EIRENE post-processing with TallyViz

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TallyViz

GUI for plotting input and output Eirene tallies.

Branch: **python3**

https://jugit.fz-juelich.de/p.boerner/TallyViz/-/tree/python3

TallyViz/python3

Name
.settings
calc
tallyviz
.directory
.gitignore
.project
.pydevproject
README.txt
SettingsExplain.odt
__init__.py
colors1.tbl
exviztegral.py
requirements.txt
settvizpath.py
setuptallyviz.py
tallyviz.py

TallyViz/python3: requirements

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TallyViz/python3: requirements

Python versions: **3.6.8** - **3.7.0 - 3.8.10**

The following packages needs to be installed:

- **numpy, matplotlib**
- **cython**
- **vtk**
- **wxpython**
- **qt**

```
pip install -r requirements.txt
```

TallyViz/python3: wxpython

GUI interface for python


```python
# First things, first. Import the wxPython package.
import wx

# Next, create an application object.
app = wx.App()

# Then a frame.
frm = wx.Frame(None, title="Hello World")

# Show it.
frm.Show()

# Start the event loop.
app.MainLoop()
```

TallyViz/python3: wxpython

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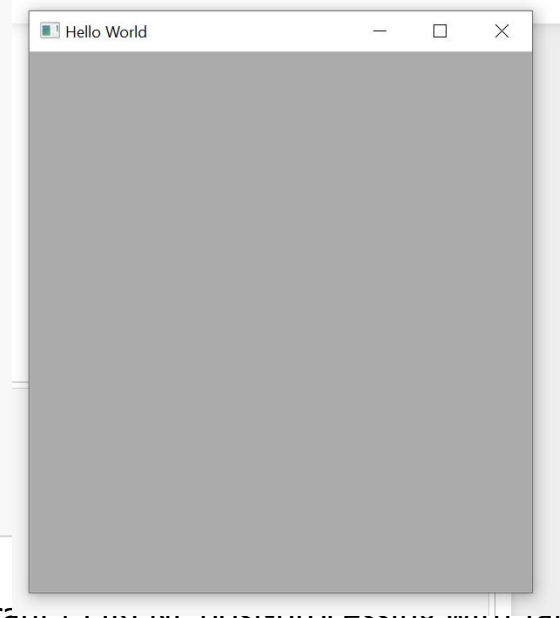
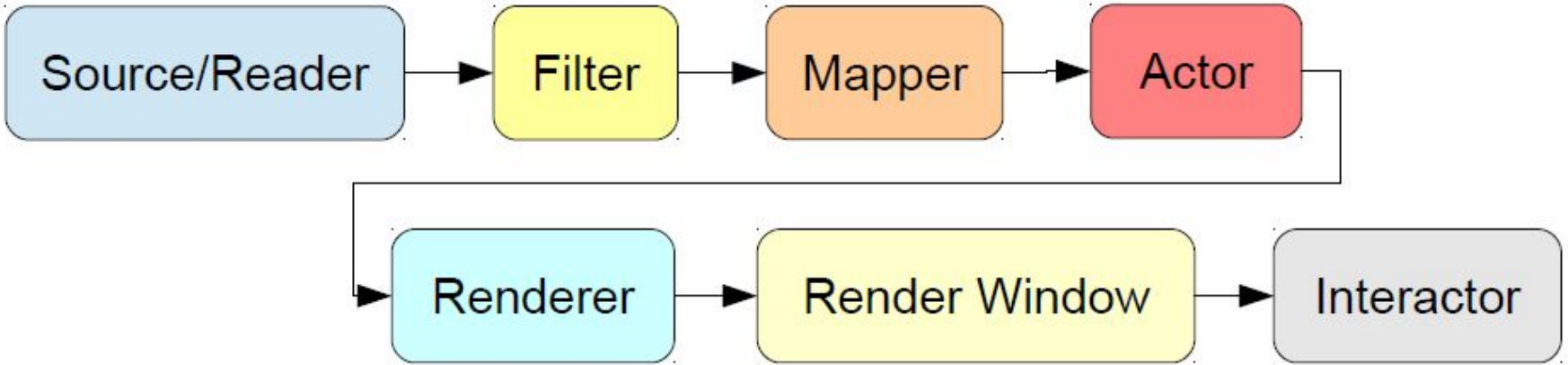


TallyViz/python3: `vtk`

3D visualization toolkit

VISUALIZATION PIPELINE



TallyViz/python3: `viztegral`

The executable `viztegral` must be generated and properly linked:

- Add the path to python packages in `settvizpath.py`
- Compile the `.pyx` files by calling

```
python setuptallyviz.py build_ext --inplace
```

If successful the viztegral executable is compiled into the `build` directory.

TallyViz/python3: `viztegral`

- build
  - lib.linux-x86_64-3.8
    - viztegral.cpython-38-x86_64-linux-gnu.so
  - temp.linux-x86_64-3.8/tallyviz
    - viztegral.o

- build
  - lib.win-amd64-3.7
    - viztegral.cp37-win_amd64.pyd
  - temp.win-amd64-3.7\Release\tallyviz
    - viztegral.cp37-win_amd64.exp
    - viztegral.cp37-win_amd64.lib
    - viztegral.obj

TallyViz/python3: classes

underline : class

MainFrame:

- geometry → geometryHandler
- _tallyHandler → tallyHandler
- on-plotButton():
  - Viz.visualize:
    - vtk: *mapper, actor, render, renderWindow, interactor*

geometryHandler:

- _points
- _elements
- _vtkObject:
    - vtk: *reader, filter*

TallyViz/python3: classes

tallyHandler:

