Introduction to scripting

NSCCS ADF/ReaxFF Workshop

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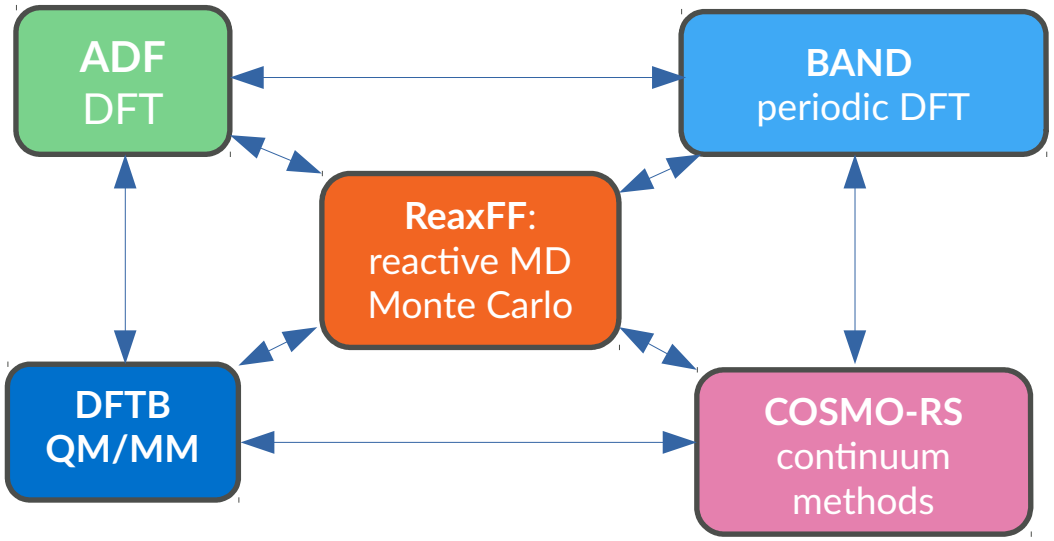
Scripting

The ADF modelling suite comes with it's own Python:

```
$ADFBIN/startpython
```



Links all program packages

→ workflows

→ custom post-processing/analysis

→ rapid prototyping in development

Available modules

NumPy

fundamental package
for scientific computing

RDKit

Cheminformatics
and Machine Learning

ASE (+ calculators)

Atomic simulation environment

PLAMS

Python Library for Automating
Molecular Simulations developed @SCM

more...

