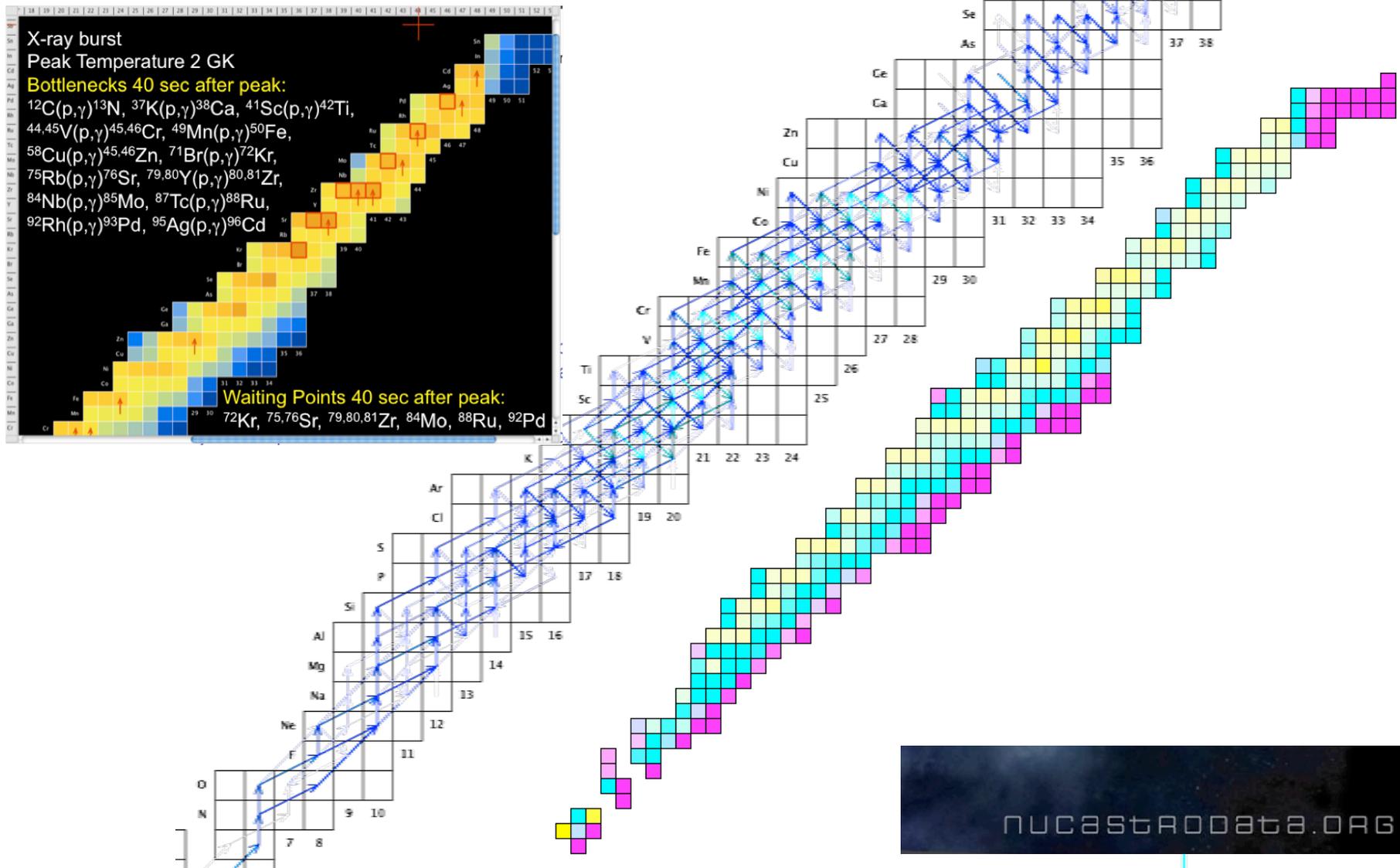


computational infrastructure for nuclear astrophysics

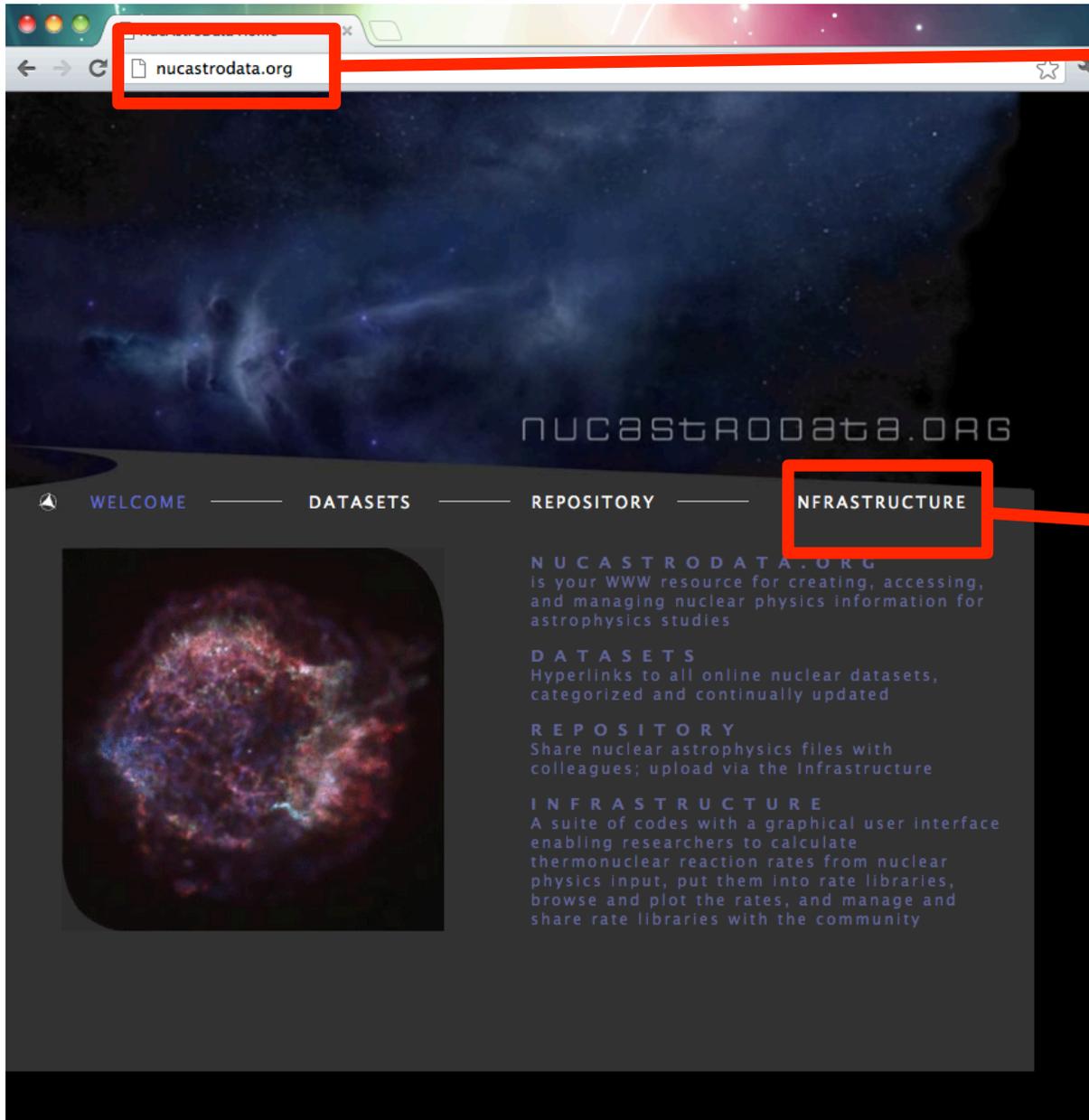
step-by-step simulation instructions



Michael Smith, Physics Division, Oak Ridge National Lab

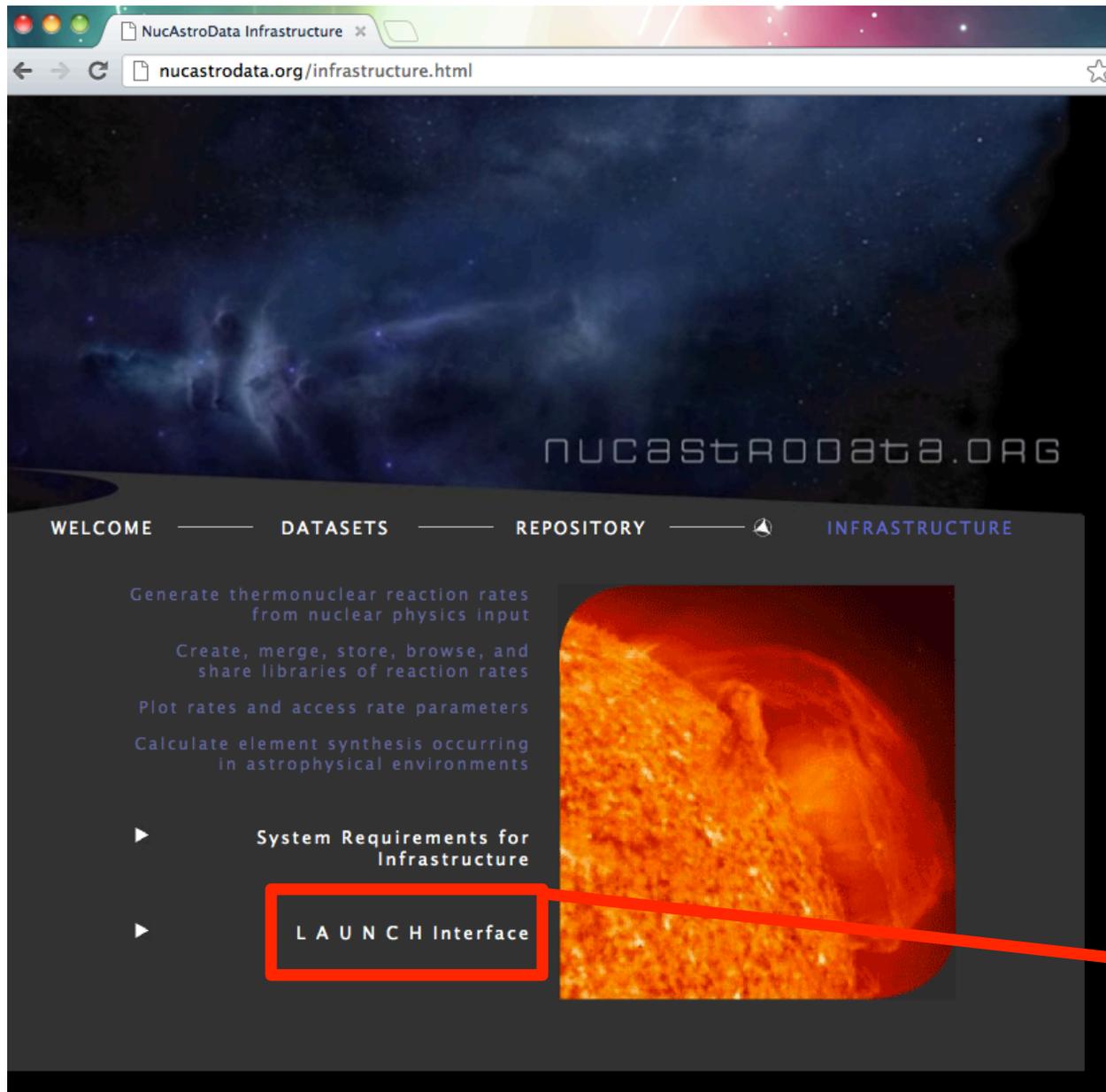
coordinator@nucastrodata.org

visit here

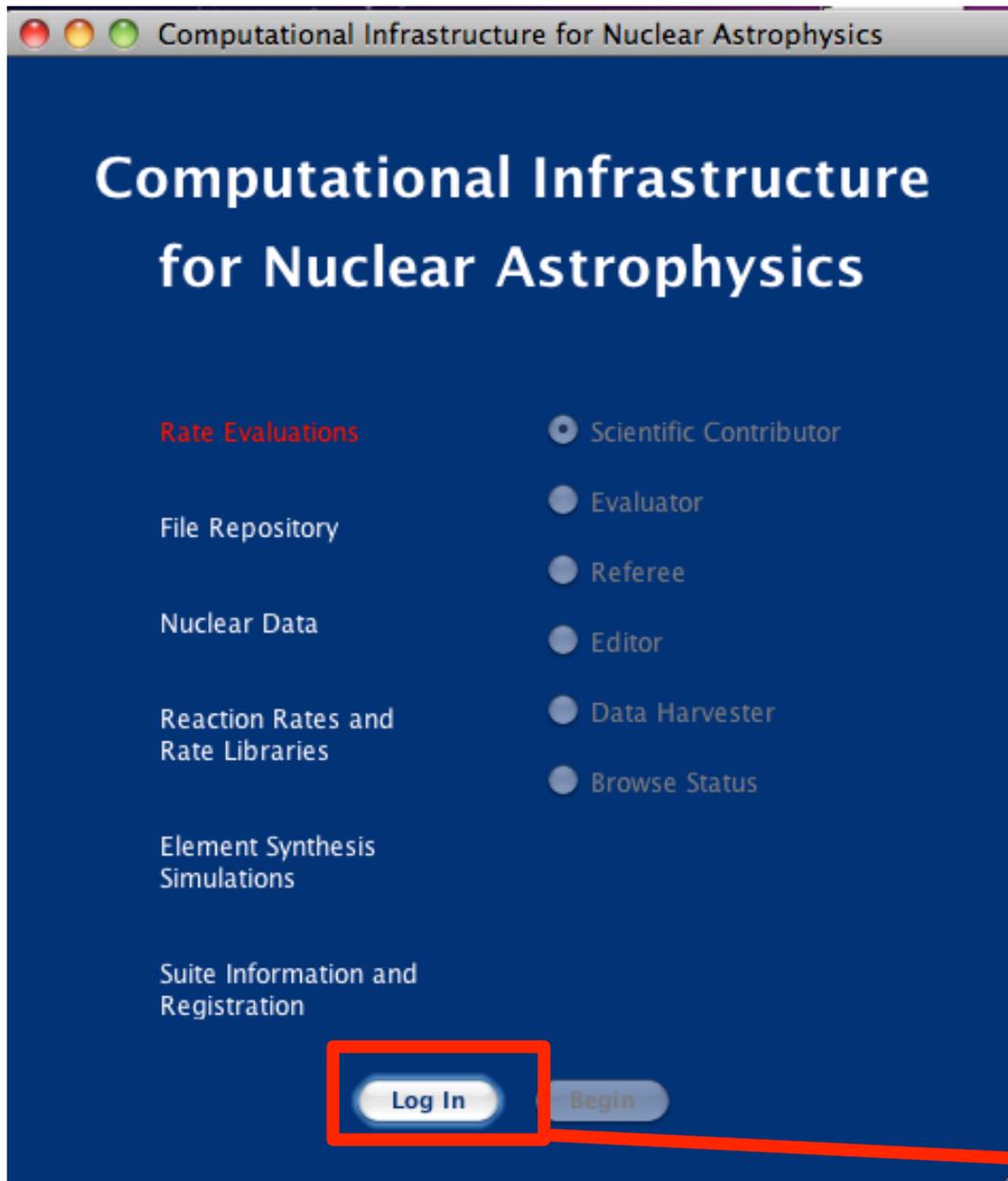


then click here

download the java application from nucastrodata.org



download the java application from nucastrodata.org



you need an internet connection to run this suite

click here

launch the platform-independent java application and log in

Computational Infrastructure for Nuclear Astrophysics

Computational Infrastructure for Nuclear Astrophysics

Rate Evaluations

- Element Synthesis Simulator

File Repository

- Element Synthesis Manager
- Element Synthesis Visuali...