- _out_tallies=[.. → out-tally]
- _in-tallies= [.. → in-tally]
- read-tally():
    - vtk: *reader*

in-tally/out-tally(tally):

- total_strata
- strata= [.. → stratum]

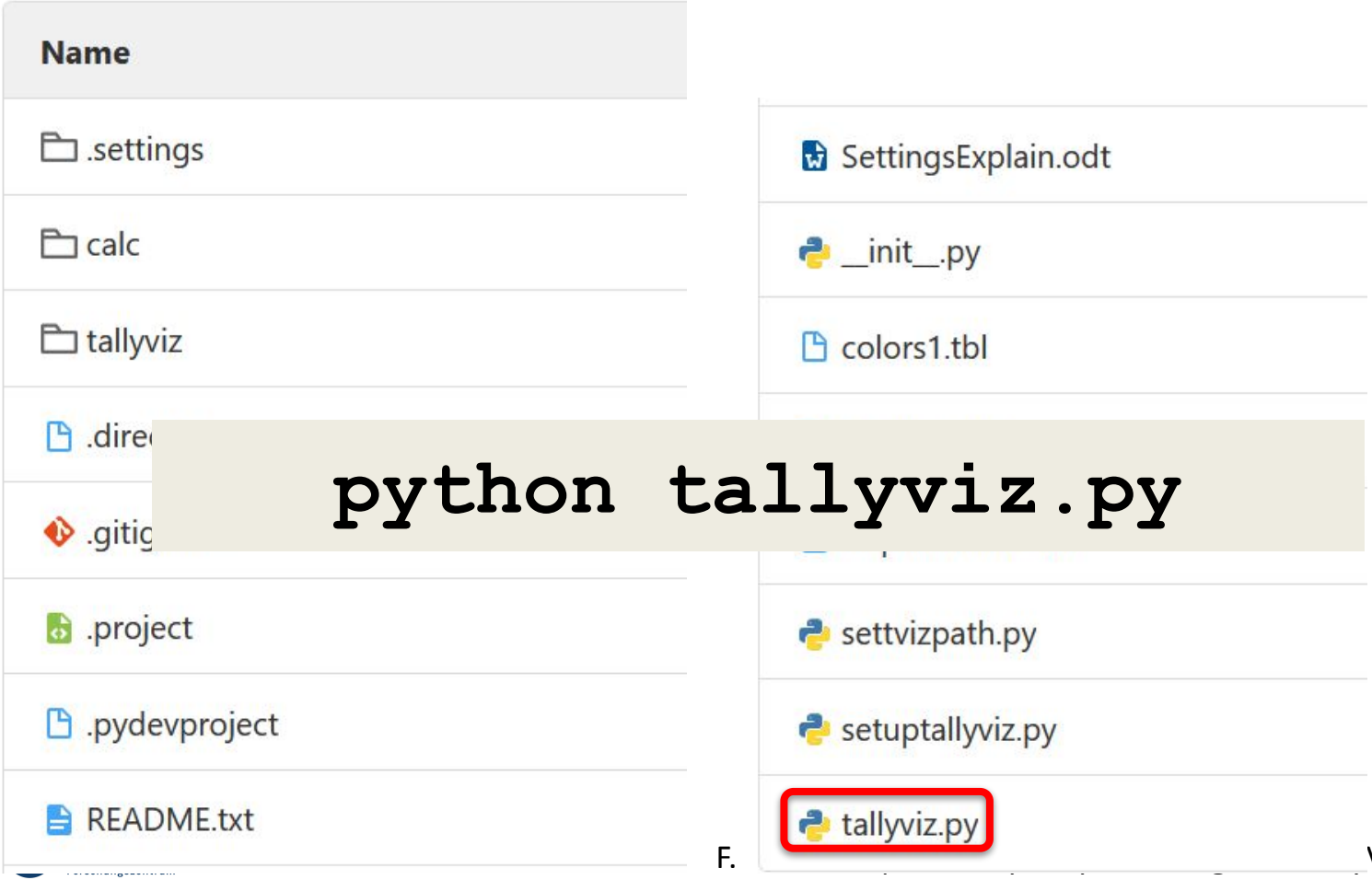
stratum:

- species → species

species:

- values

TallyViz/python3: launch



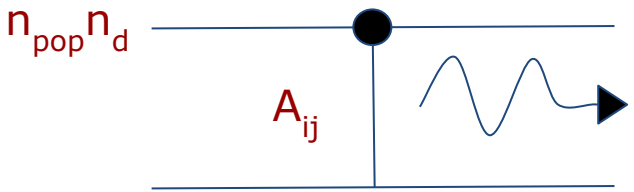
TallyViz/python3: emission rate

Emission rates:

$$\varepsilon_{ij} = n_{pop} n_d A_{ij}$$

n_{pop} pop coeff n_d donor density A_{ij} Einstein coeff

AMJUEL **TALLIES** **PHOTON**



TallyViz/python3: emission rate

Input: block 12 Diagnostic:

```
*** 12. DATA FOR DIAGNOSTIC MODULE
    6     1
* CHORD    1; LY_ALPHA
    2     0     1
    0     0     1     1     1     0
10.2375E+00  10.2357E+00
    0        2.4387E+02 -1.5164E+02  0.0000E+00
    0        3.0363E+02 -7.9405E+01  0.0000E+00
```

- predefined emissivity model (Ly-α/β Ba-α/β/γ/δ)
- user-defined emissivity model

TallyViz/python3: emission rate

Input: block 12 Diagnostic:

