Nucleosynthesis Studies

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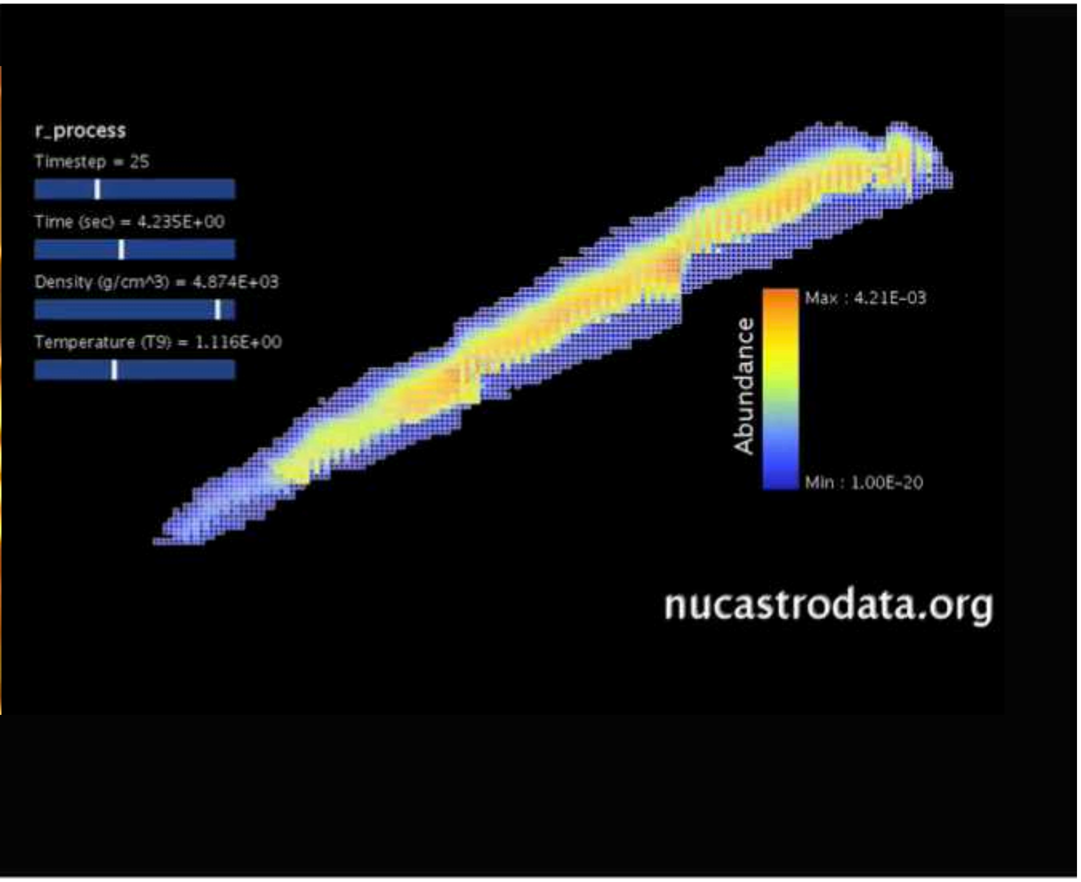
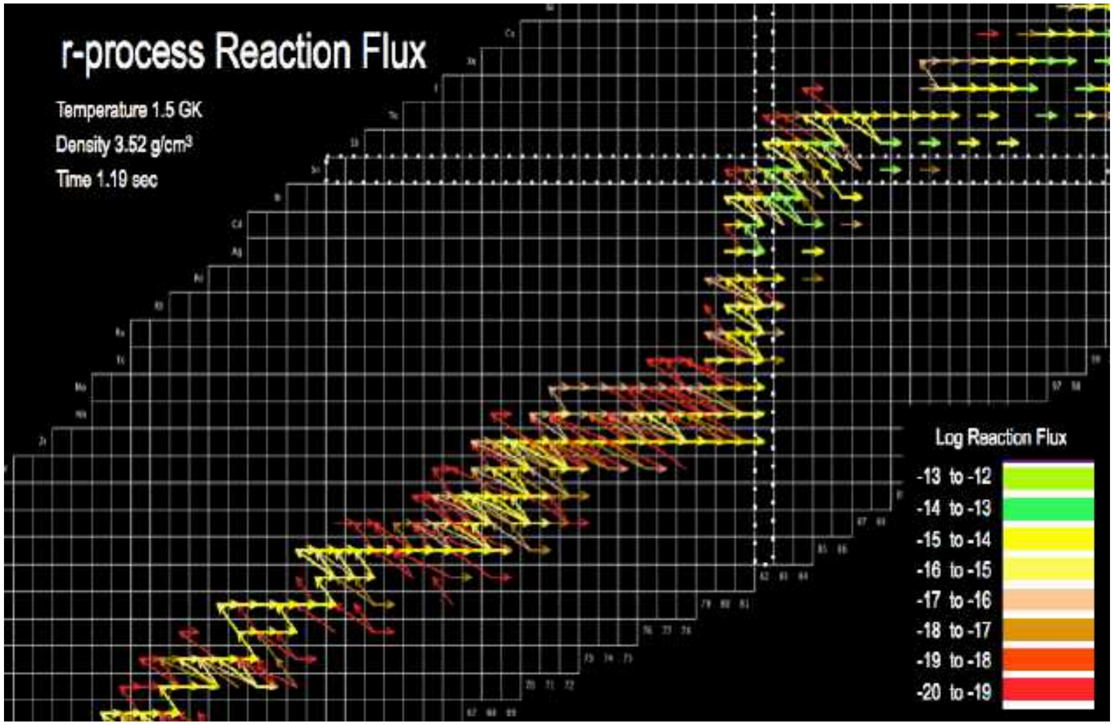
What Is Nucleosynthesis ?



- creation of elements in astrophysical environments

Outline

- Motivation & Background
- How Simulations Work
- Common Problems
- Uncertainty Quantification
- Summary & Future

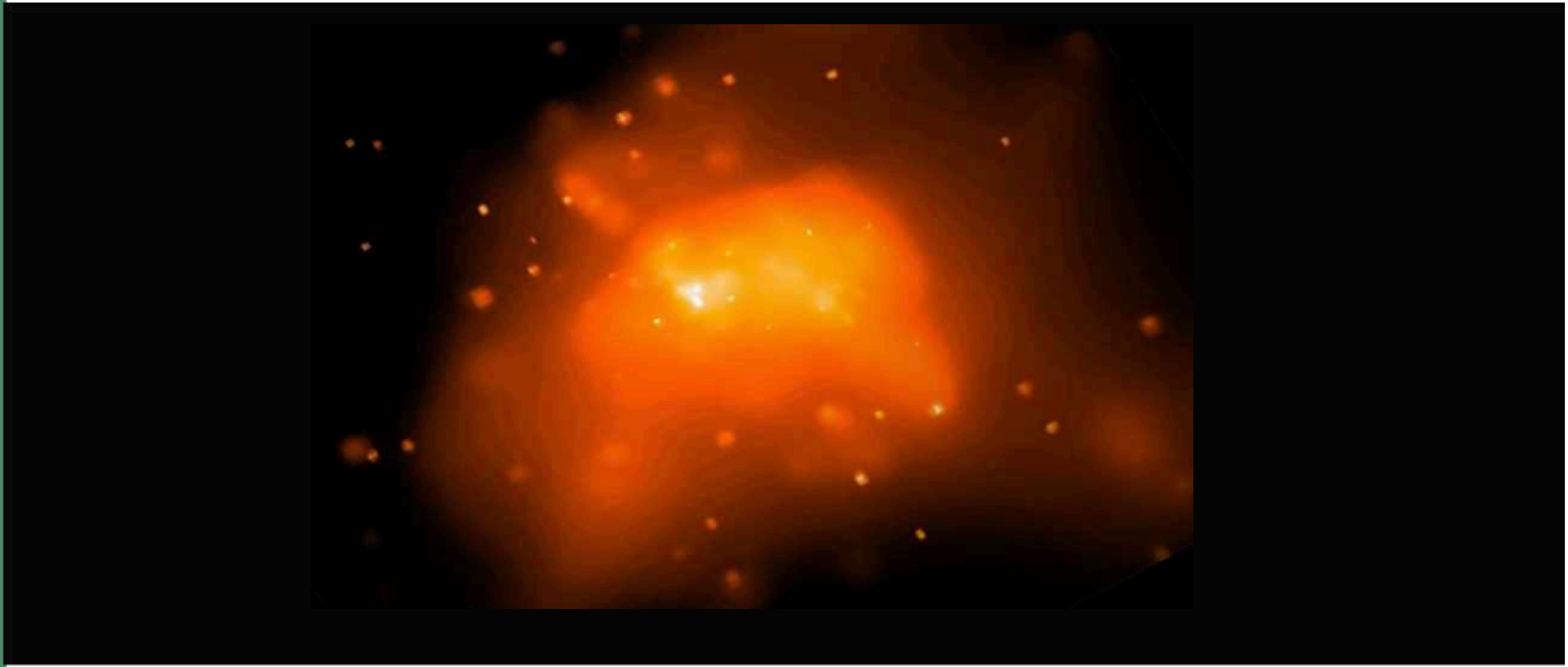


$$\begin{bmatrix} 1+Y_m(t)\,[jm,qr]\,\delta t & Y_j(t)[jm,qr]\delta t & -Y_l(t)[kl,ji]\delta t & -Y_k(t)[kl,ji]\delta t \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} \Delta_j \\ \Delta_m \\ \Delta_k \\ \Delta_l \end{bmatrix} = \begin{bmatrix} Y_k(t)\;Y_l(t)\;[kl,ji]\;\delta t\;-\;Y_j(t)\;Y_m(t)\;[jm,qr]\;\delta t \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}$$

Why Study Nucleosynthesis ?

- to understand the cosmos

Why Study Nucleosynthesis ?

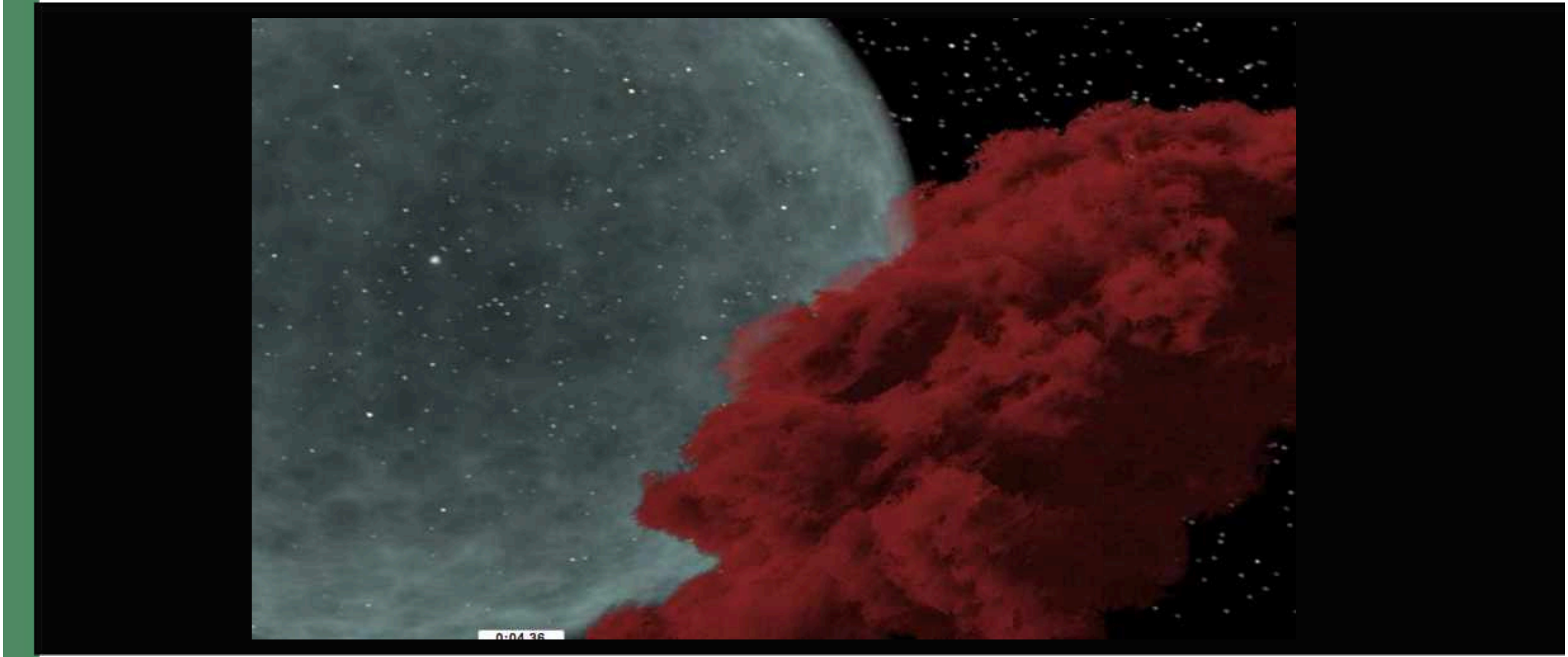


- to understand the cosmos

Why Study Nucleosynthesis ?

- to understand us …"where we came from"

Why Study Nucleosynthesis ?

