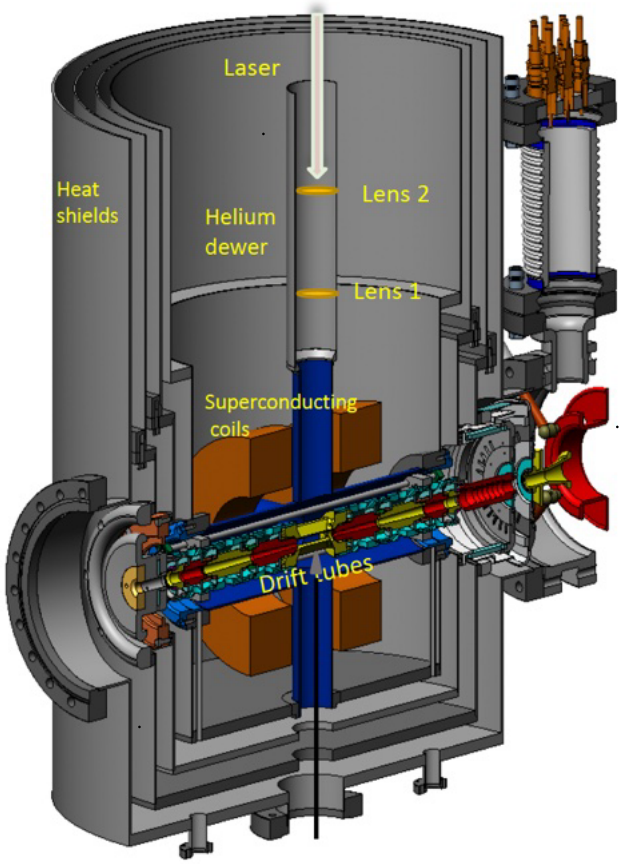
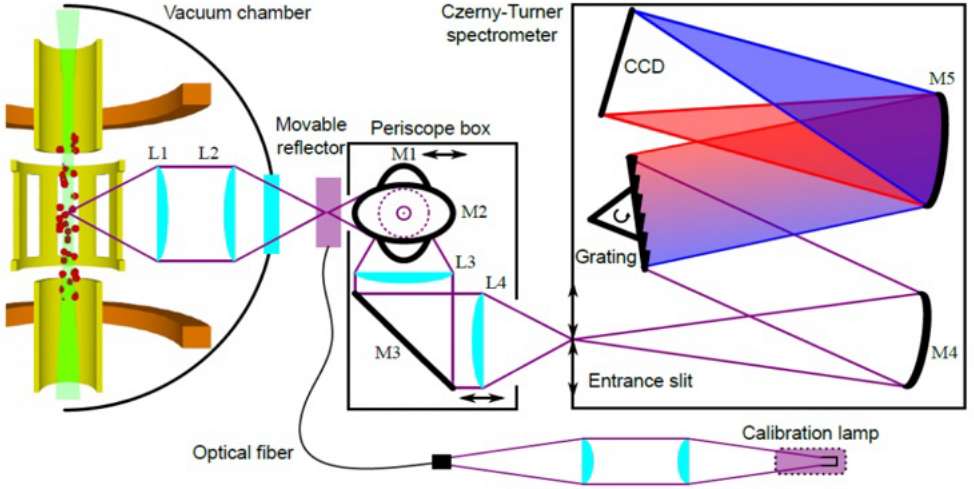
Software and Analysis Organization

Ullrich Schwanke, Jonas Kankel
Humboldt University Berlin

Motivation



- **HCI spectroscopy will be applied to a number of different HCIs**
- **Procedures for data recording well defined**
- **Here, we will be concerned with the data analysis code that might be used & adapted by more than one person at a time**
- **Jonas and I looked at the code (provided by Lakshmi)**



The Code - Scope

From HD-EBIT

- Dataset description
- Spectrometer data
- HD-EBIT Settings

From NIST

- Line data

Analysis code/scripts with command line arguments

- Cosmic removal
- Image corrections
- Line finding/fitting
- Line identification
- ....