Nuclear Data

Reaction Rates and
Rate Libraries

Element Synthesis
Simulations

Suite Information and
Registration

Log In

guests can use
some functions

Registered Users
can save their work
in their own disk
allocaiton

Log on

Log in as guest (limited access)

Log in as registered user (full access)

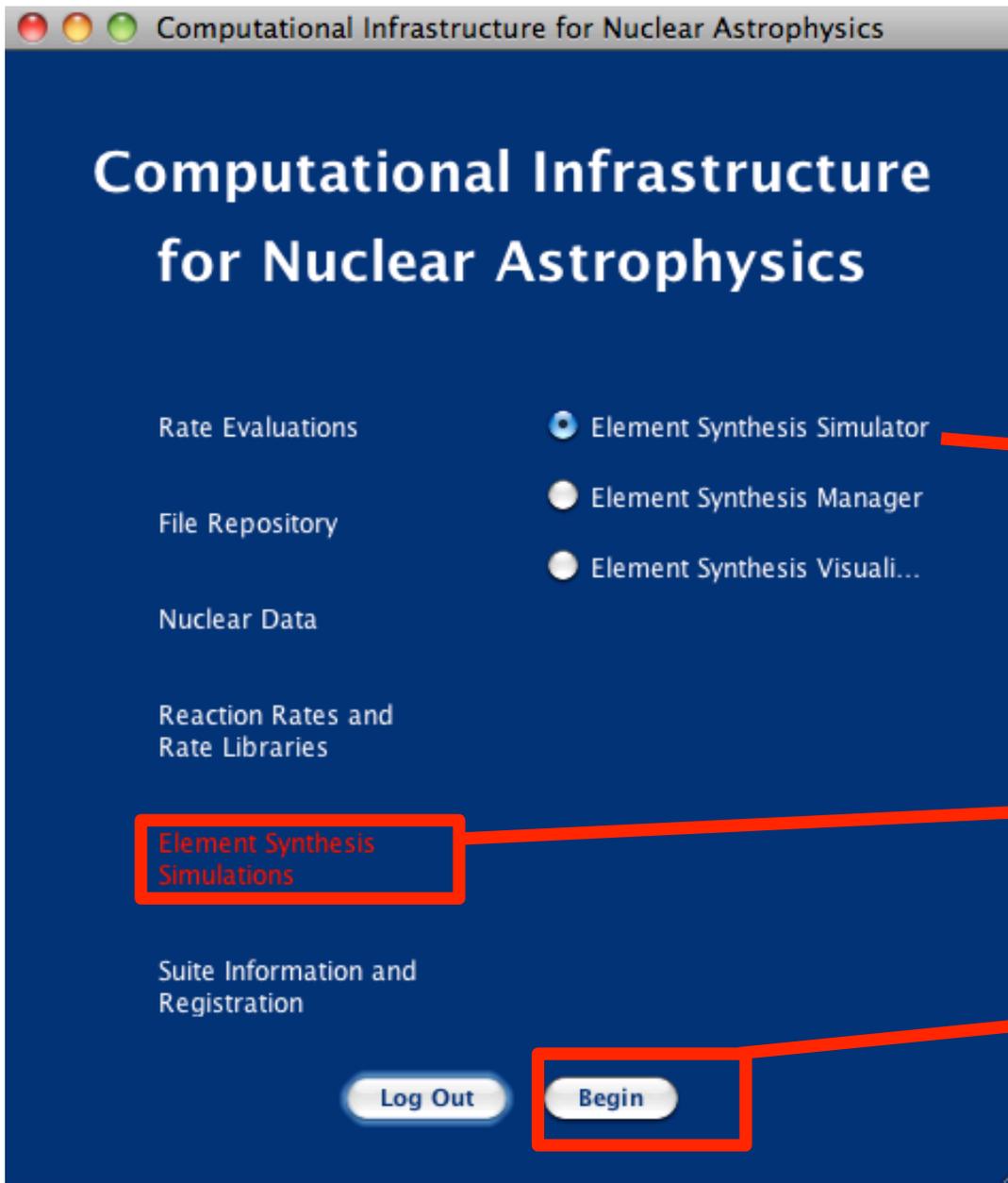
Username:

Password:

Submit

for your
first login,
use
guest,
then
register

login to the system – you need an internet connection

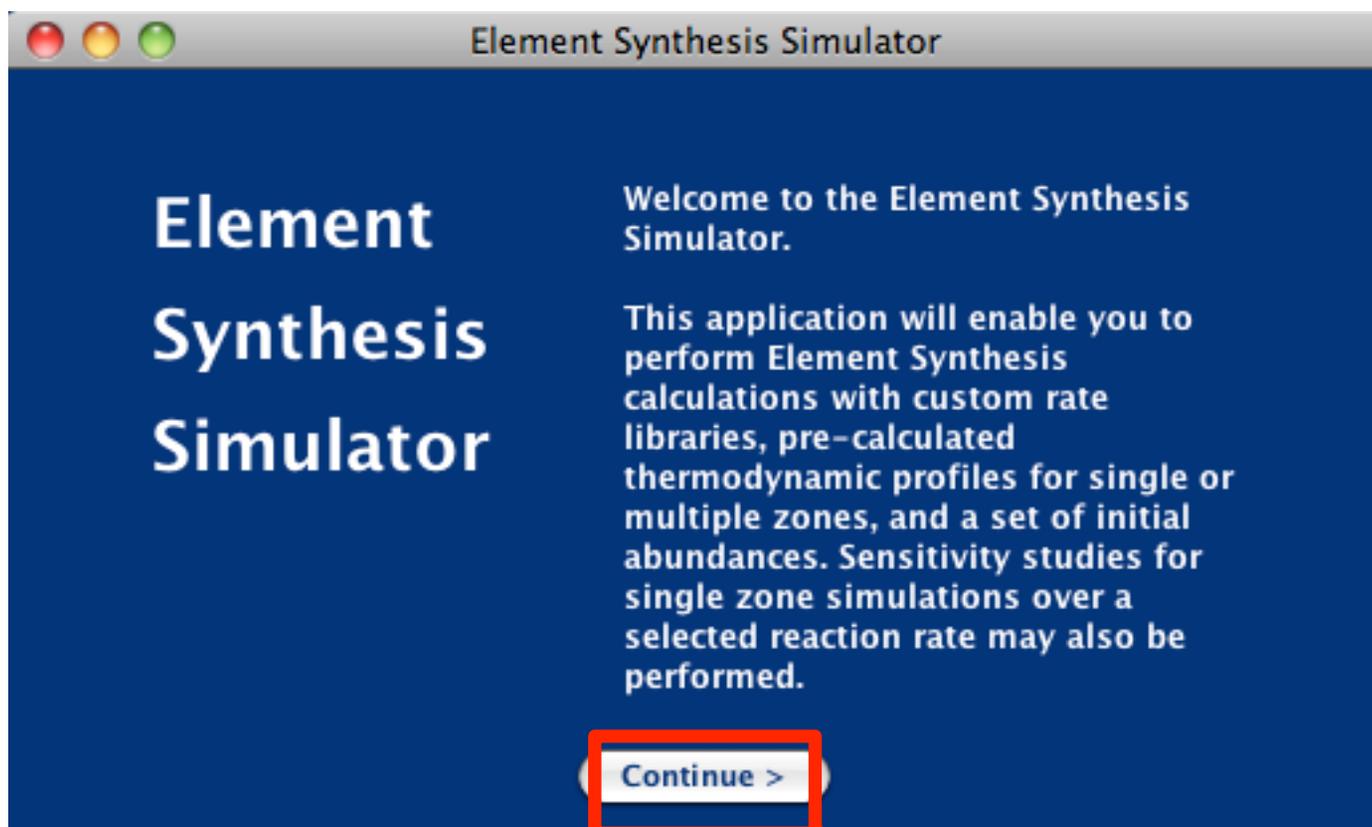


then click here

first
mouseover
here

then
finally
click here

go to Element Synthesis Simulations & Element Synthesis Simulator



click here

starting up Element Synthesis Simulator

Element Synthesis Simulator

Element Synthesis Simulator | Select Simulation Type Step 1 of 5

Please select an element synthesis simulation category and then an element synthesis simulation type from the dropdown menus below.

Simulation Category: Nova
Xray Burst
Simulation Type: Supernova
 Other

Simulation Description:

Element Synthesis Simulation Category: Nova
Element Synthesis Simulation Type: New 1.35 M Solar ONeMg WD

Element Synthesis Simulation Type Description:
New 1.35 M Nova with 50% solar + 50% ONeMg initial abundances

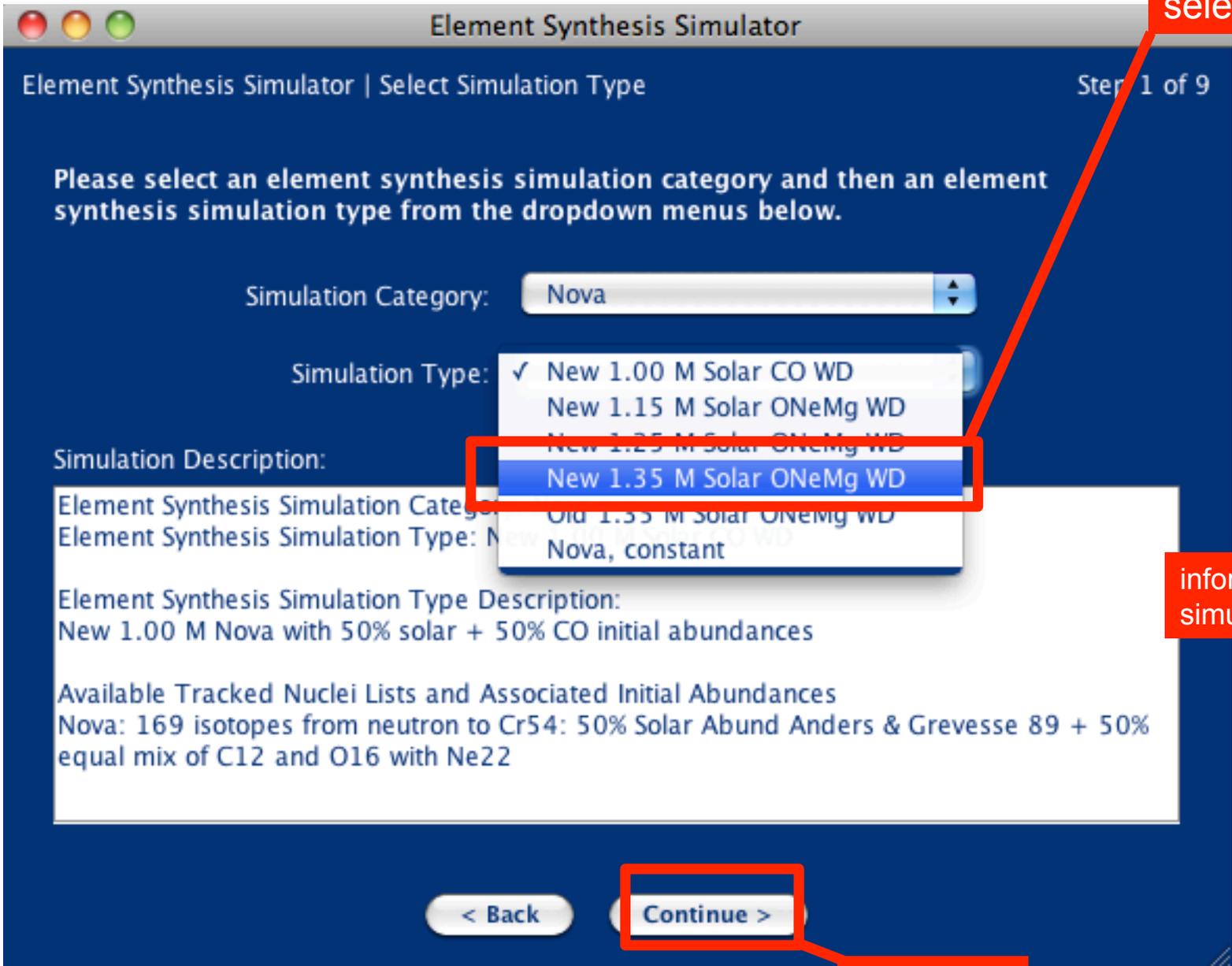
Available Tracked Nuclei Lists and Associated Initial Abundances
Nova: 169 isotopes from neutron to Cr54: 50% solar + 50% ONeMg Initial Abundances from Politano

[< Back](#) [Continue >](#)

select model category here

supernova coming soon !

choose a simulation category



select here

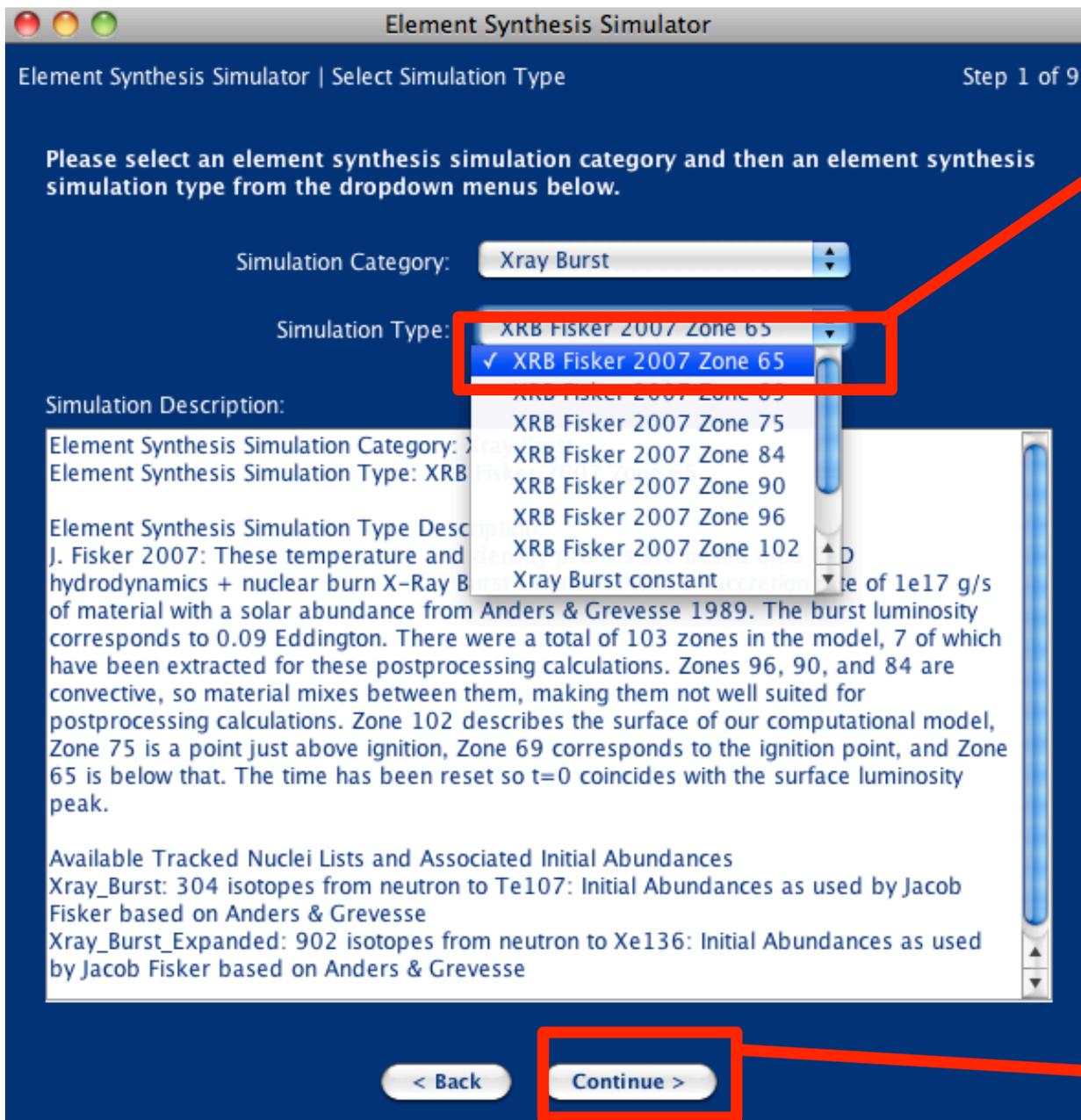
New 1.35 M Solar ONeMg WD

information on simulation is here

Continue >

click here

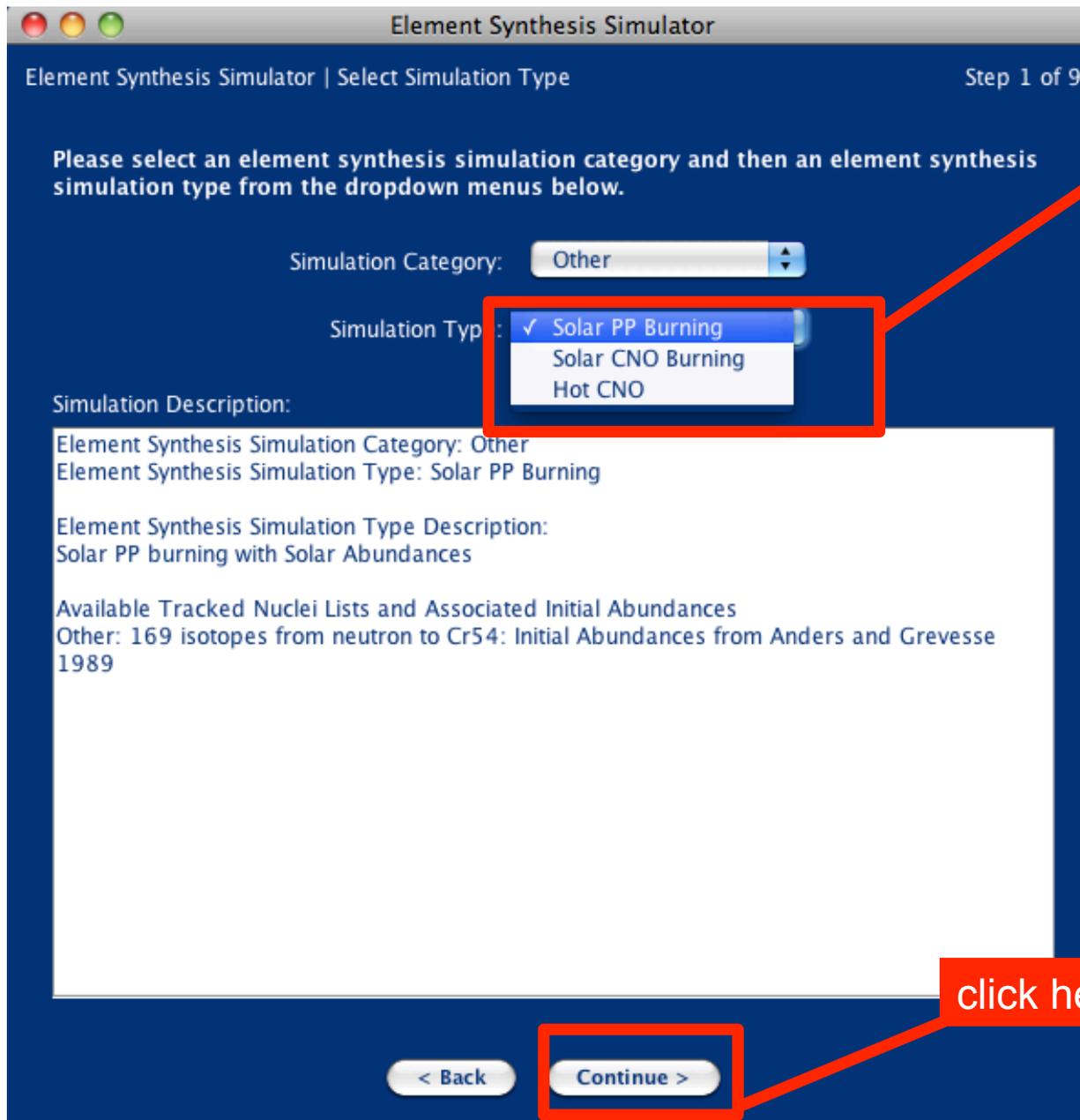
choose a particular simulation



select here

click here

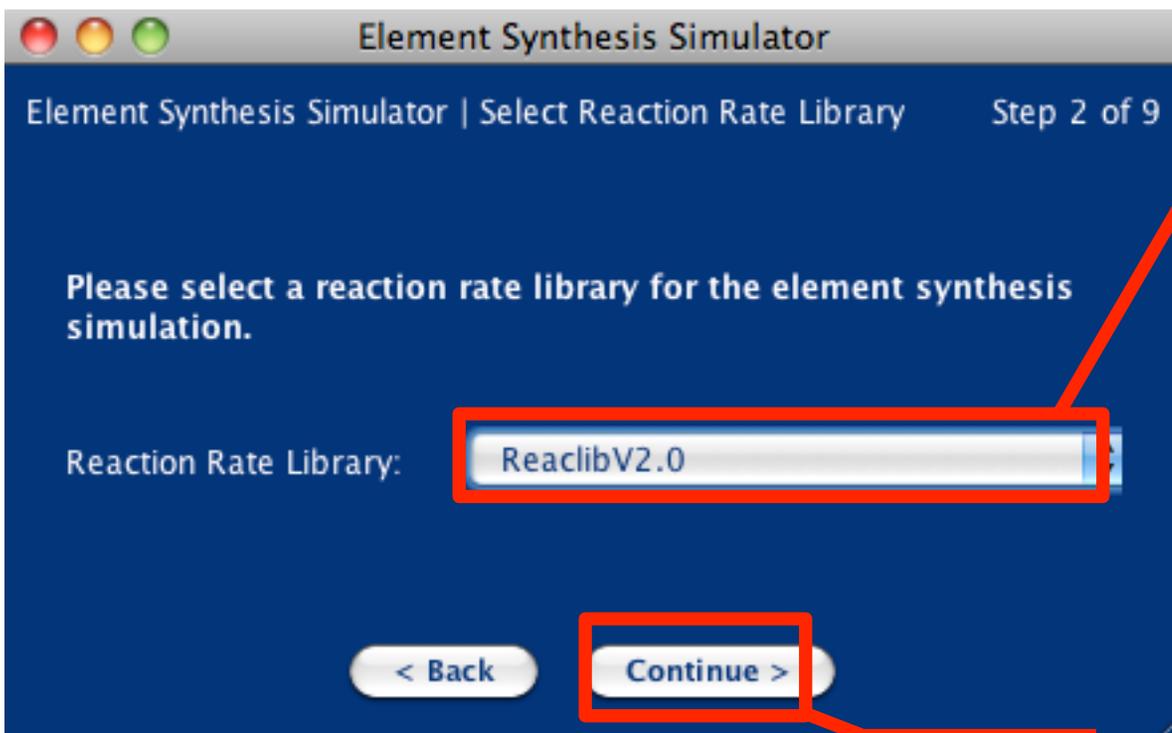
here is the simulation list for X-ray bursts



