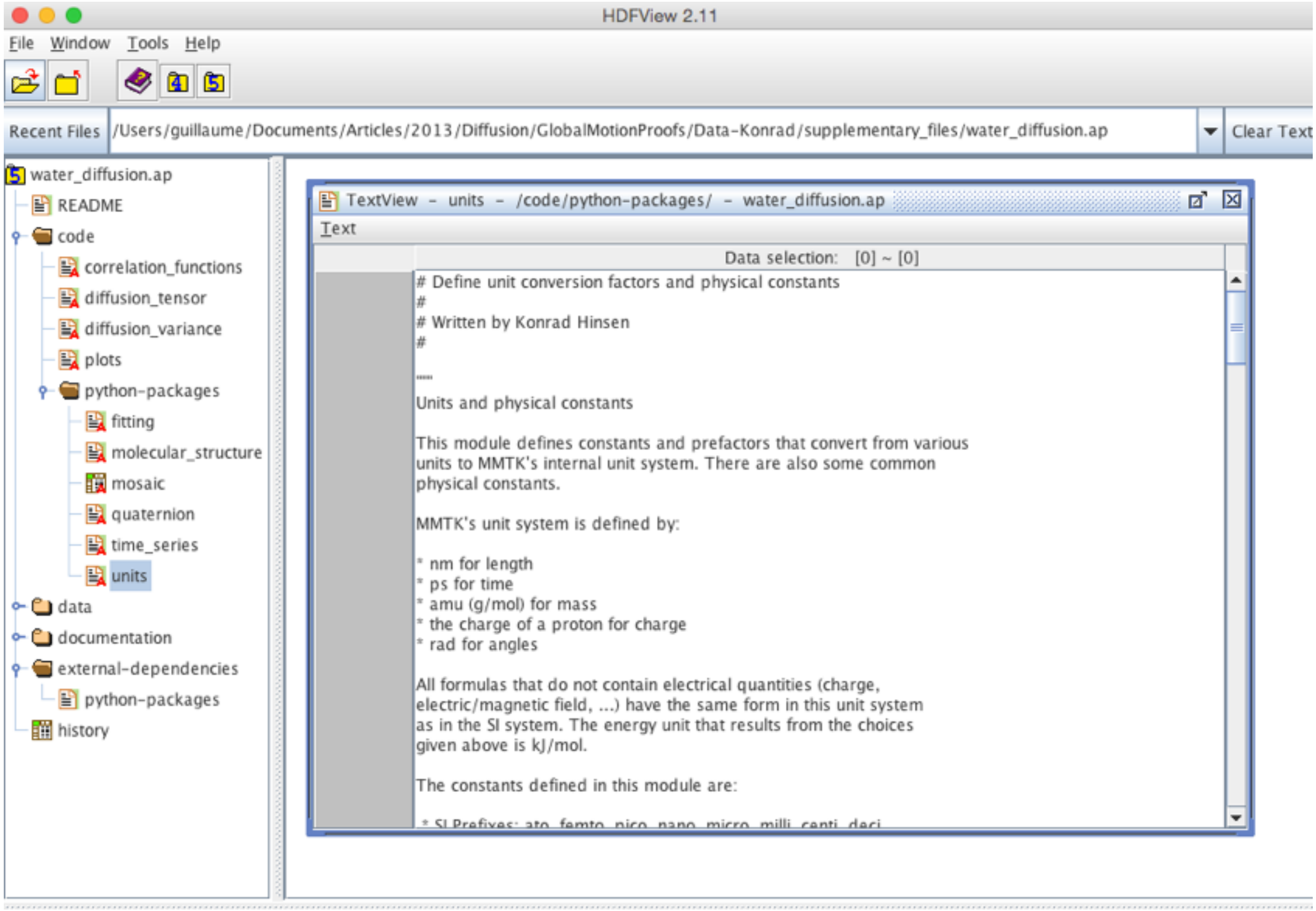
This license lets others distribute, remix, tweak, and build upon your work, even commercially, as long as they credit you for the original creation.