https://www.scm.com/doc/Scripting/index.html

ADF/ReaxFF: RXKF files

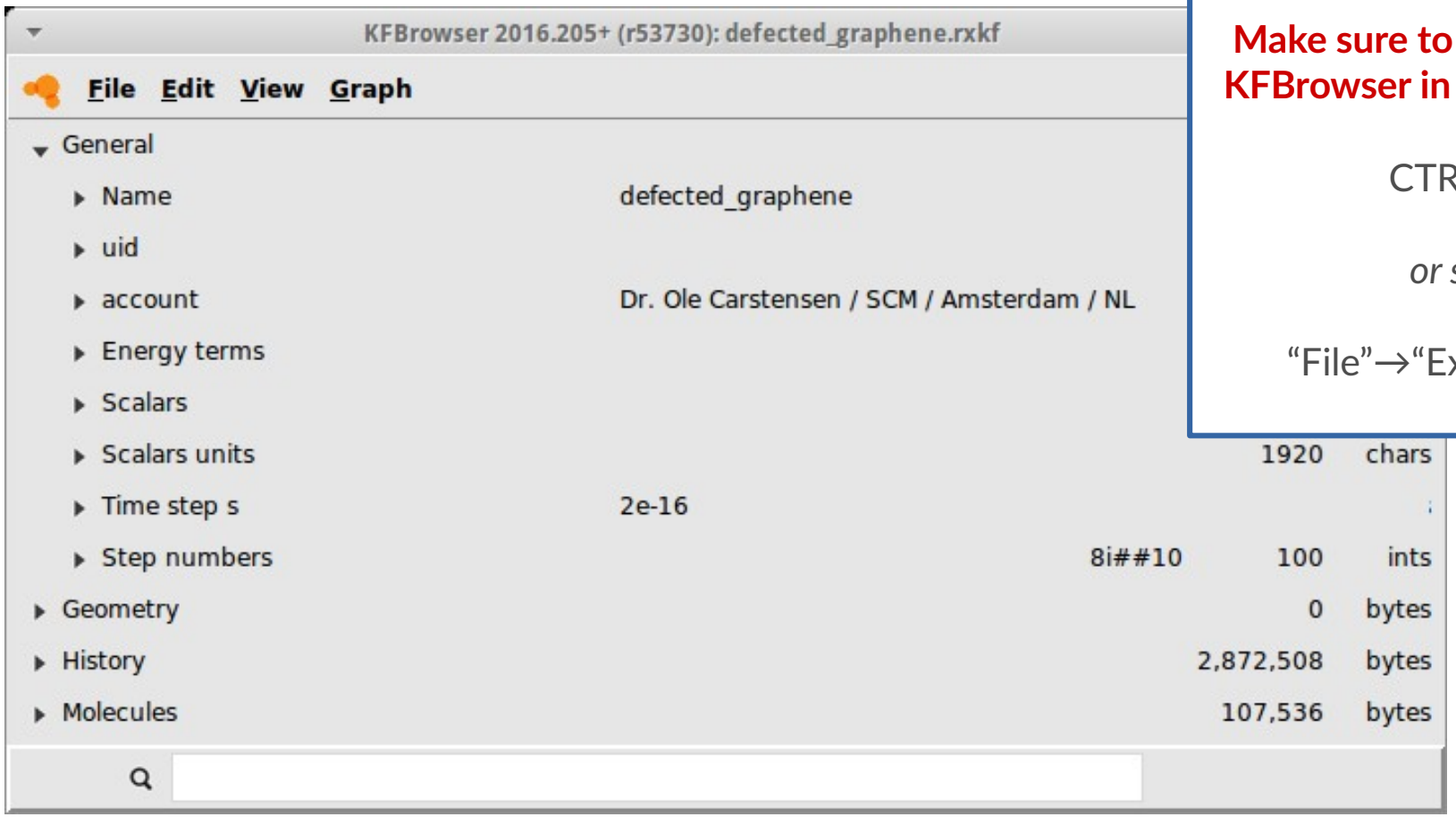
The RXKF format

Info:

The RXKF file is the general result file of an ADF/ReaxFF calculation.

It is a KF file: Direct-Access, binary, and keyword driven (see here). It contains your trajectory as well as information about the calculation.

Use the KFBrowser of the GUI to inspect RXKF files:



Make sure to always use the KFBrowser in "Expert Mode":

