UNIVERSITY OF CALGARY

# SiRop Manual

## A User's Guide to Using the r-process code SiRop

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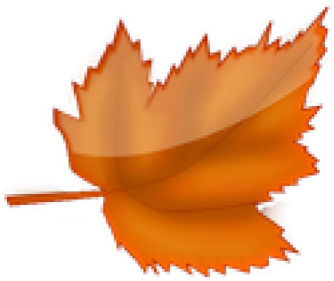

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## PREFACE

This document is meant to provide a starting place for those interested in using SiRop for running r-process simulations. SiRop is an evolution of an earlier r-process code which was developed specifically to perform sensitivity studies. In other words, we wanted a program that we could use to run automated or “script-like” execution of code. This involved a complete re-work of the user interface an addition of code to perform automated queueing, execution and analysis of r-process simulations. This manual will, as a result, be focused on the modules for sensitivity studies, but will also include a description of how to use the code for r-process simulations in general. Supplementary descriptions for the behavior of this program can be found in the two papers Kostka et al. 2014a and Kostka et al. 2014b along with the r-Java 2.0 manual available at www.quarknova.ca/rJava since it and SiRop are built on the same underlying code base.

## INTRODUCTION

The r-process, or rapid neutron capture process, is the astrophysical process which is responsible for producing some of the elements we see in the Galaxy today. Due to the shape of the nuclear binding energy curve and the high coulomb repulsion of heavy nuclei elements heavier than iron or nickel cannot be produced through regular burning phases inside of a star. Elements beyond the iron group are then assumed to be mainly produced by neutron capture processes. The r-process is one such nucleosynthesis mechanism which involves nuclear reactions in some sort of neutron rich environment where isotopes are converted into heavier and heavier isotopes through a sequence of neutron captures and beta-decays. This means the isotopes involved in simulating the r-process are frequently unmeasured and in many instances theoretical calculations must be used to supplement the existing nuclear (see Figure 1). For this reason it is of interest both on purely theoretical grounds and for planning of nuclear experiments to understand what isotopes are most important to the r-process.

Nuclear sensitivity studies are a way of understanding the role of individual isotopes and their physical characteristics like mass or half-live. When we perform a sensitivity study what we're doing is taking a set of nuclear inputs, running a simulation with these parameters and then comparing these base results to the results of simulations where we have changed a small number of inputs. Statistical analysis of this can then provide a quantitative value to the changes to the final results of a simulation of an r-process site. We could, for example, vary the masses of all unmeasured isotopes that are accessible to an experimental facility to identify more important candidates for measurement (at least most important to the r-process). Alternatively, currently measured properties of isotopes could be varied within their experimental uncertainty to test whether current measurement uncertainties are low enough to provide no measureable change to the r-process simulated results. SiRop is designed to assist in answering these questions and has a flexible design and user interface which allows for a large range studies to be performed.

Simulating this process in various different astrophysical environments requires solving differential equations numerically and this is the heart of what an r-process code like SiRop does. The details are beyond the scope of this manual and is beyond what a user needs to know, but there are a couple main features to keep in mind when running SiRop. The ordinary differential equation (ODE) SiRop solves can be written simply by listing all of the nuclear processes which transmute an isotope as follows

$$\frac{dY_i}{dt} = \sum processes\ which\ create\ Y_i - \sum processes\ which\ destroy\ Y_i\,,$$

where $Y_i$ is the abundance (or total number) of a single isotopic species. For example, a neutron capture process of iron-56 "destroys" iron-56 and creates iron-57 and so the reaction rate is

added to two pairs of coupled isotopic rate of change. So if we were only considering neutron capture, neutron photo-dissociation and beta-decay reactions the ODE for a single isotope, say tin-132 would look like the following

$$\frac{dY_{132Sn}}{dt} = n_n\langle\sigma v\rangle Y_{131Sn} + \lambda_\gamma Y_{133Sn} + \frac{\ln 2}{T_{1/2}} Y_{132In} - n_n\langle\sigma v\rangle Y_{132Sn} - \lambda_\gamma Y_{132Sn} - \frac{\ln 2}{T_{1/2}} Y_{132Sn}$$

where $n_n$ is the neutron number density, $\langle\sigma v\rangle$ is the thermally averaged cross-section, $\lambda_\gamma$ is the neutron photo-dissociation rate, $T_{1/2}$ is the beta-decay half-life and $Y_X$ is the abundance of isotope X as indicated. Each nuclear property is that of the multiplied isotope abundance, so, for example, in the term $n_n\langle\sigma v\rangle Y_{131Sn}$ , $\langle\sigma v\rangle$ is the thermally averaged cross-section of tin-131. (For a more thorough discussion see, for example, the overview provided in Hix and Thielemann 1999.) The reason for writing this out explicitly is to highlight a critical assumption used in SiRop where each nuclear quantity is assumed to be a true constant taken from a lookup table. In reality, for any parameter which has been determined theoretically using some form of nuclear model the reality is that these values are functions of the parameters used in the nuclear model. So for example, if we computed the half-lives using Fermi's Golden rule, we could right the decay rate as a function of the matrix elements, nuclear charge, and nuclear decay energy $\lambda_\beta(W_{np}, Z, Q_\beta)$ but any modification to the underlying parameters (e.g. mass) in a sensitivity study would not capture the change to the decay rate which should, in principle, be accounted for. Ideally, a code would encapsulate a model for all aspects of the r-process and include a full astrophysical explosion model and a full quantum mechanical model for nuclear parameters. Such a code would be an enormous undertaking, to say the least.