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* CHORD    1; LY_ALPHA
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```

Population of excited states from AMJUEL (Reiter/Savada/Fujimoto)

- ★ atomic transitions up to n=6 (Lyman, Balmer, Paschen ..)
- ★ molecular transitions:
  - singlet B,C→X (Lyman, Werner)
  - triplet: d → a (Fulcher)

TallyViz/python3: emission rate

Output: tally 57

- Emission rates in all the simulation domain: different donors contributions.

```
++++++++++++++++++++++++++++++++++++++++++++++++++
ISTRA =      0
++++++++++++++++++++++++++++++++++++++++++++++++++
BA_GAMMA,  SOURCE RATE
NCELLS:          4681
NSPECIES:           6
SPECIES
        ATOMIC NEUTRAL HYDR.         ATOMIC HYDR. ION DIATOMIC NEUTRAL HYDR. M   DIATOMIC HYDR. MOL ION       NEGATIVE HYDR. ION      TRIATOMIC HYDR. ION
UNITS
             PHOTONS/S/CM**3          PHOTONS/S/CM**3          PHOTONS/S/CM**3          PHOTONS/S/CM**3          PHOTONS/S/CM**3          PHOTONS/S/CM**3
TOTAL ("UNITS*CM**3), AND MEAN VALUE ("UNITS")
TOTAL
          6.3719791E+19            6.3513314E+16            7.8065833E+17            6.4873657E+18            3.0450531E+14            6.0171540E+13
MEAN
          1.2846187E+12            1.2804560E+09            1.5738412E+10            1.3078812E+11            6.1389596E+06            1.2130844E+06
================================================
        1            6.1795720E+10            2.5990364E+08            0.0000000E+00            0.0000000E+00            0.0000000E+00            0.0000000E+00
        2            7.0960755E+10            2.5990364E+08            0.0000000E+00            0.0000000E+00            0.0000000E+00            0.0000000E+00
```

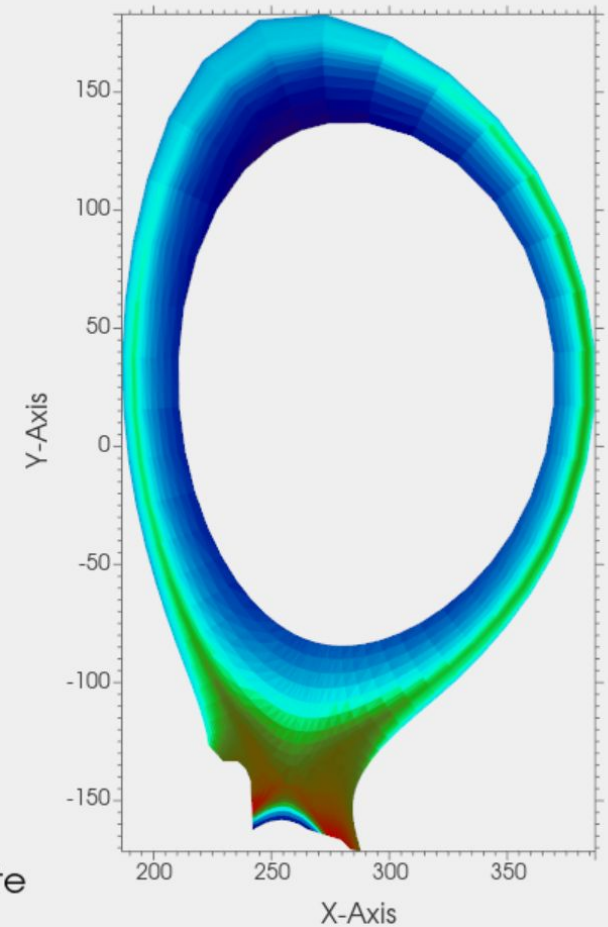
TallyViz/python3: emission rate

Output: tally 57 - minor issues

- predefined emissivity model:
  - only emission rates for last chord in output

- user-defined emissivity model
  - some emission rates missing (allocation issues)