Creative Commons Licenses

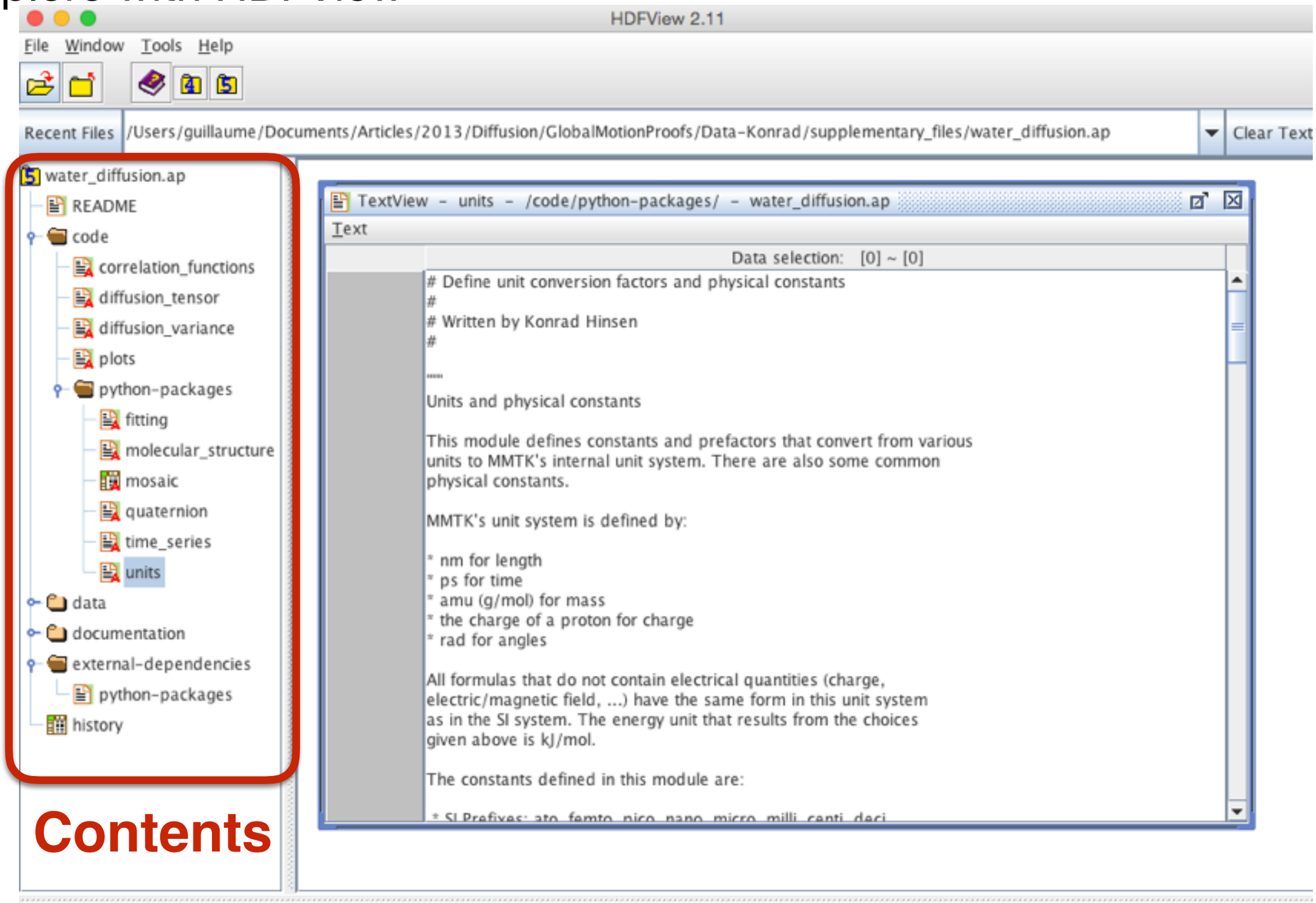
A concrete example - exploration

- Explore with HDFView



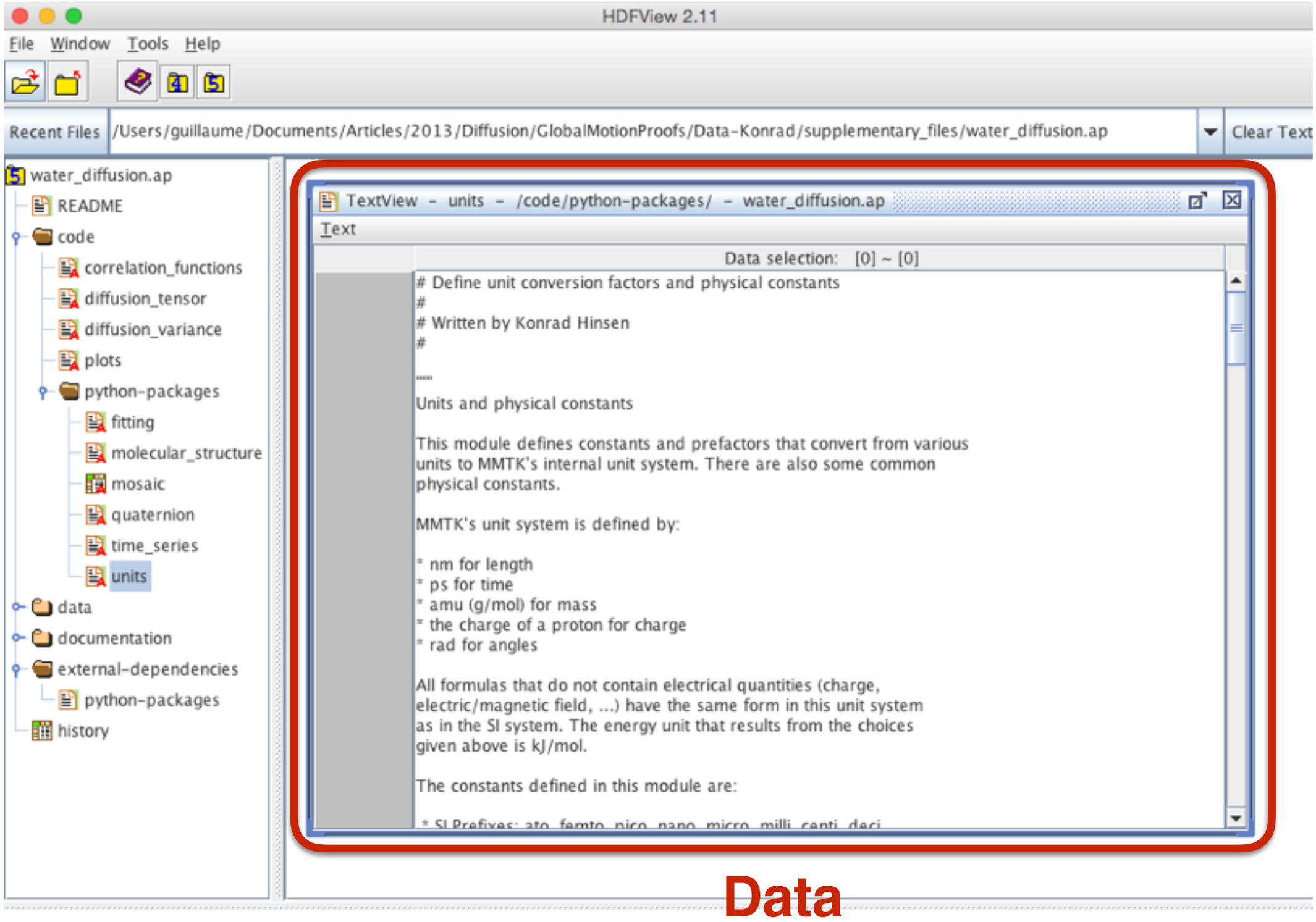
A concrete example - exploration

- Explore with HDFView



A concrete example - exploration

- Explore with HDFView



A concrete example - exploration

- Explore with HDFView

HDFView 2.11

File Window Tools Help

Recent Files /Users/guillaume/Documents/Articles/2013/Diffusion/GlobalMotionProofs/Data-Konrad/supplementary_files/Test/water_diffusion.ap Clear Text

water_diffusion.ap
- README
- code
  - correlation_functions
  - diffusion_tensor
  - diffusion_variance
  - plots
  - python-packages
    - fitting
    - molecular_structure
    - mosaic
    - quaternion
    - time_series
    - units
- data
- documentation
- external_dependencies
- history

history at / [water_diffusion.ap in /Users/guillaume/Documents/Articles/2013/Diffusion/GlobalMotionProofs/Data-Konrad/supplementary_files/Test]