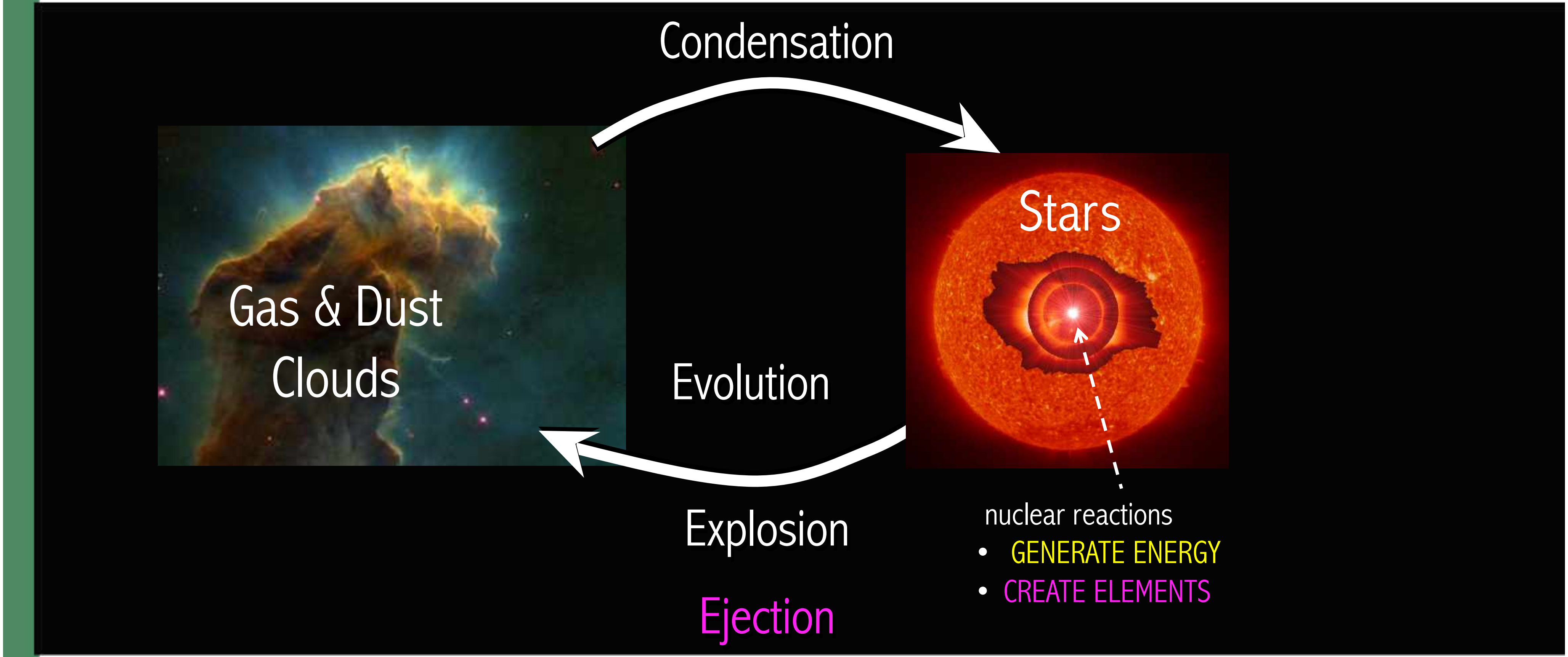


- to understand how our solar system formed

Why Study Nucleosynthesis ?

- to understand us …“where we came from”

Why Study Nucleosynthesis ?



Condensation

Gas & Dust Clouds

Stars

Evolution

Explosion

Ejection

nuclear reactions

- GENERATE ENERGY
- CREATE ELEMENTS

- to understand how stars are element factories

Why Study Nucleosynthesis ?

Carbon

Nitrogen

Iron

Calcium

- to understand the creation & dispersion of the elements of life

Why Study Nucleosynthesis ?

Aluminum

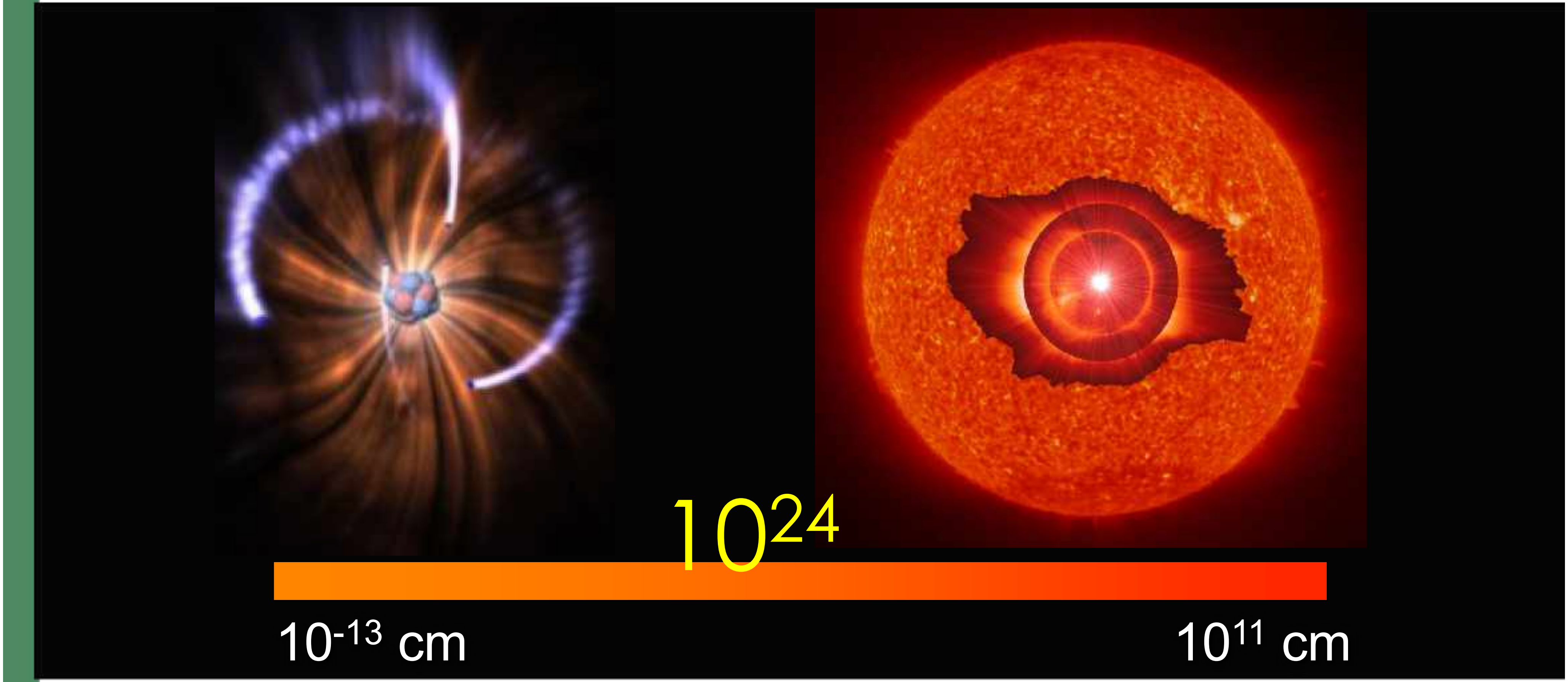
Silicon

Gold

Platinum

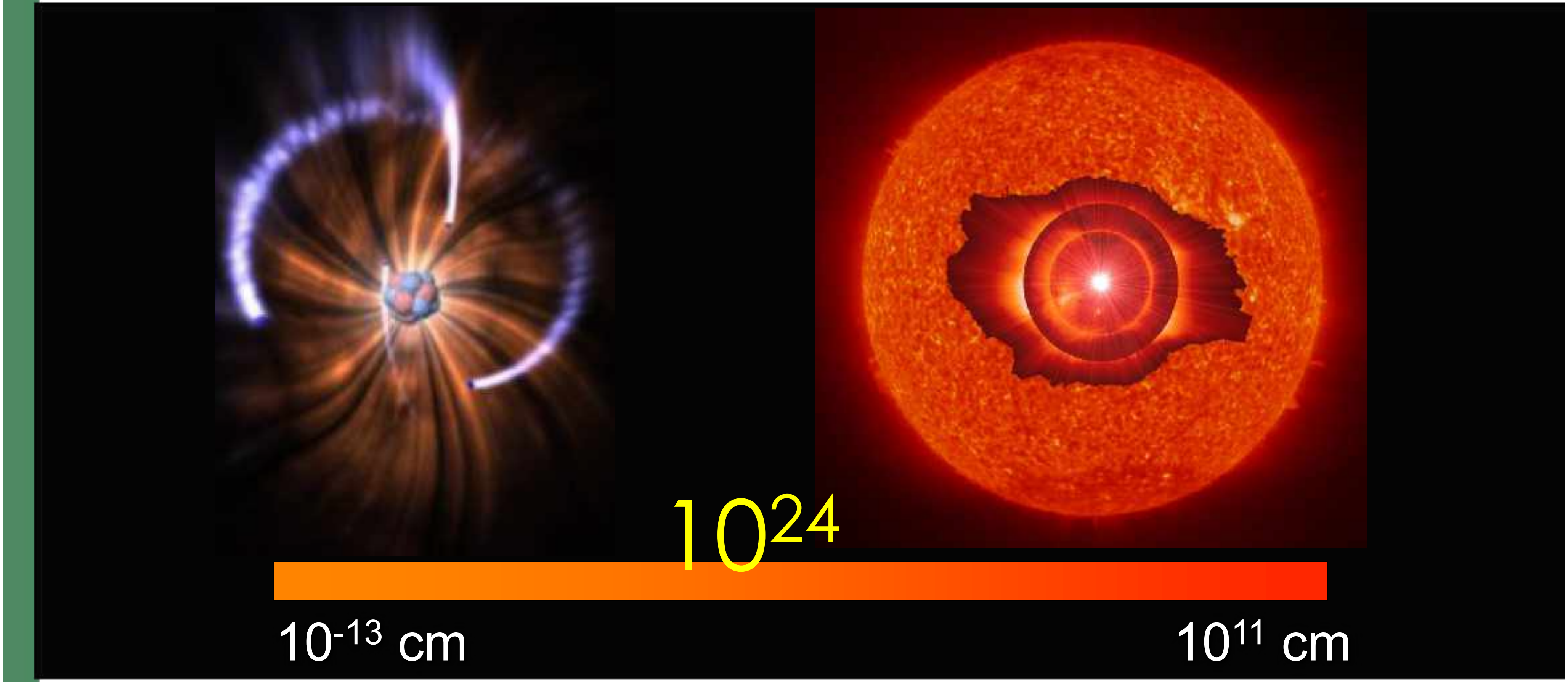
… and all the elements that make life fun!

Why Study Nucleosynthesis ?



- to understand the cosmic leverage of nuclear physics

Why Study Nucleosynthesis ?