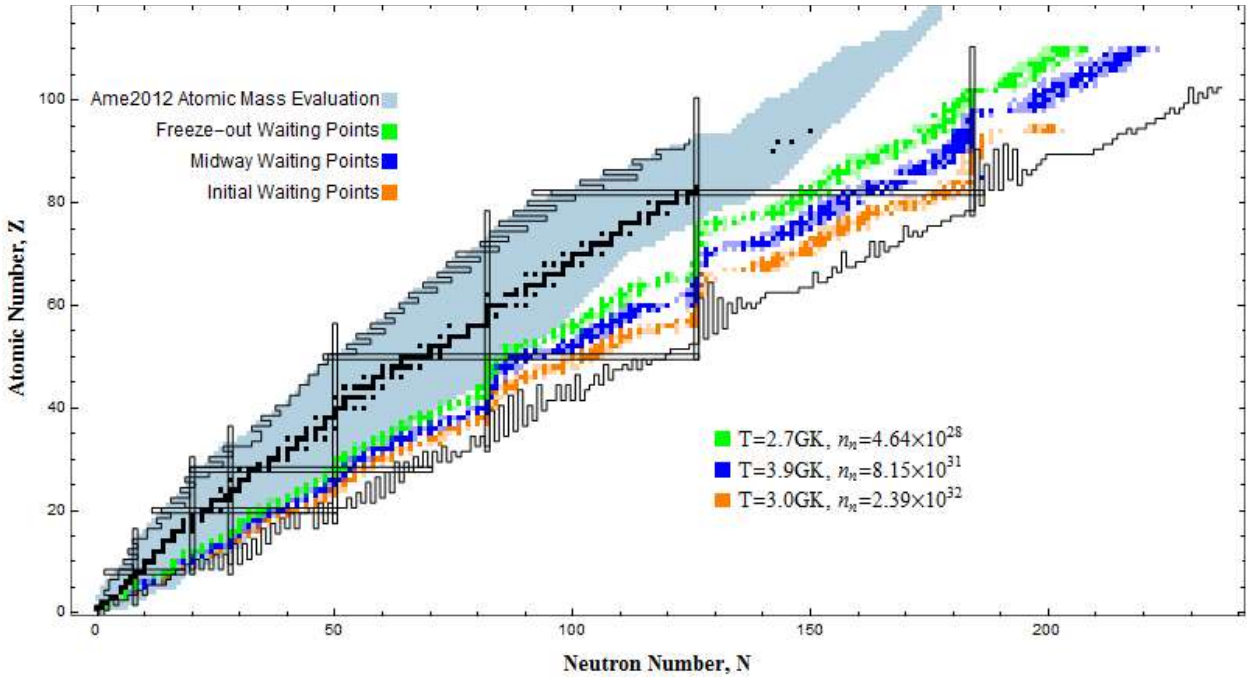


**Figure 1 Chart of nuclides displaying (in blue) the isotopes with measured masses as indicated in the 2012 Atomic Mass Evaluation along with theoretical r-process paths (in green, blue and orange). The black squares indicate stable isotopes and the naturally occurring actinides. The jagged black lines are the proton drip line (experimental) and the neutron drip (HFB21 theoretical) and the black rectangles indicate the nuclear magic numbers.**

## SIROP BASICS

SiRop provides the user with a Graphical User Interface (GUI) as opposed to a command line interface. In addition to providing a more user-friendly experience, this allows the code to provide immediate graphical feedback during execution of the code. The program groups different functionality into different modules available as different tabs or pages in the program (each can be opened as its own window which is useful in multi-monitor environments). The modules available are as follows:

**Desktop**: Home page, provides access to other modules.
**Code**: Holds parameters for running the code (e.g. initial density and temperature).
**Data**: Table of all nuclear inputs. Allows for importing and single cell editing.
**Chart**: Allows user to create useful graphs which are updated as code runs.
**Sensitivity**: Allows for setting up complex sensitivity studies.
**3D**: Presents a 3D real-time graph of the abundances on a chart of nuclides like visualization.
**Messages**: Displays messages during code execution and other information.
**R-Path**: Uses input nuclear parameters to explore the r-process path.

In addition to the modules, the program has a top and bottom ribbon which offers quick access to the different modules at the top of the window, includes a button for un-docking the individual modules into their own windows (top right) and in the bottom left provides a progress bar which indicates the execution state of the program along with an “x” icon which can be used to terminate in-progress dynamic r-process simulations.

### DESKTOP

The Desktop page is displayed after the program has finished loading after being opened. The Desktop lists all modules which can be opened from the Desktop page or from the top bar of the program. These icons can be attached (by dragging and dropping individual icons from the desktop page) to the top hot-bar for easy access from other pages in the application (see Figure 2 for a screenshot). In order to execute an r-process simulation (after setting up all the initial conditions) the Calculate command (orange maple leaf) can be pressed. Additionally, the state of the program can be saved as projects. This can be done by pressing the Save or Save As icons. This allows you to setup a complex set of parameters and perhaps defer execution until later or save results in the program for re-opening later. Any saved projects should appear in the Recent Projects section of the desktop, but can also be found at the location you saved the project to using the Open button. (The program cannot be saved mid-execution and any running calculations must be terminated before saving).


**Figure 2 SiRop Desktop screen where from which the different program modules can be accessed.**

## CODE

The Code module exposes different methods for computing nuclear abundances and all of the relevant parameters (with the exception of the values for the nuclear inputs). The left hand panel contains a queue of Operations or calculations to be chained during execution of the code. (This is mainly to allow for nuclear statistical equilibrium (NSE) to be used as an initial condition.) See Figure 3 for a screenshot. The options here are:

**r-Process**: Sets up the initial conditions for a dynamic r-process calculation.
**NSE**: Runs a (static) calculation to determine the abundances using the equations for nuclear statistical equilibrium. This can be executed on its own as a stand-alone calculation or it can be used as initial conditions for an r-process calculation by listing it immediately before an r-process calculation in the Operations sub-panel.
**Fission**: Calculates the fission yields as they are calculated in the code when full fission is selected. Uses fission barrier widths and heights along with a neutron energy to calculate the probability distribution following fission. See the r-Java 2.0 manual for more details (available at www.quarknova.ca) or the Kostka et al. 2014b paper on r-Java 2.0.
**Reset**: This is executed once at the beginning of the Calculate command by default and copies the initial mass fractions listed in the data table to the active mass fractions to be

used as initial conditions (i.e. set the initial seed nuclei). Normal usage of the code won't normally require this to be added manually.

**Waiting Point Rates**: Calculates and displays to the message module calculated results for the r-process path calculated based on the rates instead of the classical waiting point approximation (see later section for more details).

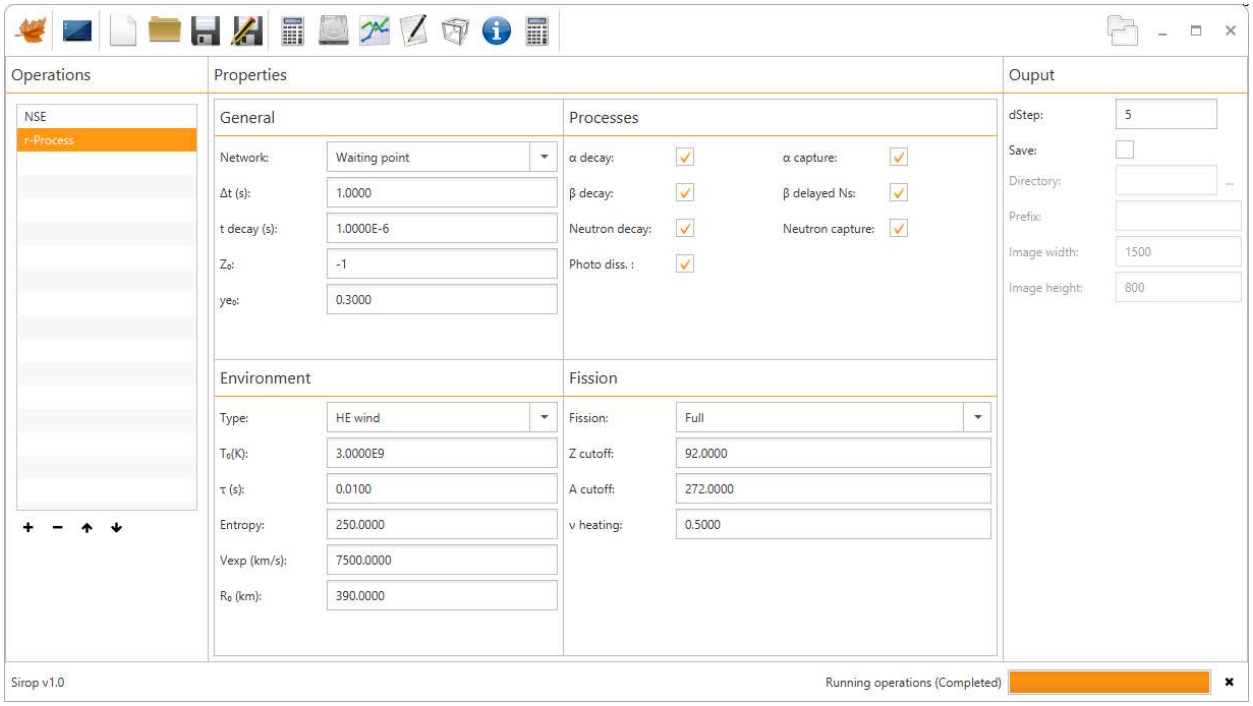


**Figure 3 Code module where the different parameters can be set for running the different calculations and simulations available in SiRop.**