select here

click here

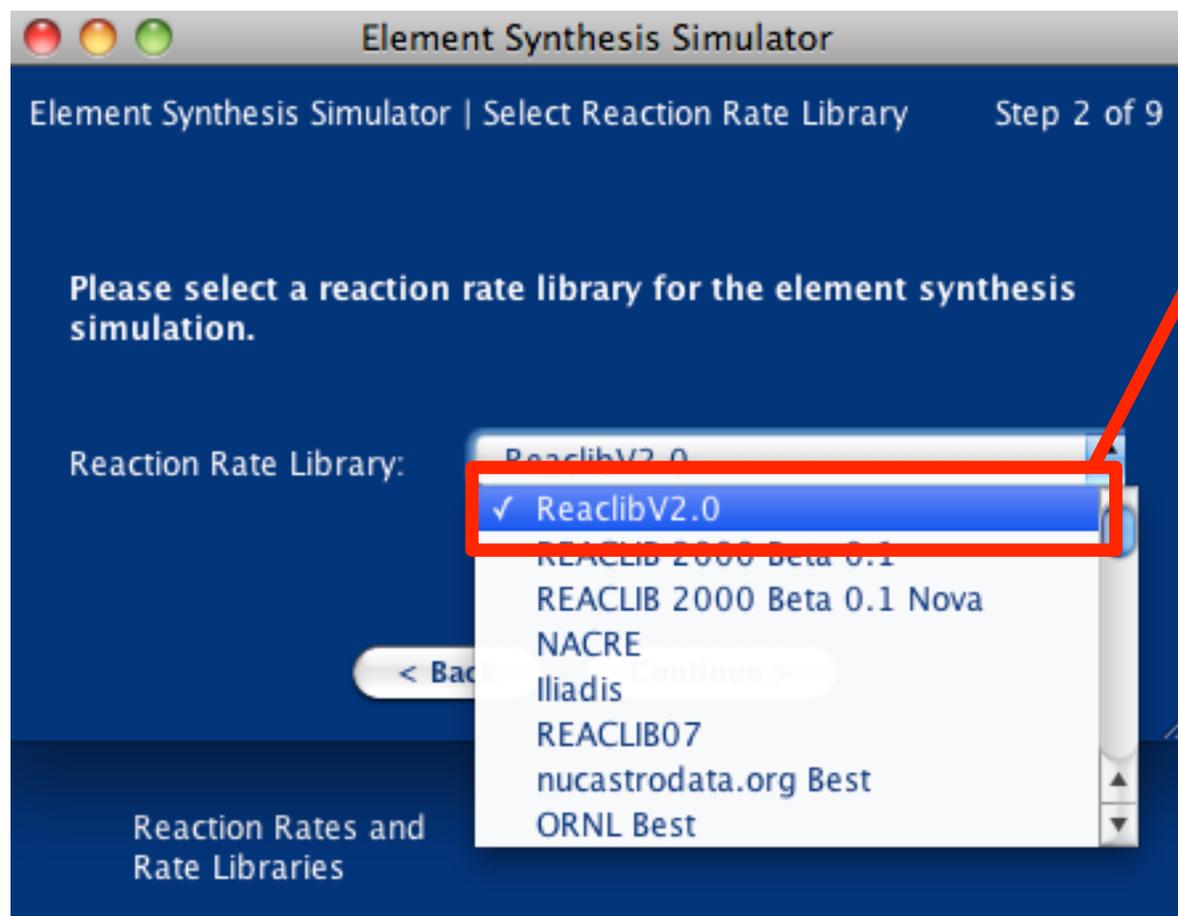
here is the simulation list for "Other" ...



select here

click here

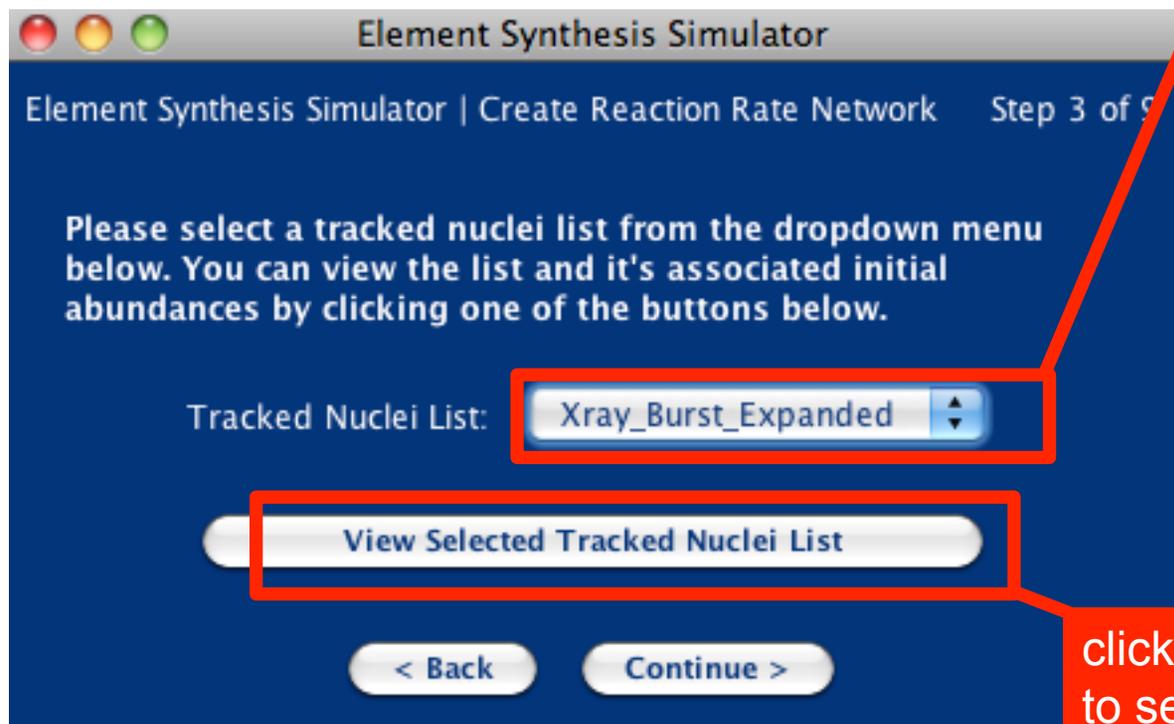
choose a library of rates – default is JINA REACLIB v2.0



select here

use a reference library or your own library of modified rates

choose a library of rates – you can choose your own library

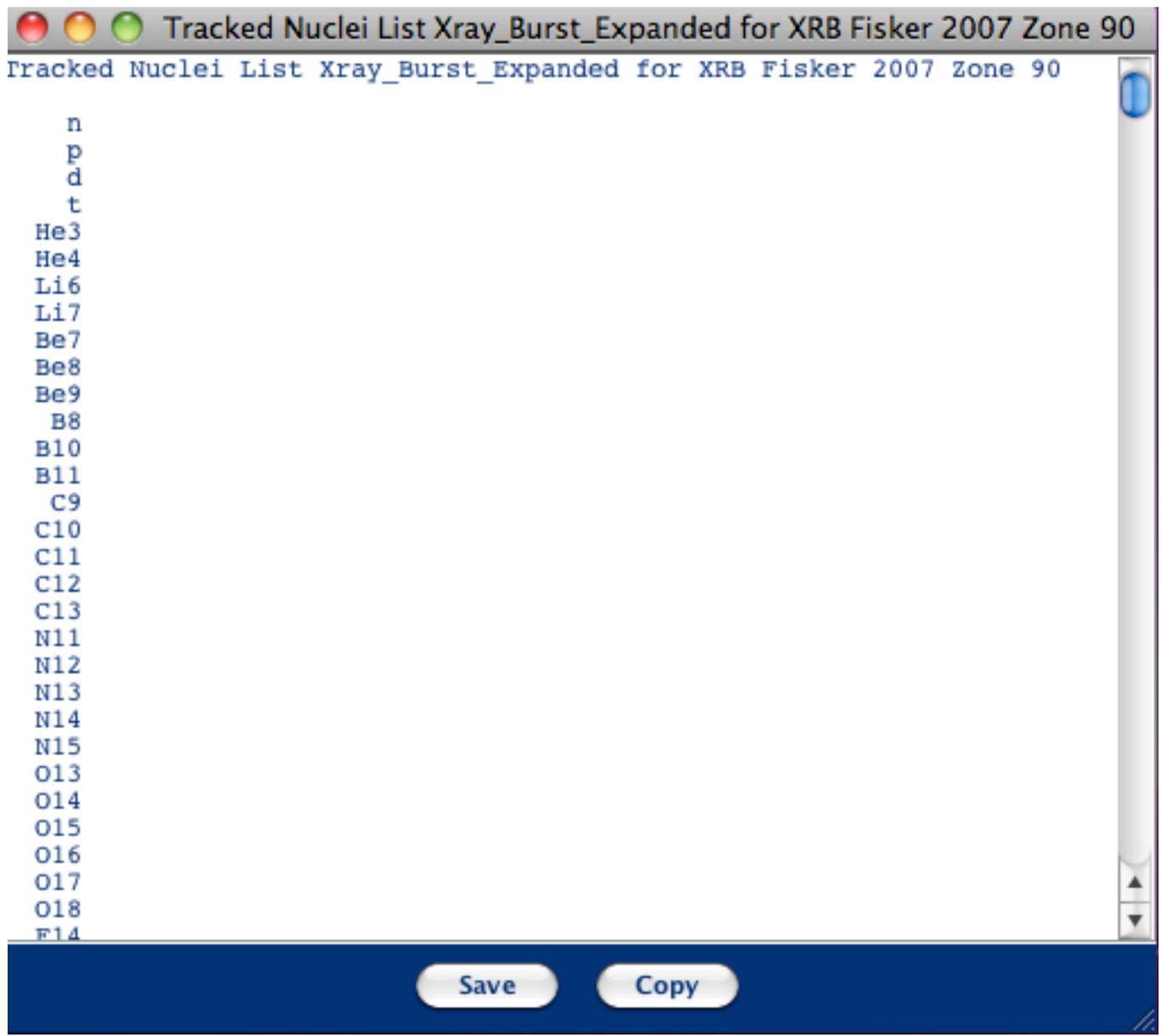


select here

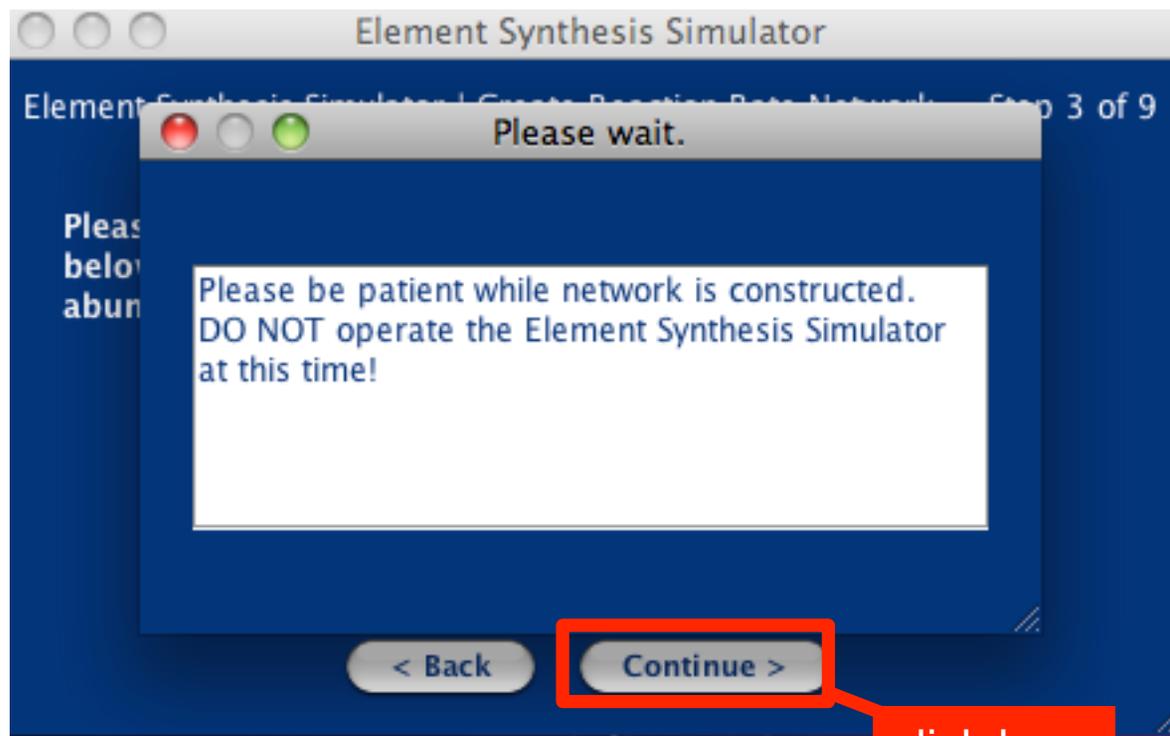
this set is compatible with J. Fisker's XRB profiles in our system

click here to see nuclei

choose a set of nuclei to track



a list of tracked nuclei



click here
to set up
network

setting up the network

Element Synthesis Simulator

Element Synthesis Simulator | Network Summary Step 4 of 9

Below is a summary and report detailing the reaction rate network.

Library: ReaLibV2.0

Network Setup Summary: Network prepared

Network Setup Report:

```
Part 4)      Running net_setup.  
Library has 898 isotopes  
Isotopes vary from  n to xe136  
Number of 7 parameter sets:  
  reaction type 1 has 741 parameter sets  
  reaction type 2 has 2726 parameter sets  
  reaction type 3 has 18 parameter sets  
  reaction type 4 has 2619 parameter sets  
  reaction type 5 has 4752 parameter sets  
  reaction type 6 has 20 parameter sets  
  reaction type 7 has 6 parameter sets  
  reaction type 8 has 26 parameter sets  
Number of rates not parameterized: 0  
Network prepared for simulation
```