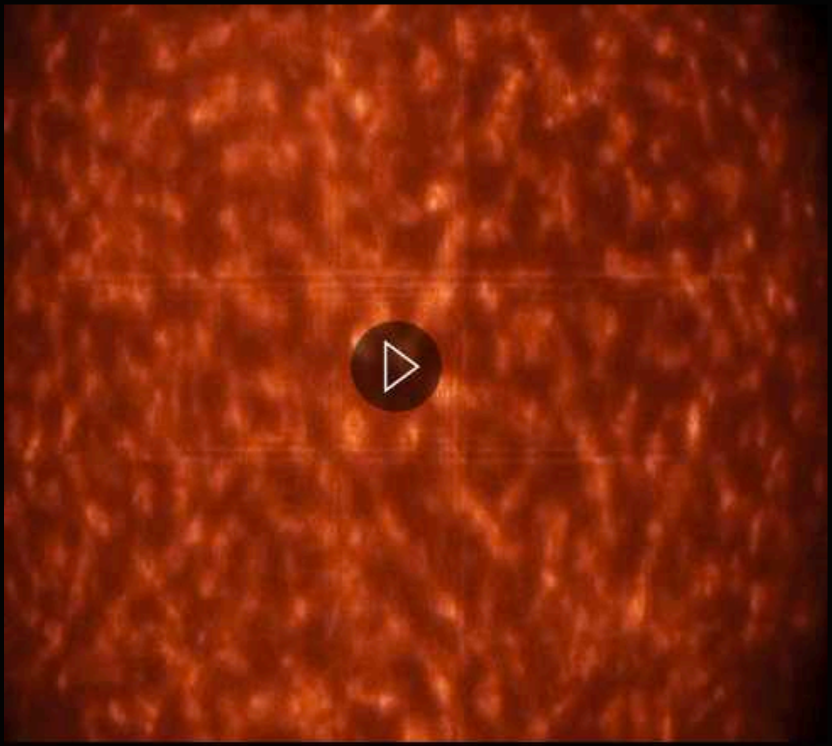
10^{24}

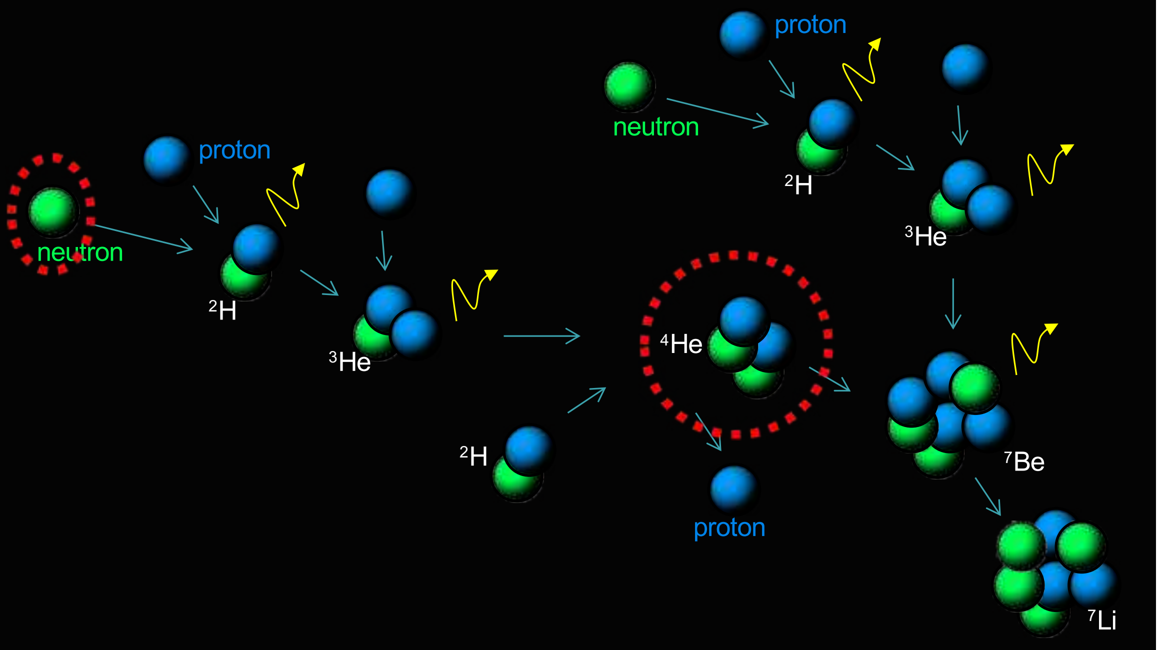
10^{-13} cm

10^{11} cm

- to understand the micro – macroscopic cosmic connection

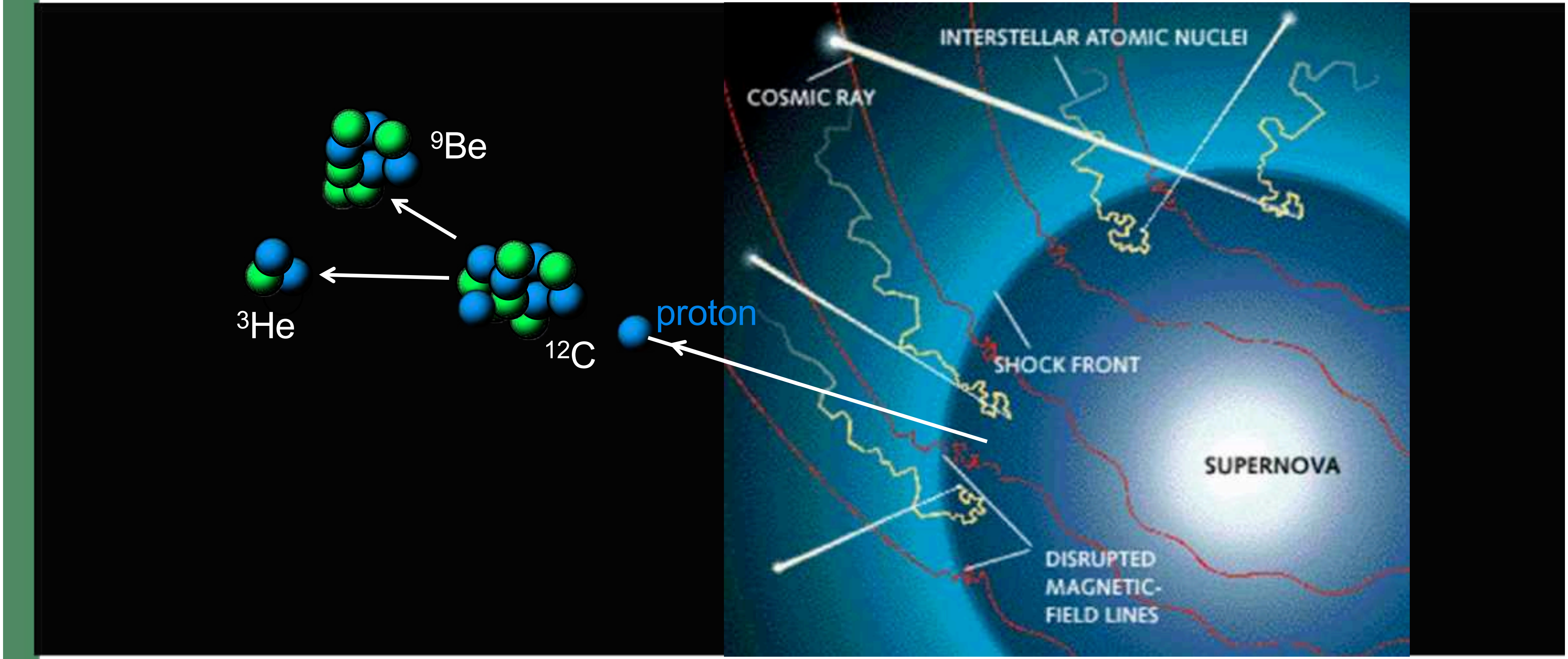
Major Nucleosynthesis Sites





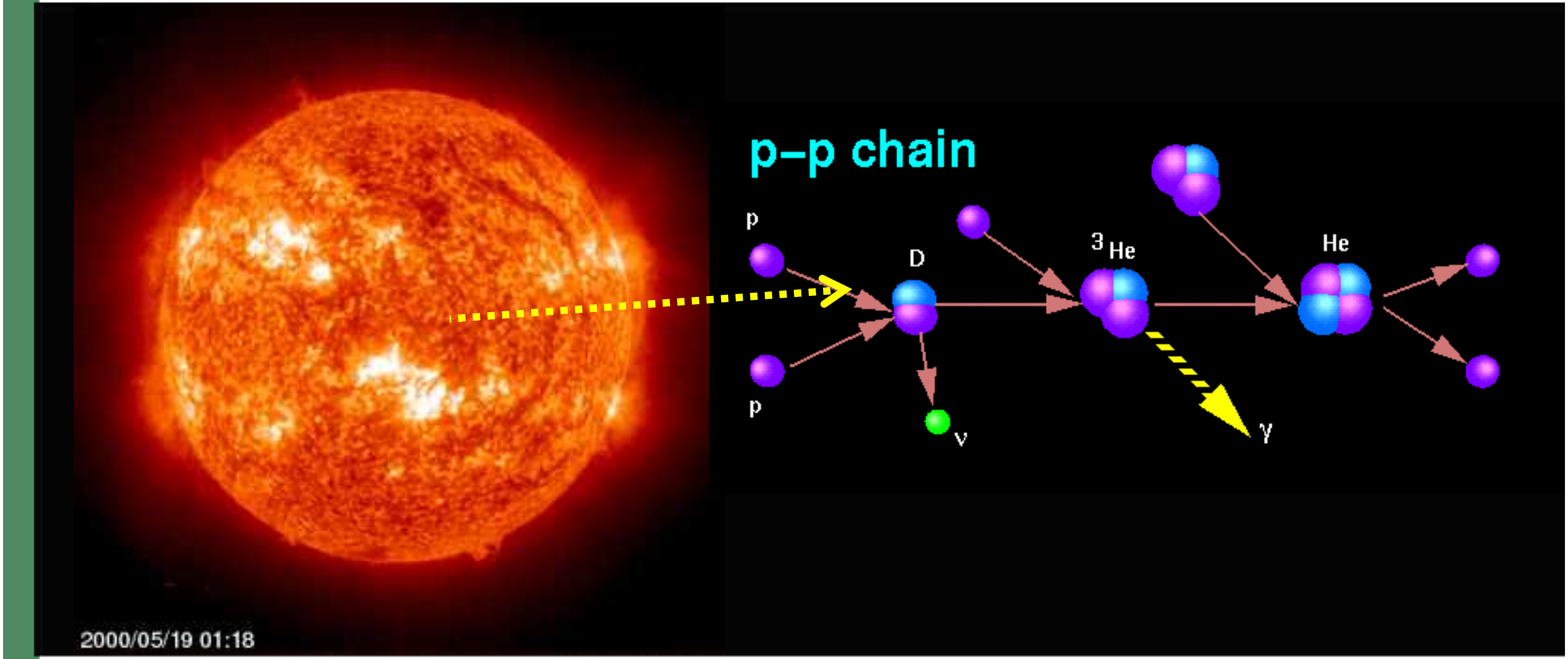
- big bang

Major Nucleosynthesis Sites



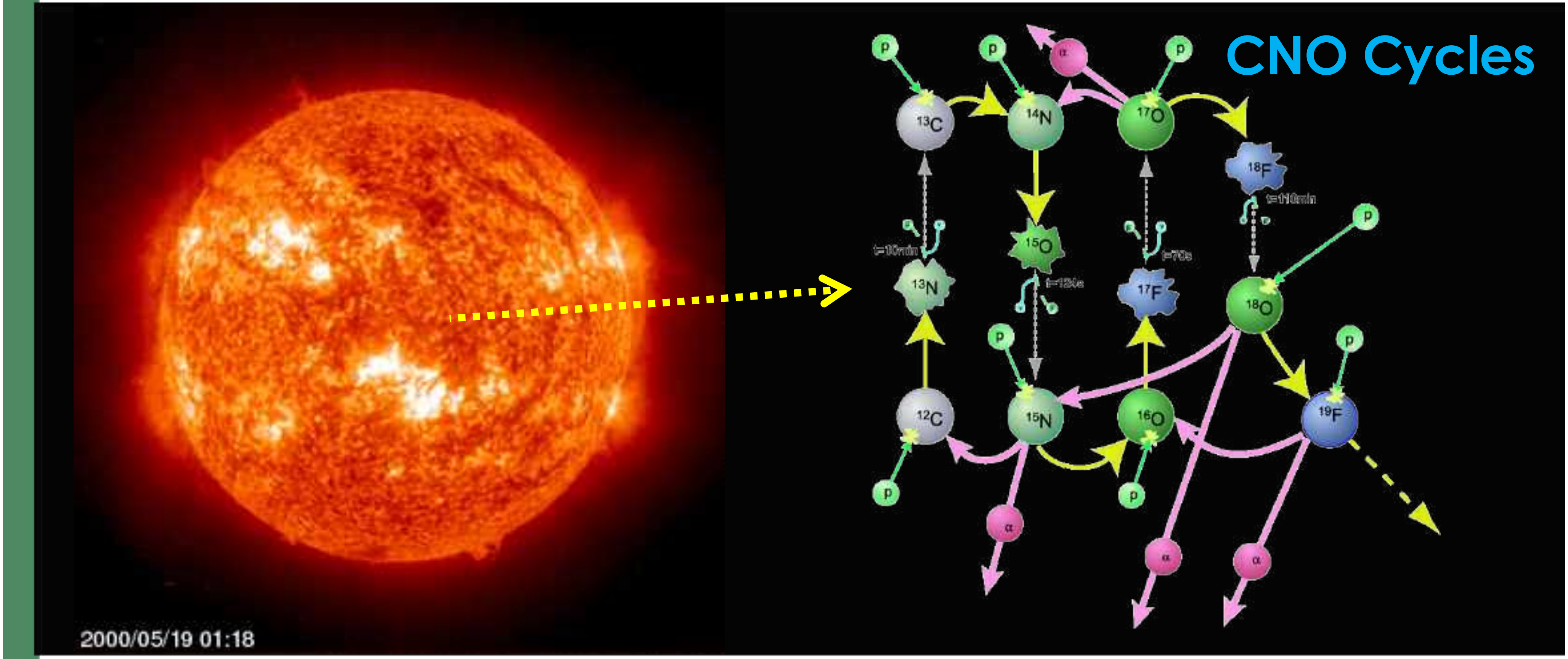
- cosmic rays

Major Nucleosynthesis Sites



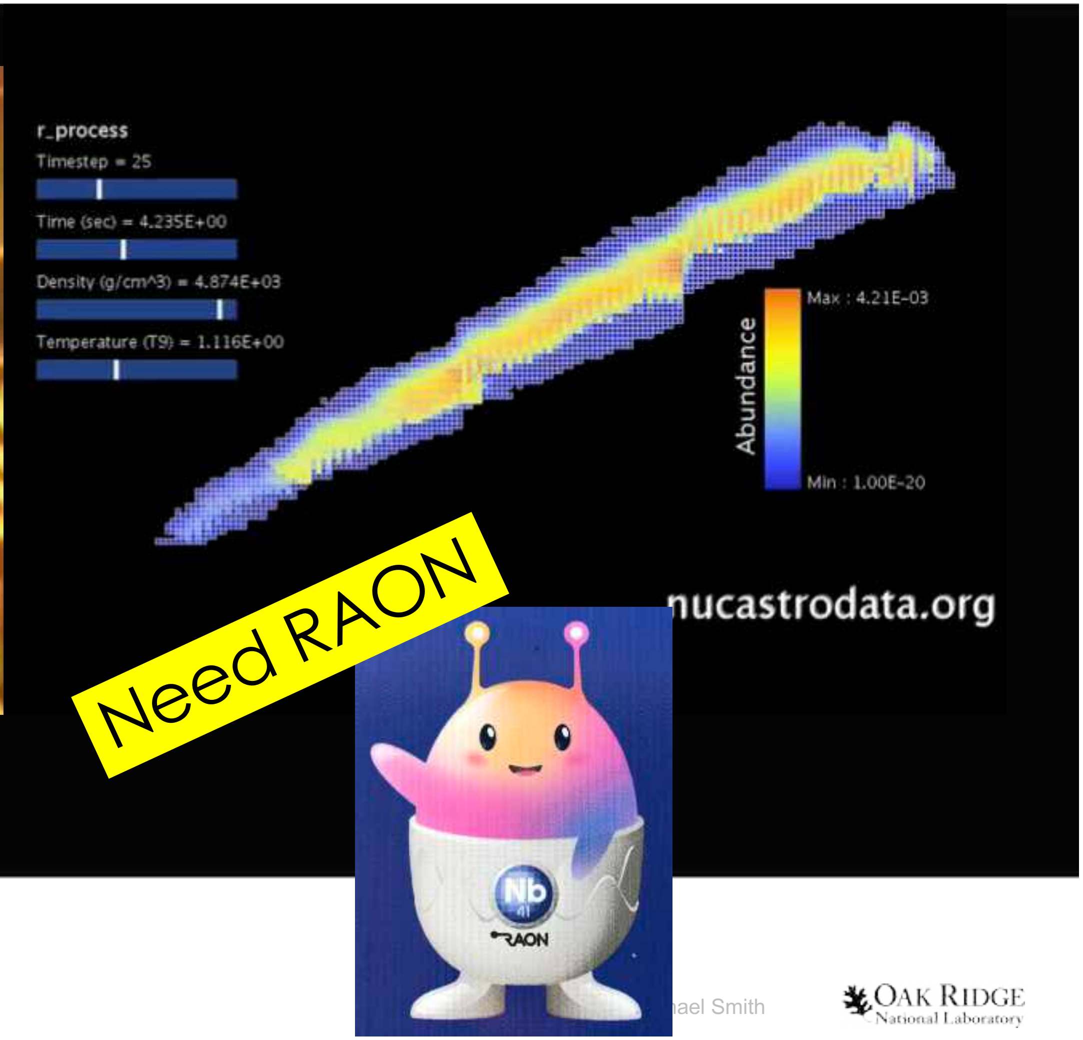
- Stars

Major Nucleosynthesis Sites



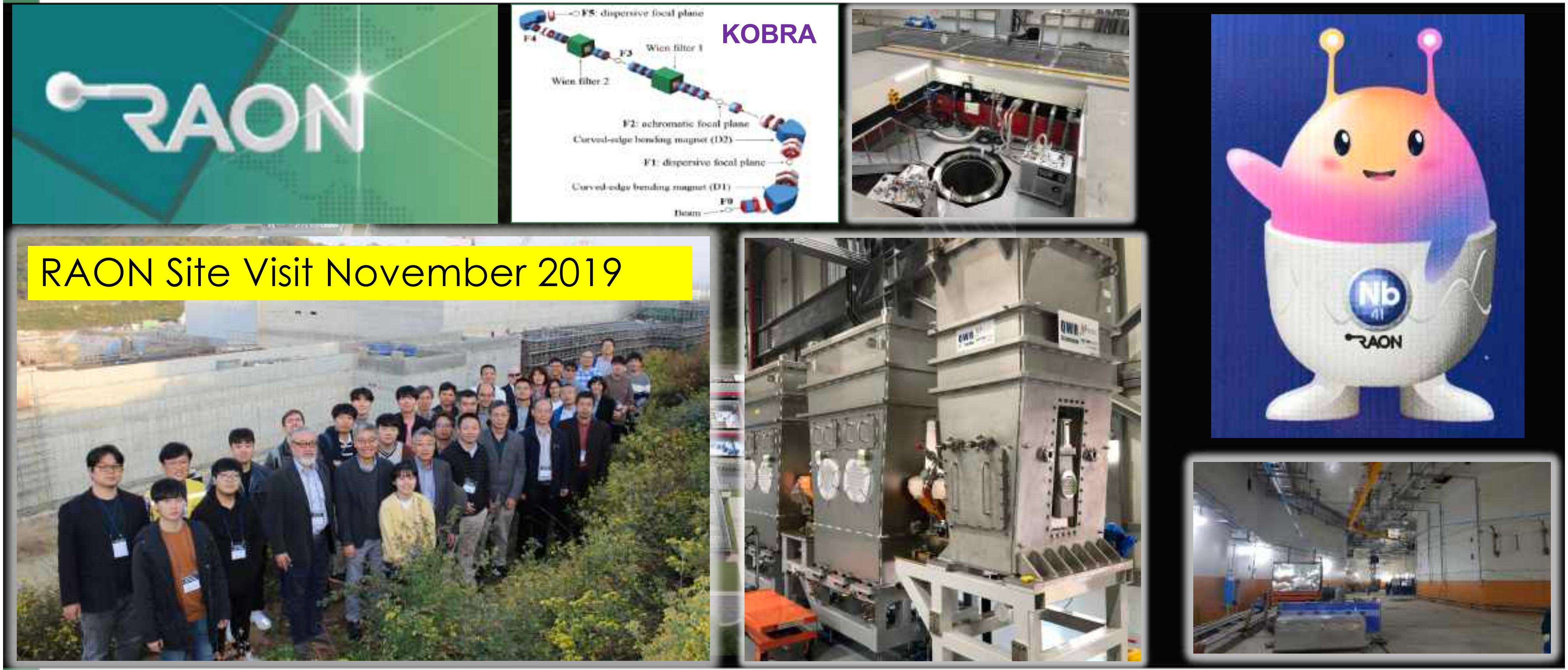
- Stars

Major Nucleosynthesis Sites



- stellar explosions

Major Nucleosynthesis Sites

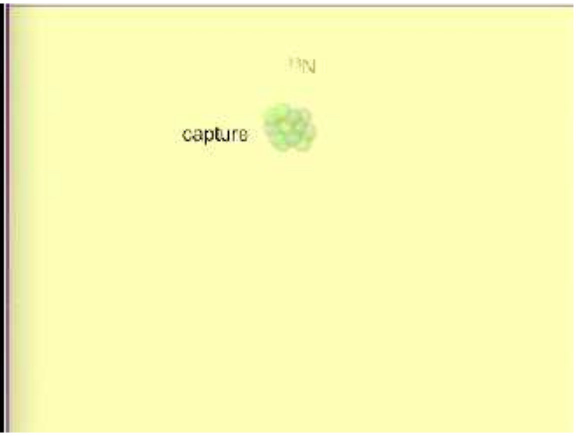


RAON Site Visit November 2019

