UTILIZING NUCLEOSYNTHETIC MODELS AND JUPYTER NOTEBOOKS TO CONSTRAIN THE BUILDING BLOCKS OF THE SOLAR SYSTEM.
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Introduction: The stellar building blocks of the Solar System can be constrained using the nucleosynthetic isotopic composition of meteorites. In an accompanying study [1], high precision nucleosynthetic isotope variations are synthesized with new nucleosynthesis models, where correlations between interelement isotopic variations are used to infer stellar building blocks. Based on our findings, the likely nucleosynthetic source for the Solar System's supply of ^{48}Ca and other neutron-rich iron-group isotopes, is a white dwarf star. We use the term NRLEE (Neutron- Rich Low-Entropy matter Ejector) to denote this astrophysical site generically. The nucleosynthetic pathways in a NRLEE are investigated using nuclear reaction network calculations generated in C/C++ with NucNet Tools [see accompanying abstract 2].

Despite the utility of nucleosynthesis calculations, such as those from NucNet Tools, in constraining the nature of the Solar System's building blocks, these calculations can seem inaccessible for the non-specialized scientist. Here, we show how we make results from NucNet Tools more accessible by using Python's Jupyter notebook user interface. Through the use of this interface, code can be stored, and figures plotted inline along with accompanying text and images. This allows for an interactive visual tool that scientists from a wide range backgrounds and expertise can access. By making NucNet Tools results more accessible to a broader part of the community, we expand the tools available to isotope cosmochemists investigating the building blocks and evolution of the Solar System.

Jupyter: Jupyter is an open-source computational notebook that can be used to present and work with data in a human-readable format. These notebooks allow for the combination of software code, text, and multimedia images with editing enabled. Jupyter notebooks can also be used to seamlessly import and download necessary data packages that could otherwise require multiple steps to attain. Studies have shown Jupyter to be the computational notebook of choice for students and professionals alike due to its ability to provide open science [3, 4]. It has been used in different fields as a way to visualize the more difficult aspects of science and allow for the reproducibility of the analysis and key plots [5, 6].

Tracing Isotope Abundances Using NRLEE Simulations: To provide the community with reproducible, open science, we present a set of cosmochemistry notebooks focused on nucleosynthesis during NRLEEs (e.g., thermonuclear supernovae; **Fig. 1.**) from [1, 2]. The notebooks are an easy to use, publicly accessible tool that can be manipulated to demonstrate and analyze nucleosynthetic processes and the resulting isotopic abundances based off calculations used in [2]. The notebooks import, download, and run python scripts analyzing the NucNet tools output for the user, and provide example calculations. The notebooks also allow for modification through the editing of command lines, where example isotopes can be replaced or parameters can be adjusted to alter the resulting plots and calculations.
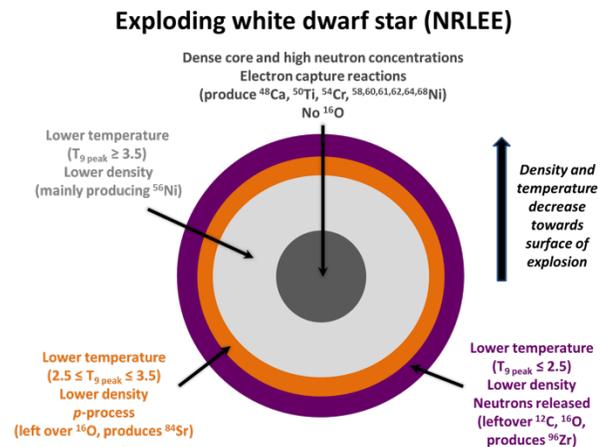

Fig. 1. Schematic nucleosynthetic structure of the ejecta from an exploding white dwarf star (a NRLEE).

The nucleosynthesis model of an NRLEE used in this notebook centers on a C-O white dwarf star in the stages leading up to, during, and immediately after a thermonuclear supernova explosion. The calculation sets up a schematic representation of the explosion, following the complex mixing and nuclide production in different layers of the star. The code can be used to match and compare observed meteorite isotope abundances to their potential nucleosynthetic sources and analyze the context of the coupling of neutron-rich species and its contribution to presolar grain mineralogy.

Jupyter Notebook Examples: These notebooks can be used to plot the mass fractions of different isotopes with time during various burning stages and in distinct areas of the star, providing a key visual for students learning about cosmochemistry. An example being the