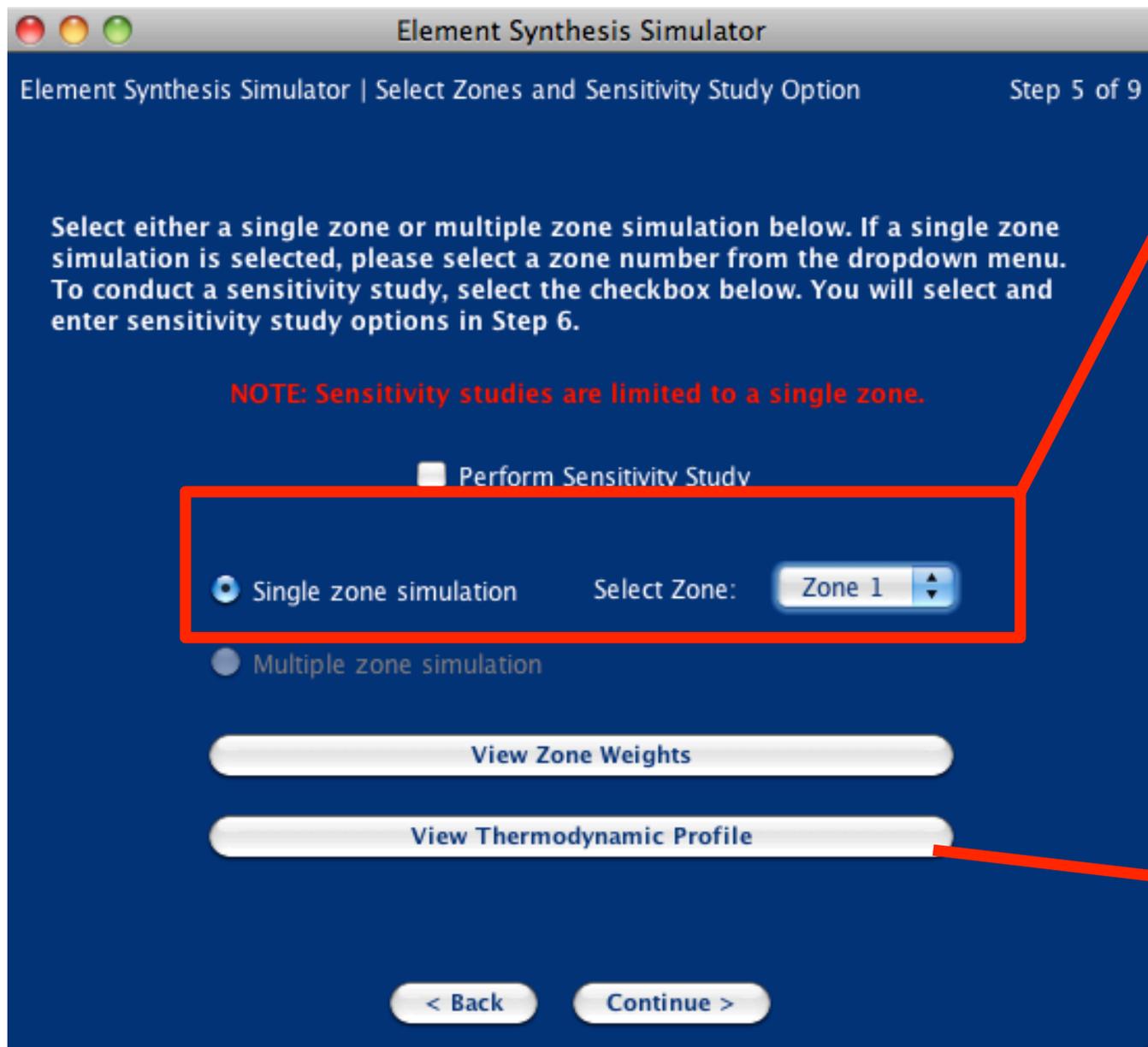
< Back **Continue >**

check here

this shows network is ready

click here

network is set up



some models have many zones

run zones one at a time OR have the system run them back to back

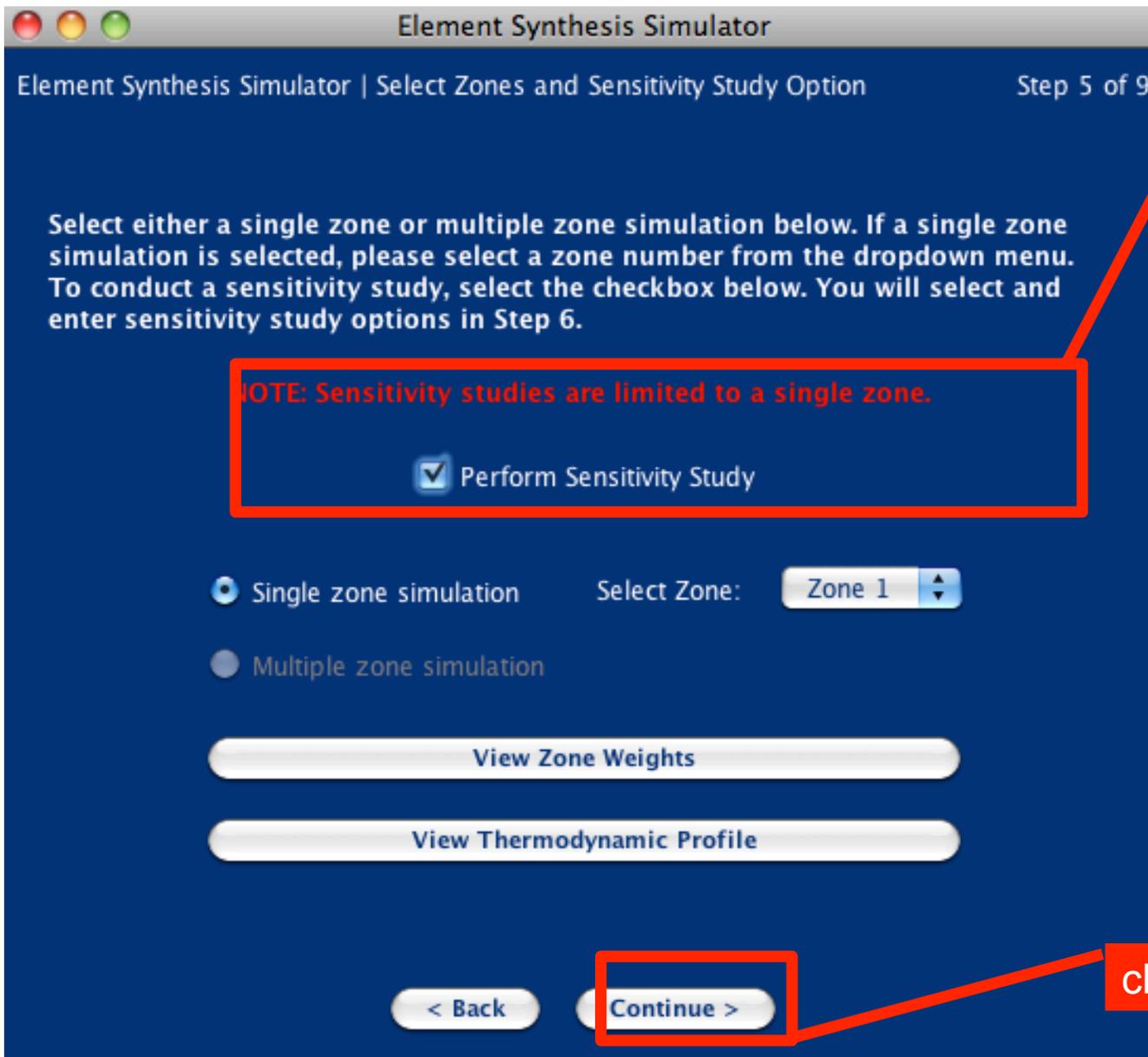
see the chosen profile (temperature vs. time, density vs. time)

set up single- or multi-zone, view thermo history

```
Thermo Profile for XRB Fisker 2007 Zone 90 for Zone Zone 1
Thermo Profile for XRB Fisker 2007 Zone 90 for Zone Zone 1

Zone 90
Start Time= -4.912623D+01 Stop Time= 1.060070D+04 Init Del t= 4.
-4.912623000000E+01 2.26000000E-01 1.29000000E+05
-4.800466400000E+01 2.26000000E-01 1.29000000E+05
-4.688309700000E+01 2.27000000E-01 1.29000000E+05
-4.594845800000E+01 2.27000000E-01 1.29000000E+05
-4.501382000000E+01 2.27000000E-01 1.28000000E+05
-4.407918100000E+01 2.28000000E-01 1.28000000E+05
-4.295761400000E+01 2.28000000E-01 1.28000000E+05
-4.161173400000E+01 2.29000000E-01 1.28000000E+05
-4.049016800000E+01 2.29000000E-01 1.28000000E+05
-3.936860100000E+01 2.30000000E-01 1.28000000E+05
-3.843396200000E+01 2.30000000E-01 1.28000000E+05
-3.749932400000E+01 2.30000000E-01 1.28000000E+05
-3.656468500000E+01 2.31000000E-01 1.27000000E+05
-3.563004600000E+01 2.31000000E-01 1.27000000E+05
-3.469540700000E+01 2.32000000E-01 1.27000000E+05
-3.376076900000E+01 2.32000000E-01 1.27000000E+05
-3.282613000000E+01 2.32000000E-01 1.27000000E+05
-3.170456300000E+01 2.33000000E-01 1.27000000E+05
-3.058299700000E+01 2.34000000E-01 1.27000000E+05
-2.964835800000E+01 2.34000000E-01 1.26000000E+05
-2.871371900000E+01 2.35000000E-01 1.26000000E+05
-2.777908000000E+01 2.35000000E-01 1.26000000E+05
-2.684444100000E+01 2.36000000E-01 1.26000000E+05
-2.590980300000E+01 2.37000000E-01 1.26000000E+05
-2.497516400000E+01 2.37000000E-01 1.25000000E+05
-2.419629800000E+01 2.38000000E-01 1.25000000E+05
-2.341743300000E+01 2.39000000E-01 1.25000000E+05
-2.263856700000E+01 2.39000000E-01 1.25000000E+05
-2.185970100000E+01 2.40000000E-01 1.25000000E+05
-2.108083600000E+01 2.41000000E-01 1.24000000E+05
-2.030197000000E+01 2.42000000E-01 1.24000000E+05
```

view chosen thermodynamic history for this post-processing calc



select here for sensitivity study

sensitivity studies vary one rate by a set of factors you supply and **automatically** run a series of simulations with those different rates, leaving all other rates unchanged

click here

setting up a sensitivity study

Element Synthesis Simulator

Element Synthesis Simulator | Sensitivity Study Options Step 6 of 9

Select a rate for the sensitivity study from a tree or a nuclide chart by clicking one of the buttons below. Then enter up to ten scale factors for this rate as a comma-separated list. Scale factors will be automatically reordered from smallest to largest and each corresponding, one-zone simulation will be calculated in that order.

NOTE: A sensitivity study may take up to an hour to complete.

Selected Rate:

Scale Factors (comma separated list):

choose a reaction to vary

setting up a sensitivity study

Select Reaction with a Nuclide Chart

0 1 2 3 4 5 6 7 8 9 10 11 12 13

Na Na

Ne Ne

F F

O ¹⁴O

N N

C C

B B

Be Be 9 13

Li Li 7 10 11 12

He He 3 5 8

H H 4 6

n 0 2

1

List of Reactions

- 14O --> 14N
- 14O --> p + 13N
- 14O --> n + 13O
- n + 14O --> 15O
- 4He + 14O --> 18Ne
- n + 14O --> 4He + 11C
- n + 14O --> p + 14N
- p + 14O --> n + 14F
- 4He + 14O --> p + 17F**
- 4He + 14O --> n + 17Ne

Selected Reaction

4He + 14O --> p + 17F

Select Reaction

Submit Reaction

Close Window

choose reaction to vary

then finally click here

Element Synthesis Simulator

Element Synthesis Simulator | Sensitivity Study Options Step 6 of 9

Select a rate for the sensitivity study from a tree or a nuclide chart by clicking one of the buttons below. Then enter up to ten scale factors for this rate as a comma-separated list. Scale factors will be automatically reordered from smallest to largest and each corresponding, one-zone simulation will be calculated in that order.

NOTE: A sensitivity study may take up to an hour to complete.

Selected Rate:

Scale Factors (comma separated list):

enter your
desired rate
variations here

click here

setting up a sensitivity study

Element Synthesis Simulator

Element Synthesis Simulator | Simulation Options Step 7 of 9

Enter simulation options and simulation notes below. Click *Continue* to begin the simulation.

Number of timesteps before exit: Include weak reactions

Start time (sec): Include screening

Stop time (sec):

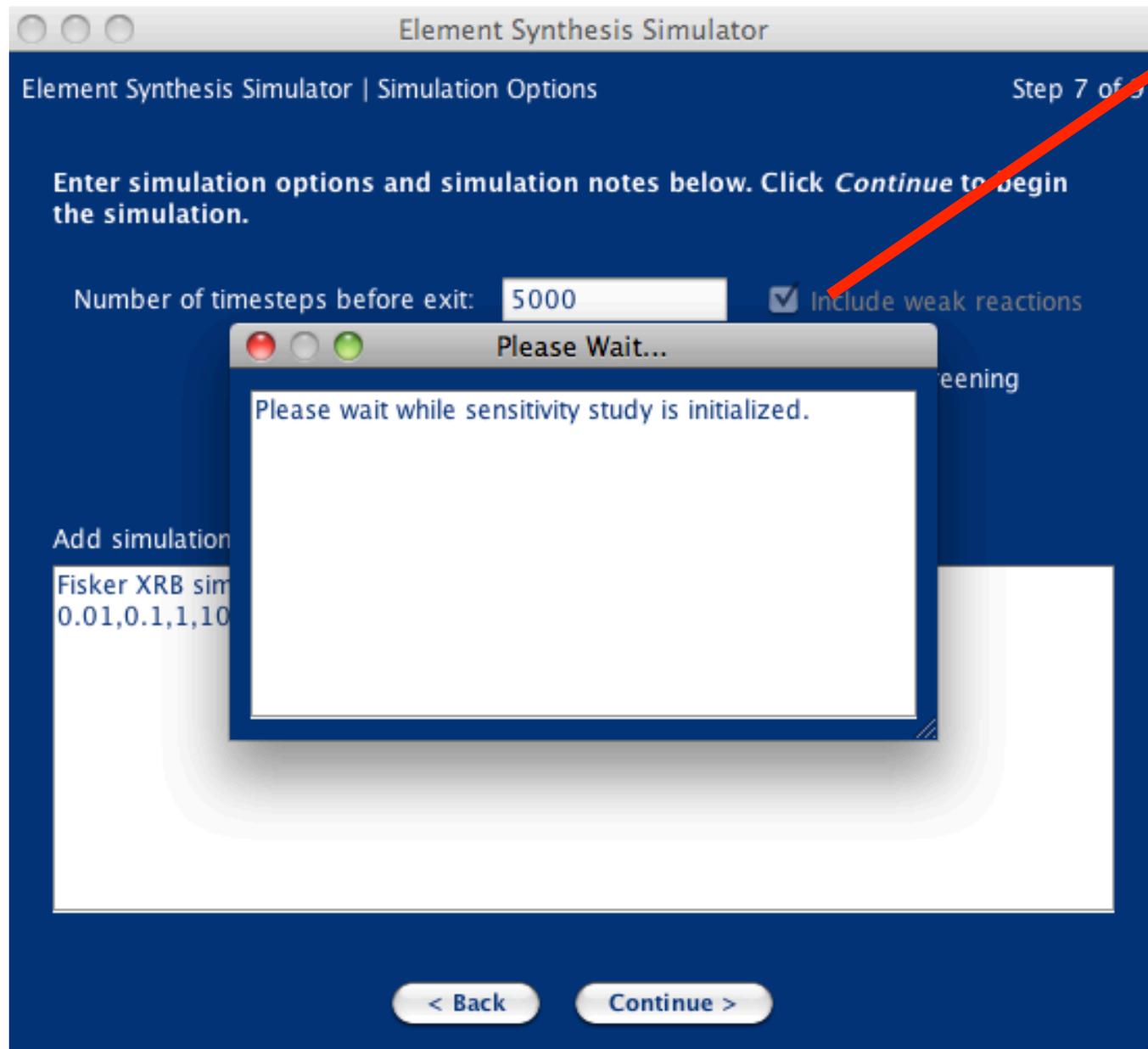
Add simulation notes below:

Fisker XRB simulation zone 90 sensitivity study 14O(alpha,p) variation
0.01,0.1,1,10,100 |

add notes here

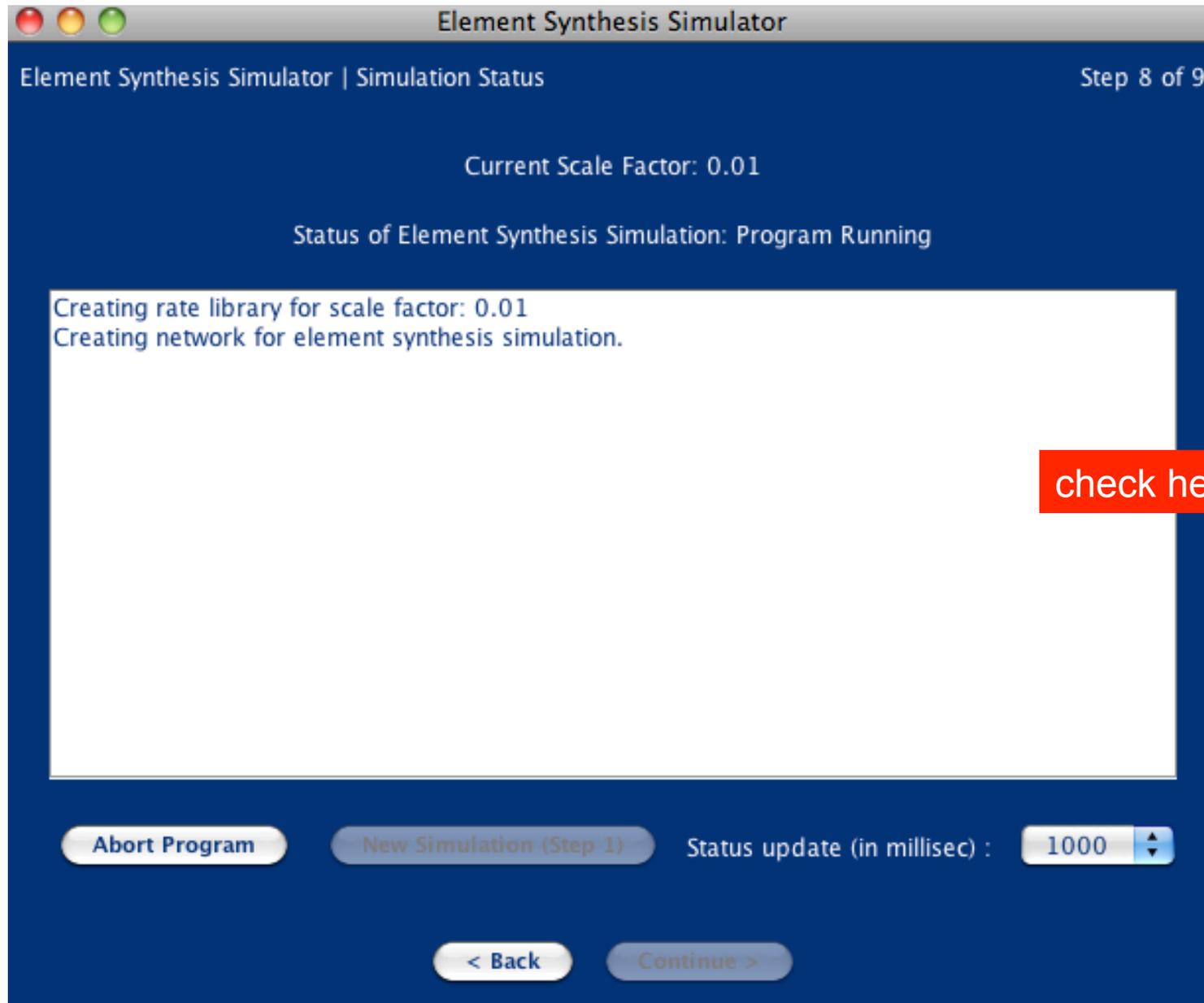
click here
to start

simulation options, notes attached to simulation, and starting run



wait a bit...