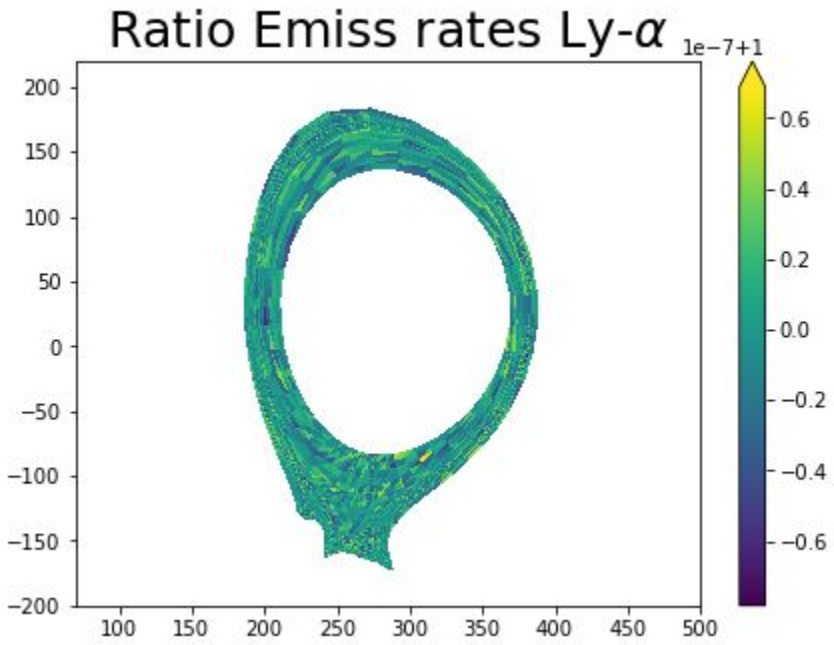
TallyViz/python3: emission rate

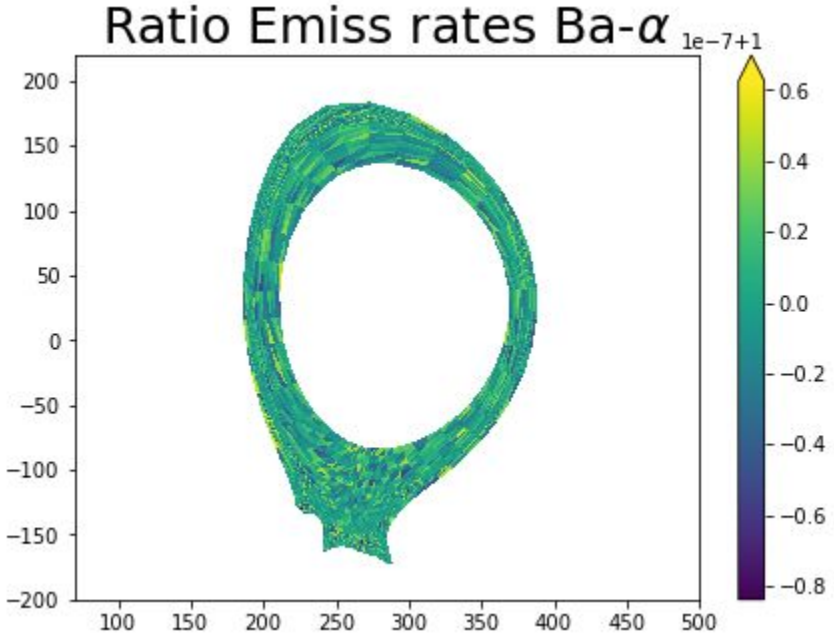


Ly-alpha, emission rate

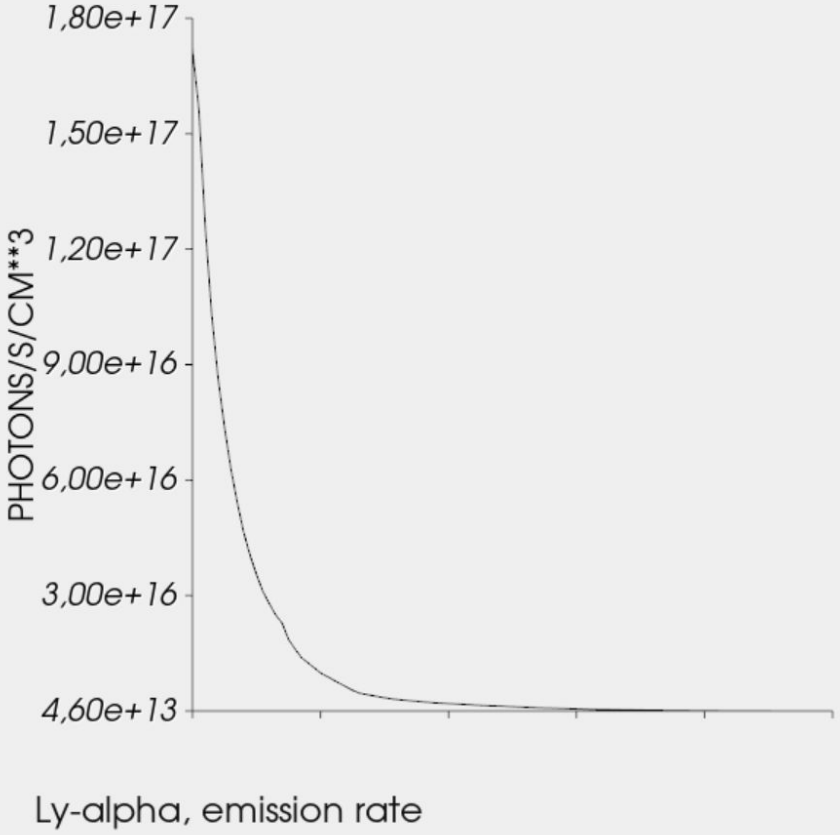
TallyViz/python3: emission rate

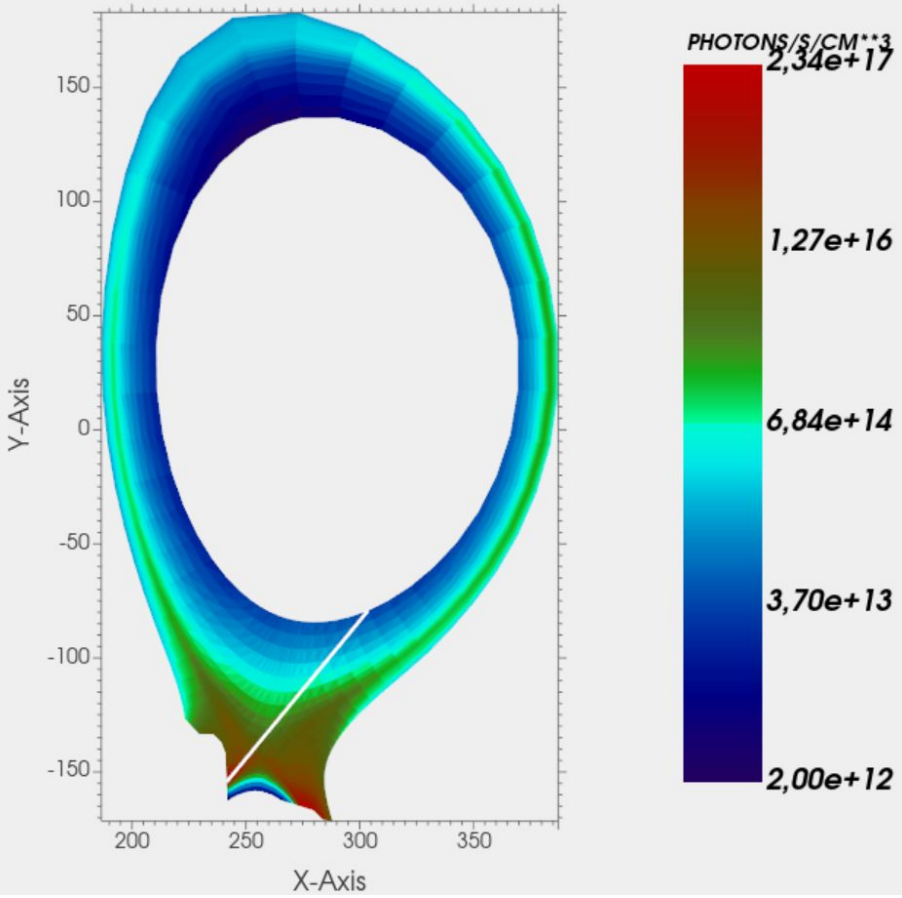
Sanity-check: comparison outtal 57 and data computed directly from AMJUEL.



