COMPUTATIONAL INFRASTRUCTURE FOR NUCLEAR ASTROPHYSICS AT OAK RIDGE NATIONAL LABORATORY

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Overview

→ Laboratory experiments at ORNL and facilities worldwide

→ Data evaluations by USNDP & others

→ Processing & disseminating data in formats for astrophysics simulations.

→ Run & visualize astrophysics simulations

STARS

We have created the world's FIRST, easy, user friendly, uniform, reliable way to get recent nuclear results into astrophysical models

nucastrodata.org

Computational Infrastructure Components

Nuclear Data →

- **Nuclear Data Evaluator's Toolkit**
- **Mass Model Evaluator**
- **Nuclear Data Manager**
- **Nuclear Data Viewer**
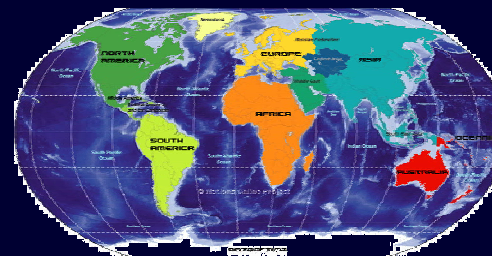
Reaction Rates & Rate Libraries →

- **Rate Generator**
- **Rate Manager**
- **Rate Commentor**
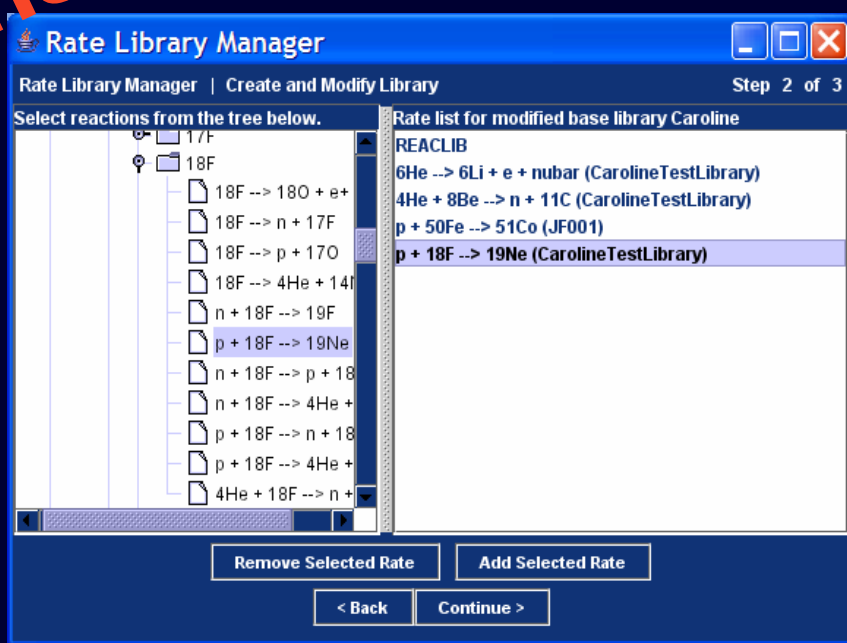- **Rate Library Manager**
- **Rate Viewer**
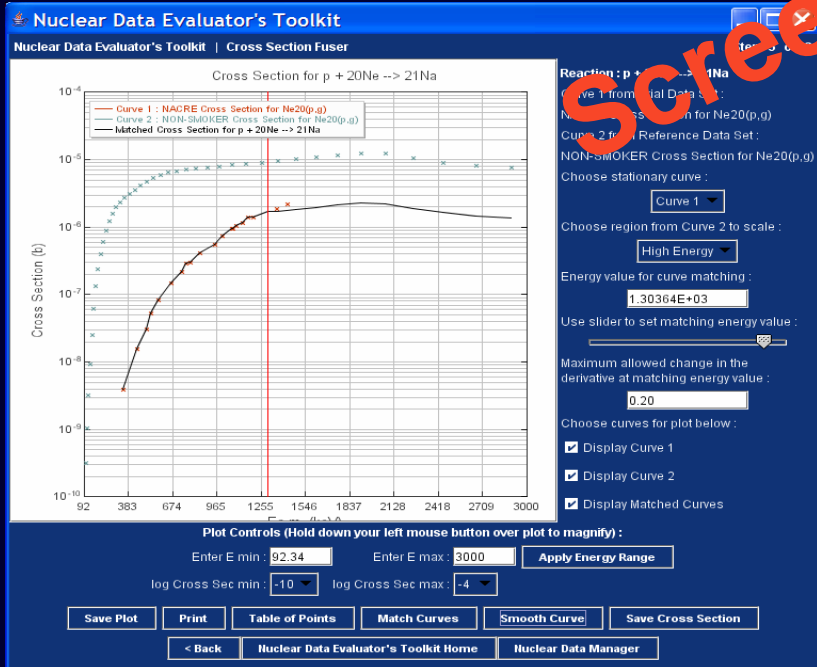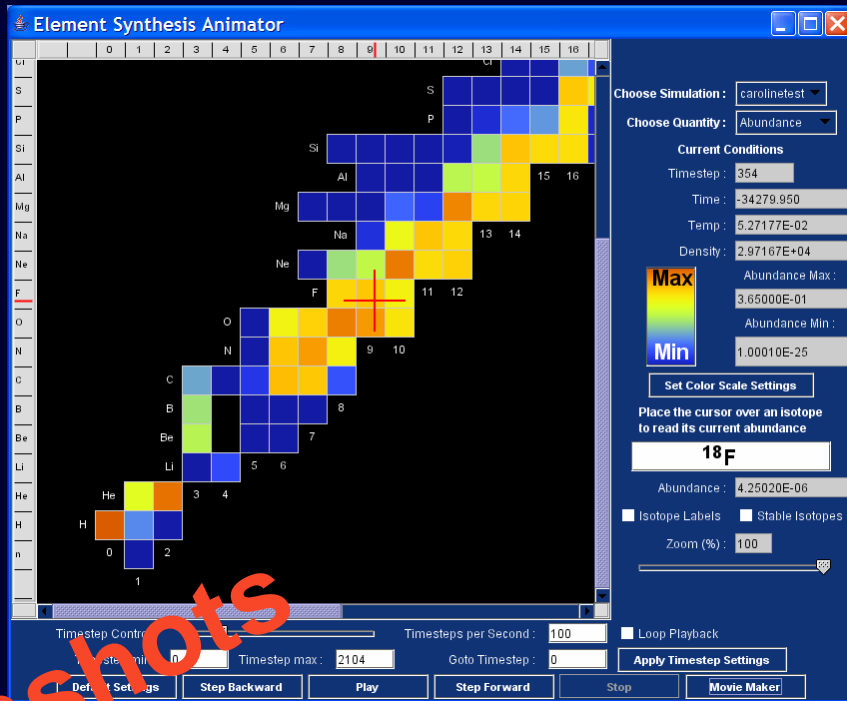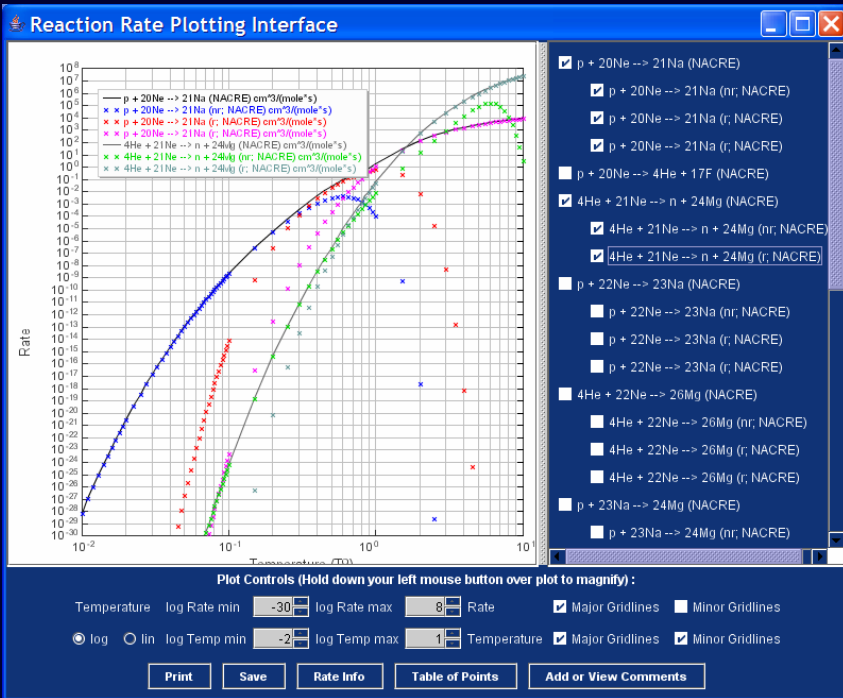
Element Synthesis →