initializing the chosen sensitivity study



running the simulation – status report

Element Synthesis Simulator

Element Synthesis Simulator | Simulation Status Step 8 of 9

Current Scale Factor: 0.01

Status of Element Synthesis Simulation: Program Running

Step	Time(sec)	Temp(T9)
...		
Step = 633	Time(sec) = -4.912513727E+01	Temp(T9) = 2.26000E-01
Step = 634	Time(sec) = -4.912512737E+01	Temp(T9) = 2.26000E-01
Step = 635	Time(sec) = -4.912511742E+01	Temp(T9) = 2.26000E-01
Step = 636	Time(sec) = -4.912510742E+01	Temp(T9) = 2.26000E-01
Step = 637	Time(sec) = -4.912509734E+01	Temp(T9) = 2.26000E-01
Step = 638	Time(sec) = -4.912508719E+01	Temp(T9) = 2.26000E-01
Step = 639	Time(sec) = -4.912507696E+01	Temp(T9) = 2.26000E-01
Step = 640	Time(sec) = -4.912506664E+01	Temp(T9) = 2.26000E-01
Step = 641	Time(sec) = -4.912505622E+01	Temp(T9) = 2.26000E-01
Step = 642	Time(sec) = -4.912504568E+01	Temp(T9) = 2.26000E-01
Step = 643	Time(sec) = -4.912503502E+01	Temp(T9) = 2.26000E-01
Step = 644	Time(sec) = -4.912502421E+01	Temp(T9) = 2.26000E-01
Step = 645	Time(sec) = -4.912501323E+01	Temp(T9) = 2.26000E-01

check here

Abort Program New Simulation (Step 1) Status update (in millisec) : 1000

< Back Continue >

running the simulation – status report

Element Synthesis Simulator

Element Synthesis Simulator | Simulation Status Step 8 of 9

Current Scale Factor: 100.0

Status of Element Synthesis Simulation: Program Complete

```
...
Step = 3769 Time(sec) = 1.059580875E+04 Temp(T9) = 2.41000E-01
Step = 3770 Time(sec) = 1.059637732E+04 Temp(T9) = 2.41250E-01
Step = 3771 Time(sec) = 1.059702654E+04 Temp(T9) = 2.42250E-01
Step = 3772 Time(sec) = 1.059755172E+04 Temp(T9) = 2.43060E-01
Step = 3773 Time(sec) = 1.059801314E+04 Temp(T9) = 2.43771E-01
Step = 3774 Time(sec) = 1.059846919E+04 Temp(T9) = 2.44789E-01
Step = 3775 Time(sec) = 1.059883714E+04 Temp(T9) = 2.45733E-01
Step = 3776 Time(sec) = 1.059914805E+04 Temp(T9) = 2.46221E-01
Step = 3777 Time(sec) = 1.059948399E+04 Temp(T9) = 2.46581E-01
Step = 3778 Time(sec) = 1.059988116E+04 Temp(T9) = 2.47014E-01
Step = 3779 Time(sec) = 1.060031441E+04 Temp(T9) = 2.48141E-01
Step = 3780 Time(sec) = 1.060065735E+04 Temp(T9) = 2.48901E-01
Step = 3781 Time(sec) = 1.060070000E+04 Temp(T9) = 2.48996E-01
Element Synthesis Simulation Complete.
Sensitivity study complete!
```

Abort Program New Simulation (Step 1) Status update (in millisec) : 1000

< Back **Continue >**

click here

all simulations in sensitivity study completed

Element Synthesis Simulation Report

Element Synthesis Simulation Type	XRB Fisker 2007 Zone 90
Number of Timesteps Before Exit	5000
Start Time (sec)	-4.912623E+01
Stop Time (sec)	1.060070E+04
Include Weak Reactions	Y
Include Screening	Y
User Notes	Fisker XRB simulation zone 90 sensitivity study 14O(alpha,p) variation 0.01,0.1,1,10,100
Selected Zones	1
Initial Abundance Profile	Xray_Burst_Expanded_Abund
26Al State	metastable + ground
Isotope List Selected By	Sunet File
Sunet File	Xray_Burst_Expanded
Reaction Rate Library	ReaclibV2.0
Selected Reaction Rate	4He + 14O --> p + 17F
Scale Factors	0.01, 0.1, 1.0, 10.0, 100.0

 View Scaled Rate Parameters

Save as Text File

Save as HTML File

Copy

Print

Save Simulation

click here

< Back

Close Element Synthesis Simulator

Element Synthesis Simulator Home

Element Synthesis Visualizer

simulation final report – and save the simulation

de Weak Reactions | Y

Save Sensitivity Study...

Enter the principle name for the sensitivity study in the field below. This name will be appended by an underscore and then an integer corresponding to the order in which each single-zone simulation was calculated.

xrayburst_fisker_zone90_august2012

OK Cancel

click here

enter filename here

A screenshot of a software dialog box titled "Save Sensitivity Study...". The dialog has a blue background and white text. It contains a text input field with the text "xrayburst_fisker_zone90_august2012". Below the input field are two buttons: "OK" and "Cancel". A red box highlights the "OK" button with the text "click here" below it. Another red box highlights the text input field with the text "enter filename here" to its right. The window title bar shows "de Weak Reactions | Y".

Element Synthesis Simulation saved

Simulation was saved to
/USER/xrayburst_fisker_zone90_august2012_1
through
/USER/xrayburst_fisker_zone90_august2012_5

Ok

click here

A screenshot of a software dialog box titled "Element Synthesis Simulation saved". The dialog has a blue background and white text. It contains a text area with the text "Simulation was saved to /USER/xrayburst_fisker_zone90_august2012_1 through /USER/xrayburst_fisker_zone90_august2012_5". Below the text area is a button labeled "Ok". A red box highlights the "Ok" button with the text "click here" to its right. The window title bar shows "Element Synthesis Simulation saved".

saving the simulations in the sensitivity study

Element Synthesis Simulation Report

Element Synthesis Simulation Type	XRB Fisker 2007 Zone 90
Number of Timesteps Before Exit	5000
Start Time (sec)	-4.912623E+01
Stop Time (sec)	1.060070E+04
Include Weak Reactions	Y
Include Screening	Y
User Notes	Fisker XRB simulation zone 90 sensitivity study 14O(alpha,p) variation 0.01,0.1,1,10,100
Selected Zones	1
Initial Abundance Profile	Xray_Burst_Expanded_Abund
26Al State	metastable + ground
Isotope List Selected By	Sunet File
Sunet File	Xray_Burst_Expanded
Reaction Rate Library	ReaclibV2.0
Selected Reaction Rate	4He + 14O --> p + 17F
Scale Factors	0.01, 0.1, 1.0, 10.0, 100.0

 View Scaled Rate Parameters

Save as Text File

Save as HTML File

Copy

Print

Save Simulation

< Back

Close Element Synthesis Simulator

Element Synthesis Simulator Home

Element Synthesis Visualizer

proceed to visualizing the simulations

click here

Element Synthesis Visualizer

Element Synthesis Visualizer | Select Simulations

Select simulations from the tree below.

- Simulations
 - User
 - Shared

Selected Simulations

- xrayburst_fisker_zone90_august2012_1 (zone_01)
- xrayburst_fisker_zone90_august2012_2 (zone_01)
- xrayburst_fisker_zone90_august2012_3 (zone_01)
- xrayburst_fisker_zone90_august2012_4 (zone_01)
- xrayburst_fisker_zone90_august2012_5 (zone_01)

Remove Selected Simulation Add Selected Simulation

< Back Continue >

the simulations you ran are pre-loaded

you can add additional simulations to the list by using the file tree on the left

click here

Element Synthesis Visualizer – you are now using this tool

Element Synthesis Visualizer

Element Synthesis Visualizer | Visualization Tools

Step

1-D Plots

- Abundance Plotting Interface**
- Sensitivity Study Plotting Interface
- Final Weighted Abund Plotting Interface
- Thermo Profile Plotting Interface

2-D Plots

- Element Synthesis Animator
- Final Weighted Abund Nuclide Chart
- Integrated Flux Nuclide Chart

– Create 1-D plots of abundance vs. time for selected isotopes.

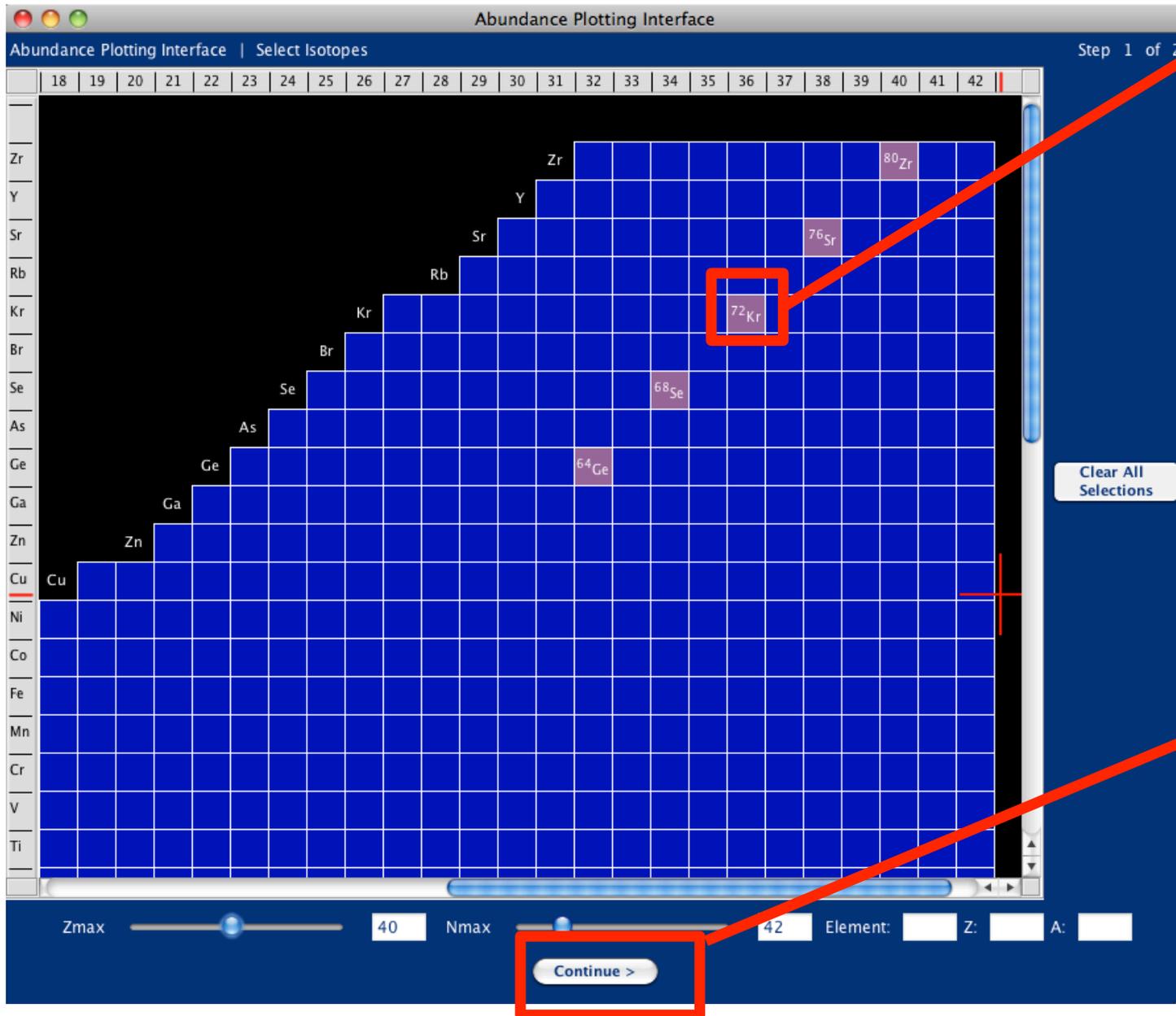
– Create 1-D plots of abundance ratio vs. mass number for selected isotopes.

View Sample

< Back Close Element Synthesis Visualizer

mouseover here to see description, click to launch plot

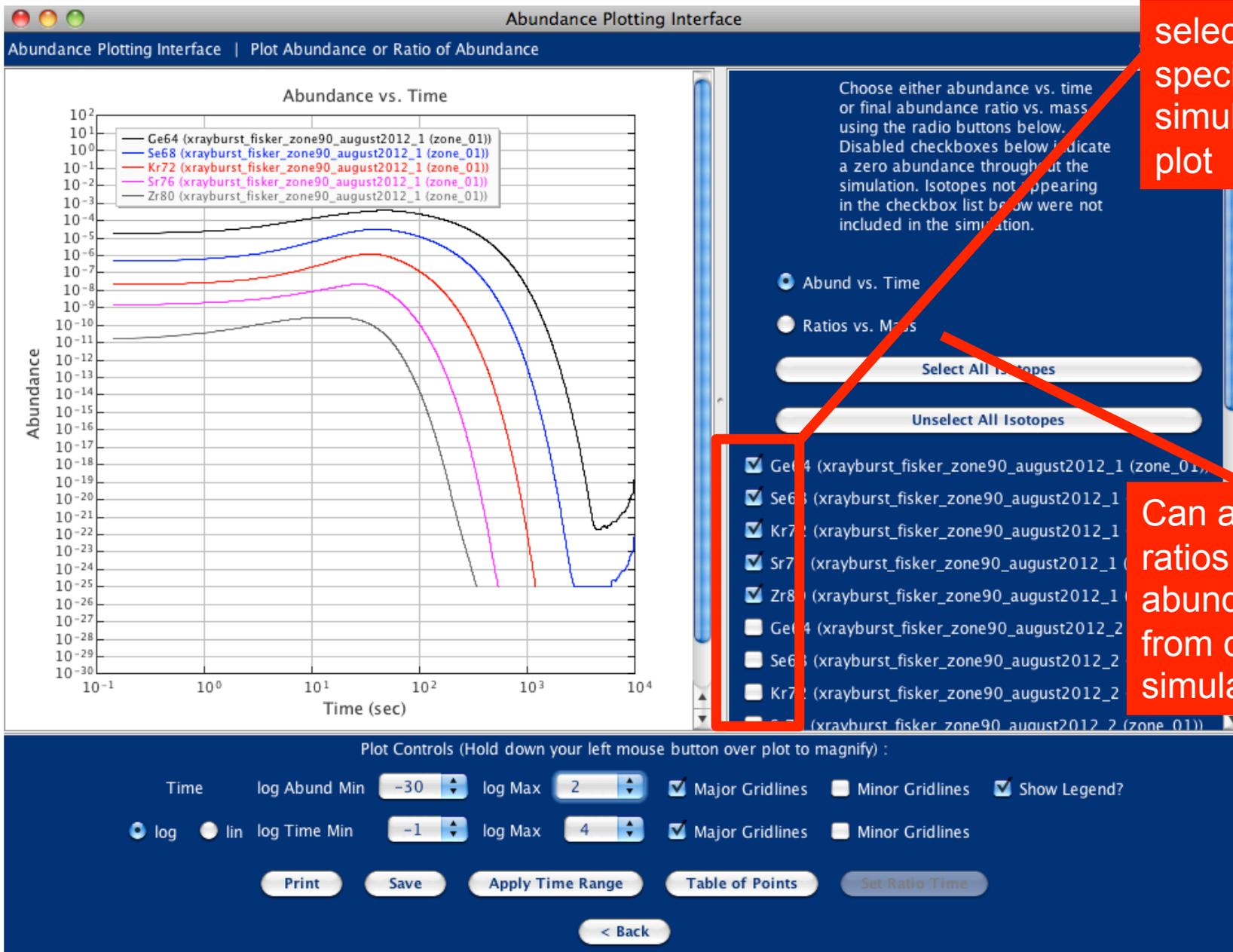
plot abundances vs. time



select nuclei here

click here

choose which nuclei to plot abundance vs. time



select nuclei in specific simulations to plot

Can also plot ratios of abundances from different simulations

view, modify, save abundance vs. time plots

Element Synthesis Visualizer

Element Synthesis Visualizer | Visualization Tools

Step

1-D Plots

Abundance Plotting Interface

Sensitivity Study Plotting Interface

Final Weighted Abund Plotting Interface

Thermo Profile Plotting Interface

2-D Plots

Element Synthesis Animator

Final Weighted Abund Nuclide Chart

Integrated Flux Nuclide Chart

- Create 1-D plots of final weighted abundance vs. rate scale factor.

