

pynucastro: Code Generation and Visualization for Nuclear Reaction Networks

Donald E. Willcox (LBNL), Adam Jacobs (MSU), Xinlong Li (SBU), and Michael Zingale (SBU)

Lawrence Berkeley National Laboratory (LBNL), Michigan State University (MSU), Stony Brook University (SBU)

Abstract

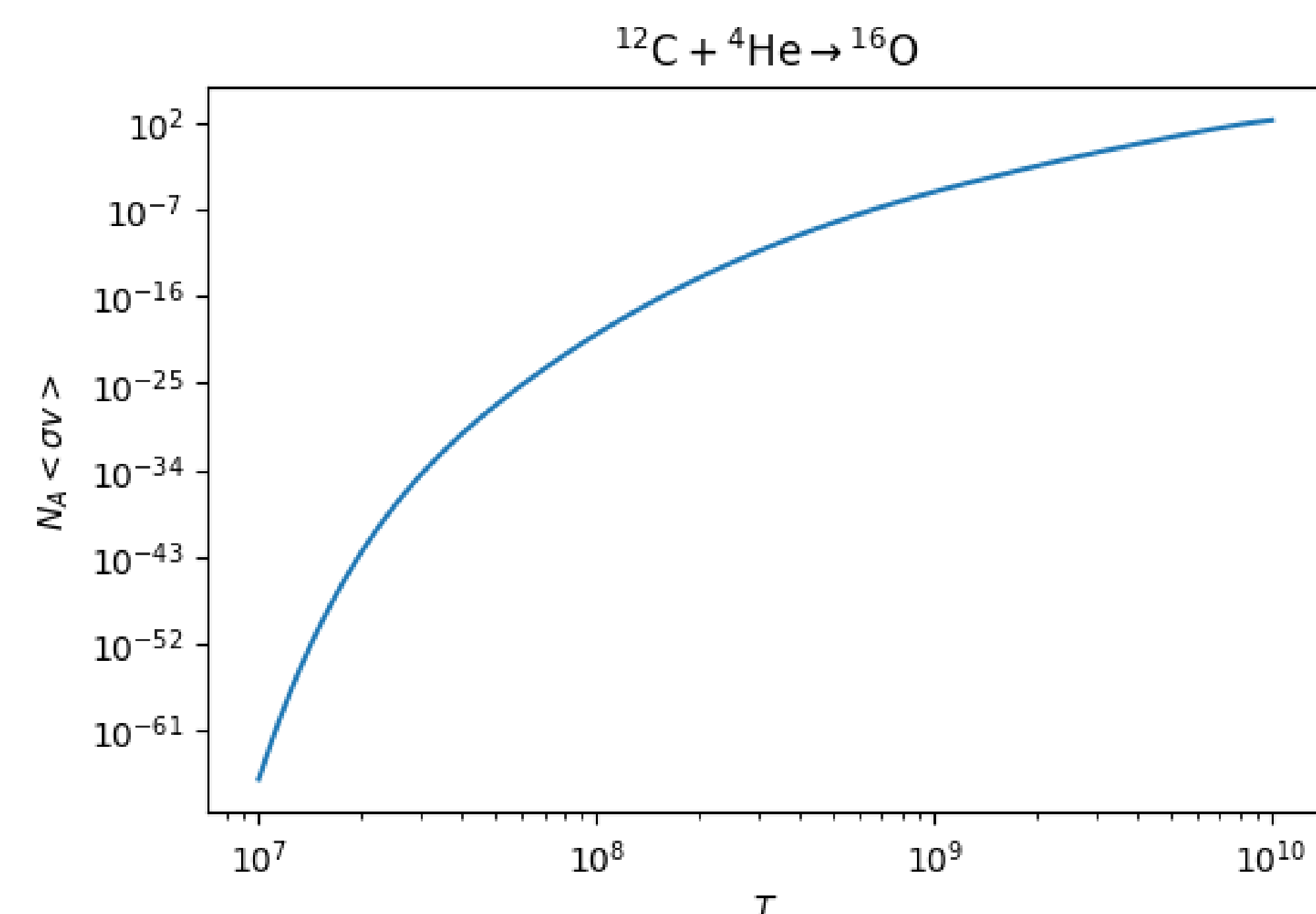
pynucastro is developed to meet both pedagogical and research needs in the field of nuclear astrophysics by providing a Python interface to nuclear reaction rate databases (including the JINA Reaclib nuclear reaction rate database). It is meant for both **interactive exploration** of reaction rates (through Jupyter notebooks) and for creating **reaction networks for simulation codes**.