- **Element Synthesis Simulator**
- **Element Synthesis Manager**
- **Element Synthesis Visualizer**

Each component enables

↓

- **Calculations**
- **File management / manipulations**
- **Data Visualization**

Registered Users
Institutes: 39
Countries: 15

Reaction Rate Plotting Interface

Rate

- p + 20Ne --> 21Na (NACRE) cm^3/(mole*s)
- p + 20Ne --> 21Na (nr; NACRE) cm^3/(mole*s)
- p + 20Ne --> 21Na (r; NACRE) cm^3/(mole*s)
- p + 20Ne --> 21Na (r; NACRE) cm^3/(mole*s)
- 4He + 21Ne --> n + 24Mg (NACRE) cm^3/(mole*s)
- 4He + 21Ne --> n + 24Mg (nr; NACRE) cm^3/(mole*s)
- 4He + 21Ne --> n + 24Mg (r; NACRE) cm^3/(mole*s)

☑ p + 20Ne --> 21Na (NACRE)
  ☑ p + 20Ne --> 21Na (nr; NACRE)
  ☑ p + 20Ne --> 21Na (r; NACRE)
  ☑ p + 20Ne --> 21Na (r; NACRE)
☐ p + 20Ne --> 4He + 17F (NACRE)
☑ 4He + 21Ne --> n + 24Mg (NACRE)
  ☑ 4He + 21Ne --> n + 24Mg (nr; NACRE)
  ☑ 4He + 21Ne --> n + 24Mg (r; NACRE)
☐ p + 22Ne --> 23Na (NACRE)
  ☐ p + 22Ne --> 23Na (nr; NACRE)
  ☐ p + 22Ne --> 23Na (r; NACRE)
  ☐ p + 22Ne --> 23Na (r; NACRE)
☐ 4He + 22Ne --> 26Mg (NACRE)
  ☐ 4He + 22Ne --> 26Mg (nr; NACRE)
  ☐ 4He + 22Ne --> 26Mg (r; NACRE)
  ☐ 4He + 22Ne --> 26Mg (r; NACRE)
☐ p + 23Na --> 24Mg (NACRE)
  ☐ p + 23Na --> 24Mg (nr; NACRE)

Plot Controls (Hold down your left mouse button over plot to magnify) :

Temperature | log Rate min -30 | log Rate max 8 | Rate | ☑ Major Gridlines | ☐ Minor Gridlines

◉ log ◯ lin | log Temp min -2 | log Temp max 1 | Temperature | ☑ Major Gridlines | ☑ Minor Gridlines

[Print] [Save] [Rate Info] [Table of Points] [Add or View Comments]

Element Synthesis Animator

Choose Simulation : carolinetest
Choose Quantity : Abundance

Current Conditions
Timestep : 354
Time : -34279.950
Temp : 5.27177E-02
Density : 2.97167E+04

Abundance Max : 3.65000E-01
Abundance Min : 1.00010E-25

[Set Color Scale Settings]

Place the cursor over an isotope to read its current abundance

18F

Abundance : 4.25020E-06

☐ Isotope Labels   ☐ Stable Isotopes

Zoom (%) : 100

Timestep Controls
Timesteps per Second : 100   ☐ Loop Playback
Timestep min : 0 | Timestep max : 2104 | Goto Timestep : 0
[Default Settings] [Step Backward] [Play] [Step Forward] [Stop] [Movie Maker]
[Apply Timestep Settings]

Nuclear Data Evaluator's Toolkit

Nuclear Data Evaluator's Toolkit | Cross Section Fuser

Cross Section for p + 20Ne --> 21Na

- Curve 1 : NACRE Cross Section for Ne20(p,g)
- Curve 2 : NON-SMOKER Cross Section for Ne20(p,g)
- Matched Cross Section for p + 20Ne --> 21Na