CTRL + E

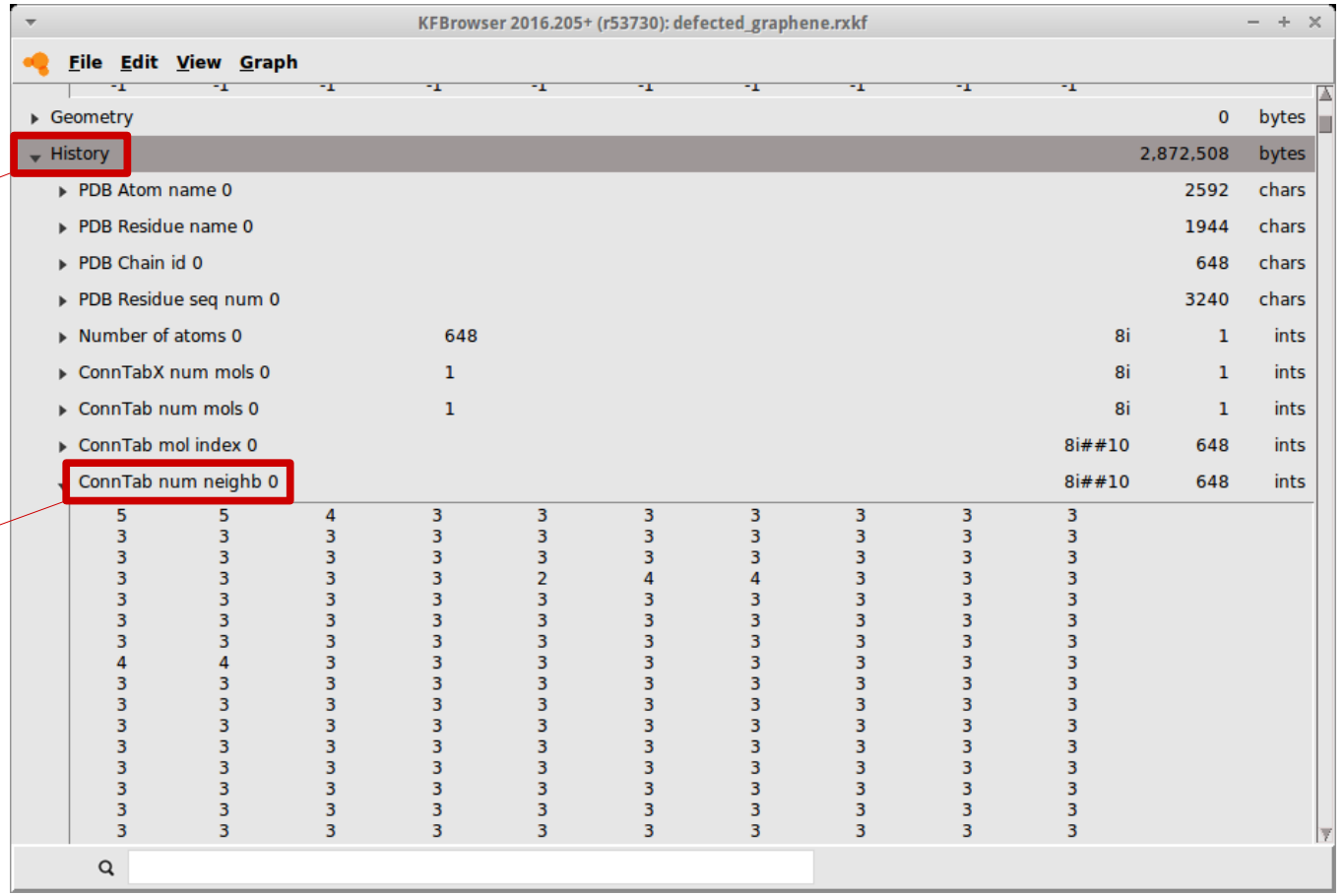
or select

"File"→"Expert Mode"

ADF/ReaxFF: RXKF files

How to look up Sections and Variables…

The data on the RXKF is organized in Sections which group together related data. Each section contains a number of variables. Each variable may be an array or a scalar and may be integer, real, logical or character type.



Here:

Number of neighbors for each atom in the first frame: Section = "History", Variable = "ConnTab num neighb 0" (in this case the variable is an array with 648 integer entries, but PYTHON will take care of this for us…)

Python Scripting
using PLAMS to read from rxkf

Data from RXKF files can easily been read and processed using PYTHON and the PLAMS library. Just modify the following template according to your own needs:

File: `plams_template.py`
Execute: `startpython plams_template.py`

Reading General Data, Examples:

```
#
# Read the timestep
#
timestep = KFReader.read('General', 'Time step s')
print timestep

[...]

#
# Read the stepnumbers
#
steps = KFReader.read('General', 'Step numbers')
print steps
```

Documentation is found here

Python Scripting
using PLAMS to read from rxkf

The most common situation will be to process some entries of an RXKF file per frame.
The following code snippet demonstrates how to read the Number of Molecules / frame:

File: `plams_template.py`
Execute: `startpython plams_template.py`

Reading Data per Frame

```
#
# Read the steps
# remove -1 from the returned list
#
Steps = KFReader.read('General', 'Step numbers')
Steps = filter(lambda a: a != -1, Steps)
#
# Loop through all frames and read
# current number of molecules
#
for step in Steps:
        NumMols = KFReader.read('History', 'ConnTab num mols ' + str(step))
        print NumMols
```

Documentation is found here

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