Results, plots

- **Theory comparison (e.g. AMBiT)**

The Code - Status

```
schwanke@polaris Spectral_analysis % pwd
/Users/schwanke/Downloads/Spectral_analysis
schwanke@polaris Spectral_analysis % ls -lrt
total 2536
-rw-r--r--@   1 schwanke  staff   32181 12 Jun  2023 Spectrometer_Sequence_creator.py
-rw-r--r--@   1 schwanke  staff   17904 13 Jun  2023 quick_spectral_viewer.py
-rw-r--r--@   1 schwanke  staff  133763 26 Jun  2023 aux_functions.py
-rw-r--r--@   1 schwanke  staff   52146 27 Jun  2023 simple_theoretical_spectrum_calibration_Mk3.py
-rw-r--r--@   1 schwanke  staff    2937  8 Aug  2024 Analyze_spectra_Ni.bat
-rw-r--r--@   1 schwanke  staff   41680 14 Jan 09:48 Energy_and_Wavelengthscan_Mk2_bismuth.py
-rw-r--r--@   1 schwanke  staff   28355 13 Feb 12:16 3_dispersion_relation_bash.py
-rw-r--r--@   1 schwanke  staff   31559 13 Feb 12:16 2b_dark_images.py
-rw-r--r--@   1 schwanke  staff   34231 13 Feb 12:16 3_dispersion_relation_Mk2_newbash.py
-rw-r--r--@   1 schwanke  staff   31908 13 Feb 12:16 3_dispersion_relation_Mk2_bash.py
-rw-r--r--@   1 schwanke  staff   29033 13 Feb 12:16 3_dispersion_relation_tophat_bash.py
-rw-r--r--@   1 schwanke  staff   10100 13 Feb 12:16 2_curvature_and_temperature_correction.py
-rw-r--r--@   1 schwanke  staff   23940 13 Feb 12:17 2_curvature_and_temperature_correction_bash.py
-rw-r--r--@   1 schwanke  staff   42307 13 Feb 12:17 5_Collective_plotter_voigttest_bash.py
-rw-r--r--@   1 schwanke  staff   26528 13 Feb 12:17 1b_after_calib_helper.py
-rw-r--r--@   1 schwanke  staff  327701 13 Feb 12:17 123_helper_Mk2.py
-rw-r--r--@   1 schwanke  staff   32001 13 Feb 12:17 3_dispersion_relation_tophat_Mk2_bash.py
-rw-r--r--@   1 schwanke  staff   35154 13 Feb 12:17 3_dispersion_relation_tophat_Mk2_newbash.py
-rw-r--r--@   1 schwanke  staff   36331 13 Feb 12:17 4_zeeman_fit_bash.py
-rw-r--r--@   1 schwanke  staff   36272 13 Feb 12:17 4_zeeman_fit_hyperfine_bash.py
-rw-r--r--@   1 schwanke  staff   25998 13 Feb 12:17 4_zeeman_fit_morethanone_bash.py
-rw-r--r--@   1 schwanke  staff   36916 13 Feb 12:17 4_zeeman_fit_voigttest_bash.py
-rw-r--r--@   1 schwanke  staff    1761 13 Feb 12:17 3b_line_refinder.py
-rw-r--r--@   1 schwanke  staff   21193 13 Feb 12:17 3b_recalibration.py
-rw-r--r--@   1 schwanke  staff   28554 13 Feb 12:17 1_correct_images_afterCalib_bash.py
-rw-r--r--@   1 schwanke  staff   52370 13 Feb 12:20 5_Collective_plotter_hyperfine_bash.py
-rw-r--r--@   1 schwanke  staff   50453 13 Feb 12:21 5_Collective_plotter_bash.py
-rw-r--r--@   1 schwanke  staff   15022 13 Feb 13:56 1_correct_images_bash.py
-rw-r--r--@   1 schwanke  staff    2397 13 Feb 14:38 Analyze_spectra_Ni.py
-rw-r--r--@   1 schwanke  staff    1153 21 Feb 11:40 readme.txt
```

The Code - Status

- **Written bei Nils Rehbehn**
- **25k lines of python code**
- **Fully procedural, long functions**

- **Easy to run on a batch system**
- **Uses standard python packages (numpy, matplotlib, argparse....)**