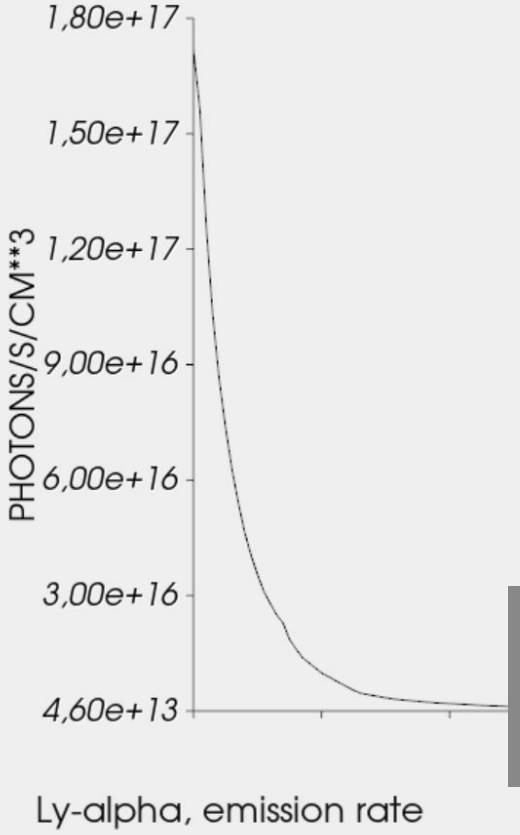


TallyViz/python3: line integral

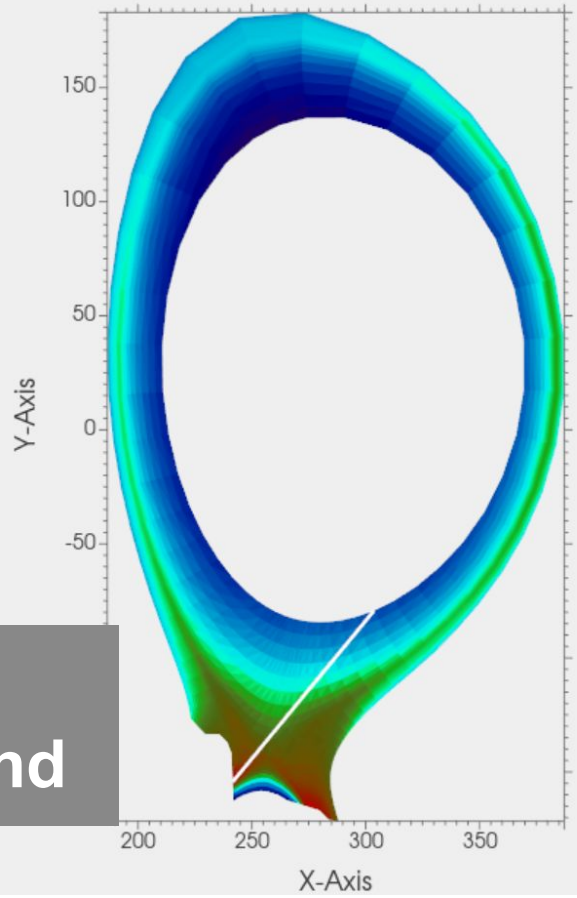




TallyViz/python3: line integral



line to be added by hand



TallyViz/python3: spectrum

Output: eirene.out

- Line integral (linint) of emission rate per sr along the chosen chords.

```
NUMBER OF DETECTOR =            5
* CHORD    5; LY_ALPHA