Table

0-base

	opened	closed	platform	hostname	username	activepap...	python_ve...	numpy_ve...	h5py_vers...	hdf5_versi...	matplotlib_version
0	1370247400257	1370247400263	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
1	1370247400844	1370247400865	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
2	1370247401362	1370247401372	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
3	1370247401881	1370247401891	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
4	1370247402387	1370247402396	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
5	1370247402899	1370247402914	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
6	1370247403420	1370247403438	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
7	1370247403934	1370247403938	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
8	1370247404420	1370247404425	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
9	1370247404913	1370247404921	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
10	1370247405414	1370494691493	linux2	isei000.hpc	hinsen	0.1.0	2.7.2	1.6.1	2.1.2	1.8.9	1.1.0
11	1370500745854	1370500746130	darwin	Konrad-H...	hinsen	0.1.0	2.7.3	1.6.2	2.1.3	1.8.11	1.2.x
12	1370500746675	1370500746681	darwin	Konrad-H...	hinsen	0.1.0	2.7.3	1.6.2	2.1.3	1.8.11	1.2.x
13	1370500747217	1370500747223	darwin	Konrad-H...	hinsen	0.1.0	2.7.3	1.6.2	2.1.3	1.8.11	1.2.x
14	1370500747757	1370500747779	darwin	Konrad-H...	hinsen	0.1.0	2.7.3	1.6.2	2.1.3	1.8.11	1.2.x
15	1370500748315	1370500800627	darwin	Konrad-H...	hinsen	0.1.0	2.7.3	1.6.2	2.1.3	1.8.11	1.2.x
16	1370500802132	1370500802151	darwin	Konrad-H...	hinsen	0.1.0	2.7.3	1.6.2	2.1.3	1.8.11	1.2.x
17	1370500802688	1370500803034	darwin	Konrad-H...	hinsen	0.1.0	2.7.3	1.6.2	2.1.3	1.8.11	1.2.x
18	1370500803586	1370500803602	darwin	Konrad-H...	hinsen	0.1.0	2.7.3	1.6.2	2.1.3	1.8.11	1.2.x
19	1370500804170	1370500804252	darwin	Konrad-H...	hinsen	0.1.0	2.7.3	1.6.2	2.1.3	1.8.11	1.2.x
20	1372849295699	1372849295951	darwin	Konrad-H...	hinsen	0.1.0	2.7.3	1.6.2	2.1.3	1.8.11	1.2.x

History

Date

Platforms

User

Packages versions

A concrete example - exploration with AP

- Explore with ActivePapers
  - open a shell window - works with the command line. You can also use a Jupyter notebook.
  - ‘unix command concept’:

    aptool -h or aptool --help

```
 [49] → aptool -h
usage: aptool [-h] [-p PAPER] [--log LOG] [--logfile LOGFILE] [--version]
              {create,ls,rm,dummy,set,group,extract,calclet,importlet,import,run,update,checkin,c
heckout,ln,cp,refs,edit,console,ipython}
              ...

Management of ActivePapers

positional arguments:
  {create,ls,rm,dummy,set,group,extract,calclet,importlet,import,run,update,checkin,checkout,ln,c
p,refs,edit,console,ipython}
                        commands
    create              Create a new ActivePaper
    ls                  Show datasets
    rm                  Remove datasets and everything depending on them
    dummy               Replace datasets by dummies
    set                 Set dataset to the value of a Python expression
```

A concrete example - exploration with AP

aptool ls -l

```
 [51] → aptool ls -l
2013-05-28/10:07:06  calclet    code/correlation_functions
2013-05-23/14:40:23  calclet    code/diffusion_tensor
2013-05-31/08:54:25  calclet    code/diffusion_variance
2013-06-03/18:24:00  calclet    code/plots
2013-05-22/11:26:53  module     code/python-packages/fitting
2013-05-21/11:34:06  module     code/python-packages/molecular_structure
2013-06-03/10:16:42  reference  code/python-packages/mosaic
2013-05-21/11:39:30  module     code/python-packages/quaternion
2013-06-03/10:16:15  module     code/python-packages/time_series
2013-05-21/11:34:06  module     code/python-packages/units
2013-06-06/06:58:09  data       data/averaged/correlation_function_laboratory_frame
2013-06-06/06:58:09  data       data/averaged/correlation_function_molecular_frame
```

Date/time of the last modification

Type of datasets

Hierarchical structure

A concrete example - datasets

8 types of datasets:

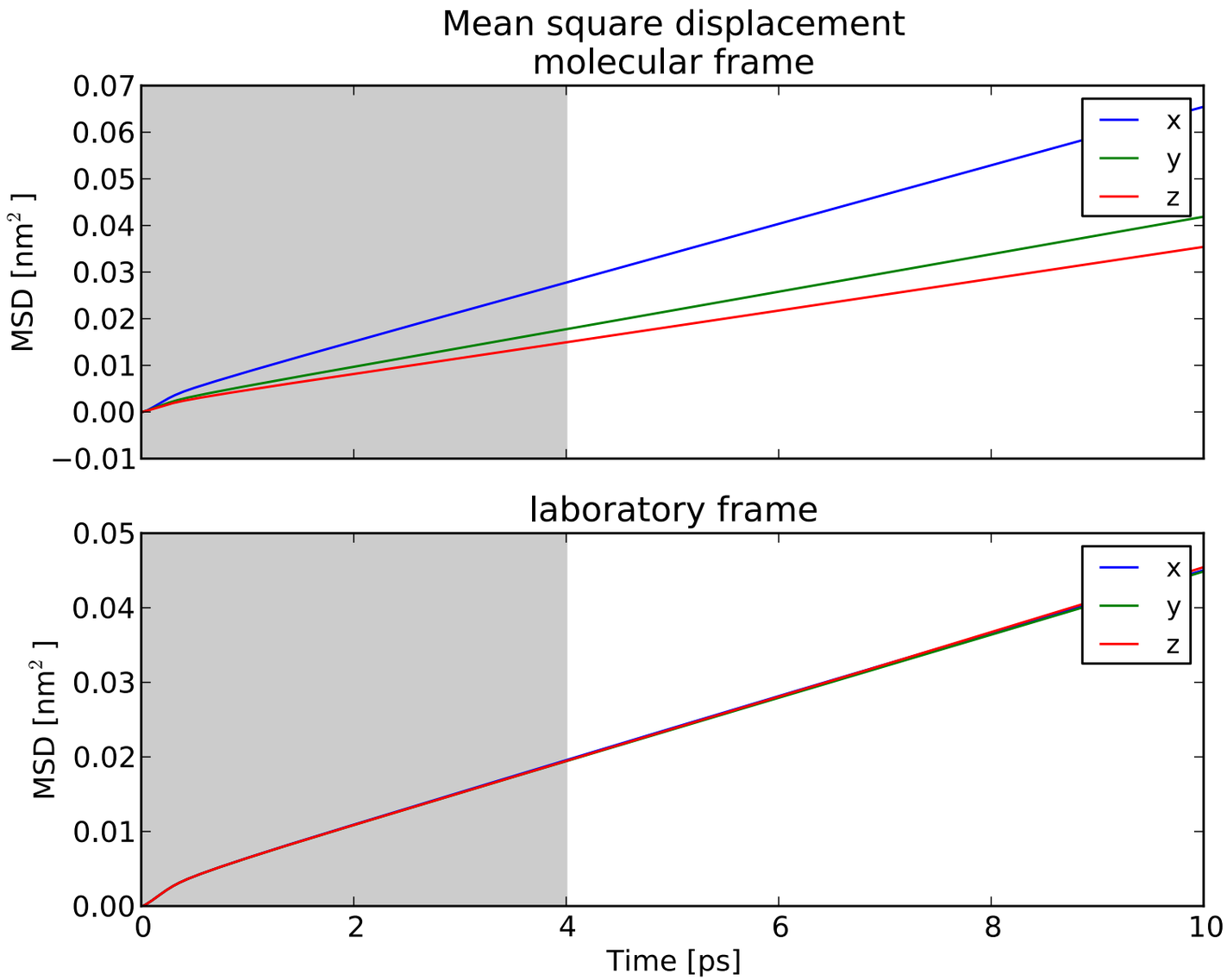
- **module**: a Python source code file to be imported by other Python code.
- **calclet**: Python script with no I/O outside of the ActivePaper.
- **importlet**: Python script without restriction (Internet, data on your computer, Python libraries).
- **reference**: to refer to datasets in other ActivePaper files.
- **data**: HDF5 dataset (array).
- **text**
- **file** (ex: PDF)
- **dummy**: a deleted dataset (to reduce the size of the file, can be restored with a calclet).

A concrete example - documentation

Extracting the documentation / plots:

- aptool checkout documentation

Get a directory containing all the PDF files. Example:



A concrete example - code

Extracting the code:

- aptool checkout code

Get a directory with the code

```
 [82] → ls -lR code/
total 64
-rw-r--r--  1 guillaume  staff  8329 May 28  2013 correlation_functions
-rw-r--r--  1 guillaume  staff  2061 May 23  2013 diffusion_tensor
-rw-r--r--  1 guillaume  staff   758 May 31  2013 diffusion_variance
-rw-r--r--  1 guillaume  staff  9195 Jun  3  2013 plots
drwxr-xr-x  8 guillaume  staff   272 Nov 28 22:31 python-packages

code//python-packages:
total 40
-rw-r--r--  1 guillaume  staff   273 May 22  2013 fitting
-rw-r--r--  1 guillaume  staff   655 May 21  2013 molecular_structure
-rw-r--r--  1 guillaume  staff     0 Nov 28 22:31 mosaic
-rw-r--r--  1 guillaume  staff  2741 May 21  2013 quaternion
-rw-r--r--  1 guillaume  staff  2983 Jun  3  2013 time_series
-rw-r--r--  1 guillaume  staff  3772 May 21  2013 units
```

A concrete example - code

Modifying the code.