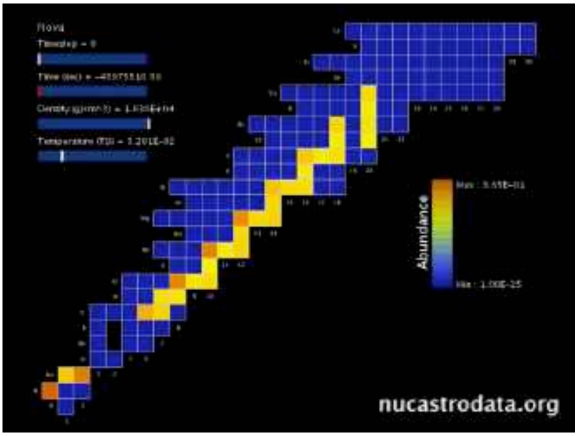
- stellar explosions

Nucleosynthesis Simulations


macrophysics



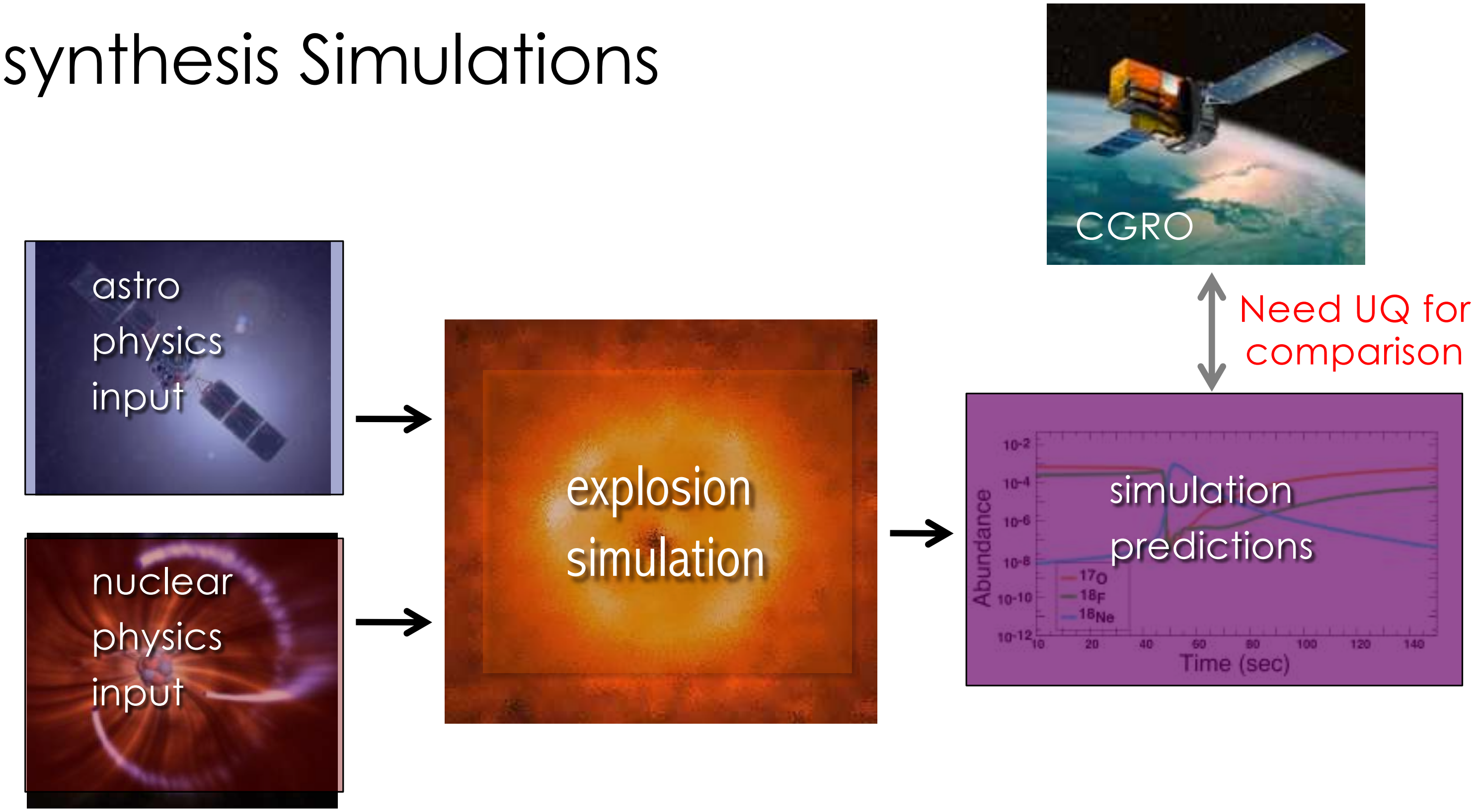
microphysics



simulation

- simulations capture the detailed microphysics of a system or event
- compress this detailed information into predictions of only a small number of observables

Nucleosynthesis Simulations


CGRO

Need UQ for comparison

astro physics input

nuclear physics input

explosion simulation

simulation predictions

- a simplified flowchart of these studies looks like this
- improving the simulation requires *quantitative* comparisons with observations …
- this requires uncertainty quantification UQ in the predictions … usually not given