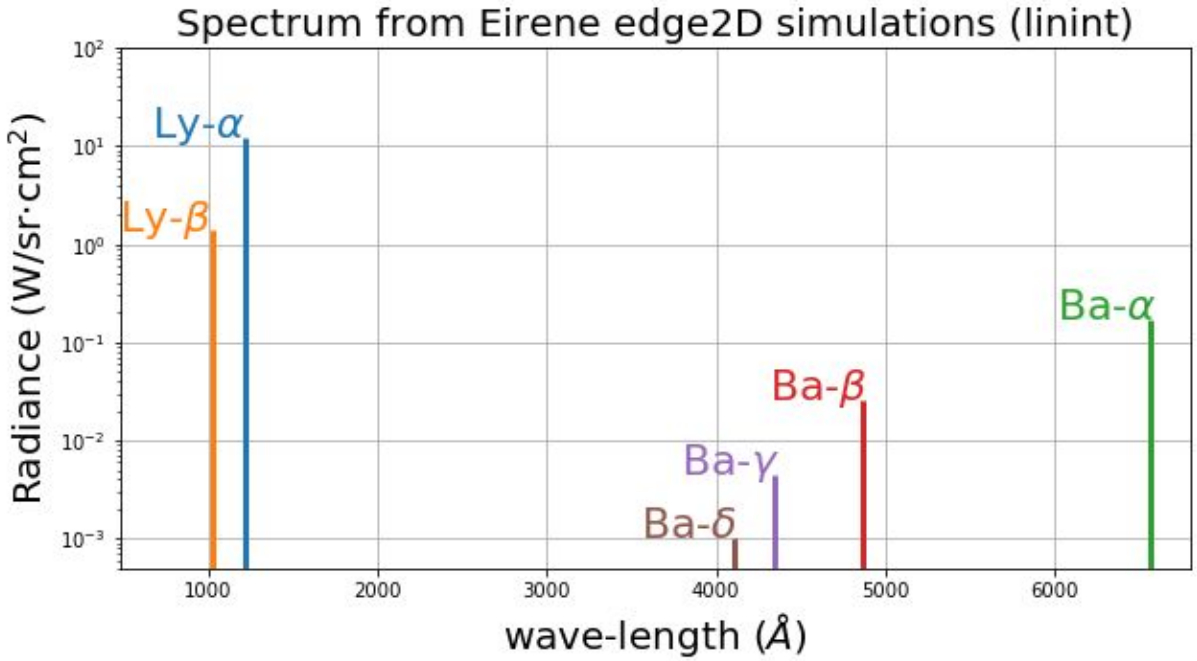
H emission SIGNAL: #/S/CM2/STERAD
=========================================



1ST POINT,"PIVOT POINT"    2.4387E+02    -1.5164E+02     0.0000E+00
2ND POINT, INSIDE VOLUME   3.0363E+02    -7.9405E+01     0.0000E+00
H emiss       7.5813E+18
```

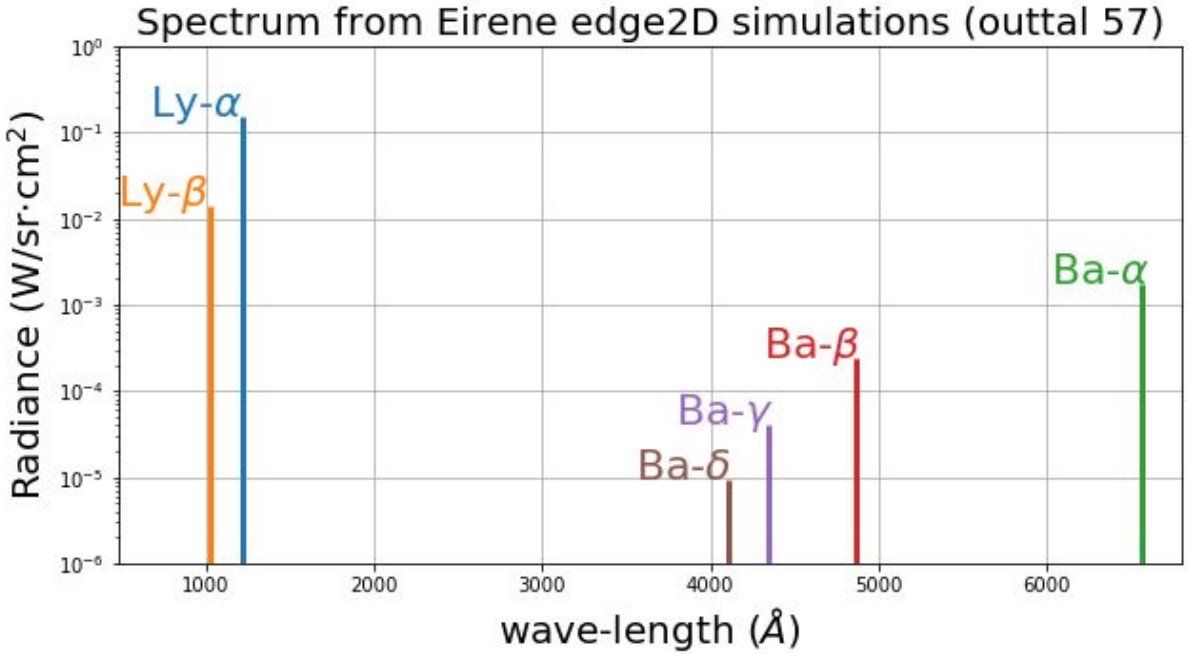
TallyViz/python3: spectrum

From Hemiss in eirene.out (linint):