Update the ActivePaper with the new code:

aptool checkin code

```
 [101] → aptool ls -l | grep \*
2013-06-06/08:39:38  file      *documentation/averaged/c_rr_diagonals.pdf
2013-06-06/08:39:39  file      *documentation/averaged/c_rr_off_diagonal.pdf
2013-06-06/08:39:36  file      *documentation/averaged/c_tt_diagonal.pdf
2013-06-06/08:39:37  file      *documentation/averaged/c_tt_off_diagonal.pdf
2013-06-06/08:39:40  file      *documentation/averaged/c_vr.pdf
2013-06-06/08:39:59  file      *documentation/averaged/msd_rr_diagonal.pdf
2013-06-06/08:39:59  file      *documentation/averaged/msd_rr_off_diagonal.pdf
2013-06-06/08:39:58  file      *documentation/averaged/msd_tt_diagonal.pdf
2013-06-06/08:39:58  file      *documentation/averaged/msd_tt_off_diagonal.pdf
```

Some files in the documentation are now marked as stale

Then you can update the files: aptool update

```
2015-11-30/17:15:18  file      documentation/averaged/c_rr_diagonals.pdf
2015-11-30/17:15:19  file      documentation/averaged/c_rr_off_diagonal.pdf
2015-11-30/17:15:16  file      documentation/averaged/c_tt_diagonal.pdf
2015-11-30/17:15:17  file      documentation/averaged/c_tt_off_diagonal.pdf
2015-11-30/17:15:20  file      documentation/averaged/c_vr.pdf
2015-11-30/17:15:43  file      documentation/averaged/msd_rr_diagonal.pdf
2015-11-30/17:15:44  file      documentation/averaged/msd_rr_off_diagonal.pdf
2015-11-30/17:15:42  file      documentation/averaged/msd_tt_diagonal.pdf
2015-11-30/17:15:43  file      documentation/averaged/msd_tt_off_diagonal.pdf
```

New dates

The files in the documentation are now updated

A concrete example - parameters

Modifying parameters.

Example: change the range of the MSD plot:

aptool set msd_plot_range ‘array([0.,200.])'

```
 [107] → aptool ls -l | grep \*
2015-11-30/17:15:43  file      *documentation/averaged/msd_rr_diagonal.pdf
2015-11-30/17:15:44  file      *documentation/averaged/msd_rr_off_diagonal.pdf
2015-11-30/17:15:42  file      *documentation/averaged/msd_tt_diagonal.pdf
2015-11-30/17:15:43  file      *documentation/averaged/msd_tt_off_diagonal.pdf
2015-11-30/17:15:46  file      *documentation/averaged/msd_vr.pdf
```

Some files in the documentation are now marked as stale

Then you can update the files: aptool update

```
2015-11-30/17:58:03  file       documentation/averaged/msd_rr_diagonal.pdf
2015-11-30/17:58:03  file       documentation/averaged/msd_rr_off_diagonal.pdf
2015-11-30/17:58:01  file       documentation/averaged/msd_tt_diagonal.pdf
2015-11-30/17:58:02  file       documentation/averaged/msd_tt_off_diagonal.pdf
2015-11-30/17:58:04  file       documentation/averaged/msd_vr.pdf
```

New dates

The files in the documentation are now updated

http://www.activepapers.org/python-edition/tutorial.html

A concrete example - interactive exploration

jupyter ActivePapers Last Checkpoint: 2 minutes ago (autosaved)

File Edit View Insert Cell Kernel Help Python 3

Code Cell Toolbar: None

```
In [2]: %matplotlib notebook
        from activepapers.exploration import ActivePaper
        import matplotlib.pyplot as plt
        import numpy as np

In [3]: ap = ActivePaper("doi:10.6084/m9.figshare.808595")

In [4]: ?ap

In [ ]:
```

Download and open the ActivePaper via its DOI

```
Type:        ActivePaper
String form: <activepapers.exploration.ActivePaper object at 0x103940b00>
File:        ~/anaconda/envs/activepapers/lib/python3.4/site-packages/ActivePapers.Py-0.1.4-py3.4.egg/activepa
pers/exploration.py
Docstring:
Datasets in this file
=====================

The input data to the computations in this file are rigid-body
trajectories for each of the 511 water molecules in the original MD
trajectory. This input data is too big to be provided here.  The
correlation functions and mean-square displacements are first computed
individually for each water atom and then averaged. The
single-molecule functions are also too big to be provided here, exceot
for a subset of five water molecules for demonstration.

All single-molecule data has a numerical suffix. In the following
list, only the first one ("_0") is shown.
```