These different calculations can be added to the Operations queue by clicking on the plus icon at the bottom of the window on the left. Similarly, operations added can be removed by selecting them (by clicking on them with the cursor) and pressing the minus button. The order of operations can be changed by selecting an added operation and pressing the up or down arrows.

The main (central) portion of the window presents different options based on the selected Operation. The r-Process operation options include temperature and density evolution parameters, lists of nuclear reactions to include, fission parameters and the option to be run using the full rate equation or using the Waiting Point Approximation (WPA). For NSE operation the options are density, temperature and electron fraction. The Fission operation lists standard channel I and II barrier heights and widths in addition to incident neutron energy. The Reset operation has no options. The Waiting Point Rates operation requires temperature, neutron number density and elemental bounds (minimum and maximum Z). In most cases the default

values are what you might want to try and start with until you're more familiar with the program.

The right hand panel has a few options relevant to dynamic calculations. The dStep option controls the number of steps in between GUI update events which refresh the charts with current data from the simulation. The save checkbox indicates whether the data should be saved to a directory in files to catalogue the evolution of the simulation data. When enabled, the data will be output to the specified directory with the supplied prefix and images will be generated at the specified size. The program will output these files (if enabled) at every update step.

## DATA

All nuclear inputs are summarized in this (large) table of values. By default, no data exists and all relevant data must be imported. By default, however, some preset values can be imported. These values include the masses, neutron cross sections and photo-dissociation rates from the HFB21 mass model in addition to the neutron induced fission rates calculated using the HFB14 mass model (available at www.astro.ulb.ac.be/bruslib) and the beta-decay half-lives and beta-delayed neutron emission probabilities calculated using the FRDM mass model (see Möller et al. 2003). If custom data is to be imported, each category must be imported from a file individually starting with a file containing all isotopes to be listed in the network. Each category can be imported by right clicking the table header (grouped by color) and clicking import in the context menu which appears. A wizard with a preview of the results of the importer will appear.

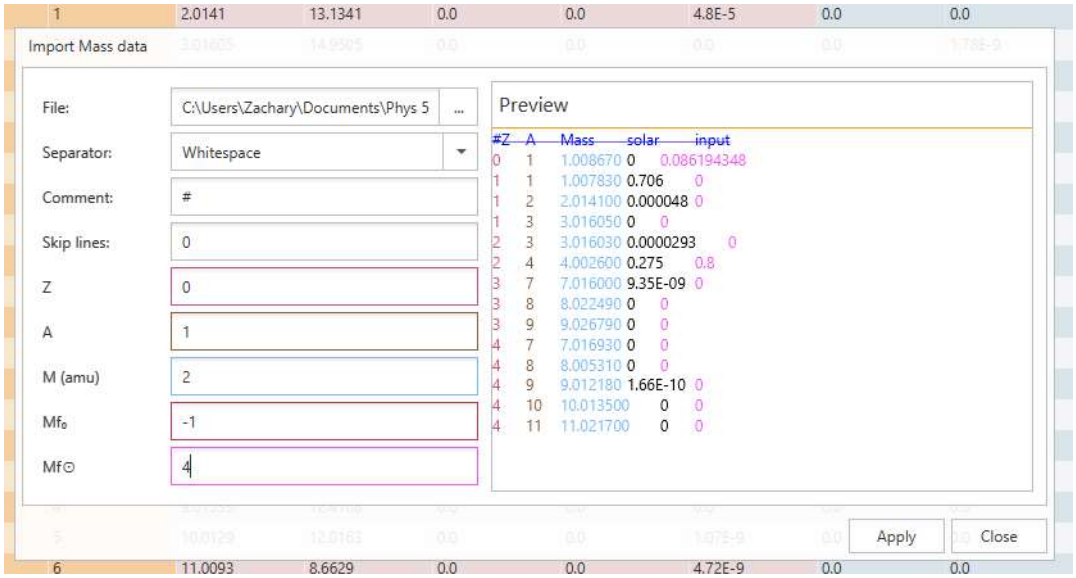


**Figure 4 Import wizard which opens a file and has partially selected columns of a sample data file shown.**

The importer (and data file in turn) requires text based tabular data organized in rows. In each category, the atomic number (Z) and atomic mass (A) must be included. Each category requires the user to specify a file to parse, the separating characters (spaces, tabs, commas, or generic whitespace), any comment characters (which must be at the beginning of a line) and any number of lines to skip. After these options, the columns of the required data must be specified (the column indexing scheme is zero based so 0 is column 1) where a value of -1 indicates that the column will be skipped during this import (except Z and A MUST be provided). This allows for data in one category in the code could be imported from multiple files. After entering a column number the preview pane should highlight the column in the same colour outlining column input box. A screenshot of a partially complete mass import can be seen in Figure 4.

The temperature dependent cross-sections and rates follow a similar import process, but due to the requirement for indicating the temperature grid points where the values were calculated the import process is slightly more complicated. The file these values are being imported from needs a row which indicates the temperatures which begins with “T9” and has all the temperatures (these temperatures must be given in units of GK). This row must be indicated to the importer and the first column of rate/cross-section data must be listed. An example of a valid text file format is in Table 1. If you are only interested in importing a single property (for e.g. half-lives) then the default values can be exported and re-imported or the default values can be simply overwritten by importing the values after a “Reset” to the default values.

| | | | | |
|---|---|---|---|---|
| T9 | 0.1 | 1 | 10 | |
| #Z | A | | | |
| 56 | 70 | Value at T=0.1 | Value at T=1 | Value at T=10 |
| 56 | 71 | Value at T=0.1 | Value at T=1 | Value at T=10 |

**Table 1 Schematic example of a file structure for importing temperature dependent cross sections or rates.**

## CHART

The charting module is rather simple and automatically sets some appropriate defaults. The graphs which SiRop can generate are and abundance vs mass number graph, a color coded Z vs A vs Abundance graph, and a [density, temperature, electron fraction, neutron number density] vs. time graph (where any or all of these values may be plotted on a graph vs time). These are the Isotope Graph, Chart of Nuclides and Time Dependent Graphs which are available to add by

clicking the plus sign in the top left corner next to the tab names. Several graphs can be generated and are available in different tabs. An important thing to note about the X vs time graphs is that they only plot points during update steps (as set in the code panel) and so if these quantities are of interest the graph must be added before running the code as this data cannot be plotted retroactively. A sample graph from midway through an r-process calculation is shown in Figure 5.