Major Goals of Nucleosynthesis Studies

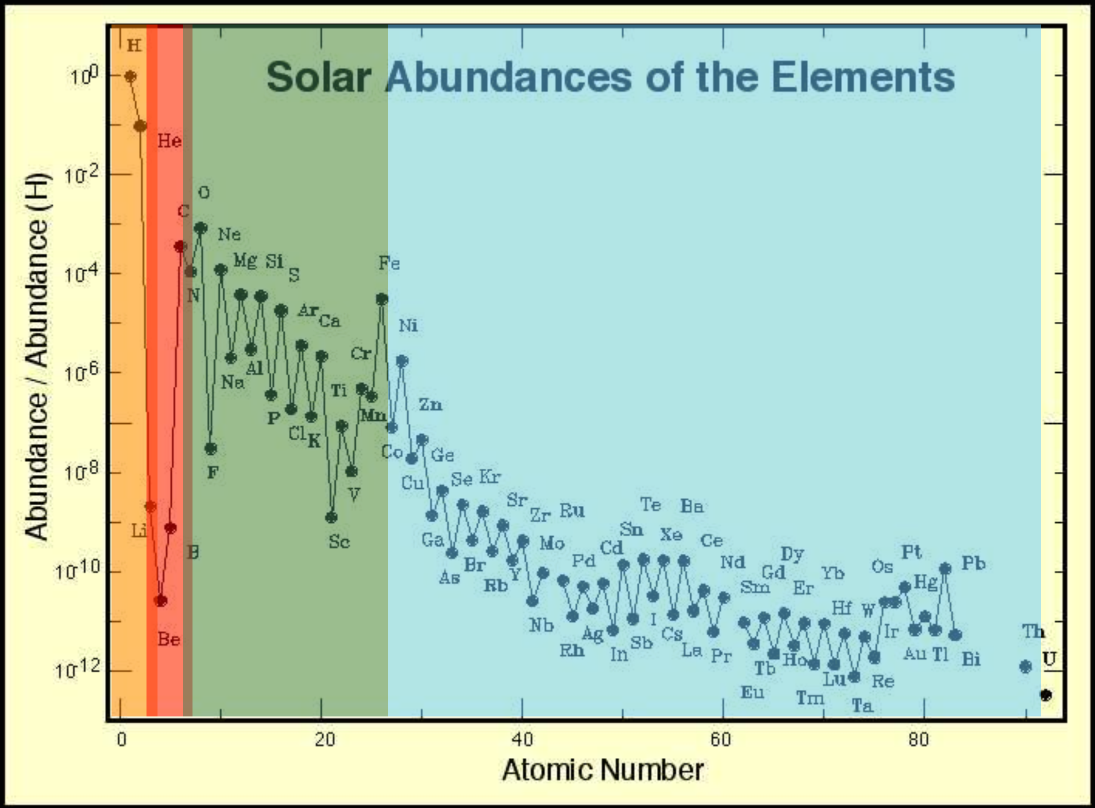
Isotope perspective

Big Bang: H, He, Li

Cosmic rays: Li, Be, B

Massive Stars … A < 56

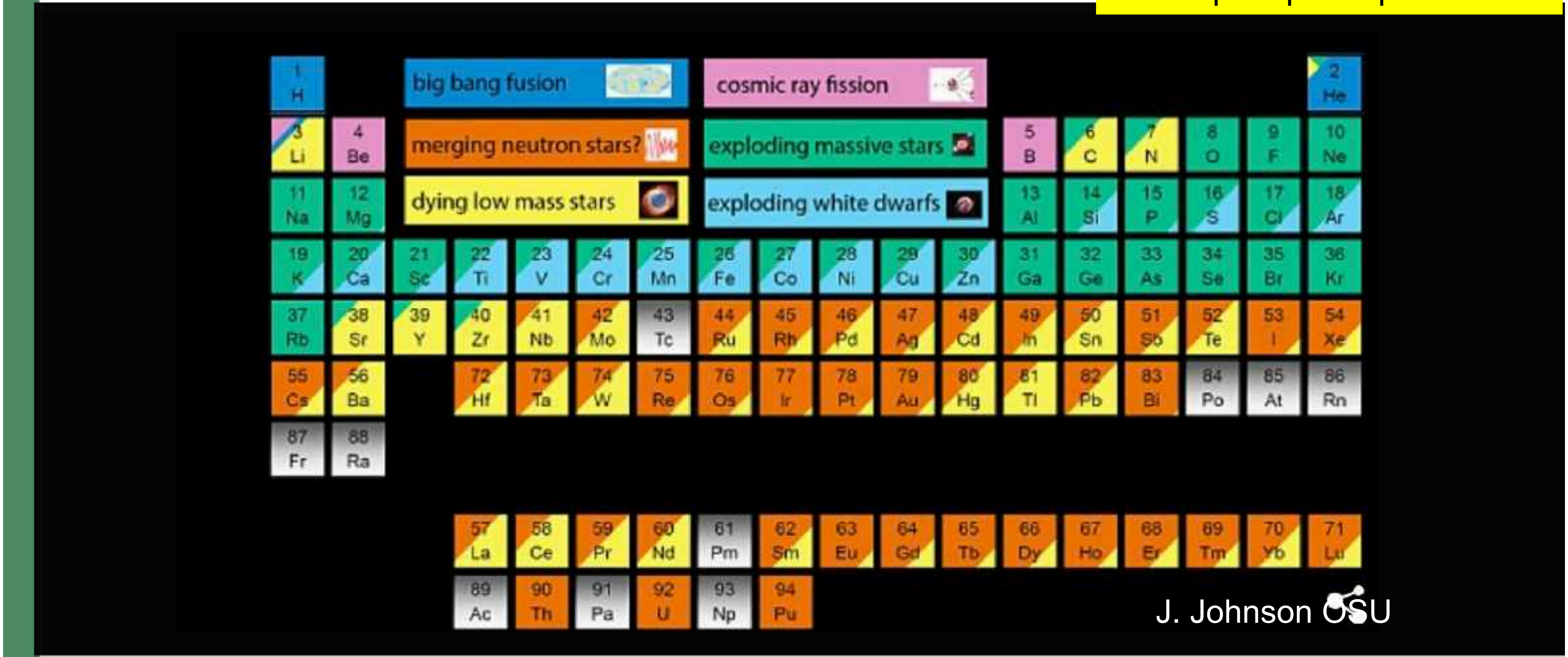
Red Giants, Supernovae,
Neutron Star Mergers … A > 56



- determine cosmic origins of all isotopes

Major Goals of Nucleosynthesis Studies

Isotope perspective



J. Johnson OSU

- determine cosmic origins of all isotopes

Major Goals of Nucleosynthesis Studies

Isotope perspective

^{19}F

24th most common element

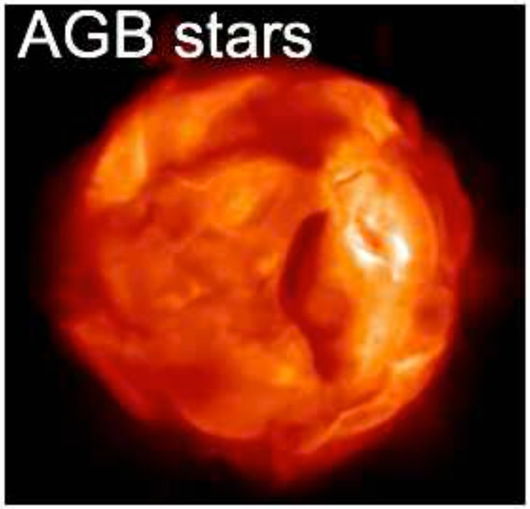
- determine cosmic origins of particular isotopes

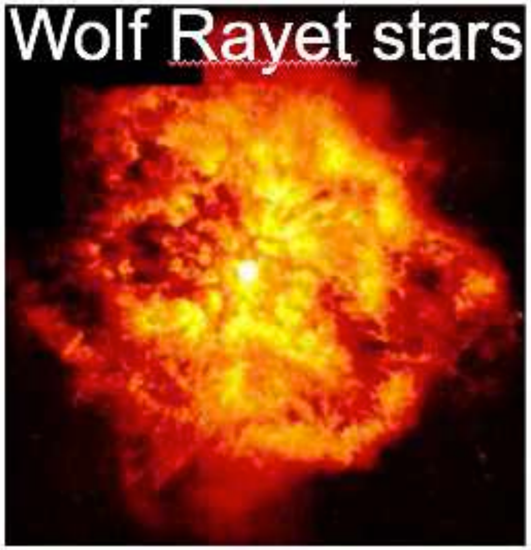
Major Goals of Nucleosynthesis Studies

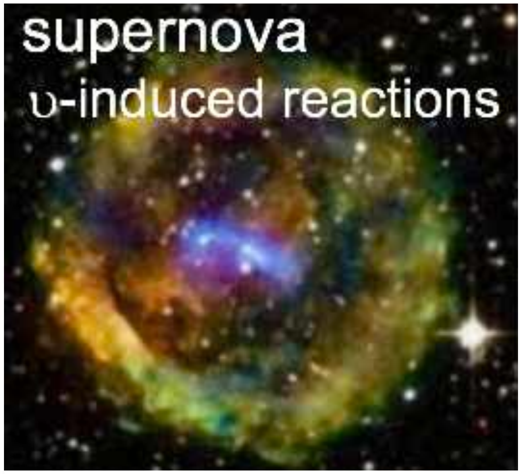
Isotope perspective

^{19}F

24th most common element







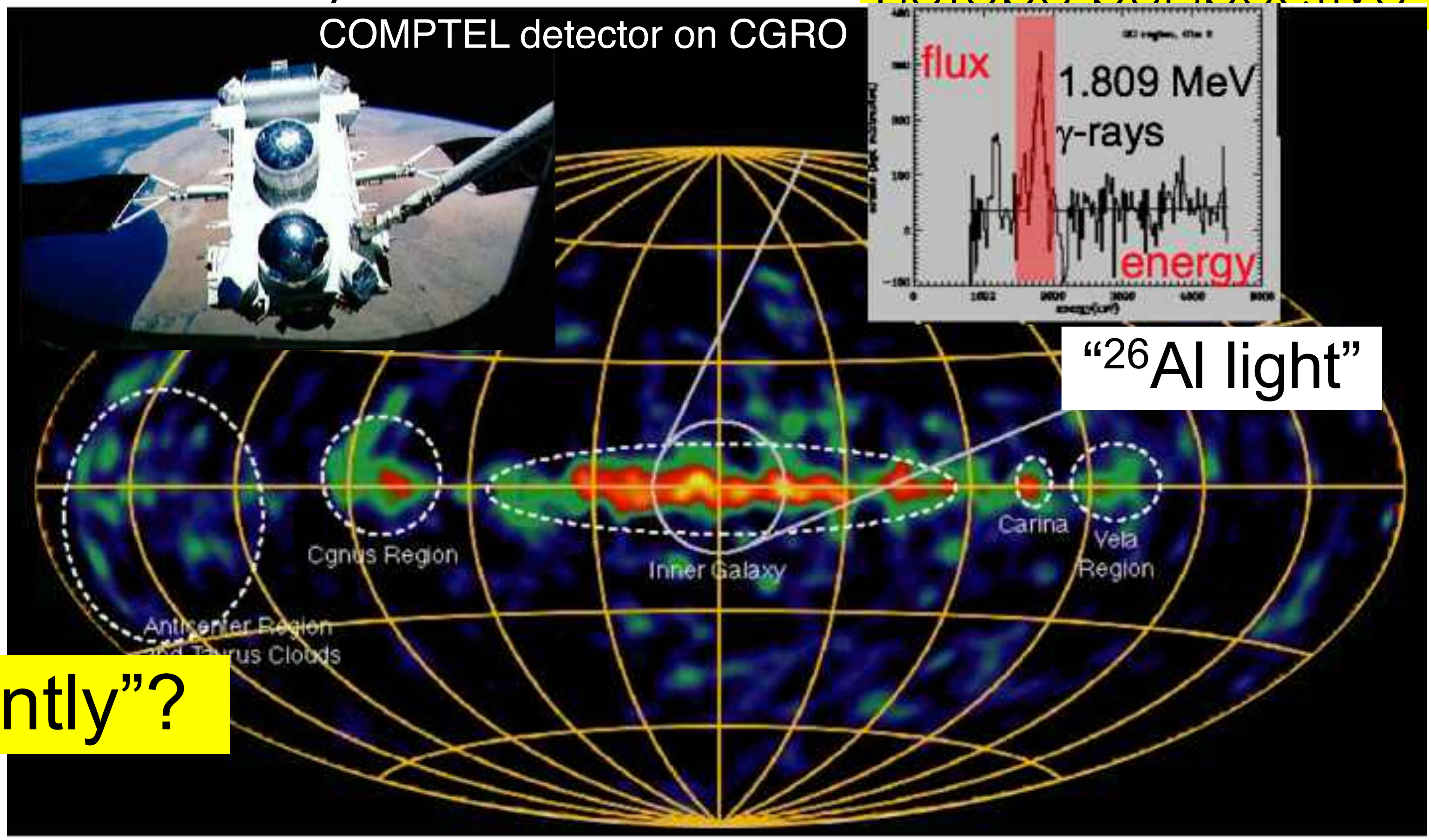
- determine cosmic origins of particular isotopes

Major Goals of Nucleosynthesis Studies

Isotope perspective

^{26}Al

radioactive
~10^6 years



made “recently”?