Explore the README

A concrete example - interactive exploration

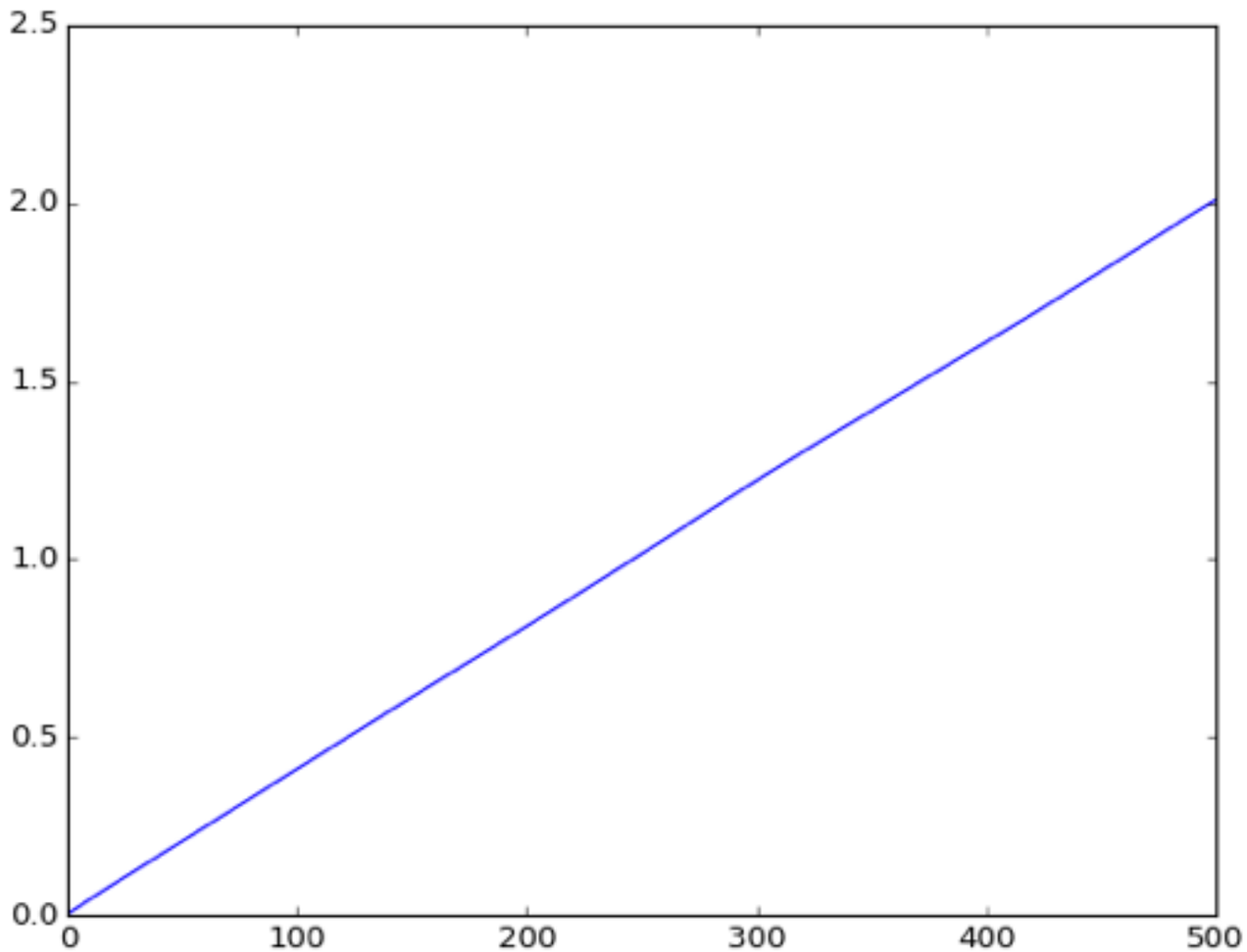
jupyter ActivePapers Last Checkpoint: 3 minutes ago (unsaved changes)

File Edit View Insert Cell Kernel Help Python 3

Code Cell Toolbar: None

```
In [4]: ?ap
```

```
In [5]: msd_time = ap.data['mean_square_displacement_time'][...]
        msd_averaged_lab_xx = ap.data['averaged/mean_square_displacement_laboratory_frame'][0, 0]
        plt.plot(msd_time, msd_averaged_lab_xx)
```



Make a plot from the data inside the ActivePaper

A concrete example - interactive exploration

jupyter ActivePapers Last Checkpoint: 16 hours ago (unsaved changes)