Reaction : p + 20Ne --> 21Na

Curve 1 from Initial Data Set :
NACRE Cross Section for Ne20(p,g)
Curve 2 from Reference Data Set :
NON-SMOKER Cross Section for Ne20(p,g)

Choose stationary curve :
[Curve 1]

Choose region from Curve 2 to scale :
[High Energy]

Energy value for curve matching :
1.30364E+03

Use slider to set matching energy value :

Maximum allowed change in the derivative at matching energy value :
0.20

Choose curves for plot below :
☑ Display Curve 1
☑ Display Curve 2
☐ Display Matched Curves

Plot Controls (Hold down your left mouse button over plot to magnify) :

Enter E min : 92.34 | Enter E max : 3000 | [Apply Energy Range]
log Cross Sec min : -10 | log Cross Sec max : -4

[Save Plot] [Print] [Table of Points] [Match Curves] [Smooth Curve] [Save Cross Section]
[< Back] [Nuclear Data Evaluator's Toolkit Home] [Nuclear Data Manager]

Rate Library Manager

Rate Library Manager | Create and Modify Library   Step 2 of 3

Select reactions from the tree below.

- 17F
- 18F
  - 18F --> 18O + e+
  - 18F --> n + 17F
  - 18F --> p + 17O
  - 18F --> 4He + 14N
  - n + 18F --> 19F
  - p + 18F --> 19Ne
  - n + 18F --> p + 18
  - n + 18F --> 4He + 1
  - p + 18F --> n + 18
  - p + 18F --> 4He +
  - 4He + 18F --> n +

Rate list for modified base library Caroline

REACLIB
6He --> 6Li + e + nubar (CarolineTestLibrary)
4He + 8Be --> n + 11C (CarolineTestLibrary)
p + 50Fe --> 51Co (JF001)
p + 18F --> 19Ne (CarolineTestLibrary)

[Remove Selected Rate] [Add Selected Rate]

[< Back] [Continue >]

New features added since last USNDP meeting

Nuclear Data ⟶ **Mass Model Evaluator**

- Compare and Visualize difference between theoretical & measured
  - masses
  - S_n, S_{2n}, S_p, S_{2p} and S_α
  - $Q(\alpha,p)$, $Q(\alpha,n)$ and $Q(p,n)$

Reaction Rates & Rate Libraries ⟶ **Rate Commentor**

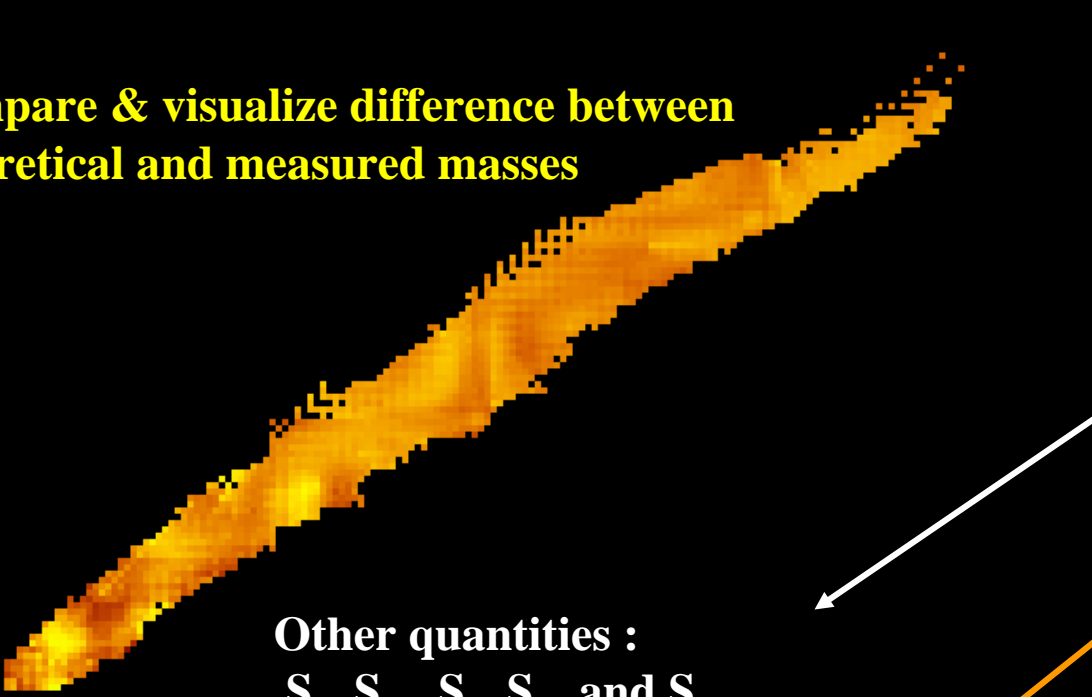- View, add, and post comments to a reaction