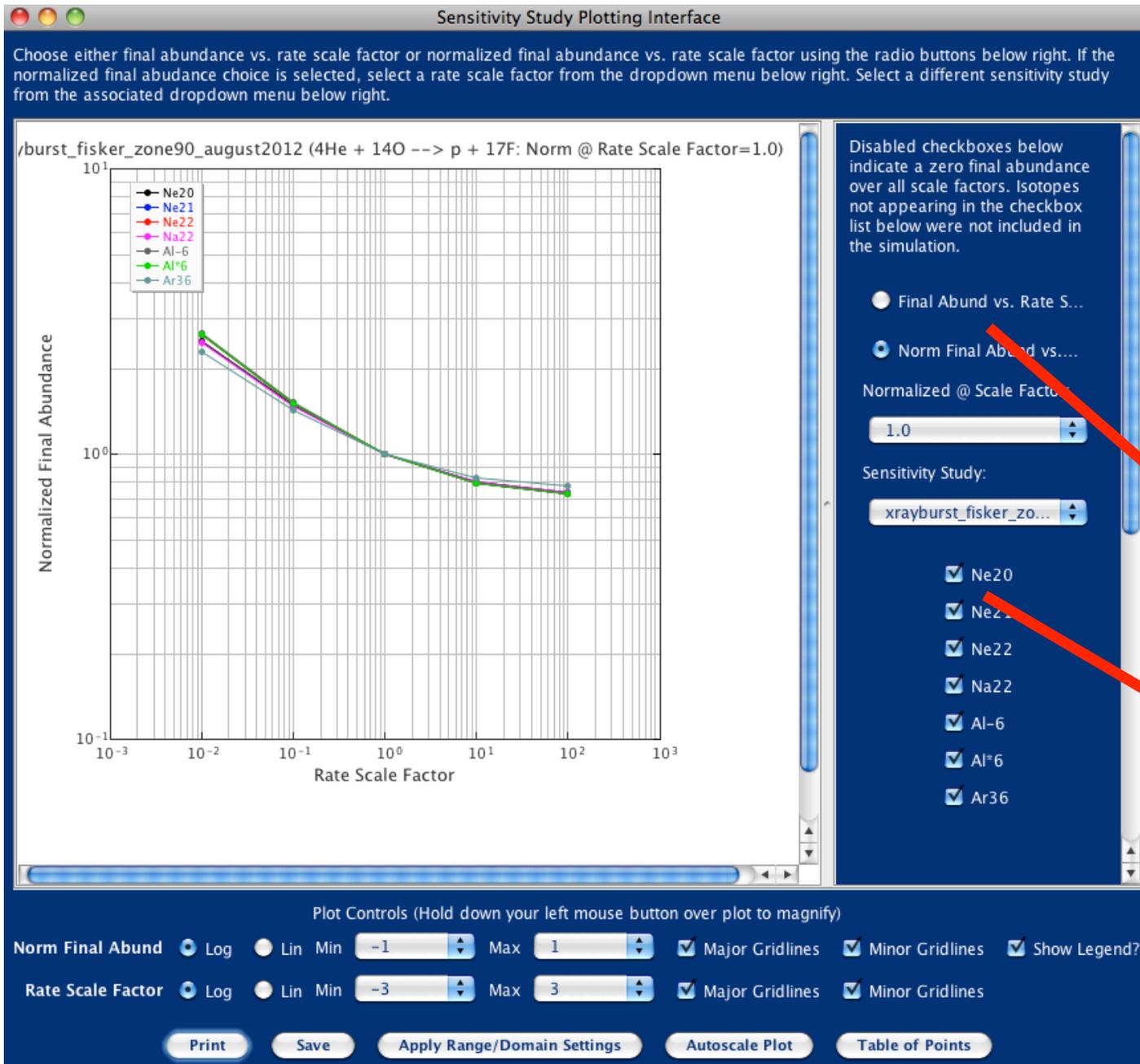
View Sample

< Back

Close Element Synthesis Visualizer

mouseover here to see description, click to launch plot

plot abundance vs. rate variation for a sensitivity study

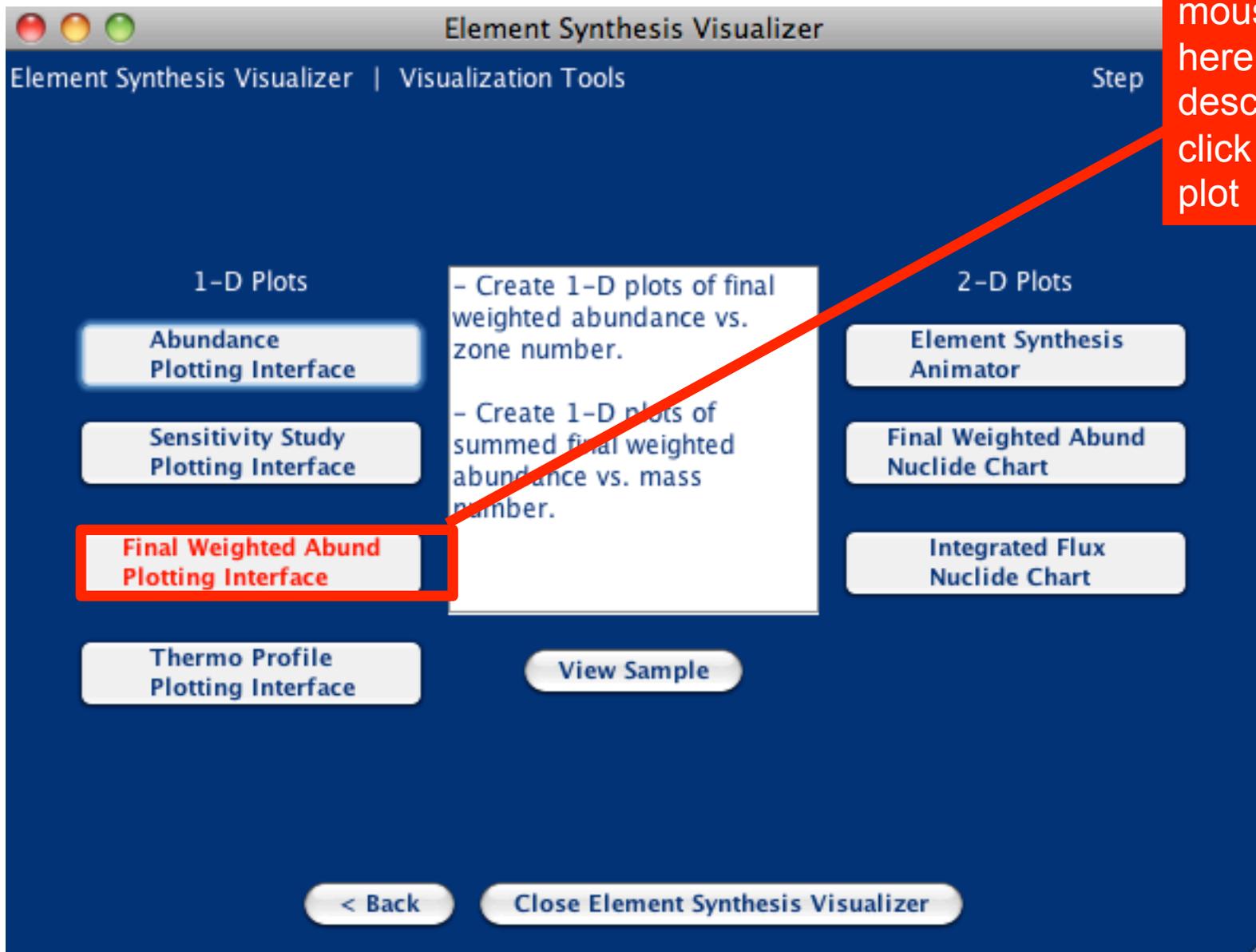


this shows the dependence of predicted abundances on variation of input reaction rate

choose to normalize rates

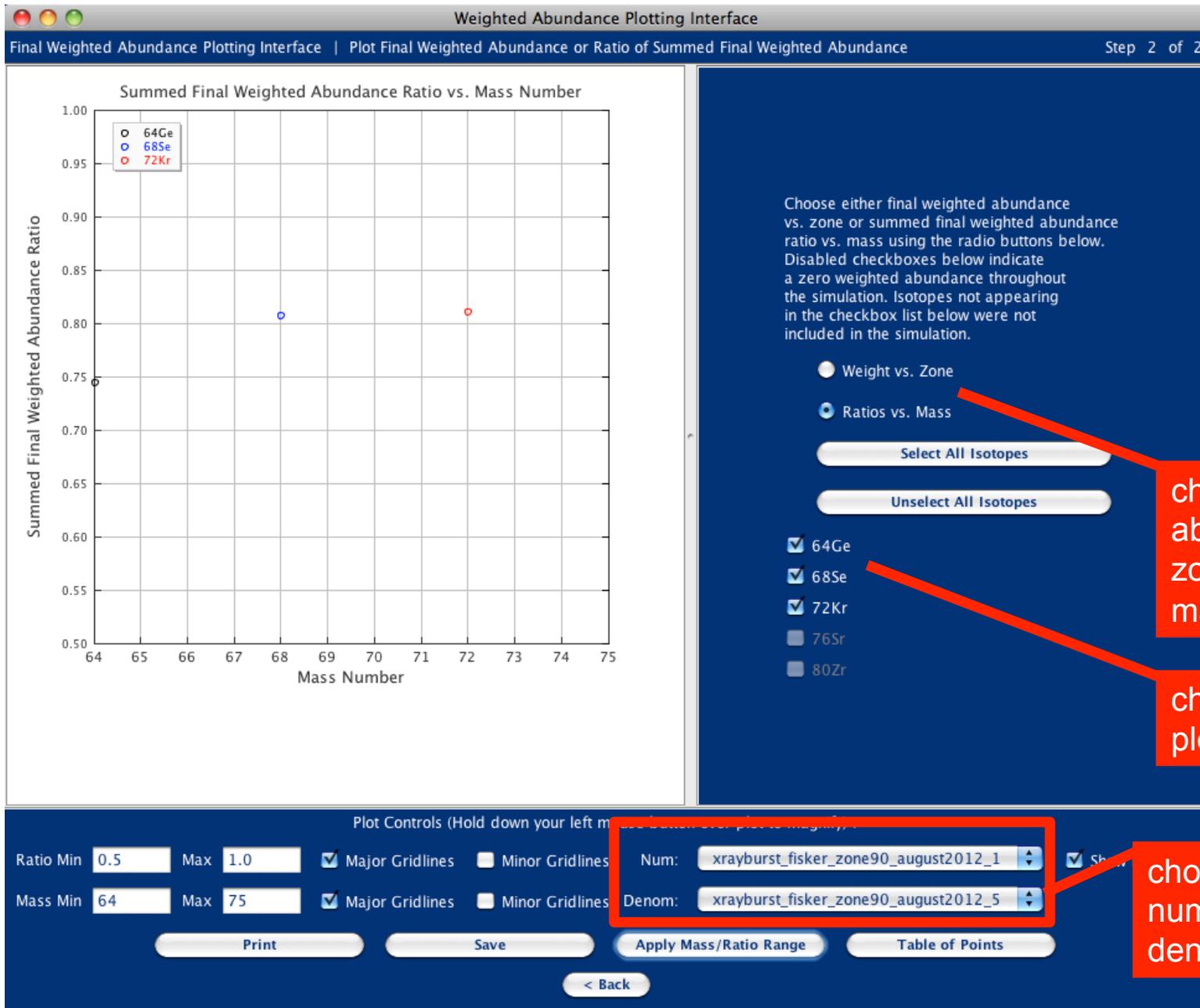
choose nuclei to plot

plot abundance vs. rate variation for a sensitivity study



mouseover here to see description, click to launch plot

plot final weighted abundances vs. zone, for multizone runs

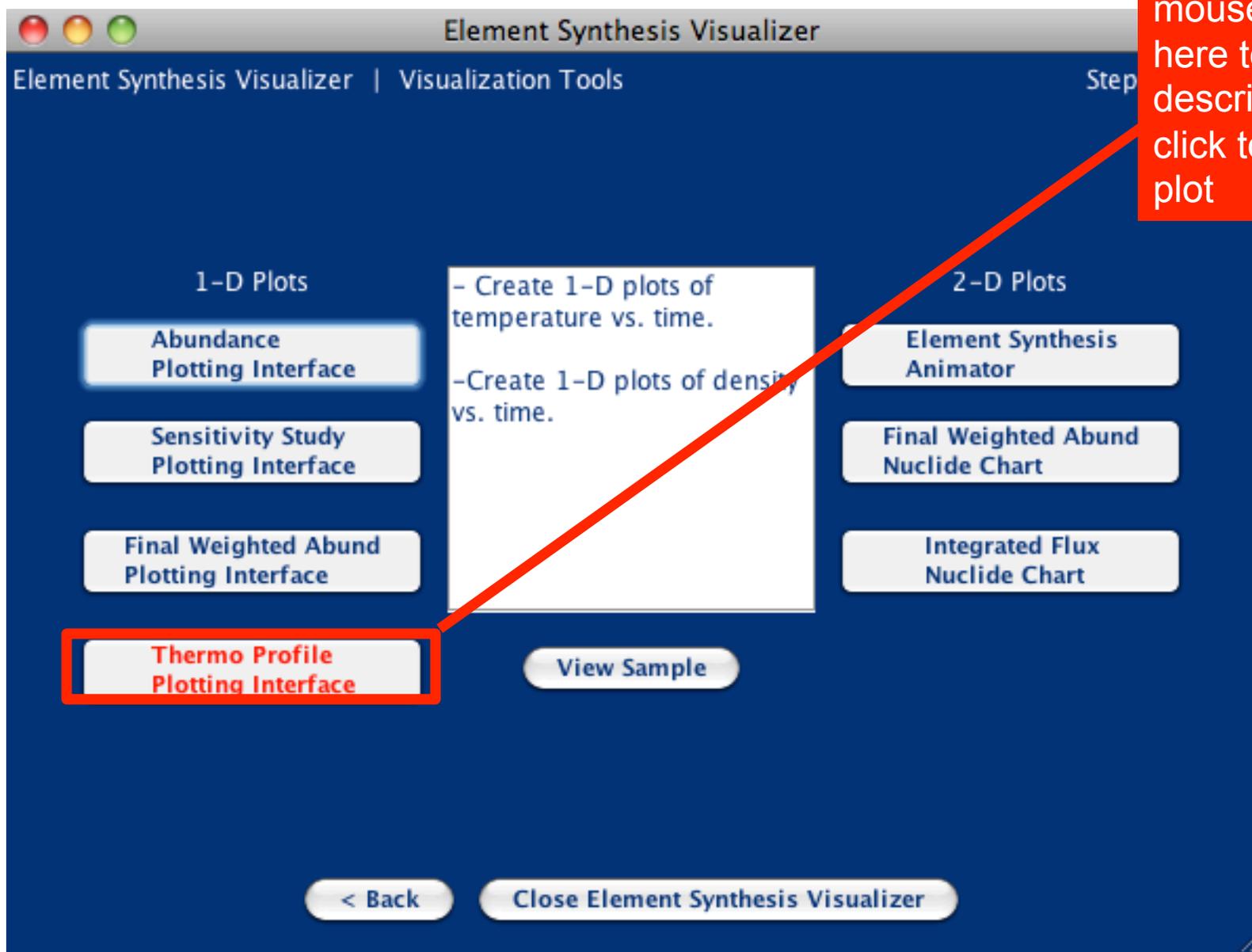


choose to plot abundance vs. zone or ratio vs. mass

choose nuclei to plot

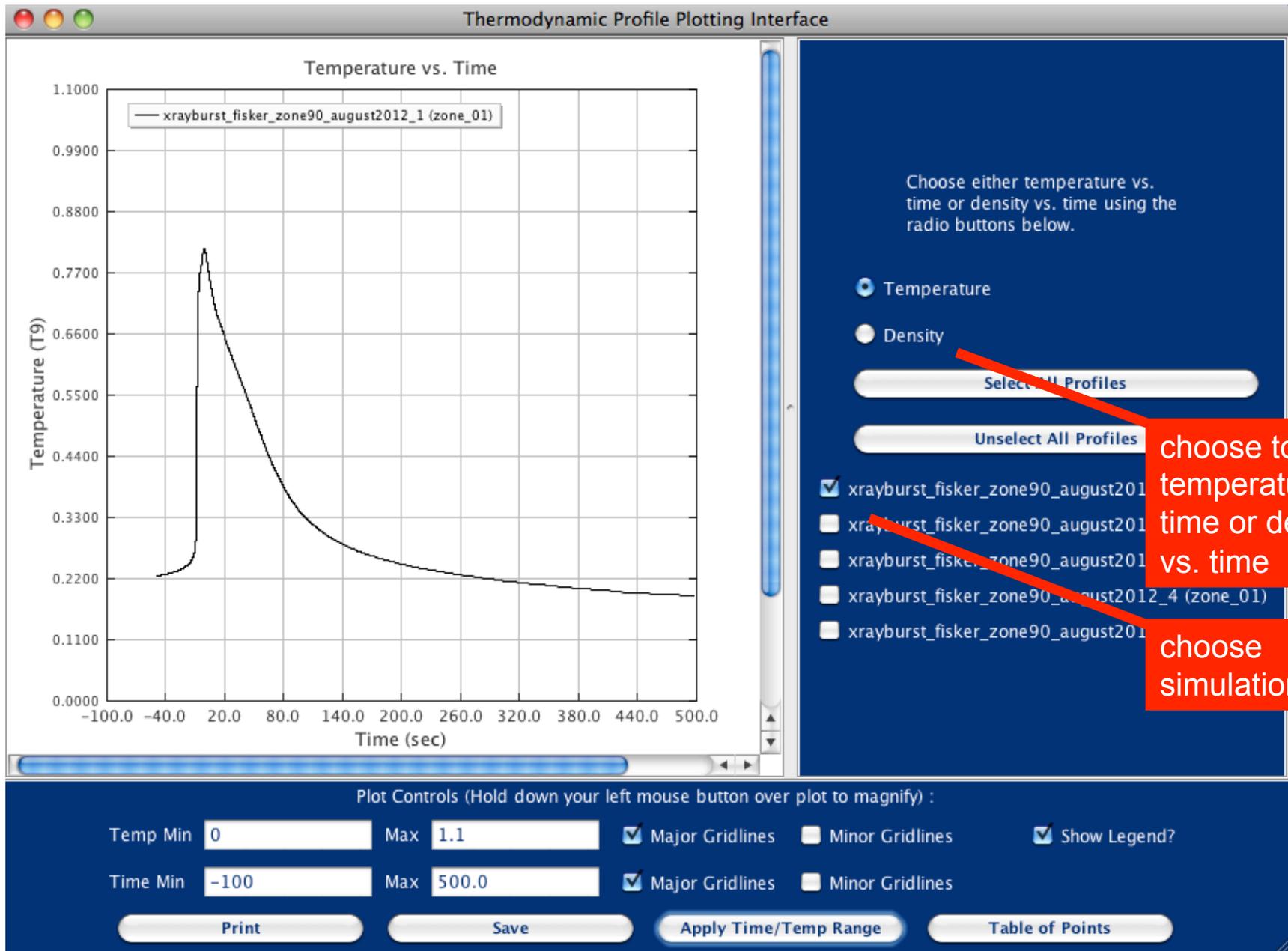
choose numerator and denominator

plots a ratio of abundances in different sensitivity study runs



mouseover here to see description, click to launch plot

plot the thermodynamic profiles



choose to plot temperature vs. time or density vs. time

choose simulation to plot

plot the thermodynamic profiles

The screenshot shows a software window titled "Element Synthesis Visualizer" with a subtitle "Visualization Tools". The interface is divided into two main sections: "1-D Plots" on the left and "2-D Plots" on the right. A central text box provides instructions for the 2-D plots. The "Element Synthesis Animator" button in the 2-D section is highlighted with a red box, and a red callout box points to it with the text "mouseover here to see description, click to launch plot".