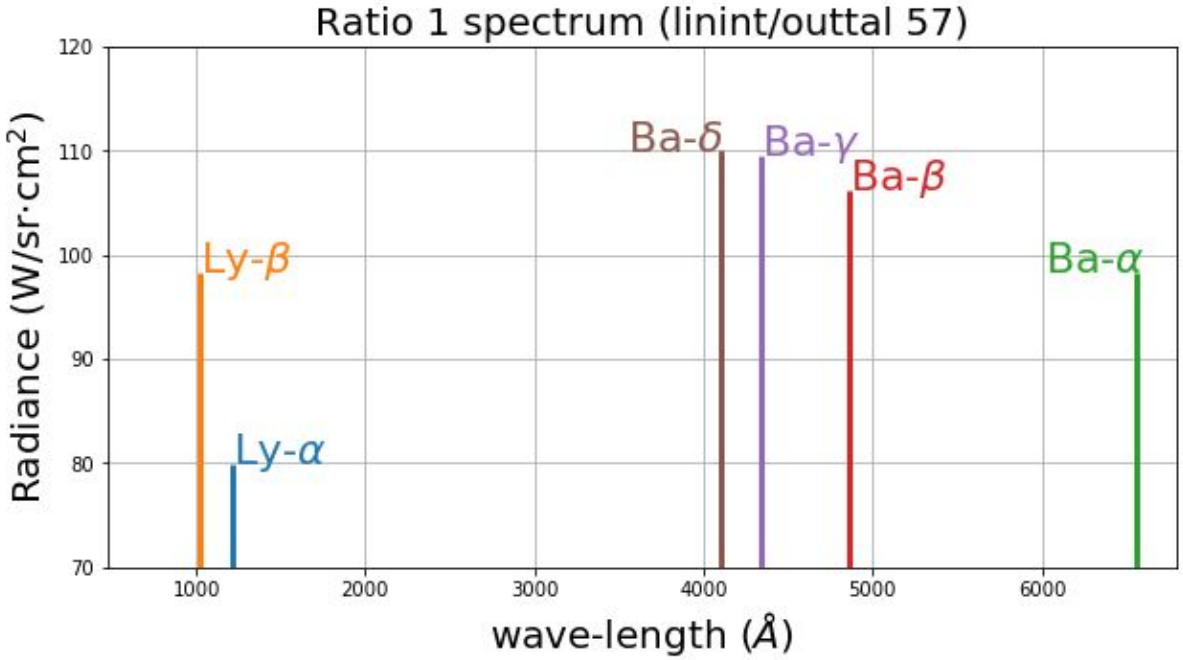
TallyViz/python3: spectrum

Line integration of outtally 57:



TallyViz/python3: spectrum-test

Problem: mismatch spectra from outtally 57 and linint.



Conclusions

TallyViz:

- Advanced and user-friendly tool for 3D postprocessing of eirene tallies.
- Integrable with other python tools, but class structure must be preserved.
- Radiation spectra: not yet implemented
  - outtally 57 for all transitions
  - load chords for lineplots and compute radiance
  - Hemiss (??).
- SOLPS-ITER:
  - run Eirene on top (having issues with reading fort.13)
  - alternative: start post-processing with VTK.

Thanks for the attention!

TallyViz/python3: spectrum-test

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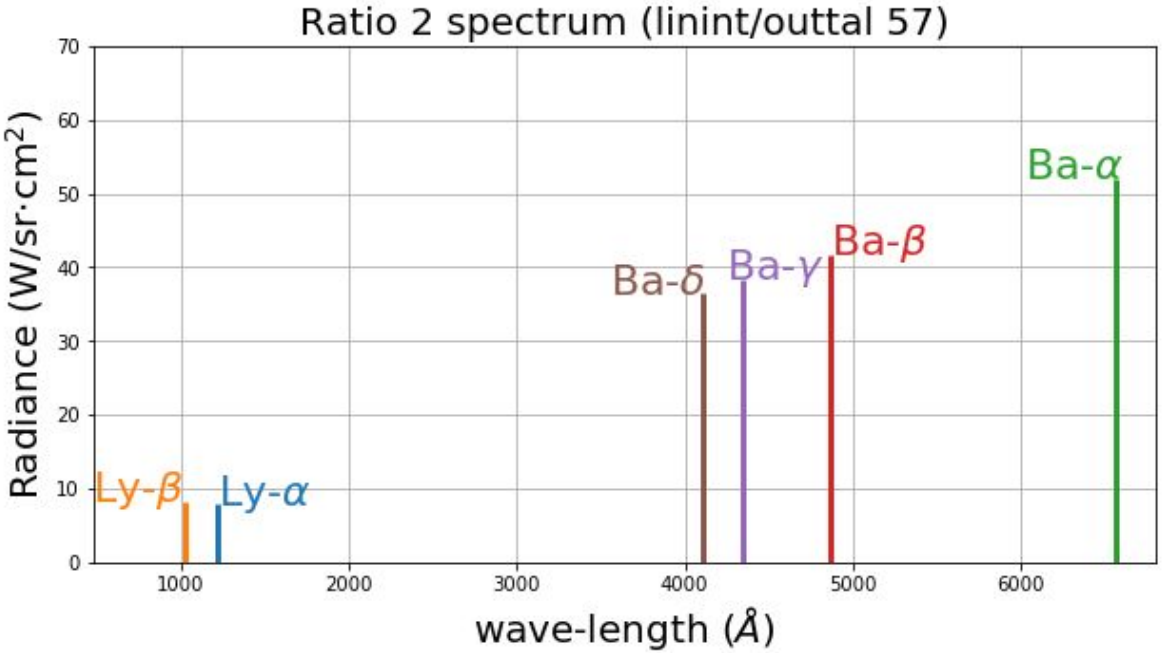
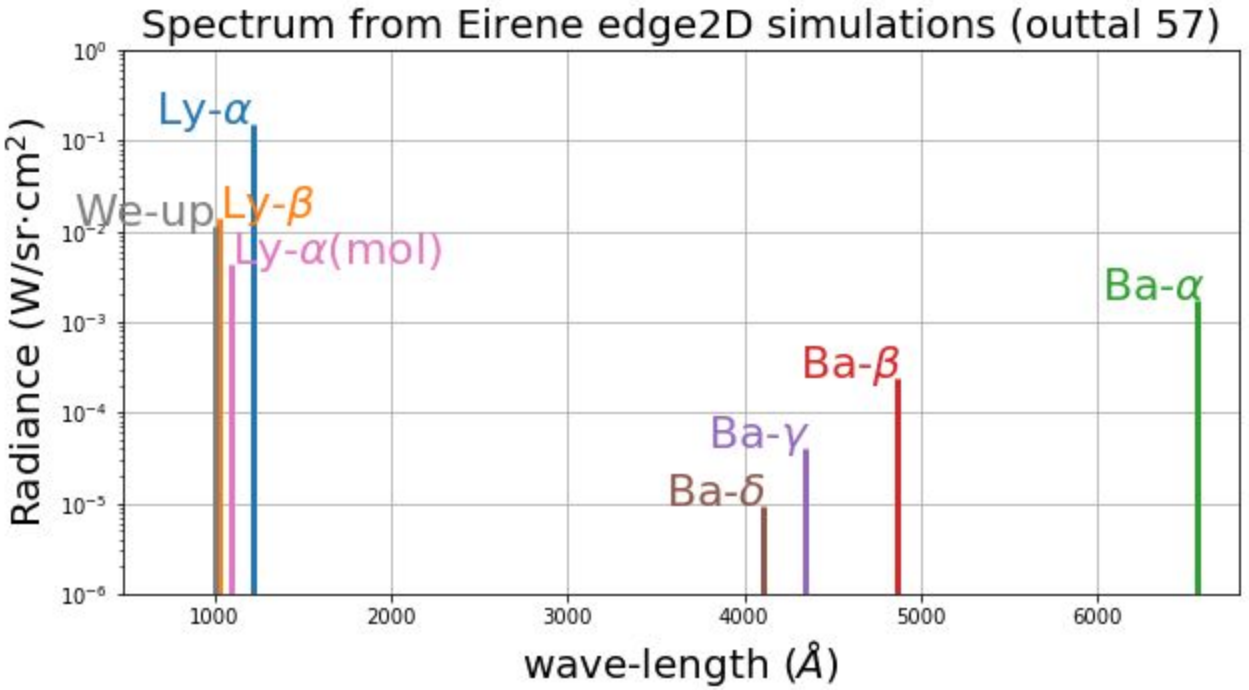