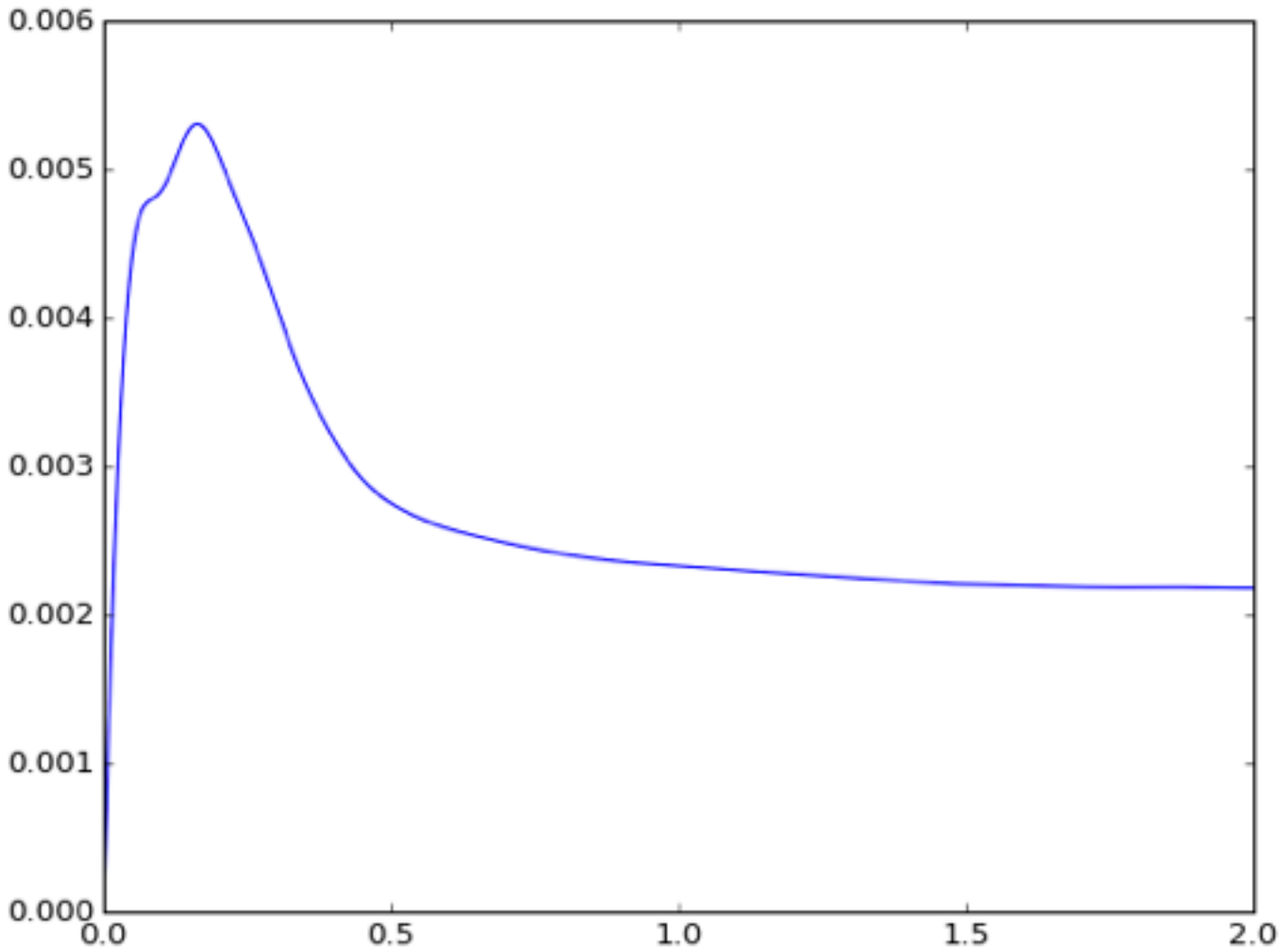
File Edit View Insert Cell Kernel Help | Python 3

Code | Cell Toolbar: None

```
In [6]: import time_series

In [7]: vacf_time = ap.data['correlation_function_time'][:2000]
        vacf_averaged_lab_xx = ap.data['averaged/correlation_function_laboratory_frame'][0, 0, :2000]

In [10]: dt = vacf_time[1]-vacf_time[0]
         plt.plot(vacf_time, time_series.integral(vacf_averaged_lab_xx, dt))
```



Import Python modules stored in the ActivePaper

Interact with the module

Limitations

- Data limit that can be stored online. In the example, we start from the simulations data (>10Gb)

- Python only

- Dependences: Numpy, h5py + external libraries

- How many years your ActivePaper will be stable? (Scientific Python ecosystem has proven to be moderately stable in the past)

Conclusions

- ActivePaper store all your data in a single file

- Python edition is operational - Number of publications available as an ActivePaper: 4

- Next developments:
  - interaction with notebooks
  - other language

- Reproducible research on the web: ActivePaper and Exec&Share
  http://www.univ-orleans.fr/misc-orleans-tours

  http://www.activepapers.org/

  GitHub https://github.com/activepapers/activepapers-python

  twitter @ActivePapers