The Journal of Open Source Software

pynucastro: an interface to nuclear reaction rates and code generator for reaction network equations

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DOI: 10.21105/joss.00588

Software

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Submitted: 15 February 2018
Published: 10 March 2018

Summary

pynucastro addresses two needs in the field of nuclear astrophysics: visual exploration of nuclear reaction rates or networks and automated code generation for integrating reaction network ODEs. pynucastro accomplishes this by interfacing with nuclear reaction rate parameterizations published by the JINA Reaclib project (Cyburt et al. 2010).

Interactive exploration is enabled by a set of classes that provide methods to visualize the temperature dependency of a rate, evaluate it at a particular temperature, and find the exponent, n, for a simple T^n parameterization. From a collection of rates, the flow between the nuclei can be visualized interactively using Jupyter widgets. These features help both with designing a network for a simulation as well as for teaching nuclear astrophysics in the classroom.

After selecting a set of rates for a given problem, pynucastro can construct a reaction network from those rates consisting of Python code to calculate the ODE right hand side. Generated Python right hand sides evolve species in the reaction network, and pynucastro includes a Python example integrating the CNO cycle for hydrogen burning.

pynucastro can also generate Fortran code implementing reaction networks, using SymPy (Meurer et al. 2017) to determine the system of ODEs comprising the network. From the symbolic expressions for the ODE right hand side, pynucastro also generates a routine to compute the analytic Jacobian matrix for implicit integration.

Fortran networks incorporate weak, intermediate, and strong reaction rate screening for the Reaclib rates (Graboske et al. 1973; Alastuey and Jancovici 1978; Itoh et al. 1979). These networks can also include selected weak reaction rate tabulations (Suzuki, Toki, and Nomoto 2016). To calculate energy generation in Fortran networks, pynucastro uses nuclear binding energies from the Atomic Mass Data Center (Huang et al. 2017; Wang et al. 2017) and the 2014 CODATA recommended values for the fundamental physical constants (Mohr, Newell, and Taylor 2016).

pynucastro is capable of generating two kinds of Fortran reaction networks. The first type is a standalone network with a driver program to integrate species and energy generation using the variable-order ODE integration package VODE (Brown, Byrne, and Hindmarsh 1989). This Fortran driver program is designed to be easy to use and can integrate reaction networks significantly faster than is possible for the generated Python networks.

Secondly, pynucastro can generate a Fortran network consisting of right hand side and Jacobian modules that evolve species, temperature, and energy generation for the StarKiller Microphysics code. Via StarKiller Microphysics, astrophysical simulation codes such as Castro (Almgren et al. 2010) and Maestro (Nonaka et al. 2010) can directly use pynucastro reaction networks. pynucastro includes a carbon burning network with tabulated

A = 23 Urca weak reactions currently used for studying white dwarf convection with Maestro (Zingale et al. 2017).

Future work will focus on implementing nuclear partition functions to compute reverse reaction rates in the Reaclib library (Rauscher and Thielemann 2000; Rauscher 2003). It is also in some cases necessary to compute reverse reaction rates using detailed balance with a consistent nuclear mass model instead of using the parameterized reverse reaction rates in Reaclib (Lippuner and Roberts 2017). Additionally, work is ongoing to port the networks generated for StarKiller Microphysics to CUDA Fortran to support parallel reaction network integration on GPU systems (Zingale et al. 2017). We intend to implement this port directly into the pynucastro-generated networks.

This work was supported by DOE/Office of Nuclear Physics grant DE-FG02-87ER40317.

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