The values in these graphs are updated at each update step so the state of the program can be monitored. This is especially useful for those new to running r-process simulations or for trying to setup initial conditions with a specific goal in mind. At any time during the program (although updates will interrupt this if they are set to rapid intervals) a right click on the graphs will bring up a context menu which allows the user to change plotting options or save the data points which are plotted.


**Figure 5 Abundance vs Mass graph partway through a NS merger r-process simulation.**

## SENSITIVITY

This module contains a Setup and Results page. This module allows for setting up complex sensitivity study parameters before executing a sequence of simulations in batch followed by statistical analysis of the data. This module mainly consists of a user interface designed to set up many Operations which are groups of changes to the nuclear parameters which will be used

during the batch execution of the code. For more details see the section below “Running a Sensitivity Study.”

### 3D

Displays a 3D chart of nuclides-like graph. The plot shows a color coded graph of the abundances on a log-scale which is updated along with the charts in the Chart module during update steps as set in the Code module.

### MESSAGES

The messages module displays text based output from the code during its execution. The data here is typically available in graphical form through the various charts available or through the automatic file output created through the code module. Nevertheless, this can be a good place to find information about the code. In addition, if any errors do occur during the execution of the code they will be pushed to this module. Under normal execution this should not be a problem, however, should this occur this can offer the development team information which can assist in troubleshooting and correction of the problem.

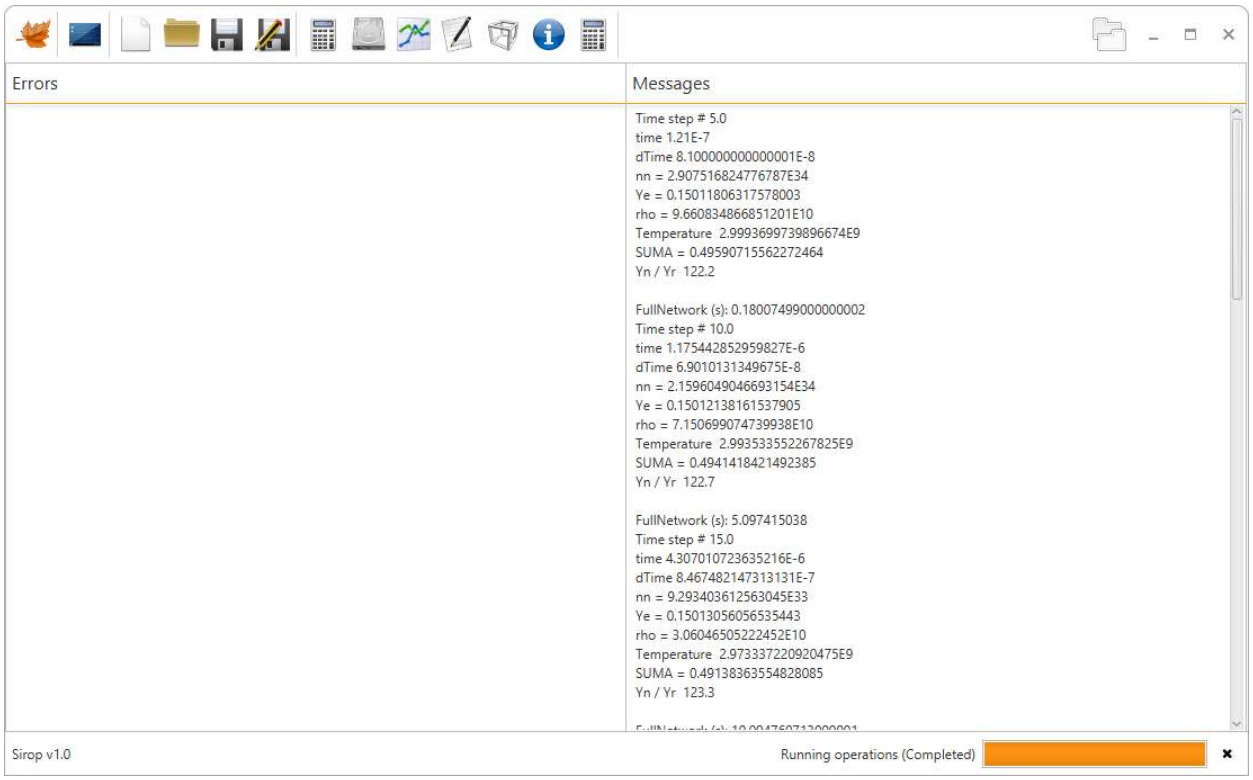


**Figure 6 Screen capture of the output in the Messages module during an r-process simulation.**

## R-PATH

This module is an entirely new addition to SiRop and has been added to assist in understanding the r-process using computationally cheap methods to estimate the isotopes of importance by calculating and plotting the r-process path. This is done using three different methods and all three are plotted together. Each method requires temperature and neutron number density as inputs and so require knowledge of these parameters during a particular r-process environment (which could be found using the data from an execution of the code which lists these values during the simulation).

The first is calculated using the classical WPA which produces population coefficients. Isotopes with population coefficients above 10% are plotted and outline the r-process path which is relevant at high temperatures (above about 1GK). The second is a bracketing method of sorts which identifies the transition regimes where the rates switch from being dominated by neutron capture rates, to beta-decay dominated to photo-dissociation dominated. These boundaries are calculated using the explicit rates and cross sections provided to the program in the Data module. Instances where the classical WPA and this method do not overlap indicate regimes where the WPA fails. The third method is a random walk computed with the cross sections and rates in the Data module. This method is not quite as cheap as the first two, but provides a “dynamic” method for determining the isotopes which will be involved in the r-process. An example of the graph from the Rates module is shown in Figure 7Figure 6.