- **Very sparse documentation/comments**
- **Does not reside in a software repository (no versioning)**
- **No software tests defined (e.g. a fixed analysis that must not be broken by code changes)**

```
(base) schwanke@polaris Analysis code % python 1_correct_images_afterCalib_bash.py -h
usage: 1_correct_images_afterCalib_bash.py [-h] date Folder calibration_threshold after_calib

Correct images of cosmics

positional arguments:
  date                  date of the measurement
  Folder                Folder name of the measurement
  calibration_threshold
                        Threshold of the calibration images
  after_calib           Use additional Calibration Data to improve dispersion function

optional arguments:
  -h, --help            show this help message and exit
```

The Code – Proposal: what to do

- **Store the code in a repository (DESY gitlab requires DESY account…)**
- **Give it a name!**
- **Apply limited versioning**
- **Document code changes (change log)**
- **Document installation, inputs/outputs and basic usage (README file or web page?)**
- **Document analysis procedures (e.g. for specific HCIs)**
- **Add a complicated test (e.g. a previous analysis)**
- **Assign someone responsible for the code**
- **Add slowly more in-line documentation (e.g. docstrings)**

```
def square(n):
    '''Take a number n and return the square of n.'''
    return n**2
```

The Code – Proposal: what to AVOID

- **Motivation: lack of manpower and limited number of code users**

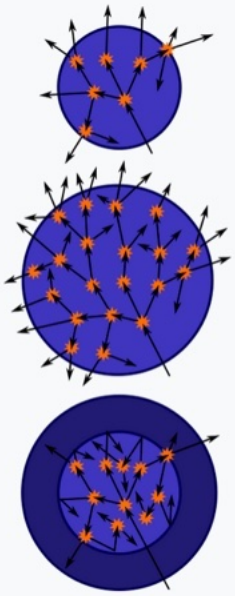
- **Re-write the code in an oo fashion**
- **Improve the code using tools like pylint**
- **Setup a system for continuous testing (software is compiled and tested at regular intervals)**
- **Add standard testing procedures (e.g. pytest)**

Critical Mass 🤓

Critical mass of a bare sphere [edit]

The shape with minimal critical mass and the smallest physical dimensions is a sphere. Bare-sphere critical masses at normal density of some actinides are listed in the following table. Most information on bare sphere masses is considered classified, since it is critical to nuclear weapons design, but some documents have been declassified.[3]

Nuclide	Half-life (y)	Critical mass (kg)	Diameter (cm)	Ref
uranium-233	159,200	15	11	[4]
uranium-235	703,800,000	52	17	[4]
neptunium-236	154,000	7	8.7	[5]
neptunium-237	2,144,000	60	18	[6][7]
plutonium-238	87.7	9.04–10.07	9.5–9.9	[8]
plutonium-239	24,110	10	9.9	[4][8]
plutonium-240	6561	40	15	[4]
plutonium-241	14.3	12	10.5	[9]
plutonium-242	375,000	75–100	19–21	[9]
americium-241	432.2	55–77	20–23	[10]
americium-242m	141	9–14	11–13	[10]
americium-243	7370	180–280	30–35	[10]
curium-243	29.1	7.34–10	10–11	[11]
curium-244	18.1	13.5–30	12.4–16	[11]
curium-245	8500	9.41–12.3	11–12	[11]
curium-246	4760	39–70.1	18–21	[11]
curium-247	15,600,000	6.94–7.06	9.9	[11]
berkelium-247	1380	75.7	11.8-12.2	[12]
berkelium-249	0.9	192	16.1-16.6	[12]
californium-249	351	6	9	[5]
californium-251	900	5.46	8.5	[5]
californium-252	2.6	2.73	6.9	[13]
einsteinium-254	0.755	9.89	7.1	[12]



Top: A sphere of fissile material is too small to allow the chain reaction to become self-sustaining as neutrons generated by fissions can too easily escape.

Middle: By increasing the mass of the sphere to a critical mass, the reaction can become self-sustaining.

Bottom: Surrounding the original sphere with a neutron reflector increases the efficiency of the reactions and also allows the reaction to become self-sustaining.