Capabilities

- Supports Reaclib library snapshots [1]
- Supports weak rates [2] tabulated in $(T, \rho Y_e)$
- Visualizes connections between nuclei as a network graph
- Evaluates rates as a function of temperature
- Symbolically constructs the ODE right hand side and Jacobian
- Generates Python or Fortran code implementing the network

Working with Reaclib

pynucastro can interpret reaction rates parameterized in the standard Reaclib formats, storing each rate internally using the **Rate** class. **Rate** interprets the Reaclib format and knows how to evaluate the rate as a function of temperature.



Creating a Network

The **Library** class allows pynucastro to work easily with files containing multiple rates, including Reaclib snapshots. We use **Library** to obtain the CNO rates linking our desired nuclei in just a few lines of Python in the following Jupyter notebook:

```
%matplotlib inline
import pynucastro as pyna

mylibrary = pyna.rates.Library('20180201ReaclibV2.22')

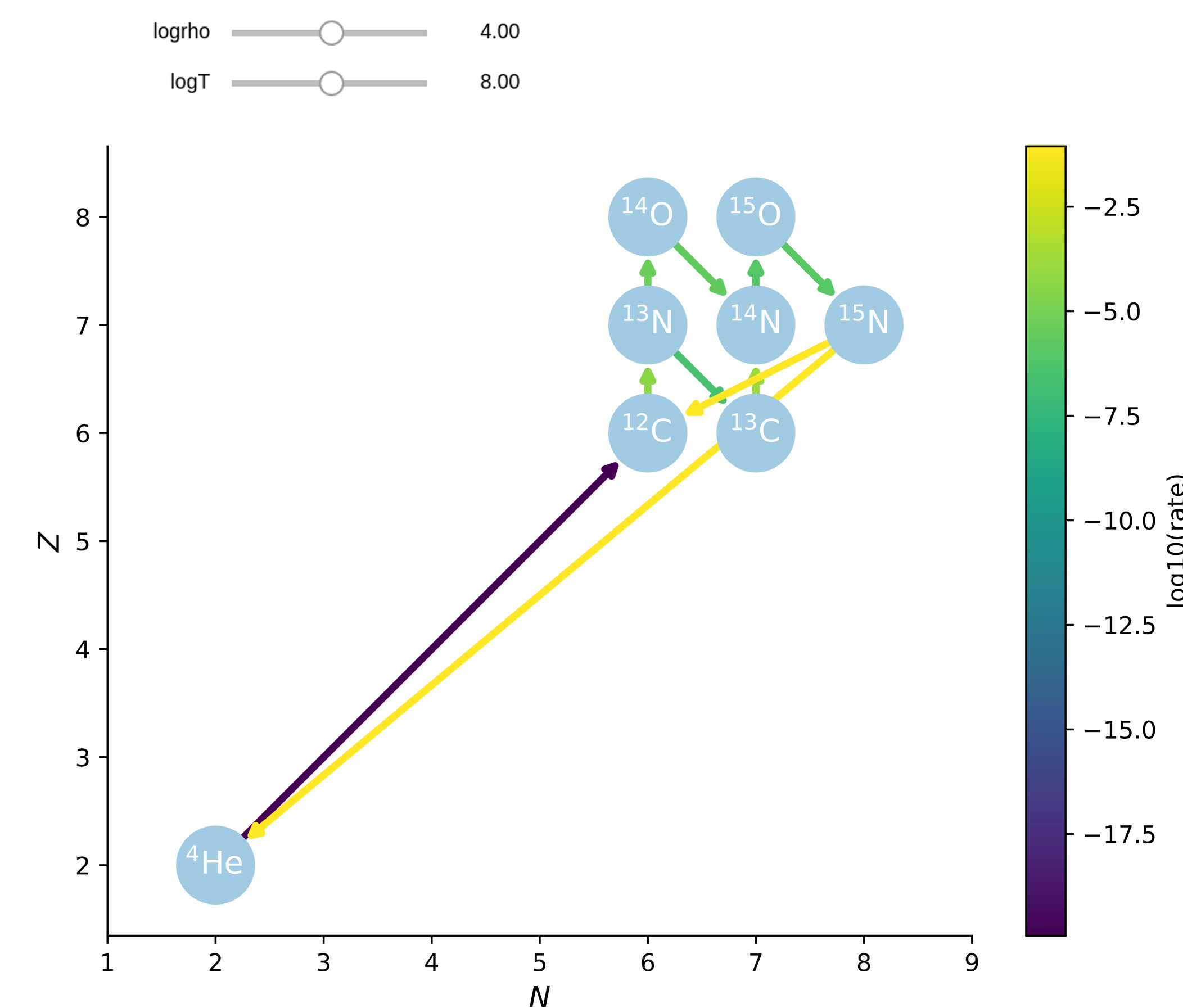
all_nuclei = ["p", "he4", "c12", "n13", "c13", "o14", "n14", "o15", "n15"]

cno_library = mylibrary.linking_nuclei(all_nuclei, with_reverse=False)

cno_network = pyna.networks.PythonNetwork(libraries=cno_library)
cno_network.write_network('network_module.py')

comp = pyna.Composition(cno_network.get_nuclei())
comp.set_solar_like()

re = pyna.Explorer(cno_network, comp)
re.explore()
```