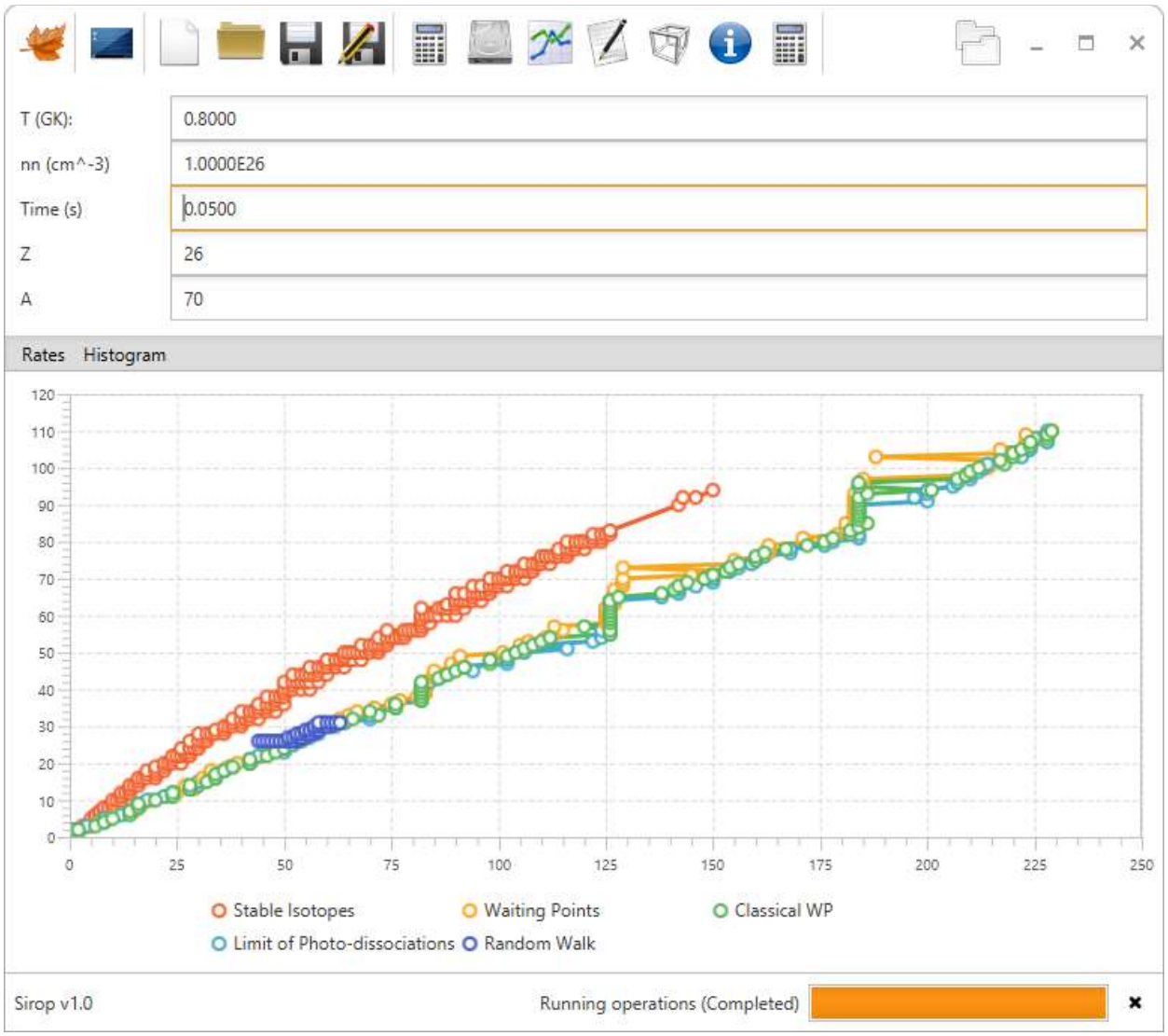


**Figure 7 Graphs showing a sample of the calculated r-process paths in the Rates module using iron-70 as a test isotope. The graphs shows the average path such an isotope would spend over 0.05 seconds.**

## PROGRAM USAGE: R-PROCESS SIMULATIONS

SiRop was built on r-Java 2.0 so can continue to be used as an r-process code in the same fashion. It is recommended that a user interested in using SiRop for sensitivity studies be familiar with running the program for non-batch execution to because the sensitivity module simply runs the program in serial with varied parameters as indicated by the setup in the Sensitivity module. When beginning an r-process simulation it is important to identify the initial conditions for the astrophysical site to be used. This includes identifying the initial temperature and density, the parametric evolution for the density to be used during the evolution of the r-process, and the initial nuclear composition and neutron richness. All these quantities should be based on reference material indicating the conditions using some sort of astrophysical model. As a reference we will outline some salient features of a few popular r-process models.

### OVERVIEW OF POPULAR R-PROCESS SITES

SiRop comes with some built-in models for the density and temperature evolution of come r-process sites. A screen-shot of the selection menu is available in Figure 8 and each option is discussed in detail below. Some order or magnitude estimates for these values are also presented to assist those less familiar with these parameters and r-process codes.

### HIGH-ENTROPY WINDS OF CORE-COLLAPSE SUPERNOVAE

Supernovae are arguable the oldest and most extensively studies r-process site and it continues as an active are of research to determine the nucleosynthetic yield of these environments. The nucleosynthesis occurs in a low density environment between the proto-neutron star and the outer supernova ejecta. Here, the predicted high temperatures lead to complete dissociation of elements from the iron core into constituent neutrons and protons. The high-entropy descriptor or requirement comes was introduced when original hydrodynamic parameters failed to lead to r-process elements being formed. It was found that an increase in the predicted entropy could lead to successful fusion of the free protons and neutrons into heavy seed nuclei while still retaining a high number of free neutrons for the remainder of the main r-process in the supernova model. These seed nuclei are formed by helium or alpha particle fusion into heavier and heavier isotopes where a large majority of the material is converted into inert (with respect to neutron capture) helium-4. Consequently this environment is sometimes referred to as an alpha-rich freeze-out (e.g. Woosley and Hoffman 1992). Additionally, the assumption of high-entropy provides a simplifying assumption about the density and temperature evolutions which is attractively simple as it is a simple polynomial function (or almost polynomial in the HEW model of Farouqi et al. 2010 provided in SiRop).

Some rough order of magnitude estimates for the physical initial conditions (at the onset of the r-process) for this scenario put the density at around $10^5$ g $cm^{-3}$, temperatures around 3 GK, and neutron number densities with a large range from about $10^{22}$ $cm^{-3}$ to $10^{26}$ $cm^{-3}$ depending on physical parameters (e.g. entropy) employed in the charged particle reaction phase of the model. Because SiRop is purely an r-process code, initial seed compositions and neutron richness or neutron to seed ratios must be taken from sources which have computed these values (see Woosley and Hoffman 1992 for an example of suitable tabulated data).

## NEUTRON STAR MERGERS

Neutron star (NS) mergers provide an obvious mechanism for providing free neutrons and seed nuclei through the ejection of the outer crust of a neutron star. The surface crust of a neutron star is expected to be composed of heavy neutron rich isotopes in NSE which provides the seed isotopes which can capture the neutrons ejected along with this outer crust. The merger types can be between two NS (NS-NS) or a NS and a black hole (BH) (NS-BH). The expansion of the ejected material can be modelled in SiRop as an expanding polytope whose details can be found in the paper “r-Java 2.0: the Astrophysics” (Kostka et al. 2014). The initial densities and temperatures should be around $10^{11}$ g $cm^{-3}$ to $10^{14}$ g $cm^{-3}$ and around 1 GK to 3 GK. The corresponding neutron number densities are also quite high at around $10^{34}$ $cm^{-3}$. The initial nuclear composition are frequently found using NSE which for low electron fraction parameters predicts a very strong r-process.

## QUARK NOVAE

The third site which has pre-set hydrodynamic properties included in SiRop is a Quark Nova (QN). A QN is the explosion of a NS due to a phase transition from hadronic to free quark matter. The phase change and resulting quark deconfinement is theoretically expected to release an enormous amount of energy which can eject an outer layer of the neutron star at relativistic speeds. This scenario has similar initial conditions as a NS merger scenario in terms of initial temperatures, densities and nuclear composition, but has a different evolution in time. The presets in the code list physical parameters of the parent NS in addition to a parameter, zeta, which determines the predicted fraction (In percent) of the energy transferred to the QN ejecta (around 1% is typical).

