pynucastro 2.0: New Features and Implementation of a Python Library for Nuclear Astrophysics

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Introduction

- `pynucastro` is an open-source python library with the main purpose of providing visualization of rates and nuclei properties, given a particular set of rates or the nuclei involved in the reaction network of interest, and its composition.

- In addition, `pynucastro` provides an interface of the first-order stiff differential system of equations provided by the selected reaction network, to C++ and python. The C++ interface also provides GPU offloading techniques making it suitable for Hydro+Reactive sources calculations.

$$\frac{dY_i}{dt} = \rho N_A \langle \sigma v \rangle_{ijk\ldots} Y_i Y_j Y_k \cdots$$

- In this new version of `pynucastro`, we have implemented high temperature burning support for $\sim 10^9\,\mathrm{K}$ environments, including the nuclear partition function in baryonic inverse rates calculations, the nuclear statistical equilibrium (NSE) composition determination, and implementations for classical electron screening.

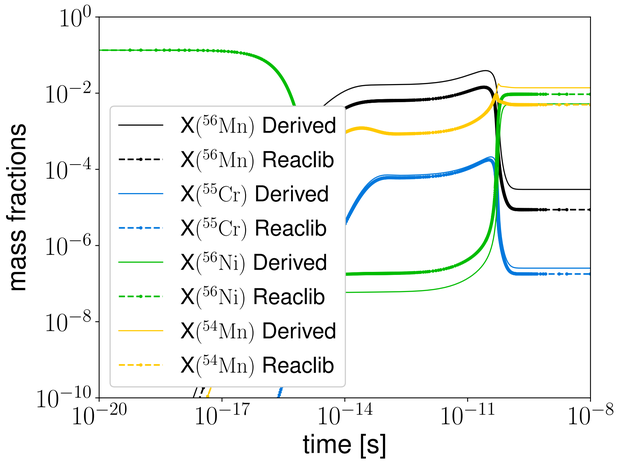
Inverse Rates

- In `pynucastro` we use the REACLIB database from which all the important rates are selected. In pynucastro, for each baryonic forward reaction (exothermic), we compute its inverse rate (endothermic) by the use of detailed balance:

$$\begin{aligned} N_a^{p-1} \langle \sigma v \rangle_{B_1,B_2,\cdots,B_p} = & \left(\frac{1}{N_a}\right)^{r-p} \frac{(2J_{C_1}+1)\cdots(2J_{C_r}+1)}{(2J_{B_1}+1)\cdots(2J_{B_p}+1)} \\ & \times \left(\frac{A_{C_1}\cdots A_{C_r}}{A_{B_1}\cdots A_{B_p}}\right)^{3/2} \left(\frac{m_u}{2\pi\hbar^2}\right)^{\frac{3}{2}(r-p)} T^{\frac{3}{2}(r-p)} \\ & \times \frac{G_{C_1}\cdots G_{C_r}(T)}{G_{B_1}\cdots G_{B_p}(T)} \frac{\prod_{B_i} c_{B_i}!}{\prod_{C_i} c_{C_i}!} \mathrm{e}^{-Q/T} \\ & \times N_a^{r-1} \langle \sigma v \rangle_{C_1,C_2,\cdots,C_r} \end{aligned}$$

where r and p are the number of reactants and products respectively, G_{N_i} are the nuclear partition functions of the nuclei N_i and the remaining quantities are just temperature independent quantities.

- The comparison between REACLIB inverse rates and the inverse rates effects obtained by pynucastro is depicted as follows:



Coulomb Screening

- Under the assumption of the linear mixing rule (Dewitt et.al 1973), the classical enhancement factor of the reaction

$$C_1 + C_2 + \cdots + C_r \rightarrow O^* \rightarrow B_1 + B_2 + \cdots + B_p$$