Using the **Composition** and **Explorer** classes, we also construct an interactive graph of the network with the value of each rate indicated by its arrow color with variable density and temperature.

Python Code Generation

The **PythonNetwork** class generates Python code to calculate each rate as a function of temperature and the ODE right hand side. pynucastro includes a sample Python integrator using SciPy.

StarKiller Microphysics

The **StarKillerNetwork** class generates Fortran reaction network code for astrophysical simulations that use the StarKiller Microphysics repository [3].

- Right hand side and Jacobian with SymPy [4]
- Couples to a stellar equation of state
- Incorporates screening and thermal neutrinos
- Supports CUDA Fortran

This short Python script builds a ^{12}C burning network with tabulated weak $A = 23$ rates:

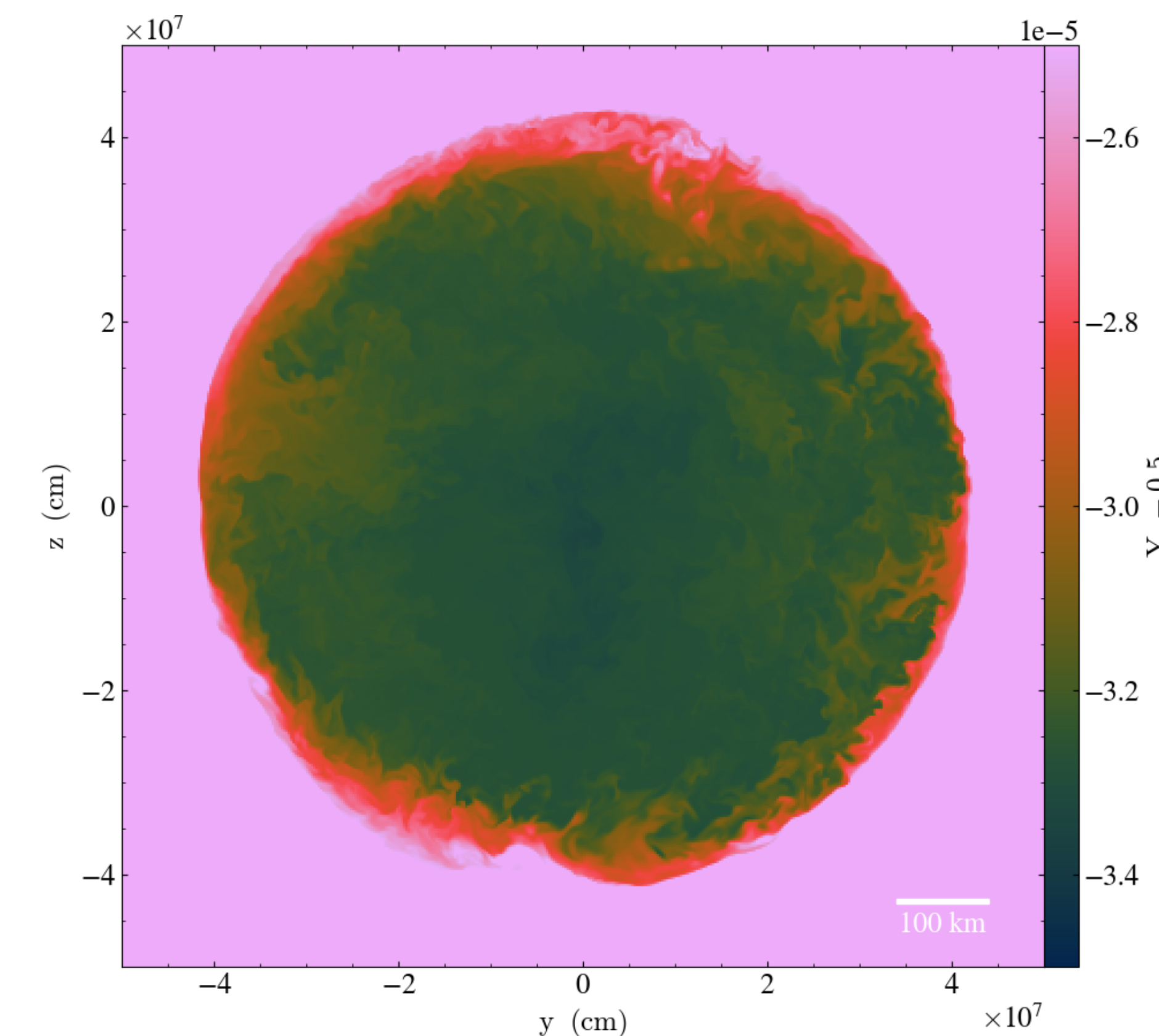
```
# C-burning with A=23 URCA rate module generator

from pynucastro.networks import StarKillerNetwork

files = ["c12-c12a-ne20-cf88",
        "c12-c12n-mg23-cf88",
        "c12-c12p-na23-cf88",
        "c12-ag-o16-nac2",
        "na23--ne23-toki",
        "ne23--na23-toki",
        "n--p-wc12"]

urca_net = StarKillerNetwork(files)
urca_net.write_network()
```