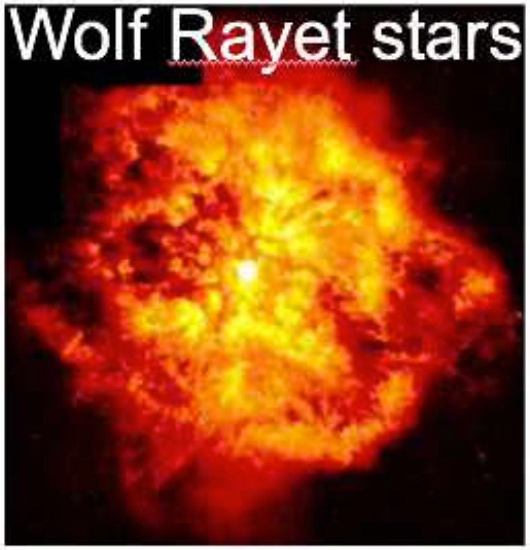
- determine cosmic origins of particular isotopes

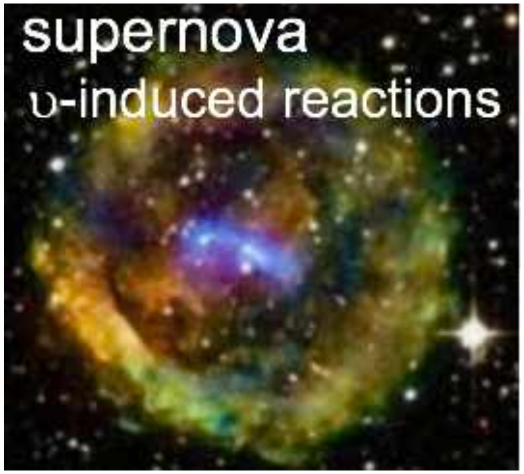
Major Goals of Nucleosynthesis Studies

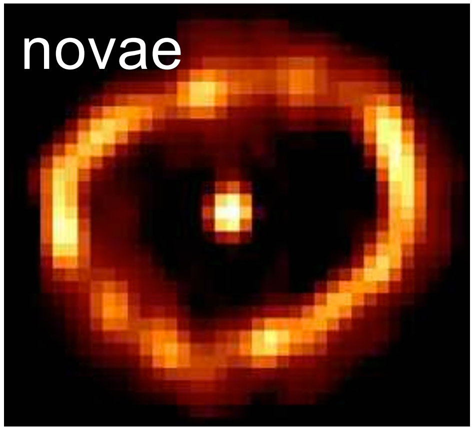
Isotope perspective

^{26}Al

radioactive
~10^6 years







made “recently”?

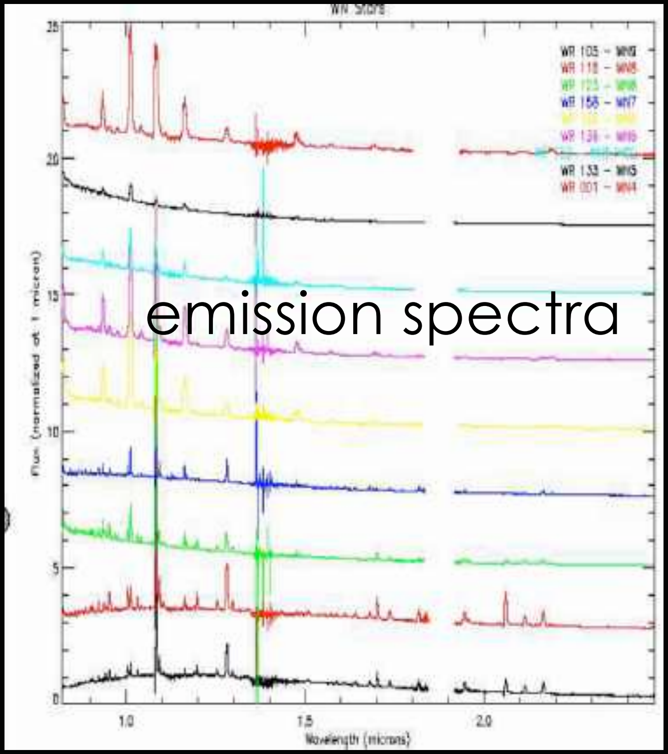
- determine cosmic origins of particular isotopes

Major Goals of Nucleosynthesis Studies

Astro perspective

Wolf-Rayet Stars

^{26}Al production?