## GENERIC ASTROPHYSICAL ENVIRONMENT

In addition to pre-canned astrophysical models above, there is an option to simply model a generic site’s density as a simple function (usually a polynomial in time). This is Custom environment and it can be used with initial conditions similar to the above sites (in terms of

temperature, density and implied neutron number density) for expansions which do not fit exactly with the other available defaults.

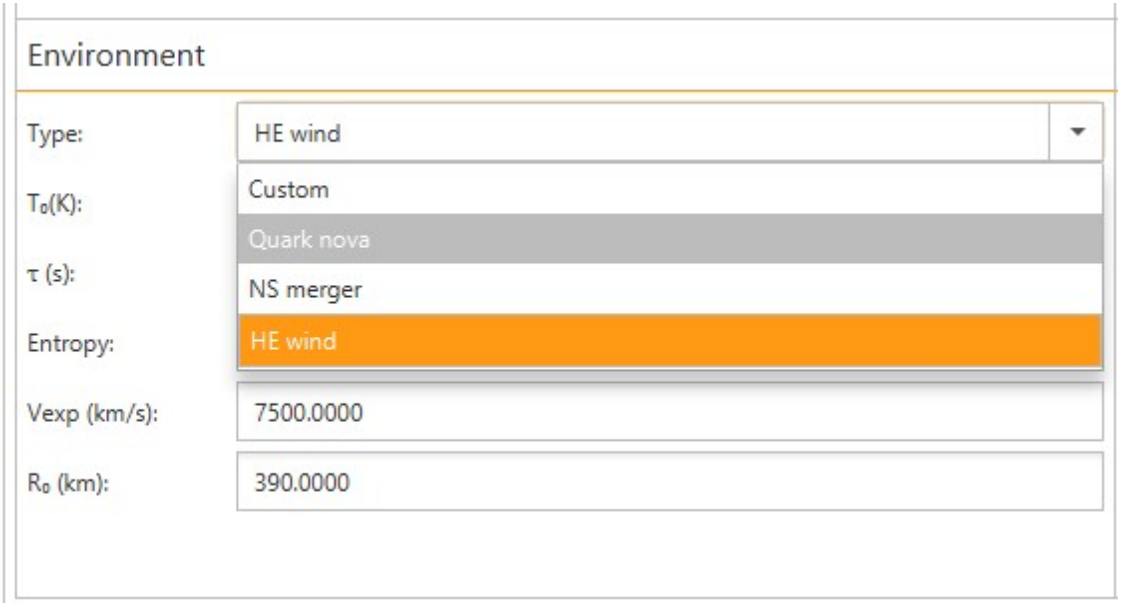


**Figure 8 A screen capture of the area in the Code module with an r-process calculation selected in the Operations queue which shows the different astrophysical models available.**

## EXECUTING THE CODE

Once the initial conditions have been set for the site and the desired nuclear parameters have been loaded into the program the settings for the r-process need to be chosen. There are two modes for running dynamic simulations: Full or Waiting Point. The Waiting Point option evolves the r-process in the WPA and is generally an outdated method. It is nevertheless an option and can be useful when you want to run a fast simulations (as the WPA is much faster as an analytic approximation to the full set of rate equations) to understand the initial conditions used or when only masses have been changed without correlations to other nuclear inputs.

The Full options runs the simulation using the full set coupled ODEs which includes only the nuclear processes available and selected in the code. SiRop includes the following nuclear reactions: neutron capture, neutron photo-dissociation, beta-decay, beta-delayed neutron emission, alpha decay, fission (spontaneous, beta-delayed and neutron induced) in addition to a rudimentary alpha capture chain (He-C-O-Ne). Any or all of these options can be turned off in the panel shown in Figure 9 (although turning off neutron capture or beta-decay don't normally make sense to disable). There are some additional options for fission which allow for fission to be turned off (None), to use a fully symmetric fission model which fission isotopes which exceed a mass and charge cutoff (Cutoff), or a non-symmetric fission model which produces a

distribution of isotopes following fission events. Unless the role of a particular reaction is under study, it is generally advised to leave all nuclear processes on.

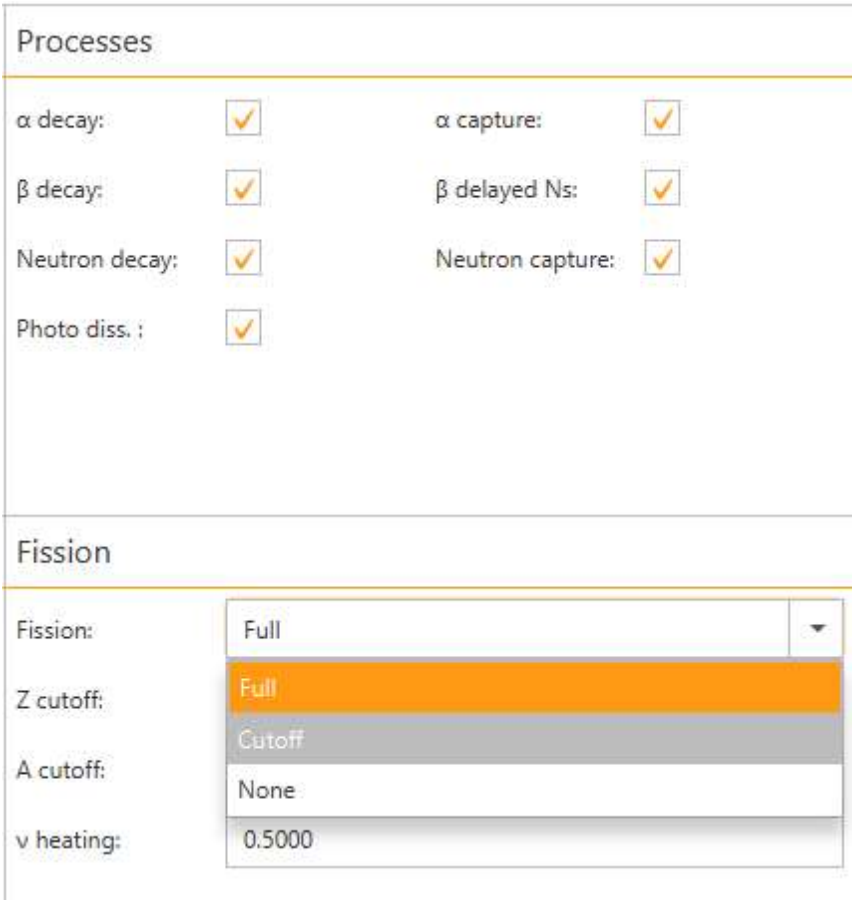


**Figure 9 Panel available after selecting an r-process calculation in the Code module. The different nuclear reactions can be turned off by clicking the checkboxes.**

Regardless of the mode selected (Full or Waiting Point) the program, upon execution, will run until the simulated time has exceeded the listed time (Δt) or the available neutrons have dropped below a threshold. The internal cutoff occurs when the neutron to seed ratio drops below 1.0 at which point the program will terminate the r-process simulation. Once the r-process is complete, the program will run the nuclear decay reactions for the specified amount of in simulation time (t decay) or until the program determines that stable isotopes have been reached. In general the defaults for the in simulation time are appropriate, but some slow expanding or very neutron rich environments may require simulations to track the r-process for more than 1 second.