Element Synthesis ⟶ **Element Synthesis Simulator & Animator**

- Run element synthesis calculation, visualize, create & export movies of
  - reaction fluxes
  - abundance & time derivatives of abundance

Screenshot: Mass Model Evaluator

Interactive Nuclide Chart for Mass Model Evaluations

Compare & visualize difference between theoretical and measured masses

Other quantities :
S_n, S_{2n}, S_p, S_{2p} and S_α
$Q(\alpha,p)$, $Q(\alpha,n)$ and $Q(p,n)$

Customize colors and ranges

Theoretical Mass Model : FRDM95
Reference Mass Model : AMDC
Select chart type below :
Difference of Data
Select quantity below :
Mass Excess

Max

Quantity Max :
3.110
Quantity Min :
-3.780

Min

Set Color Scale Settings

Place the cursor over an isotope to read its value

^{132}Sn

Value : 0.140

r-Process Path   Isotope Labels
Magic Numbers   Stable Isotopes
Zoom (%) : 16

Plot of S_n from
FRDM mass formula (P. Moller *et. al.* 1995)
shows r- process path
follows constant S_n contours in the *NZ-plane*

Sharing comments helps build the community's knowledge of these reactions, and also enables consensus to be reached on difficult issues.

Element Synthesis Animator: Abundance

Nova

Timestep = 0

Time (sec) = -43975510.39

Density (g/cm^3) = 1.636E+04

Temperature (T9) = 3.201E-02

Max : 3.65E-01

Min : 1.00E-25

Abundance

nucastrodata.org

Screenshot: Element Synthesis Animator

- **User-defined color schemes & abundance ranges**

- **can be utilized to emphasize low- or high-abundance nuclides**
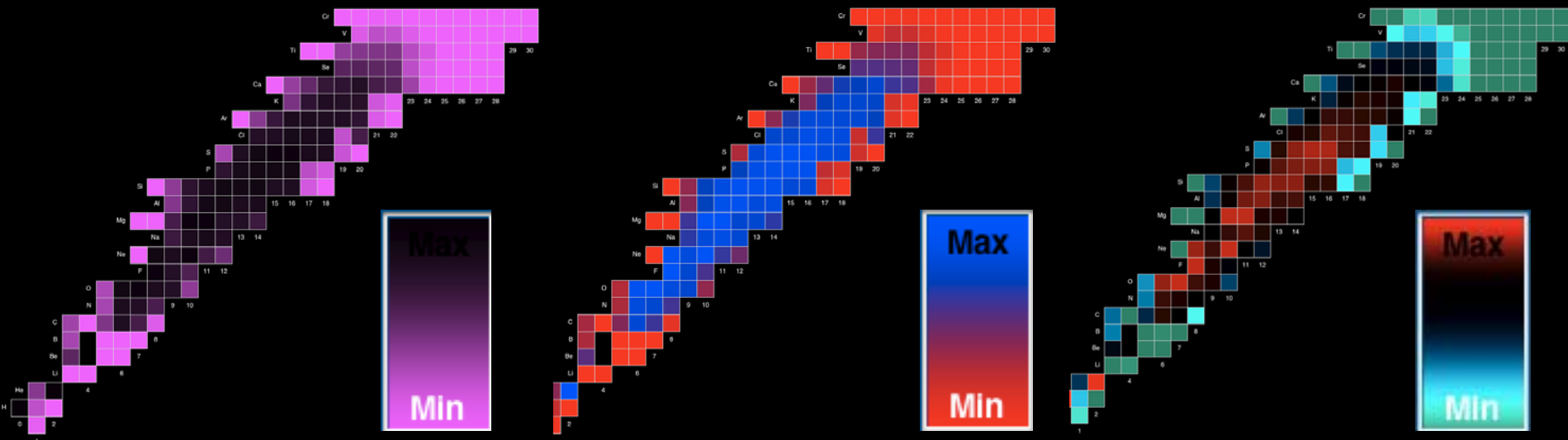
Element Synthesis Animator: Reaction Fluxes
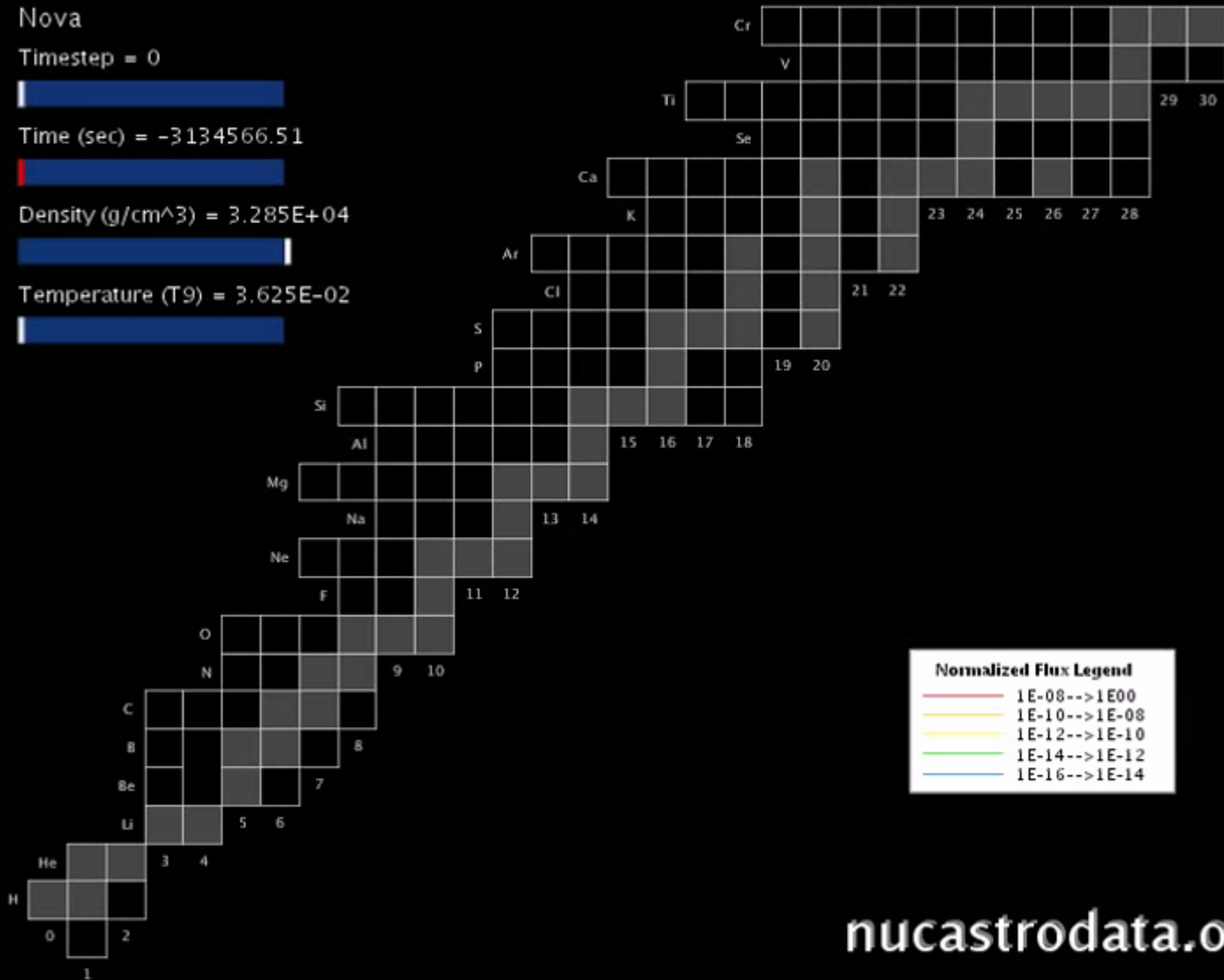
Future Work