mass fraction of isotopes during He-burning, which clearly shows the exhaustion and capture of helium by carbon to produce oxygen over time as shown in **Fig. 2**.
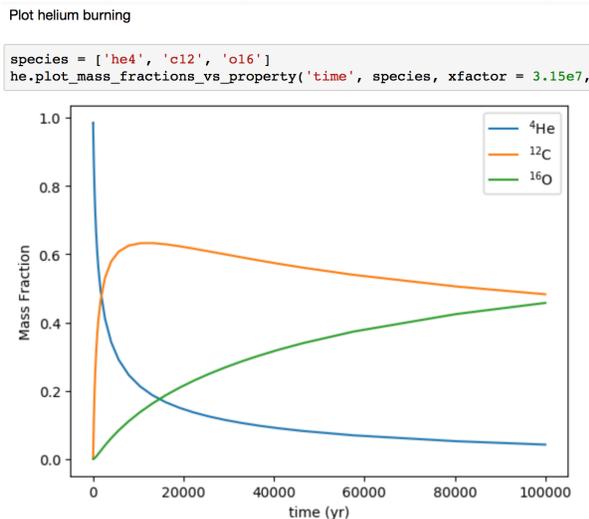
Plot helium burning

```
species = ['he4', 'c12', 'o16']
he.plot_mass_fractions_vs_property('time', species, xfactor = 3.15e7,
```


Fig. 2. He-burning excerpt from the Jupyter Notebook.

Aside from different burning stages, nucleosynthetic processes in the inner and outer layers of the star (shown in **Fig.1**) can be plotted. In **Fig. 3**, the density is fixed, and temperature varies in order to show carbon and oxygen mass fractions in the outer layers of the star for different temperatures. The exhaustion of ^{12}C for temperatures greater than 1.8 million Kelvin is shown. In **Fig. 4**, the peak temperature is fixed and the mass fractions of ^{48}Ca, ^{50}Ti, ^{54}Cr, ^{56}Ni, and ^{56}Fe are plotted against density in the interior of the star. Using the notebook, the *s*-process can also be demonstrated by plotting resulting abundances with constant neutron density averaging over all exposures.
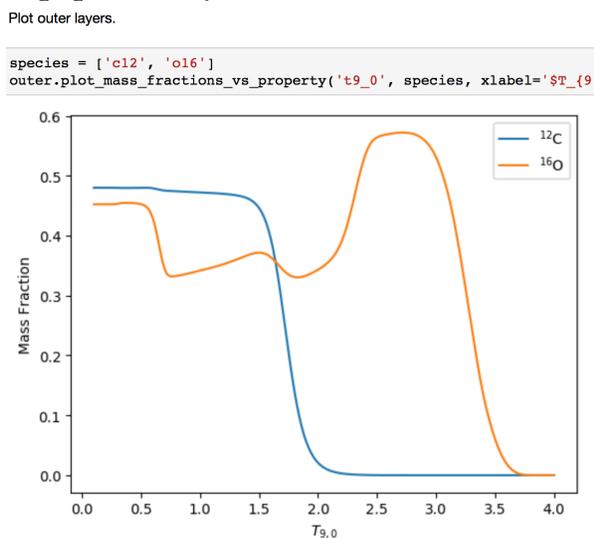
Plot outer layers.

```
species = ['c12', 'o16']
outer.plot_mass_fractions_vs_property('t9_0', species, xlabel='$T_{9
```


Fig. 3. C/O burning in the outer layers. $T_{9,0}$ is a parameter that represents the peak temperature.

Plot inner layers.

```
species = ['ca48', 'ti50', 'cr54', 'ni56', 'fe56']
inner.plot_mass_fractions_vs_property('rho_0', species, xlabel='$\\r
```
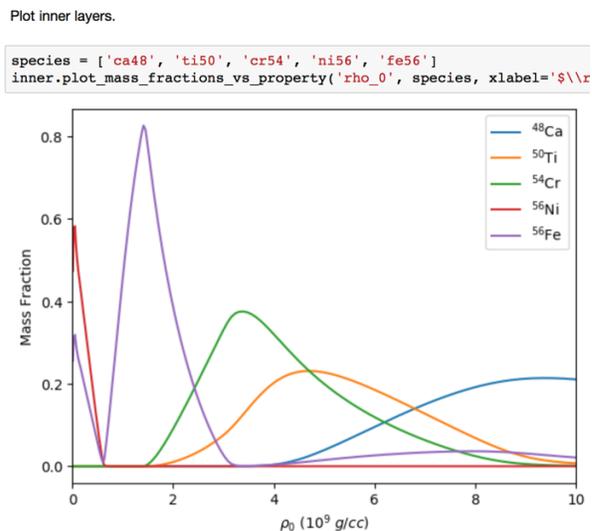

Fig. 4. Isotope mass fractions in the inner zone of the star. The variable ρ represents density.

Through the use of visuals and interactive calculations, isotope cosmochemists and students alike will be able to more easily manipulate and utilize NucNet Tools output to better understand the origin of isotope variations observed in meteorites.

References: [1] Bermingham, K. R. et al. (2021) LPSC LII [2] Meyer, B. S. et al. (2021) LPSC LII [3] Perkel J. M. (2018). *Nature 563*, 145-146. [4] Randles B. M. et al. (2017). *2017 ACM/IEEE JCDL*. [5] Rosenthal S. B. et al. (2017). *Bioinformatics, 34(1),* 126-128. [6] Loizides F. (2016*).* Players, agents and agendas; *Proceedings of the 20th International Conference on Electronic Publishing,* p. 89.