Electron fraction in a Maestro low-Mach hydrodynamics simulation of a 3-D convecting white dwarf core using the $A = 23$ Urca network:



Ongoing Development

- Implementing nuclear partition functions
- Expanding support for weak rate tabulations

Getting pynucastro

- pynucastro is freely available under the **BSD 3-Clause open source** license.
- For the companion **software paper**, see [5].
- Visit us on GitHub to **download** pynucastro or report **issues** and **request features**:

<https://github.com/pynucastro/pynucastro>

- For pynucastro **documentation** and examples, visit the pynucastro website:

<https://pynucastro.github.io/pynucastro>

Acknowledgements

This work was supported by DOE/Office of Nuclear Physics grant DE-FG02-87ER40317. This research used resources of the Oak Ridge Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

References

- [1] Richard H. Cyburt, A. Matthew Amthor, Ryan Ferguson, Zach Meisel, Karl Smith, et al. The JINA REACLIB Database: Its Recent Updates and Impact on Type-I X-ray Bursts. *The Astrophysical Journal Supplement Series*, 189(1):240, 2010.
- [2] Toshio Suzuki, Hiroshi Toki, and Ken'ichi Nomoto. Electron-capture and β -decay Rates for sd-Shell Nuclei in Stellar Environments Relevant to High-density O-Ne-Mg Cores. *The Astrophysical Journal*, 817(2):163, 2016.
- [3] M. Zingale, A. S. Almgren, M. G. Barrios Sazo, V. E. Beckner, J. B. Bell, et al. Meeting the Challenges of Modeling Astrophysical Thermonuclear Explosions: Castro, Maestro, and the AMReX Astrophysics Suite. *Journal of Physics: Conference Series*, 1031(1):012024, 2018.
- [4] Aaron Meurer, Christopher P. Smith, Mateusz Paprocki, Ondřej Čertík, Sergey B. Kirpichev, et al. SymPy: symbolic computing in Python. *PeerJ Computer Science*, 3:e103, January 2017.
- [5] D. E. Willcox and M. Zingale. pynucastro: an interface to nuclear reaction rates and code generator for reaction network equations. *Journal of Open Source Software*, 3(23):588, 2018.