Expand functionality of the Computational Infrastructure by adding new features

- theoretical Cross Section Models
- incorporate uncertainties
- resonance parameters
- improving existing features
    - enhance fitting techniques
    - file formats for exporting

Summary

- The laboratory nuclear physics results have to be **evaluated, processed, and distributed** in order to be used in astrophysics simulations

Nuclear Astrophysics Data Program at ORNL

- Computational Infrastructure with unique software tools hosted

  at **nucastrodata.org** – for creation, management and visualization of nuclear and astrophysical data
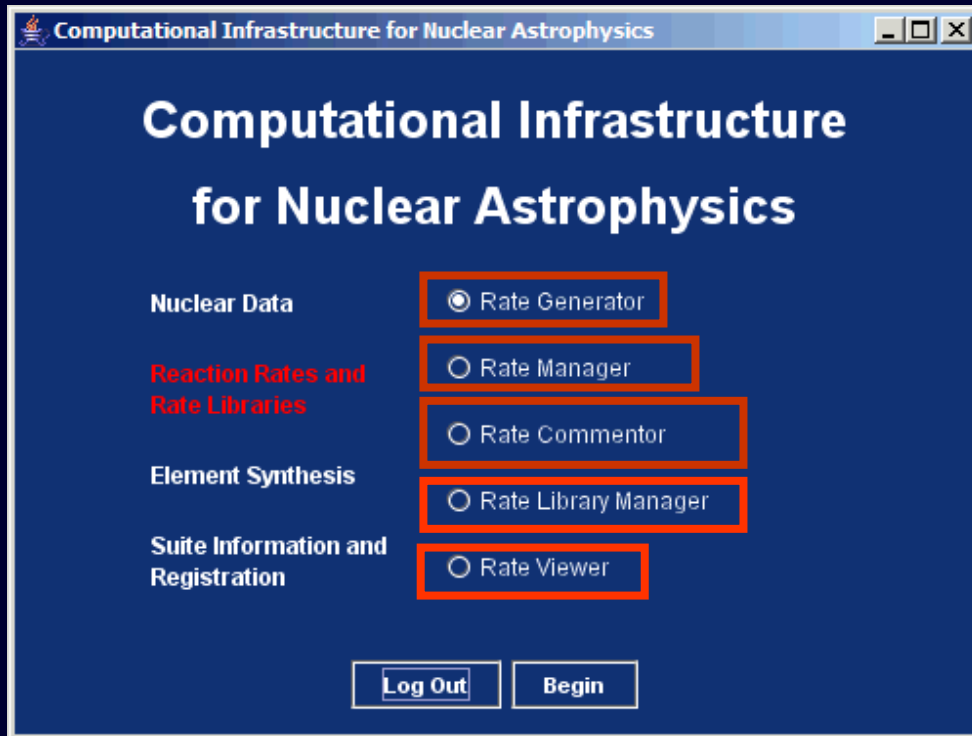
Nuclear Data
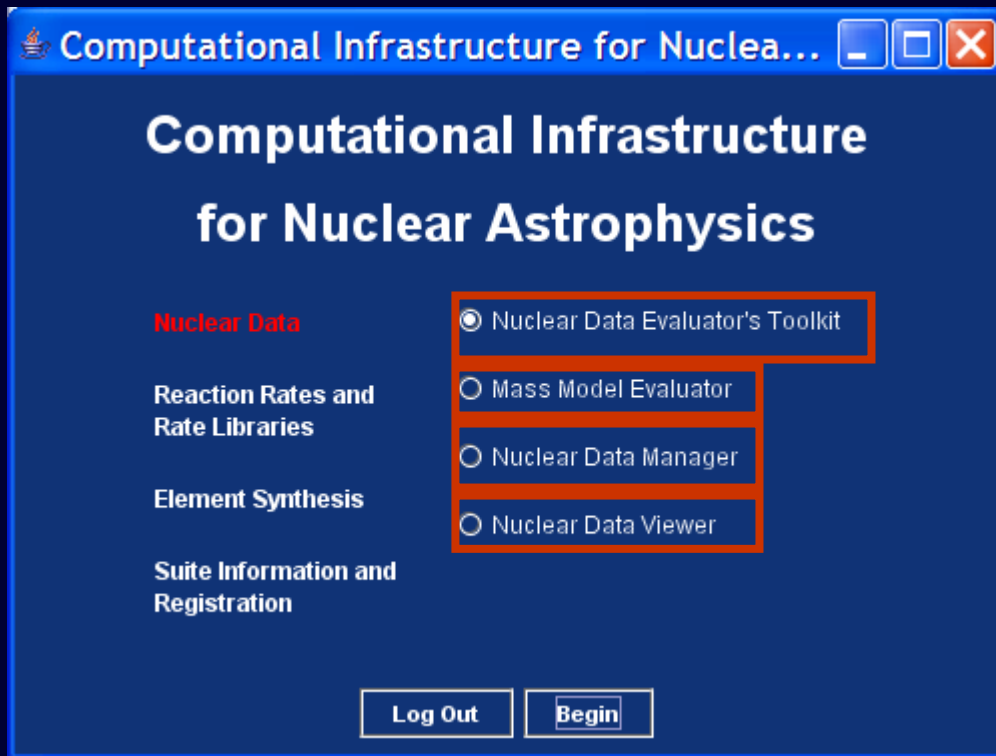
Renormalize, **extrapolate**, **merge** cross sections & S-factors;