- Is given by

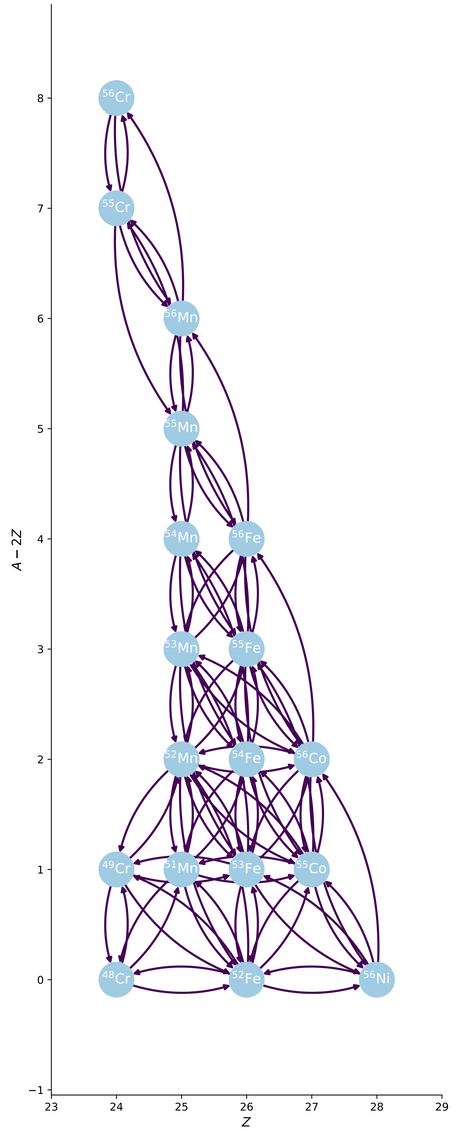
$$\begin{aligned} f^{\mathrm{cl}}_{C_1\cdots C_r \rightarrow O^*} = \exp\Bigg[& \frac{\mu^C(Z_{C_1}) + \cdots + \mu^C(Z_{C_r})}{T} \\ & - \frac{\mu^C(Z_{C_1} + \cdots Z_{C_r})}{T} \Bigg] \end{aligned}$$

where $\mu^C(Z_{C_i})$ is the free-energy excess per particle of the one component plasma (OCP) made of a negative charge background and ions of atomic number Z_{C_i}.

- Currently, pynucastro have support for two screening routines for $\mu^C(Z_{C_i})$ (Potekhin 1998, Chugunov 2009). However, there are plans to include more routines, including quantum effects (Kushnir 2020, Chugunov 2021).

Writing a Network

- As an example of `pynucastro`, we can write the following network:



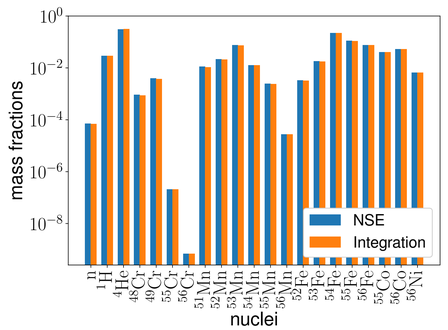
- The current network is composed by succesive alpha-capture reactions, weak-reactions and neutron captures near the iron group.

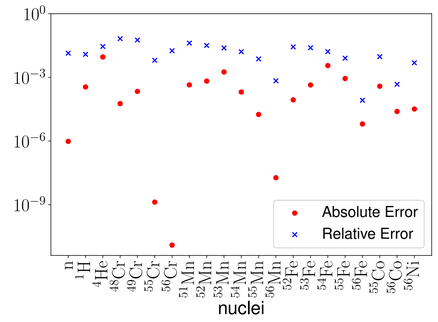
NSE Composition

- `pynucastro` provides a method to compute the mass fraction composition of a network once the nuclear statistical equilibrium is reached:

$$\begin{aligned} X_i = & \frac{m_i}{\rho}(2J_i+1)G(T)\left(\frac{m_i T}{2\pi\hbar^2}\right)^{3/2} \\ & \times \exp\left[\frac{Z_i\mu_p^{\mathrm{id}} + N_i\mu_n^{\mathrm{id}} + Q_i}{T}\right. \\ & \left. + \frac{Z_i\mu_p^C - \mu_i^C}{T}\right] \end{aligned}$$

- The difference between computing the mass fraction NSE composition and integrating the network can be seen as follows:





- https://github.com/pynucastro/pynucastro

New contributions are welcome!

This work is supported by the DOE/Office of Nuclear Physics grant DE-FG02-87ER40317; by the Chilean Government ANID grant 56160017 and the U.S Department of State, Fulbright grant PS00280789.