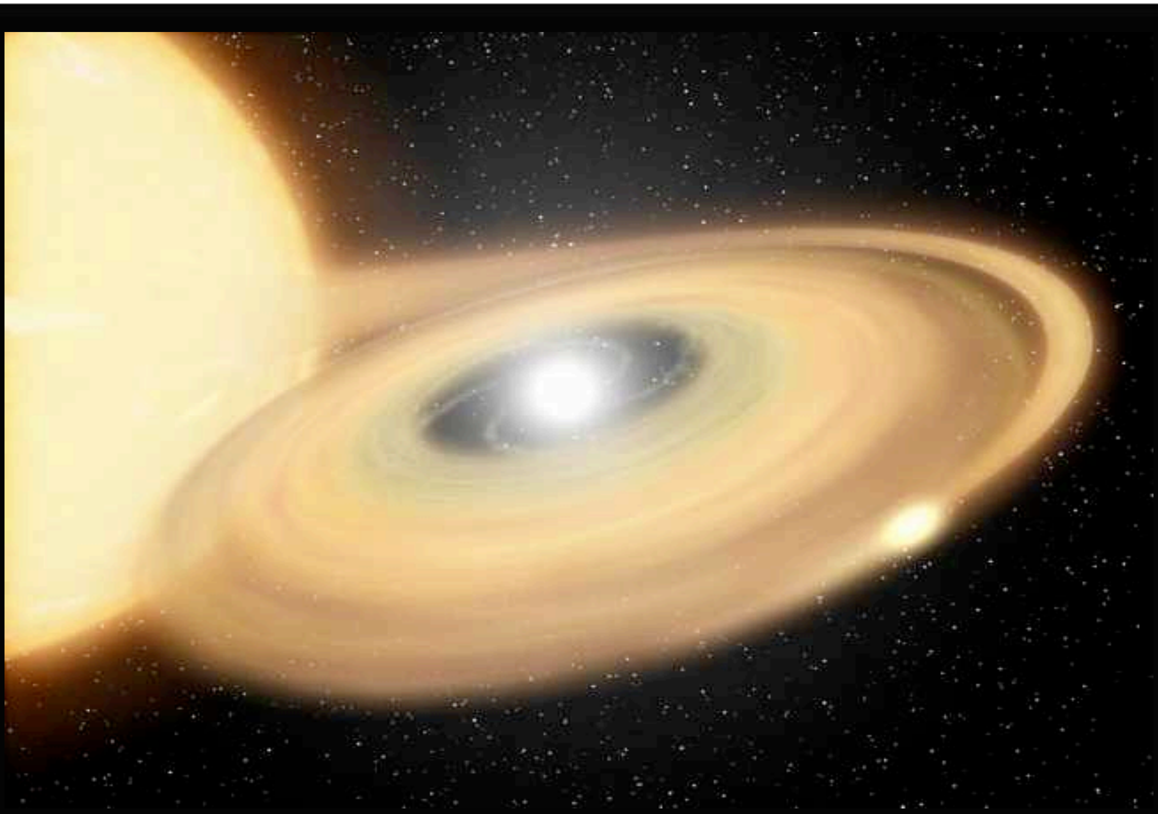


emission spectra

- determine which isotopes are produced in a given site

Major Goals of Nucleosynthesis Studies

Astro perspective



Nova Explosion

White Dwarf evolution

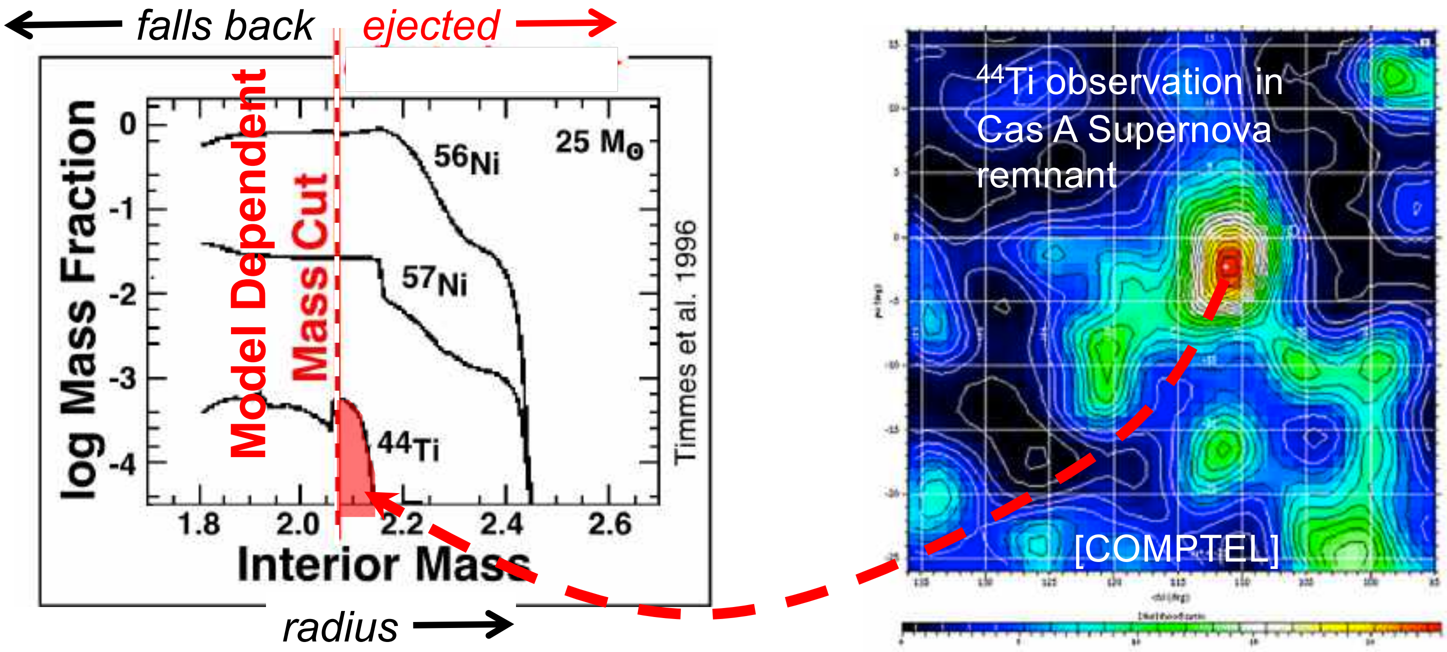
grows → Type 1a Supernova

eroded → White Dwarf

- determine how nucleosynthesis influences site evolution

Practical Goals of Nucleosynthesis Studies

Core Collapse Supernova Simulation

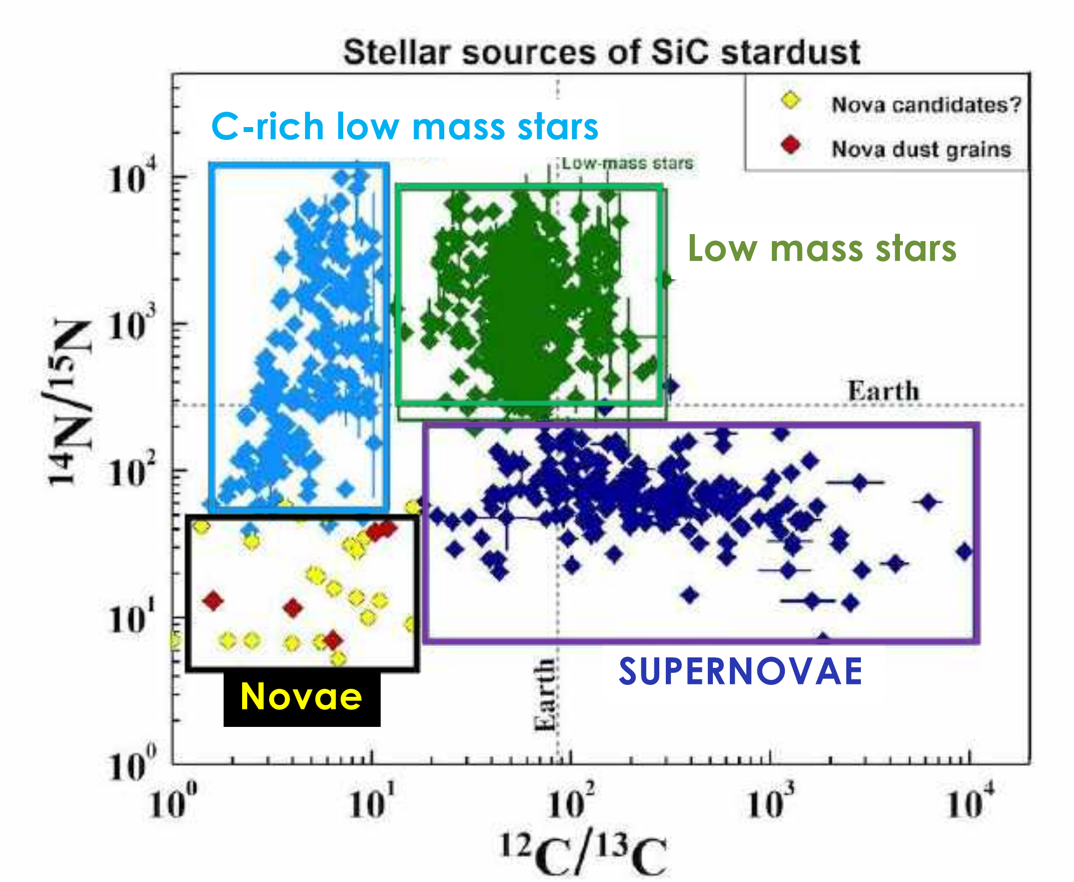


Timmes et al. 1996

^{44}Ti observation in Cas A Supernova remnant

- **explain**: connect an observation to a particular site

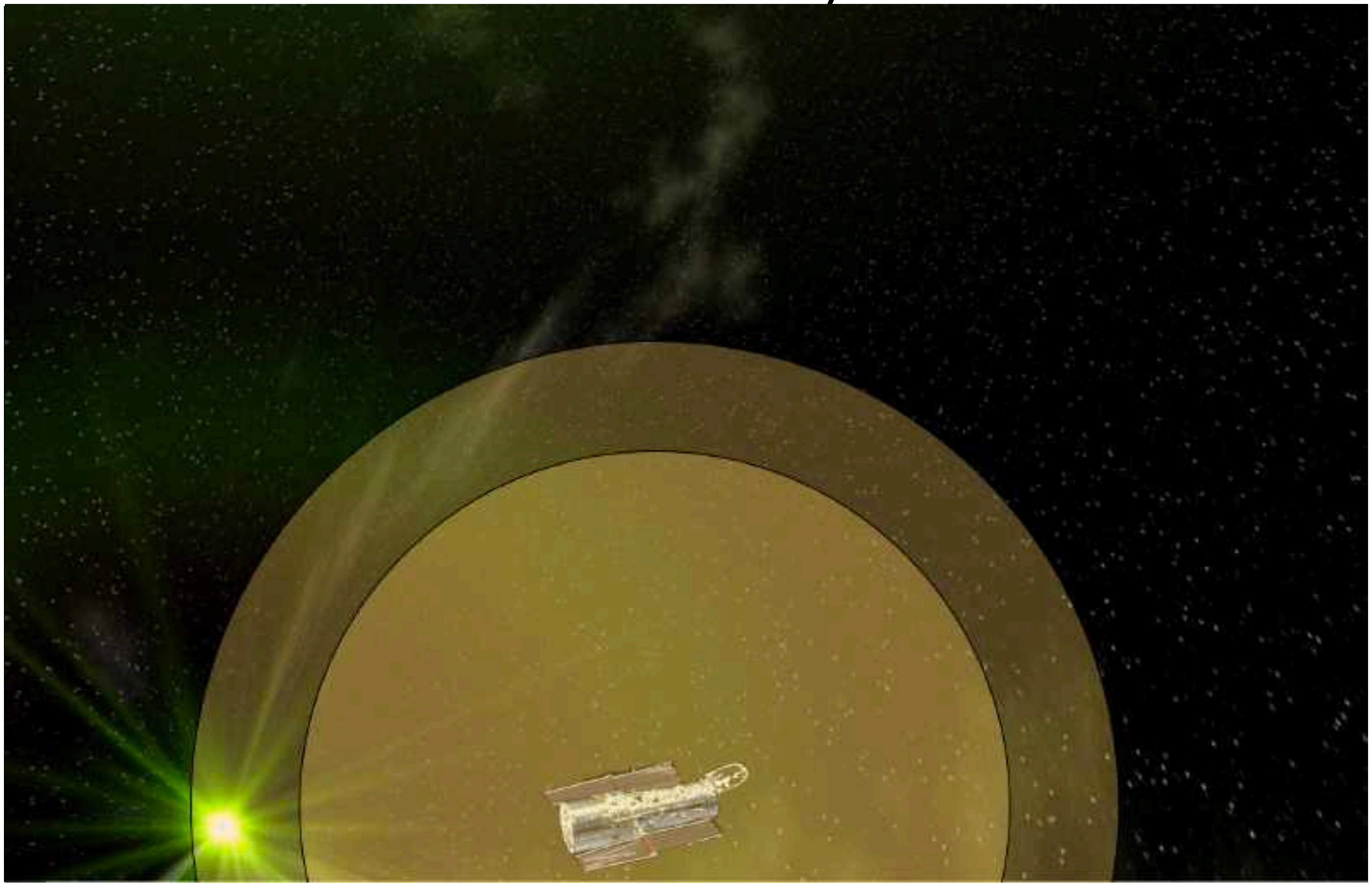
Practical Goals of Nucleosynthesis Studies



Abundance Ratios from Meteorite Grains

- **predict**: determine observational signature of a particular site

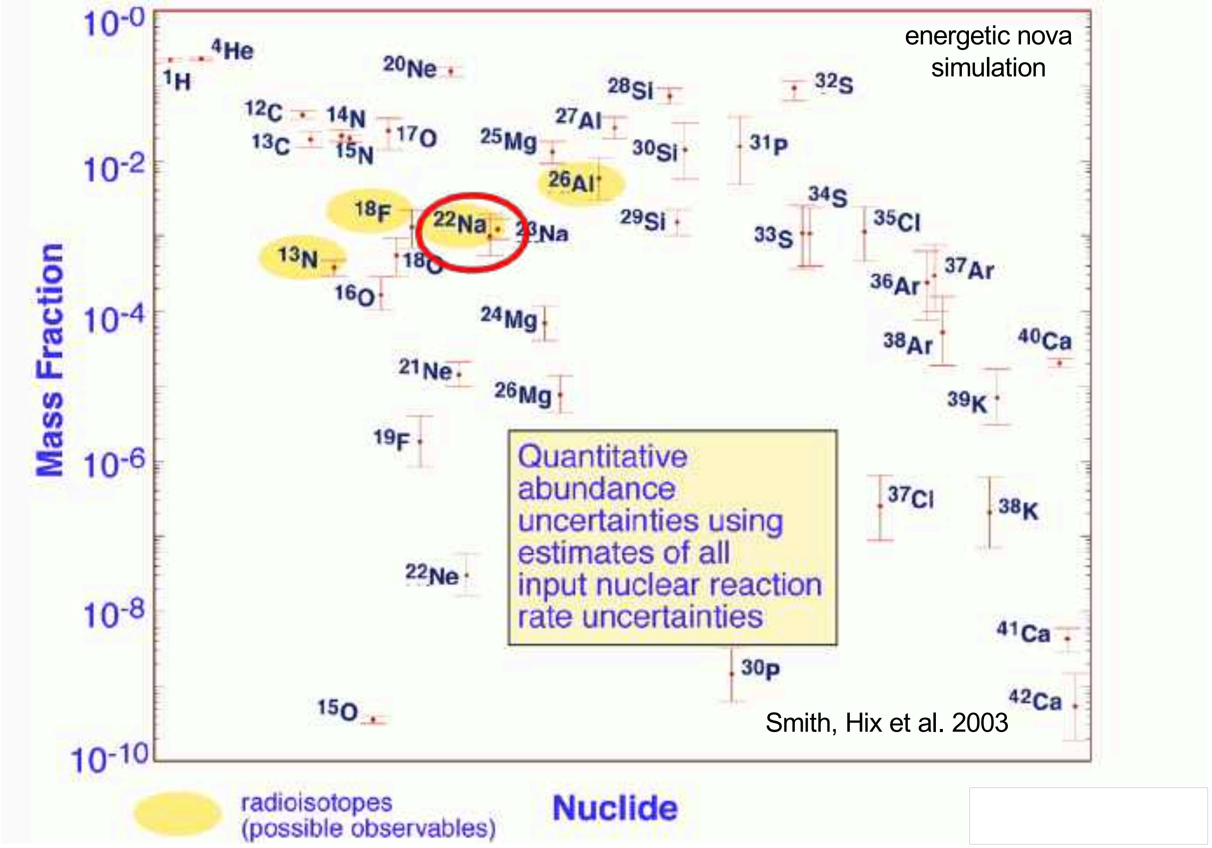
Practical Goals of Nucleosynthesis Studies



new rate
↙
simulation
↙
higher radionuclide abundance
↙
larger γ-ray emission from explosion
↙
γ-ray flux drops off more slowly
↙
can be detected from farther distance
↙
satellite sensitivity increased

- **impact**: determine the astrophysical implications of my work

Practical Goals of Nucleosynthesis Studies



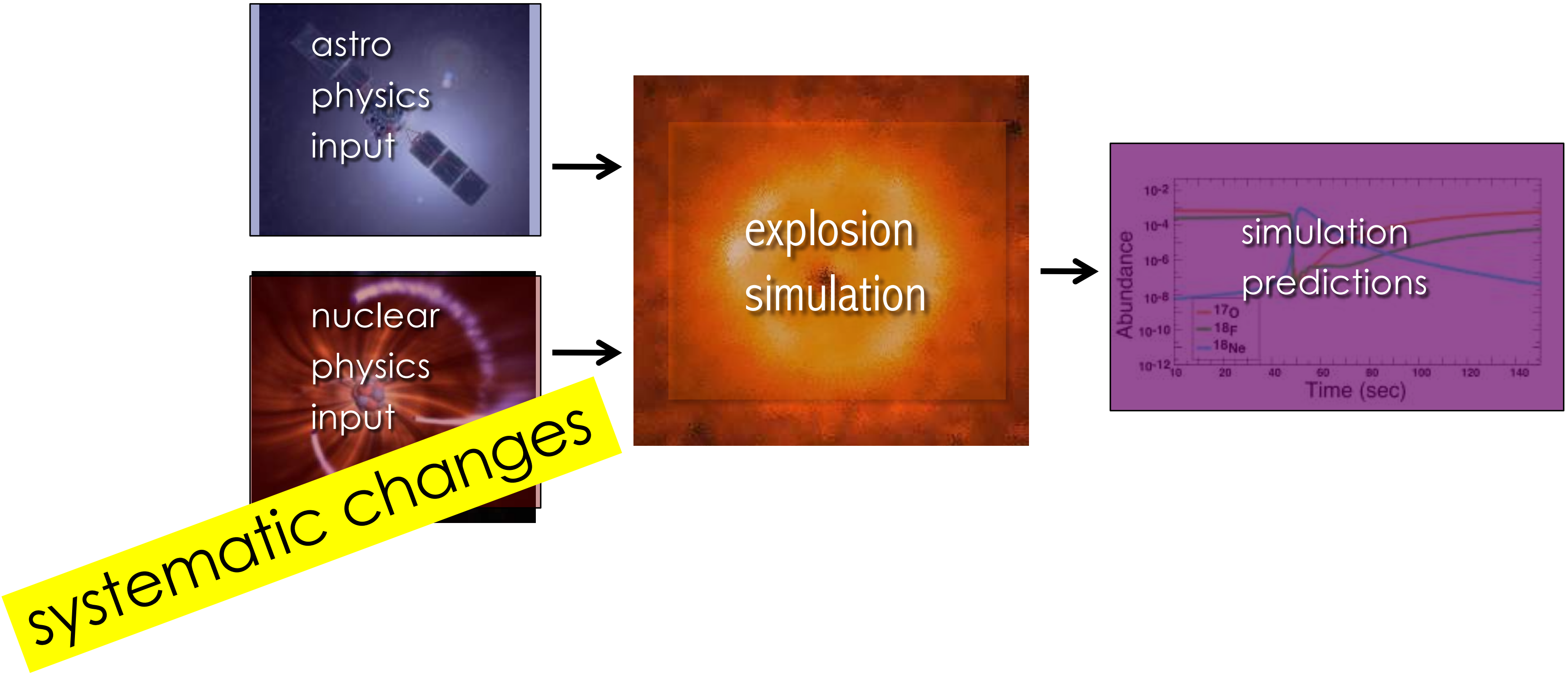
energetic nova simulation

Quantitative abundance uncertainties using estimates of all input nuclear reaction rate uncertainties