Visualize difference between theoretical / measured masses

Input, **store**, **manipulate** & **modify** cross sections & S-factors

Plot cross sections & S-factors

Reaction Rate and Rate Libraries

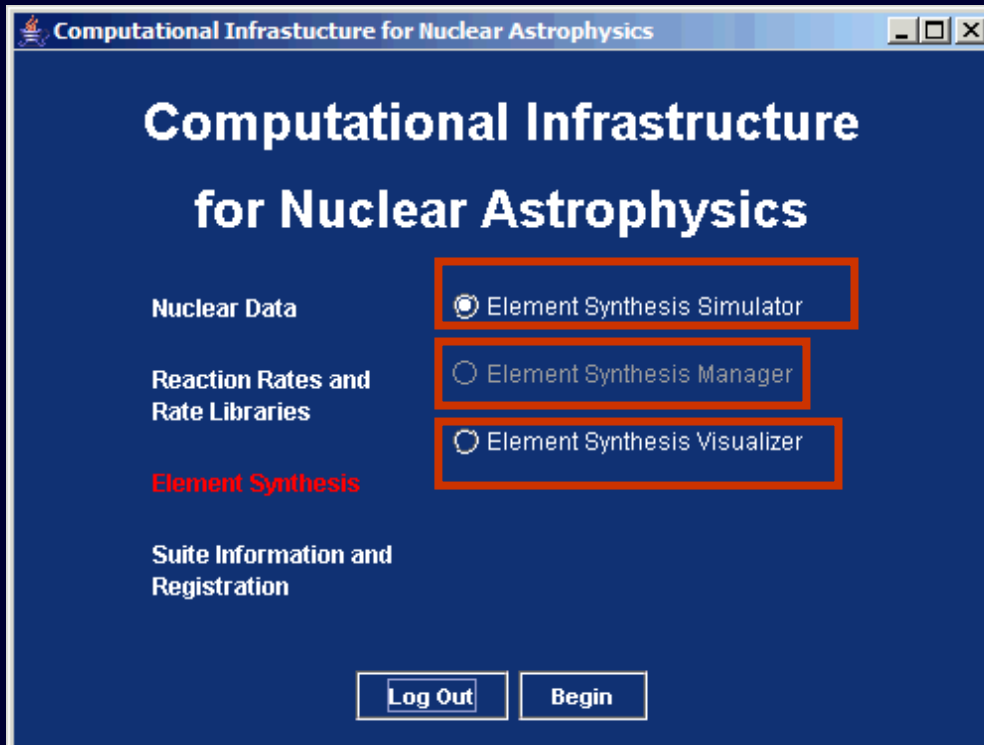**Step-by-step: calculate** reaction rates from cross sections & S-factors & **fit with parameters**

Manipulate and **modify** rates

View, add & **post comments** to a reaction

Insert reaction rates in libraries; **modify**, **merge**, **share**, **document** rate libraries

Plot rates, **access information**

Element Synthesis

Set up & run post - processing element synthesis calculations

Store and **share** element synthesis results

Visualize simulation results, quickly compare **two simulations**, **generate animations** of simulation results