Once all these settings have been selected, the program can be executed by pressing the maple leaf SiRop logo button (the Calculate button) available from the Desktop or the top left of the

top toolbar. The program takes a variable amount of time to execute depending on the site and initial conditions, but in practice can take between 30 minutes to over 24 hours. The progress of the simulation can be monitored using the Chart module and the Messages module. The final results can be saved in a number of ways including: right clicking on any of the graphs and exporting the data, copying data from the Data module, or by having selected the Save option in the Code module before executing the code.

## RUNNING A SENSITIVITY STUDY

Once a simulation setup has been chosen and initialized (as indicated above), the code is ready to run a nuclear sensitivity study. The Sensitivity module has two tabbed pages which can be accessed by selecting (mouse click) either the Setup or Results tab from the top left corner of the module page. As implied, the Setup page contains options for setting up the study and the results tab lists some textual and graphical output about the state of the batch execution and the computed statistics.

The Setup page has six different areas: Operations, Sensitivity Factors, two Properties, Output and Options. The Operations section and its Properties (to the right of Operations) contains a list of simulations to be run in sequence. The Sensitivity Factors and its Properties (to the right of Sensitivity Factors) contains a list of simple statistical metrics to be computed. The Output section allows for automatic logging of the results to a directory during the execution of the sensitivity study (similar to the Code module). The Options section contains the range of mass numbers upon which the sensitivity metrics will be calculated.

The Results page contains a Console section which prints out textural information, a Graphs section which provides graphical summary of the completed simulations from the sensitivity study being run (or completed) and a Sensitivity Results section which lists the computed statistics for each simulation queued up in the Operations section from the Setup page. This page is mainly for displaying statistics and each section has a context menu available when right-clicking which allows for manual updating and saving the sensitivity data presented.

The Sensitivity module has been designed to allow arbitrary modifications to the underlying nuclear data. To SiRop a single set of changes to nuclear parameters is referred to as an Operation. Each Operation has a name to identify it (listed under Options) and contains a list of changes in a set of Groups. Each Group contains a list of Isotopes and Values which indicate the isotopic values to change and by what amount (Add, Relative, or Percent). The setup for a particular Operation makes most sense with some examples below. Once all sensitivity Operations have been setup, they can be run by pressing the cog button located in the bottom left of the Operations panel.

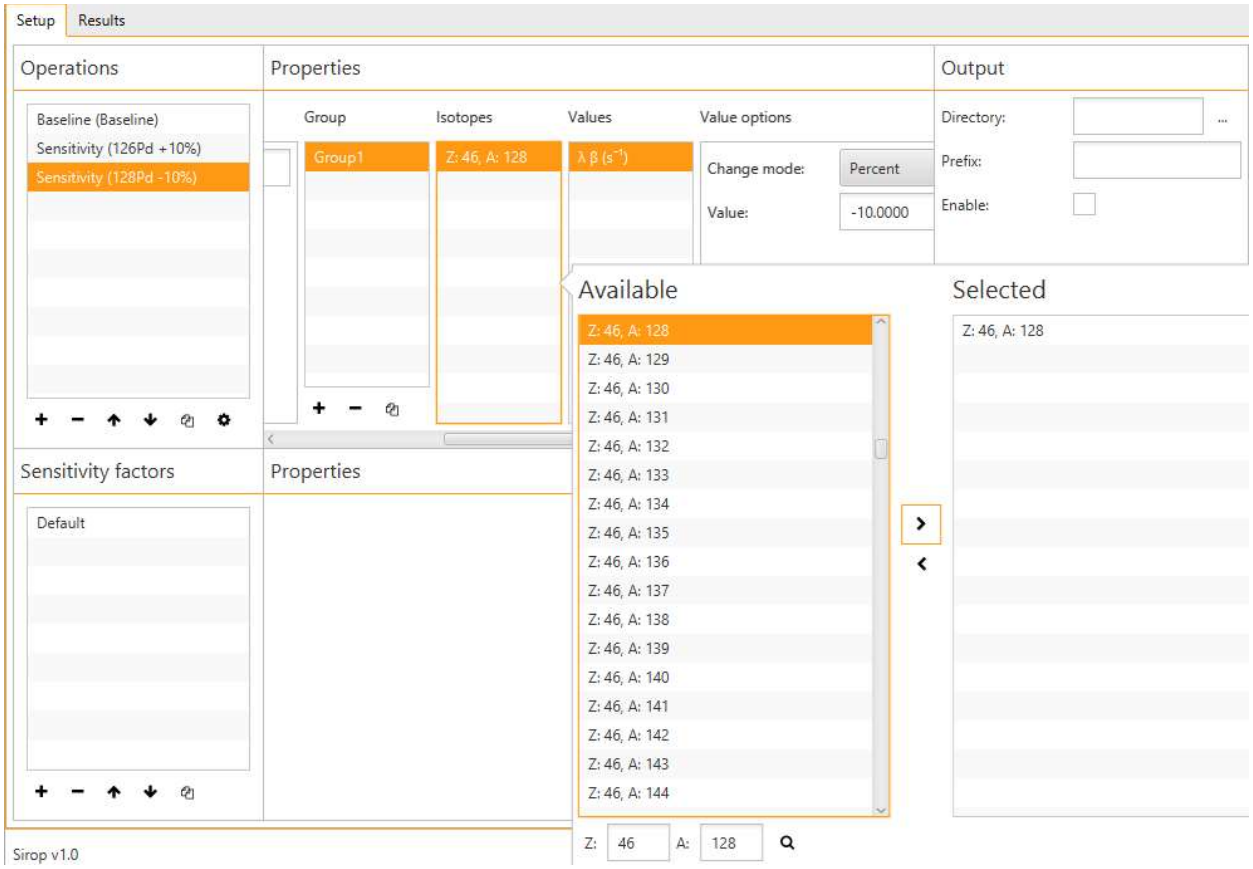


**Figure 10 Screen capture midway through setting up the sensitivity study suggested in Example 1.**

## EXAMPLE 1: CHANGES IN SINGLE ISOTOPE HALF-LIVES

Suppose we wish to identify the N=82 isotope whose half-life is most impactful to the r-process. For simplicity's sake we will only list a few of these isotopes. For this study we're going to multiply the half-lives (or the rates) by ±10% for each isotope. For 128Pd, 129Ag, 130Cd, 131In and 132Sn this means 10 different Operations. The values in each Operation will be almost identical, so we'll list the details for one. In the Options section in the Operations Properties section we'll add the name "*128Pd +10%",* in Group we'll add a group by clicking the plus button. Now that there exists a group, we ensure it is selected (click on it if it isn't highlighted in orange) and in the Isotopes section we'll right-click to bring up a context menu with the isotopes imported listed. In the search bar at the bottom I've typed in Z: 46 and A: 128 for 128Pd and after hitting enter that isotope has been selected. The right arrow in the context panel adds this isotope to the group and the context menu can be navigated away from by clicking outside of it or hitting the escape (Esc) key. Similarly, the λ β (beta-decay rate) can be added to values. Once added, the change can be specified in the Value Options: in our example, we click the drop-down menu to select percent then change the value to 10 and hitting the

enter key to confirm the entry. Now we have one operation set. For the decrease by 10% we can easily make that operation by copying the "*128Pd +10%*" operation in the Operation list and click on the copy icon at the bottom to the right of the down arrow. Once the operation is copied, we can name it "*128Pd -10%*", select the value in the only group and change the listed 10.0000 to -10 and hitting enter. An example of a partial setup and the right-click context menu is shown in Figure 10. This procedure is mimicked for the remaining isotopes and once we have set up all our operations, the sensitivity study can be run.