1-D Plots

- Abundance Plotting Interface
- Sensitivity Study Plotting Interface
- Final Weighted Abund Plotting Interface
- Thermo Profile Plotting Interface

2-D Plots

- Element Synthesis Animator**
- Final Weighted Abund Nuclide Chart
- Integrated Flux Nuclide Chart

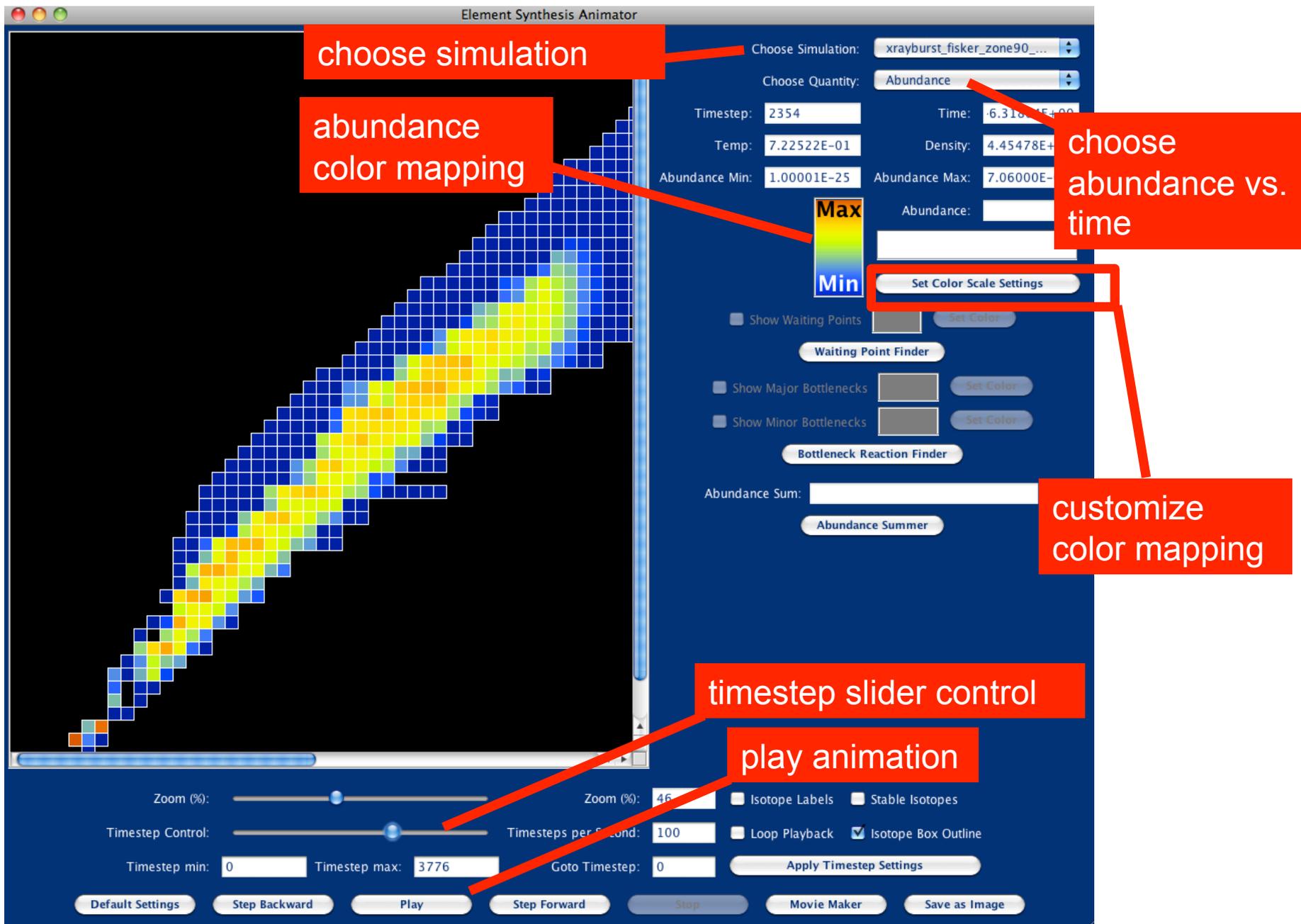
Central Text:

- Create animated 2-D plots on a nuclide chart of abundance, time derivative of abundance, or normalized reaction flux vs. time.
- Generate exportable animations.

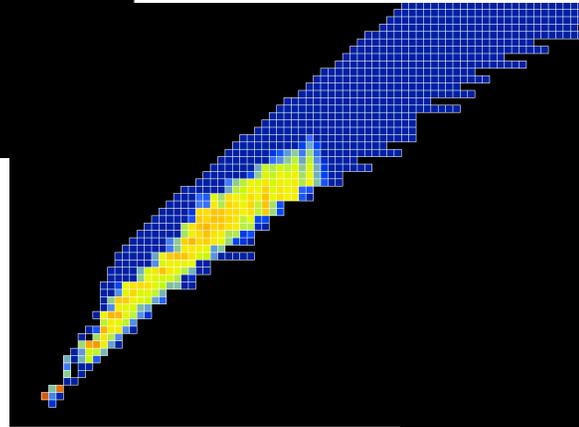
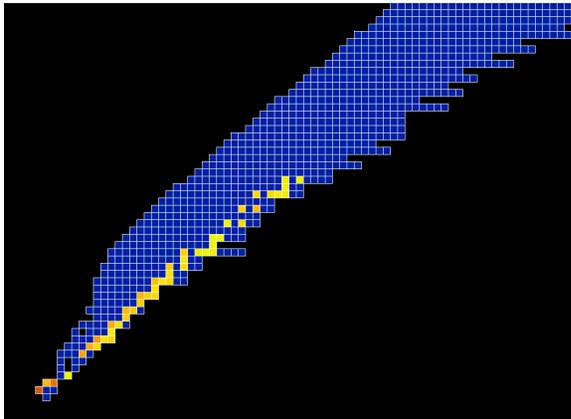
Navigation:

- View Sample
- < Back
- Close Element Synthesis Visualizer

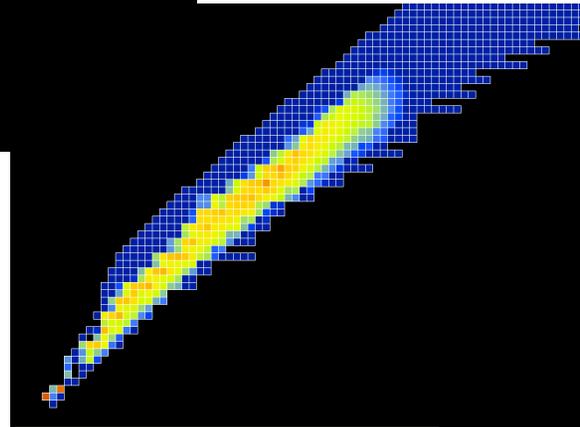
2D animated nuclide chart of abundance or flux vs. time



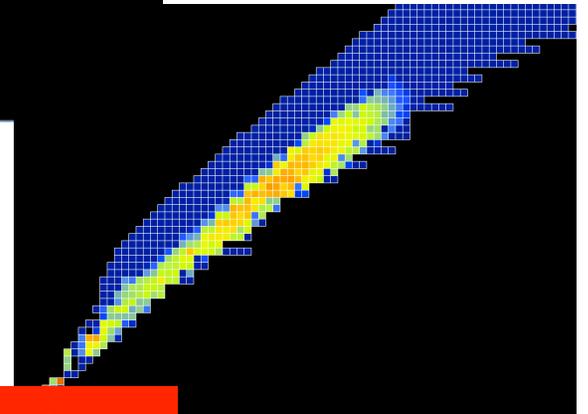
2D animated nuclide chart of abundance vs. time



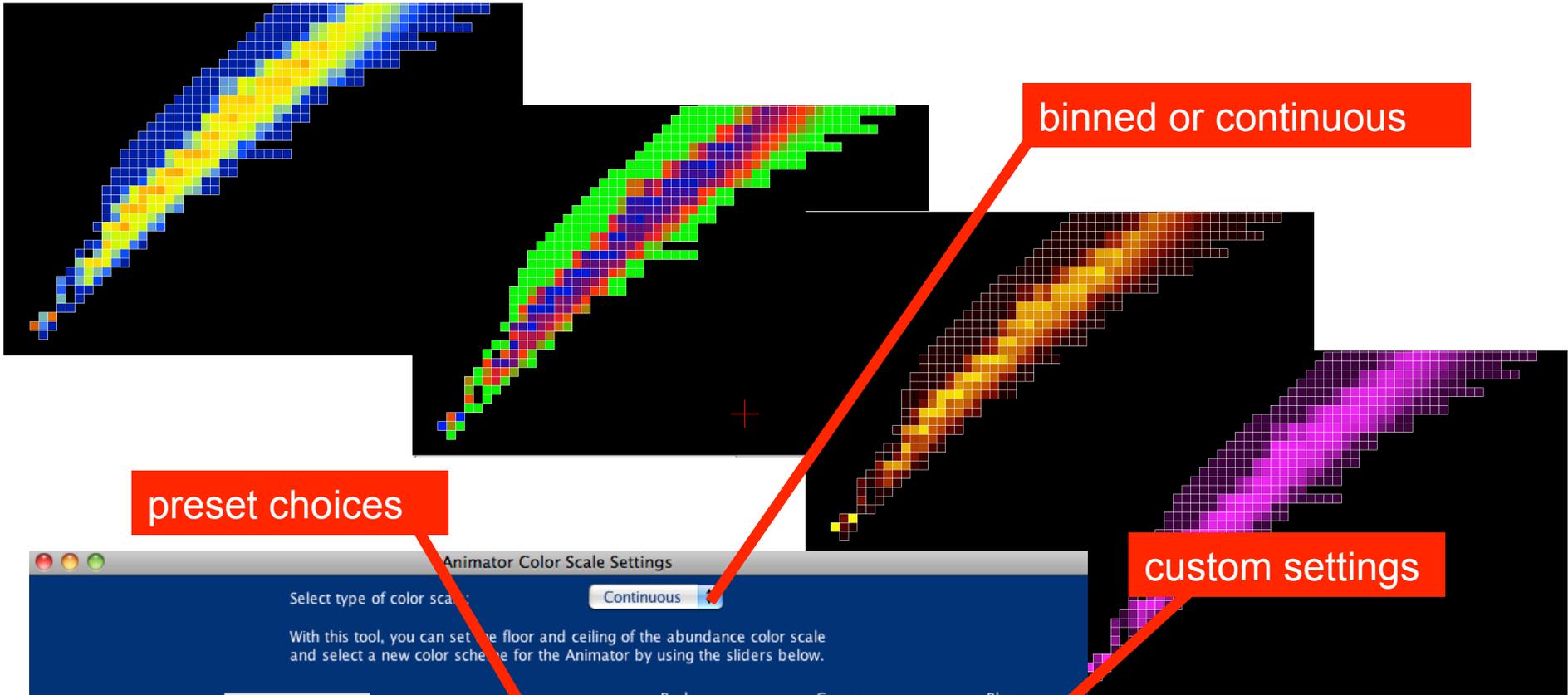
animation
screenshots



we will render a
movie of these plots
to your specifications



2D animated nuclide chart of abundance vs. time



binned or continuous

preset choices

custom settings

Animator Color Scale Settings

Select type of color scale: Continuous

With this tool, you can set the floor and ceiling of the abundance color scale and select a new color scheme for the Animator by using the sliders below.

Abundance max:

Abundance min:

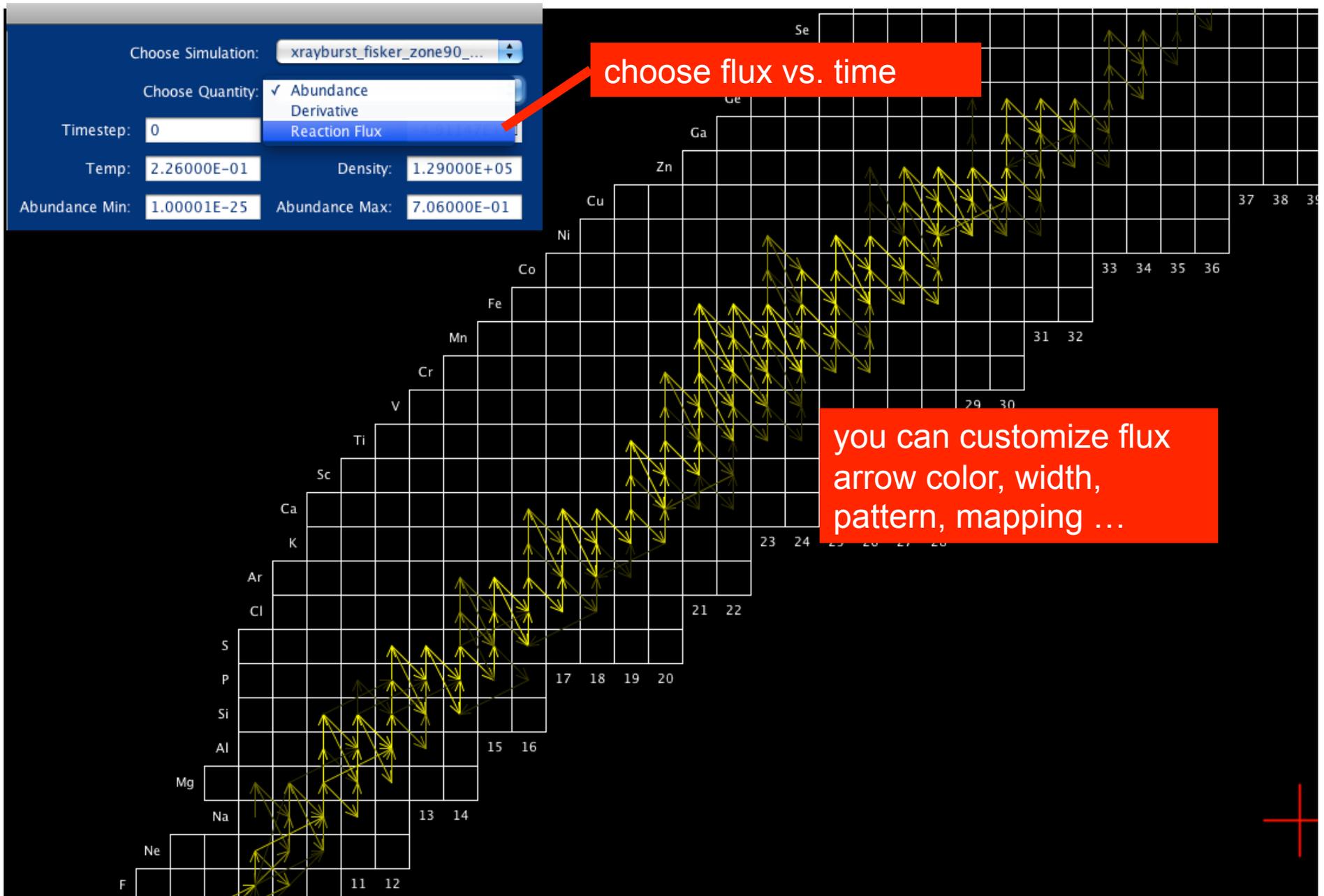
Choose a color scheme:

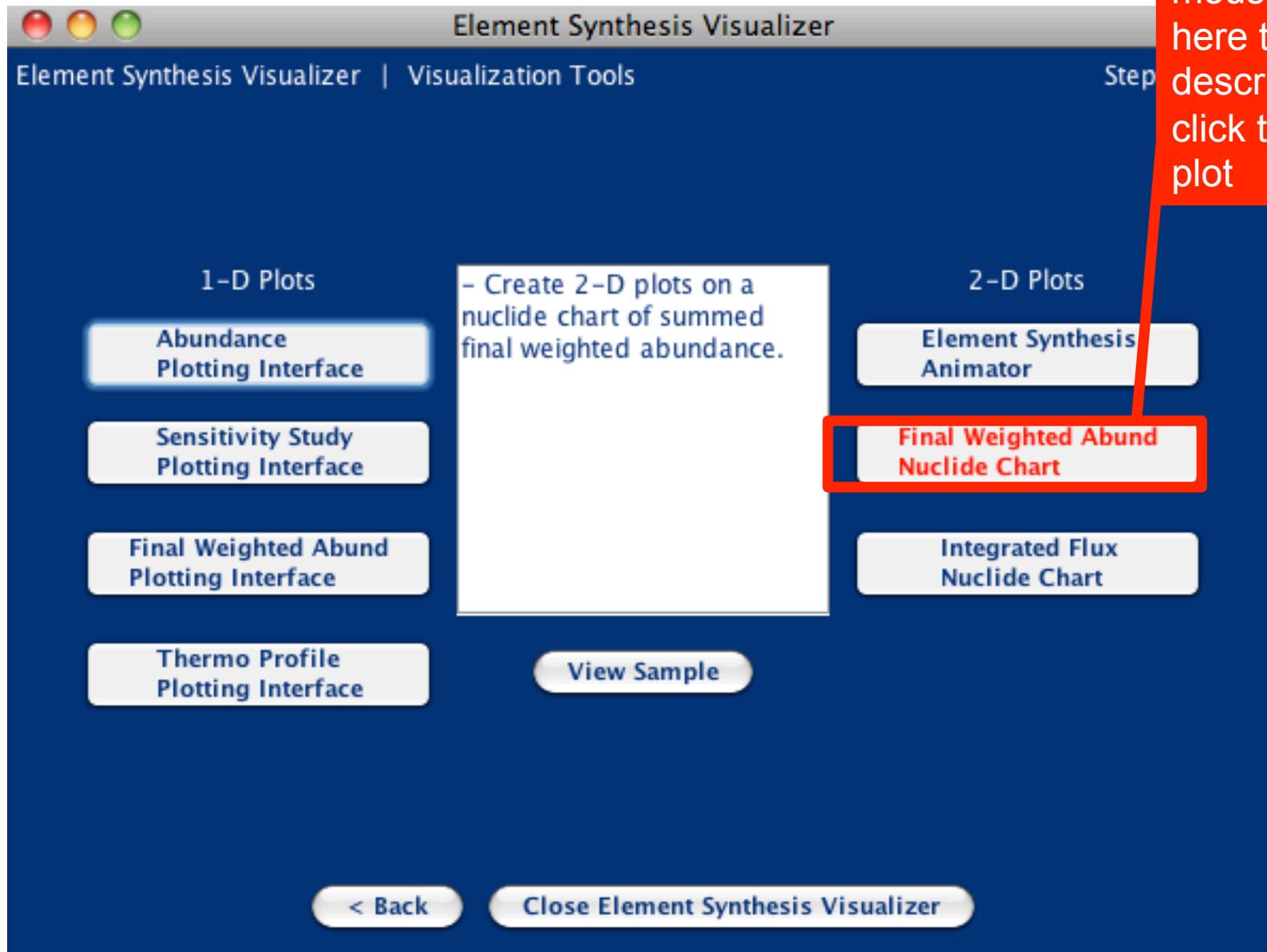
Red		Green		Blue	
Position:	Amount:	Position:	Amount:	Position:	Amount:
<input type="text" value="0.8"/>	<input type="text" value="0.5"/>	<input type="text" value="0.6"/>	<input type="text" value="0.4"/>	<input type="text" value="0.2"/>	<input type="text" value="0.3"/>