If H emiss provides radiance in eV

TallyViz/python3: spectrum (mol trans)

Line integration of outtally 57:



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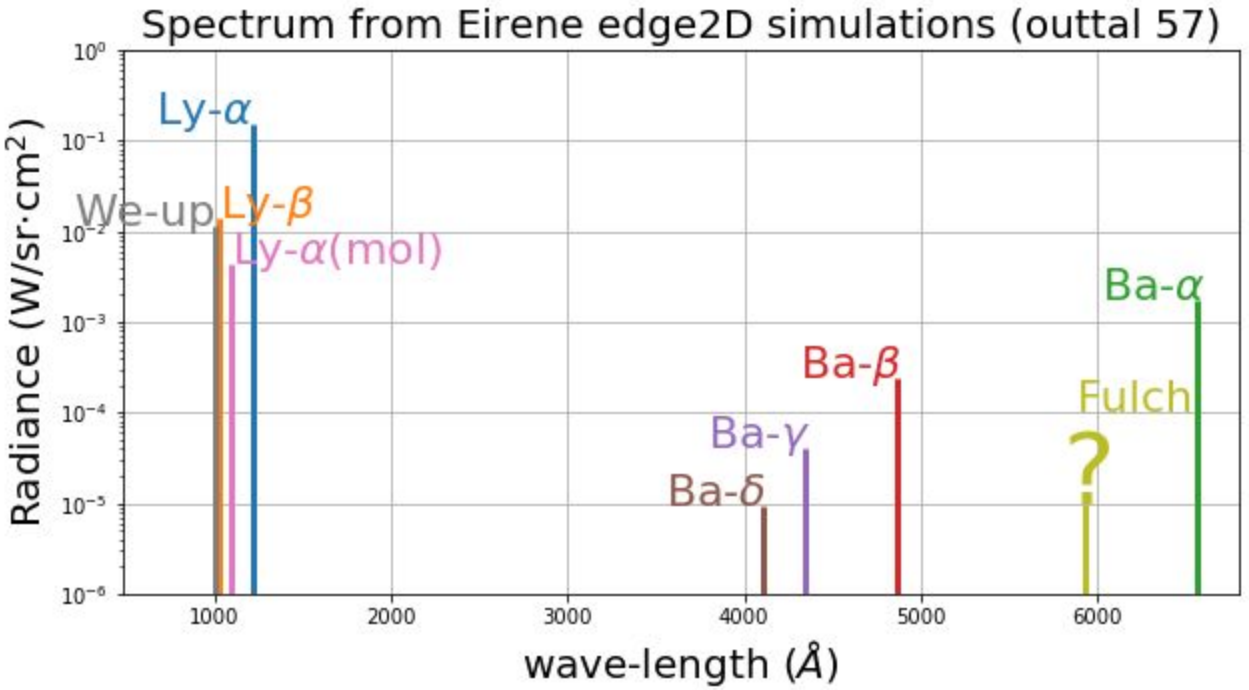

VTK: SOLPS-ITER