## EXAMPLE 2: CORRELATED NEUTRON CAPTURES AND PHOTO-DISSOCIATIONS

The principle of detailed balance implies that a change to a neutron capture cross section should correspond to the same (multiplicative) change to the reverse reaction (the neutron photo-dissociation). This can be accomplished by setting up two groups in the Group tab. If we want to change just one isotope's (e.g. 128Pd) cross section in this Operation, we can add 128Pd to the isotope list in the first Group, set the Value to "Neutron Capture Cross Sections" to be multiplied by a factor (e.g. 10). Then the second group needs to have 129Pd added with the "Photo-dissociation Rates" Value also multiplied by the same factor of 10. For each isotope in each operation this procedure must be reproduced for each Operation of interest.

## EXAMPLE 3: GROUPS CHANGES

For our last example, we won't go into as much detail, but outline an additional type of sensitivity study which is possible using SiRop. In the previous examples, only one isotope was changed per Operation (two for easily correlated values like cross-section and photo-dissociation); however, it is possible to create more complex operations. If there were evidence for shell quenching or large systematic changes to many isotopes that we were interested in, we could create this as an Operation and compare the sensitivity to the baseline and any number of additional sensitivity Operations. For the shell structure example, we could take the N=82 isotopes from "Example 1: Changes in Single Isotope Half-Lives" above, we could put 128Pd, 129Ag, 130Cd and 131In into a group together and set a multiplicative factor to the cross-sections and add a small (perhaps +0.05 MeV) the mass excess. Then in a second group, we would add 129Pd, 131Ag, 132Cd and 132In and multiply their cross sections by the same amount and subtract a small (maybe -0.05 MeV) to the mas excess. Or this change could be split into several different sub-groups for more granular control of the changes along the magic number. The flexibility to create rather complex changes in a single operation was designed into the interface to allow for arbitrary sequences of modifications.

## SUGGESTED RANGES FOR SENSITIVITY FACTORS

SiRop has been designed to allow rather large user flexibility with inputs. While this allows for numerous different possibilities for how to use the program, it comes with the programmatic difficulty of verifying that the inputs into the program make sense. While some effort has been made to programmatically detect some obvious invalid input, there is some responsibility deferred to a user to understand some of these limitations. With respect to sensitivity studies, there are some suggested ranges of modifications to the nuclear inputs which are based on nuclear theory and measurements and shouldn't be exceeded without some experience with the code and the nuclear theory.

**Measured Nuclear Masses**: See the measurement uncertainty ( <100 keV in many cases)
**Unmeasured Nuclear Masses**: ~0.5 MeV near measured masses
**Beta-Decay Half-Lives**: Factor of a few (times or divided by factors of 1-5 or 10 at the extreme range)
**Beta-Delayed Neutron Probabilities**: Probabilities must be normalized (and are automatically by the program during execution)
**Cross-Sections**: Multiplicative factors of 10-1000 are normal and strongly depend on the predictive theory used
**Beta-Decay Q Values**: See range for masses (not more than about 1 MeV even in extreme cases)

These are meant as a starting point for testing some values and better values for acceptable variation should be based on existing nuclear measurement errors, errors in model fits to existing measurements and comparisons of competing nuclear mass models.

## R-PROCESS PATH TESTING

The R-Path module is an addition to SiRop which has been designed to assist in designing sensitivity studies and help prevent some pitfalls that can be run into when using any r-process code. The idea of the r-process path is as old as the theory and is the collection of isotopes which are produced during the r-process in a particular site. The r-process path is determined by the r-process waiting points which are the isotopes which beta-decay. Historically there are two main avenues for determining these waiting points: either by equating predicted cross-sections to beta-decay rates for a sequence of isotopes, or by calculating the waiting point population coefficients using the WPA. While both methods are certainly informative, both has physical regimes where the assumptions they make break down. At high temperatures the first method (equating beta-decay with neutron capture) does not account for the significant competition with photo-dissociations which can prevent neutron captures from meeting at equilibrium with the beta-decays. The classical waiting points as computed in the WPA is only valid at high-temperatures which provide enough high-energy (MeV) photons to maintain equilibrium with the neutron captures and at temperatures much below 1 GK this assumption starts to break-down.

Access to computed rates for neutron captures, photo-dissociations and beta-decays allows for us to test when these two methods are applicable and provide better estimates for the r-process path. Since these nuclear processes are random we can simply execute a random walk with the rates. In principle this should lead to average paths and show variations in the paths, but test cases show very weak variation due to the large order of magnitudes between the different rates in the r-process.

Both the Rates module and the Waiting Point Rates calculation in the Code module can be used to calculate the r-process path to assist in identifying isotopes which can be expected to be impactful in a sensitivity study. The inputs required are the temperature, neutron number density and an initial isotope to begin the random walk. The Rates module requires specification of total simulated random walk time; whereas, the calculation in the Code module requires minimum and maximum values for the atomic number Z. The Rates module will plot in a Z vs N diagram the following: stable isotopes, waiting points calculated based on where the neutron capture rates equal beta-decay rates (“Waiting Points”), waiting points as calculated by the WPA (“Classical Waiting Points”) and the waiting points calculated using the random walk (“Random Walk”). The calculation in the Code module will list the results of the random walk in the Messages module after the program Calculate button has been pressed.

In order to determine the temperature and neutron number densities to be used, the program can be run once normally with the time plots added in the Charts module to track the evolution

in time of the temperature and neutron number density. This can be used to run the calculation of the r-process path at different points during the evolution of the r-process to identify key isotopes that will be produced during the simulation. These isotopes can then be identified for inclusion in a sensitivity study Operation list and significantly reduce the time spent executing the code by only modifying values of isotopes in through which the r-process falls on or near.

## TECHNICAL DETAILS AND NOTES

SiRop is a desktop based program written with a GUI written in Java. For this reason, the program should be available to all operating systems for which a Java Virtual Machine (JVM) exists. In practice this means we have distributions available for Windows, Mac and UNIX based operating systems and SiRop should run on any installed system with no cross platform limitations.

There are a few minor quirks which result from this technical choice that someone using SiRop may profitably be made aware of. The first is that occasionally due to the Just In Time compilation process inherent to the JVM, some portions in the GUI may respond slowly the first time they are accessed and used. The second is that all text input forms or boxes require hitting enter after the desired text (or numeric) input has been typed. Always ensure that you hit enter after typing into a text field with parameters to ensure that the changes are forwarded to the internals of the program.

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