Max
 Min

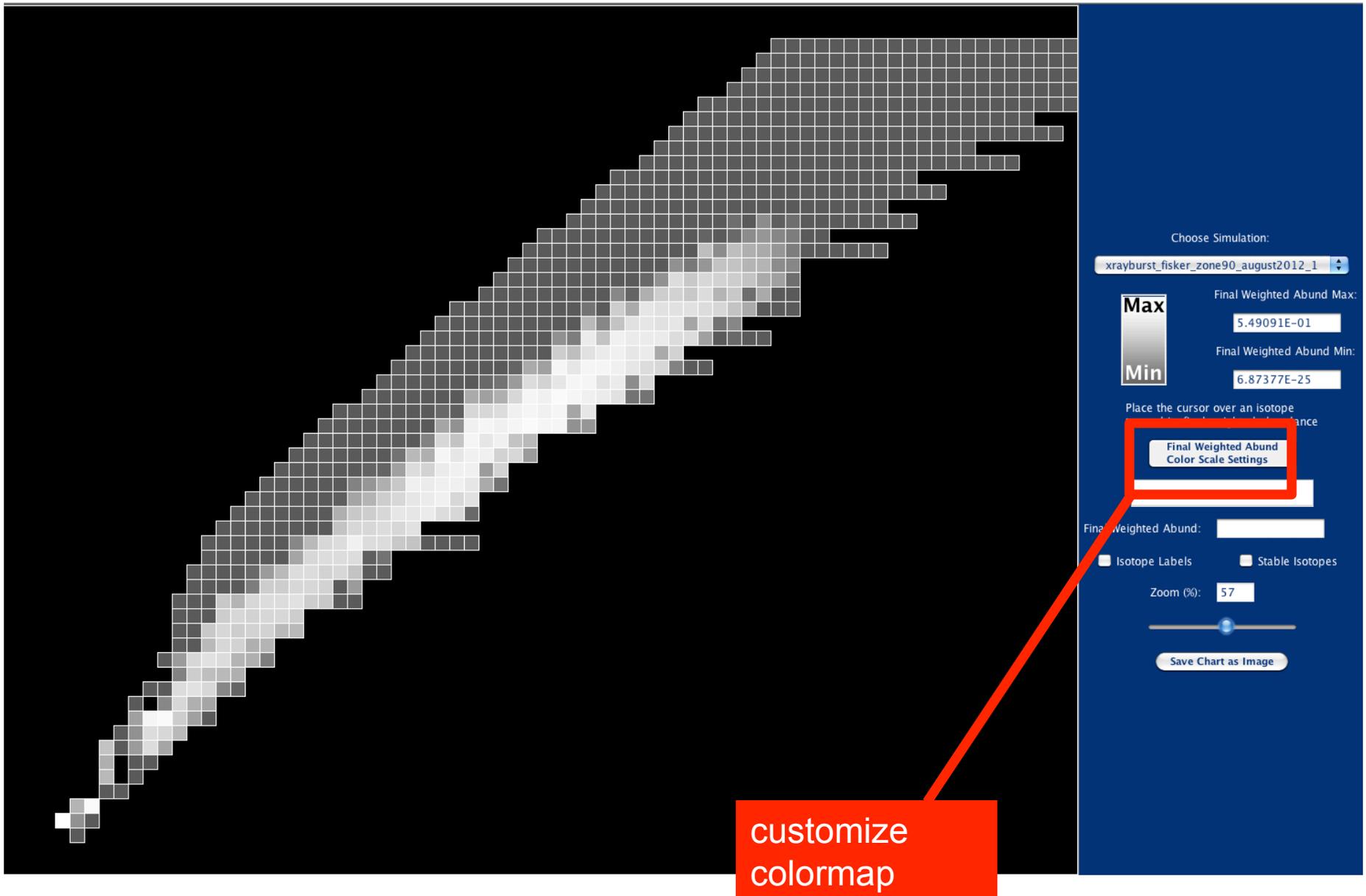
Map values outside of range to max/min color
 Show only values within this range

customizing the color mapping to look for special effects





plotting out the final abundances (weighted if a multi-zone run)



plotting out the final abundances (weighted if a multi-zone run)

Element Synthesis Visualizer

Element Synthesis Visualizer | Visualization Tools

Step

1-D Plots

- Abundance Plotting Interface
- Sensitivity Study Plotting Interface
- Final Weighted Abund Plotting Interface
- Thermo Profile Plotting Interface

2-D Plots

- Element Synthesis Animator
- Final Weighted Abund Nuclide Chart
- Integrated Flux Nuclide Chart**

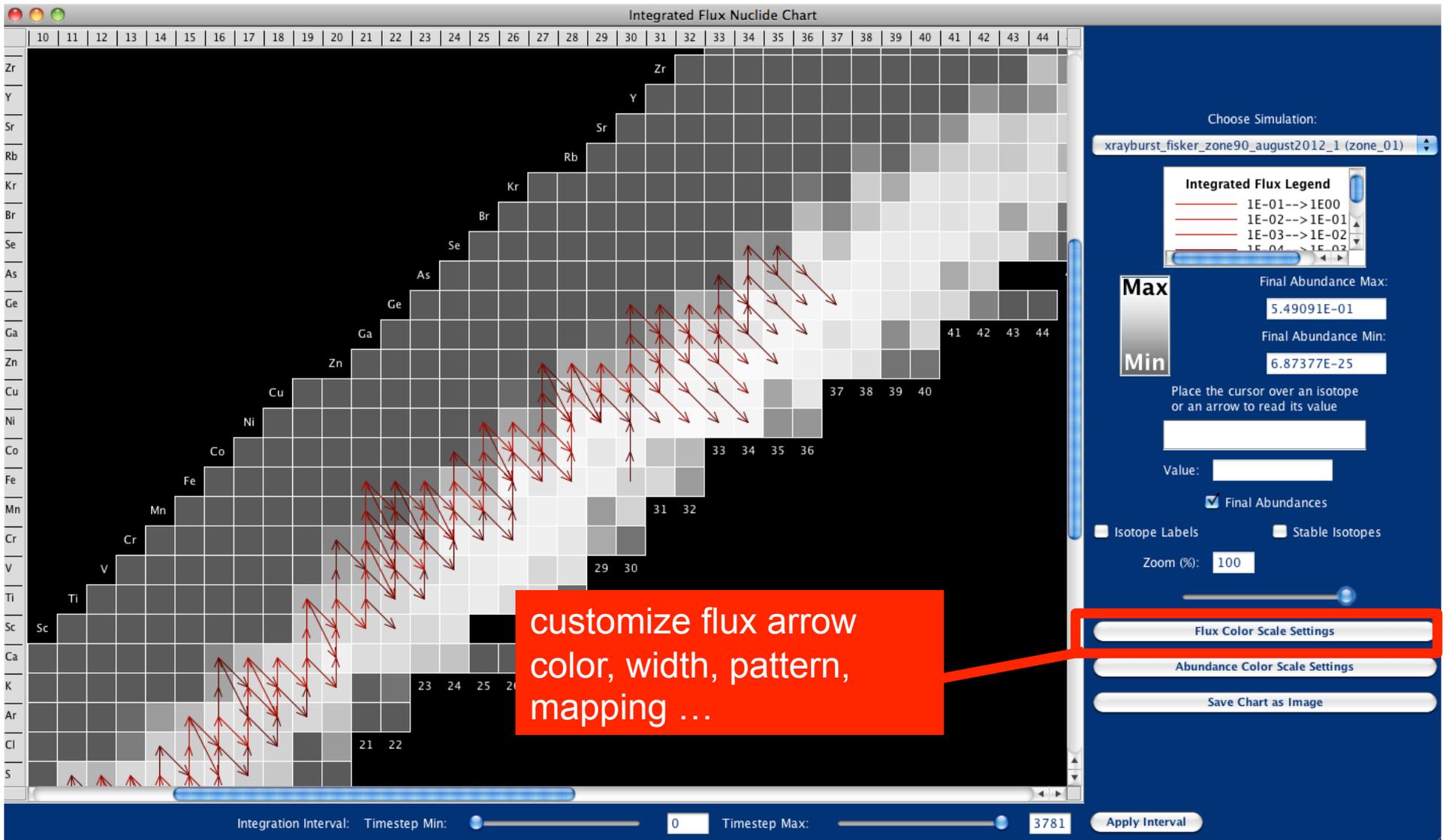
- Create 2-D plots on a nuclide chart of integrated reaction flux and final abundance.

View Sample

< Back Close Element Synthesis Visualizer

mouseover here to see description, click to launch plot

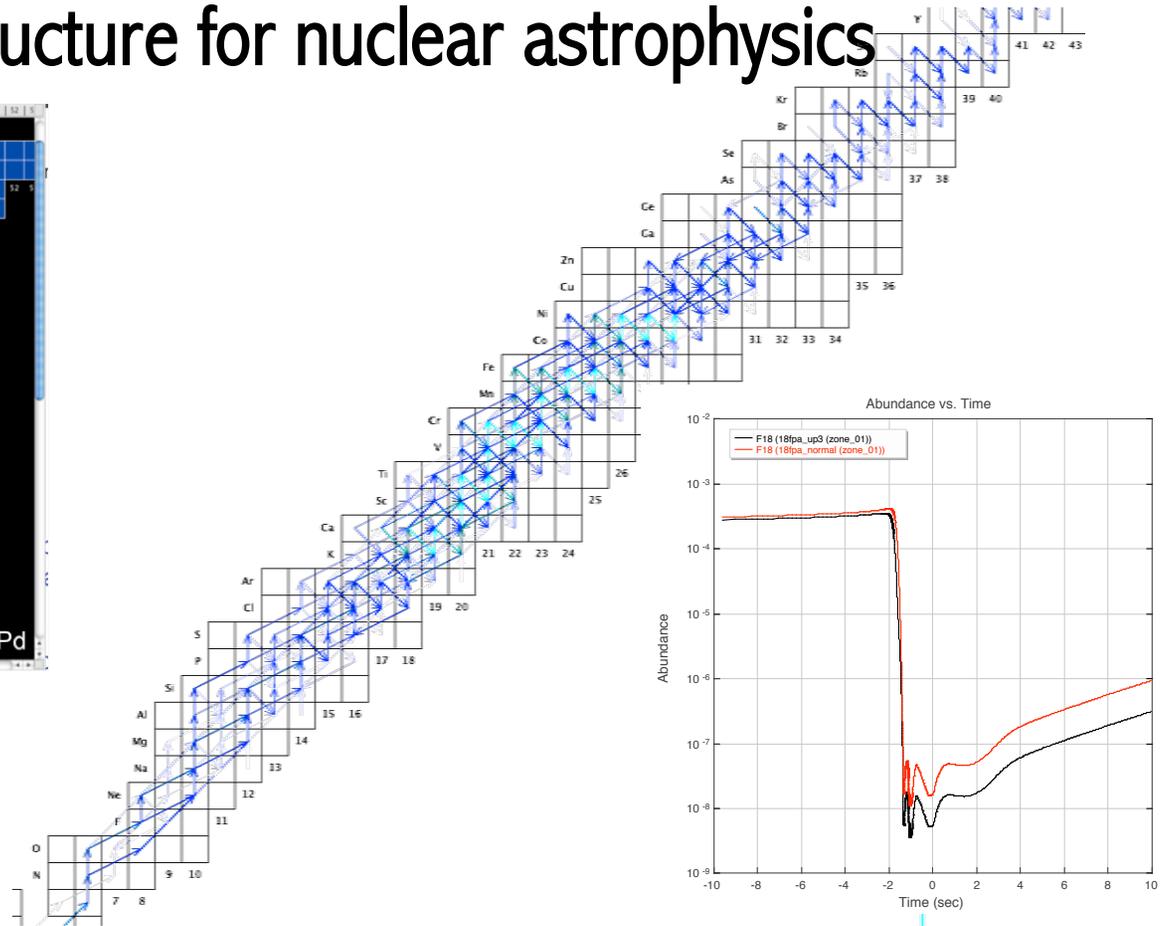
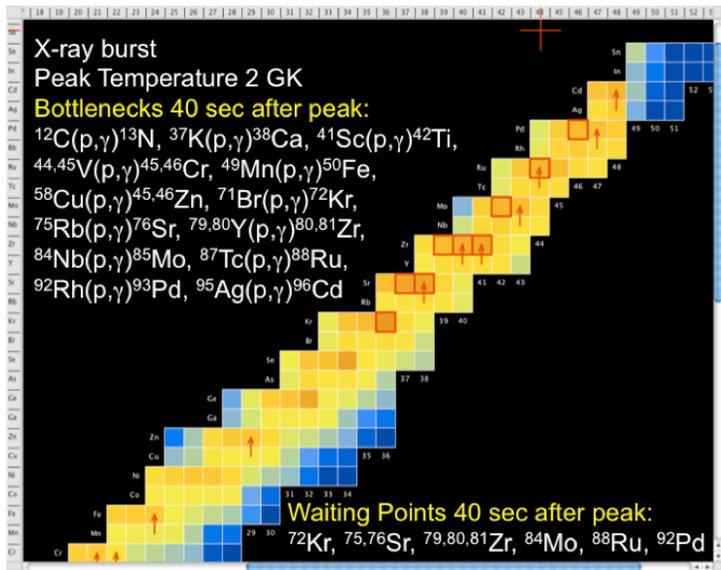
plotting out final abundances & integrated fluxes



customize flux arrow color, width, pattern, mapping ...

plotting out final abundances & integrated fluxes

computational infrastructure for nuclear astrophysics

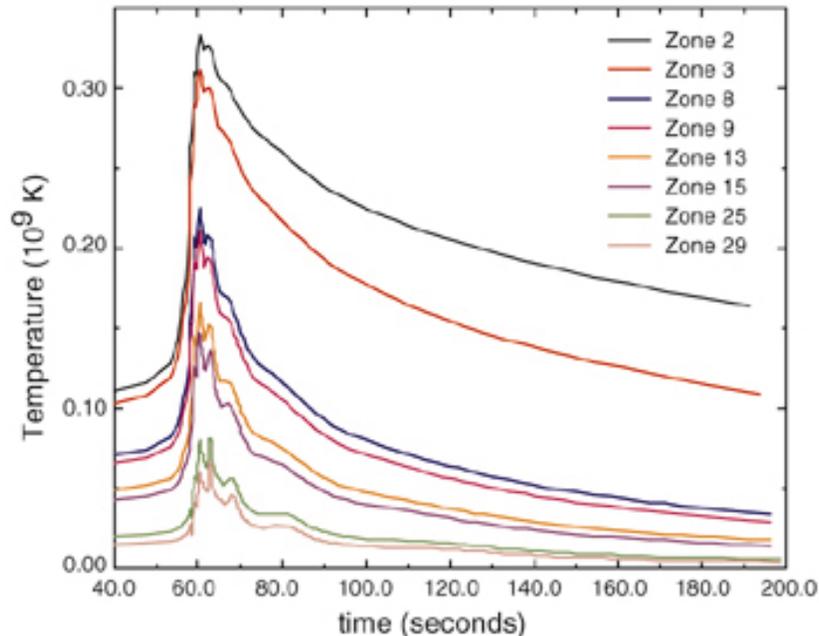


simulations overview

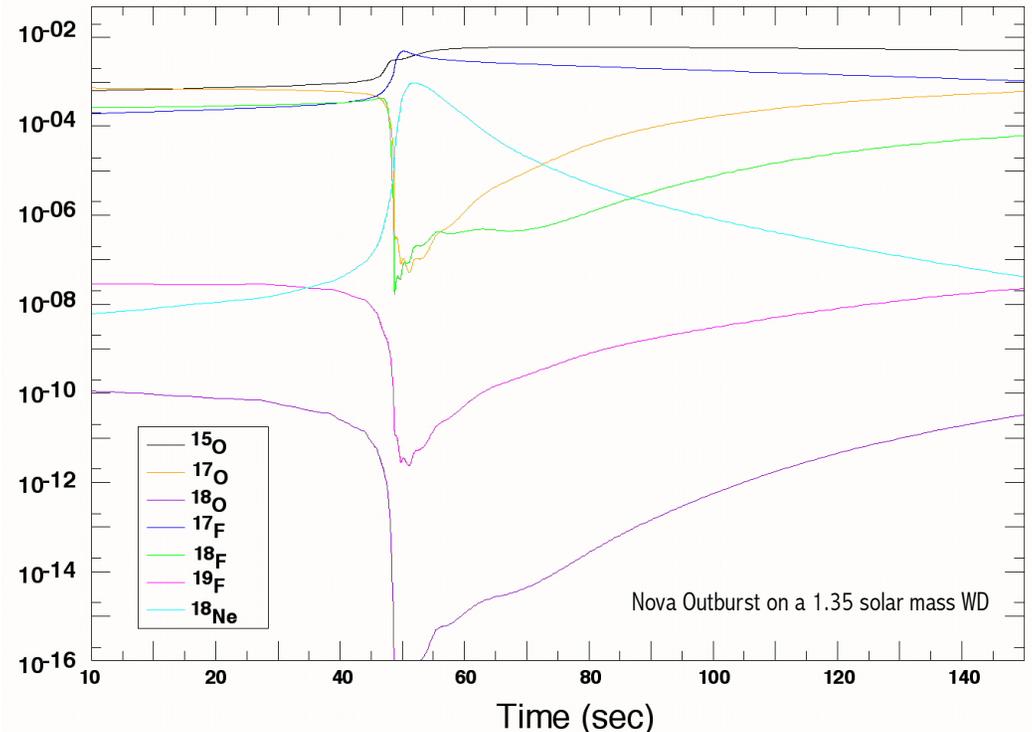
- easily set up and run simulations
- visualize simulations with 1D, 2D plots and animations
- quickly compare simulations with different input
- run automated sensitivity studies (changing input rates)
- analyze simulation results – find **bottlenecks**, **waiting points**

computational infrastructure for nuclear astrophysics

Temperature profile for different spatial zones



Abundances vs. Time



simulations overview

- post-processing code XNET from Raph Hix [ORNL / UTK]
- simulation types: novae, X-ray bursts, solar, CNO, Hot CNO
- single zone and multi-zone simulations
- some simulations with tracer particle temperature/density profiles
- coming soon (1 week): **core collapse supernova r-process**