Smith, Hix et al. 2003

- **precision**: determine the uncertainty of our predictions

Sensitivity Studies



astro physics input

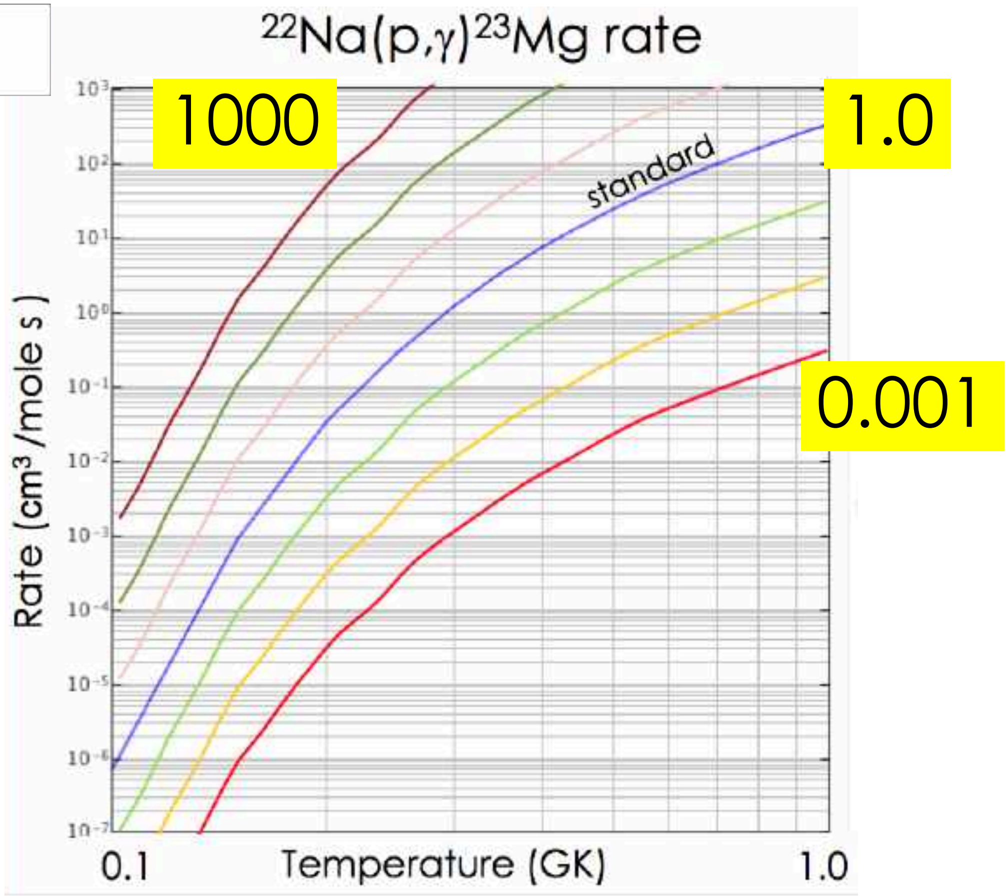
nuclear physics input

→ explosion simulation → simulation predictions

systematic changes

- sensitivity studies: examine outputs with systematic input changes

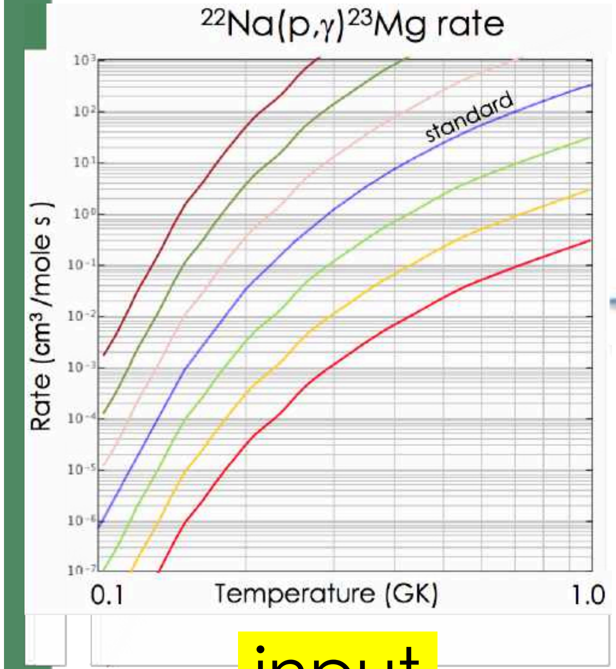
Sensitivity Studies



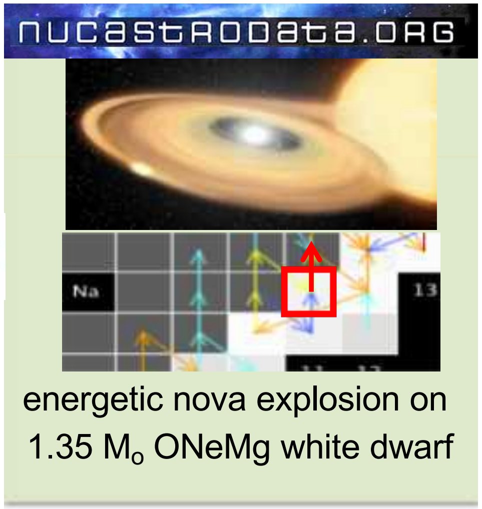
multiply
rate by
0.001
0.01
0.1
1.0
10
100
1000

- Quantitative example using the $^{22}Na(p,\gamma)^{23}Mg$ reaction rate

Sensitivity Studies

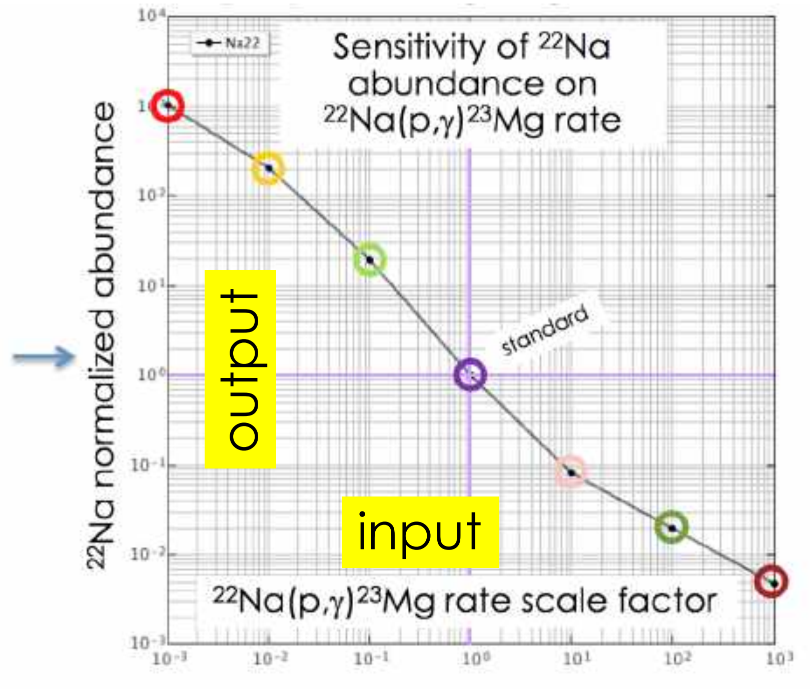


input



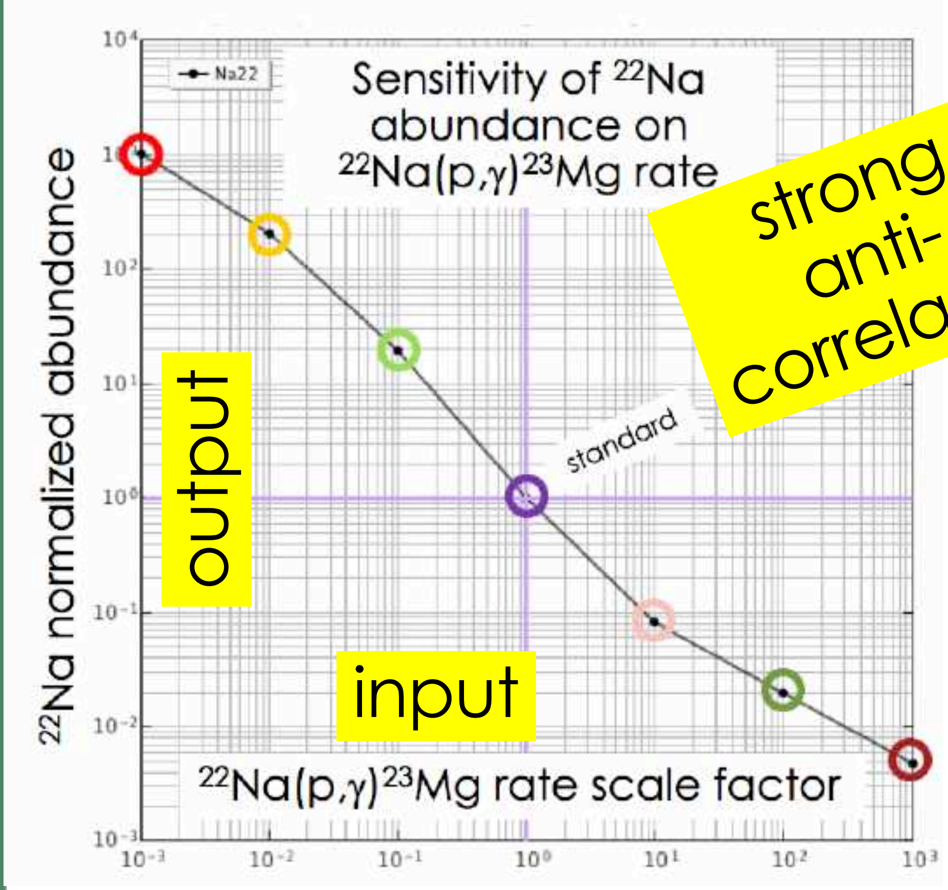
energetic nova explosion on 1.35 M_o ONeMg white dwarf

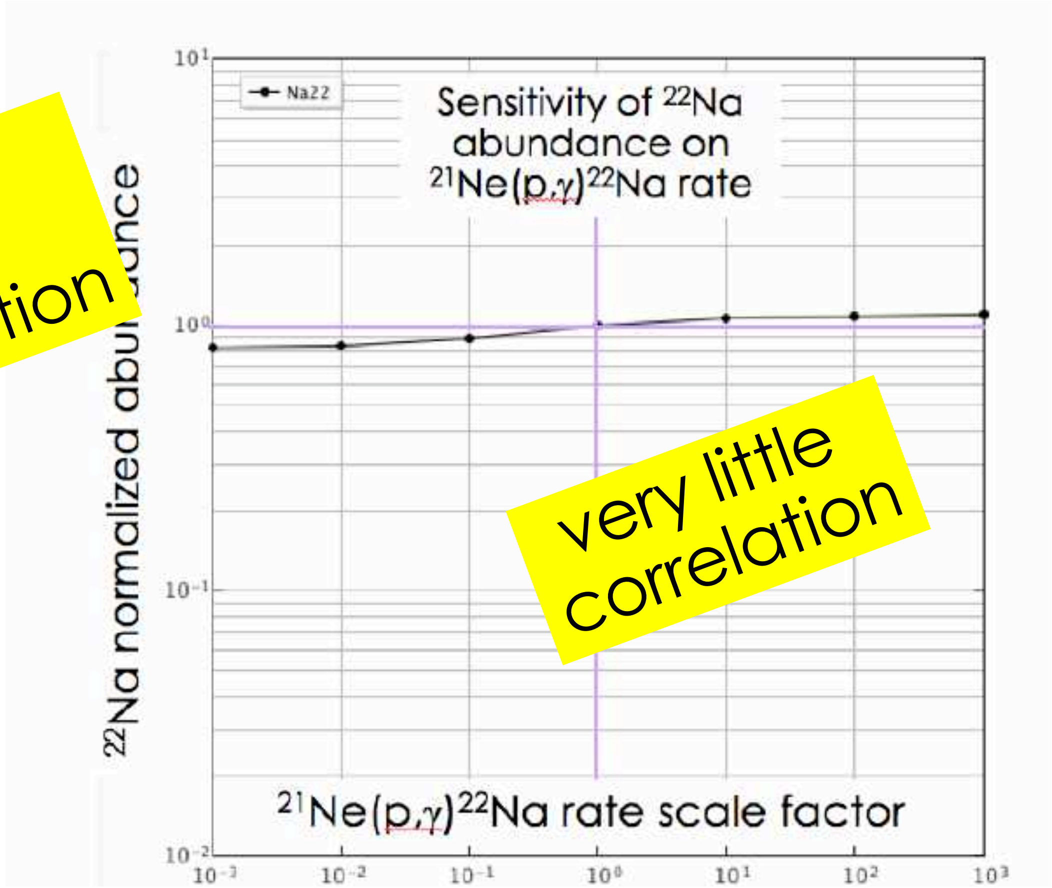
SIMULATION



- Quantitative example using the ^{22}Na(p,γ)^{23}Mg rate

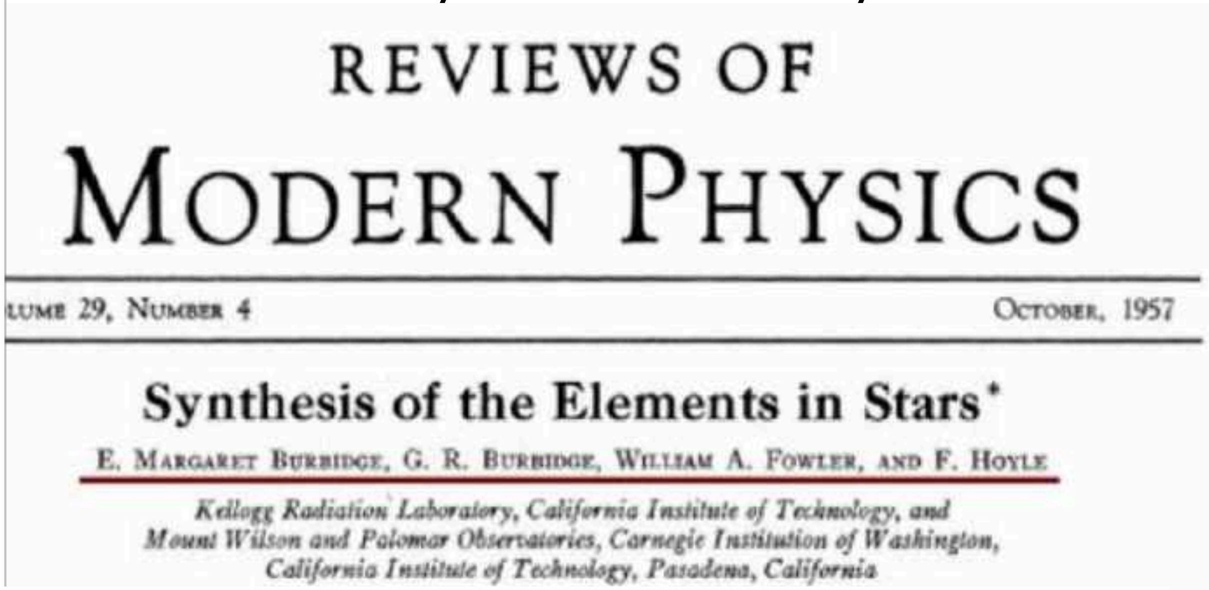
Practical Goals of Nucleosynthesis Studies





- **guide**: determine what I should study next

First Nucleosynthesis Study



REVIEWS OF

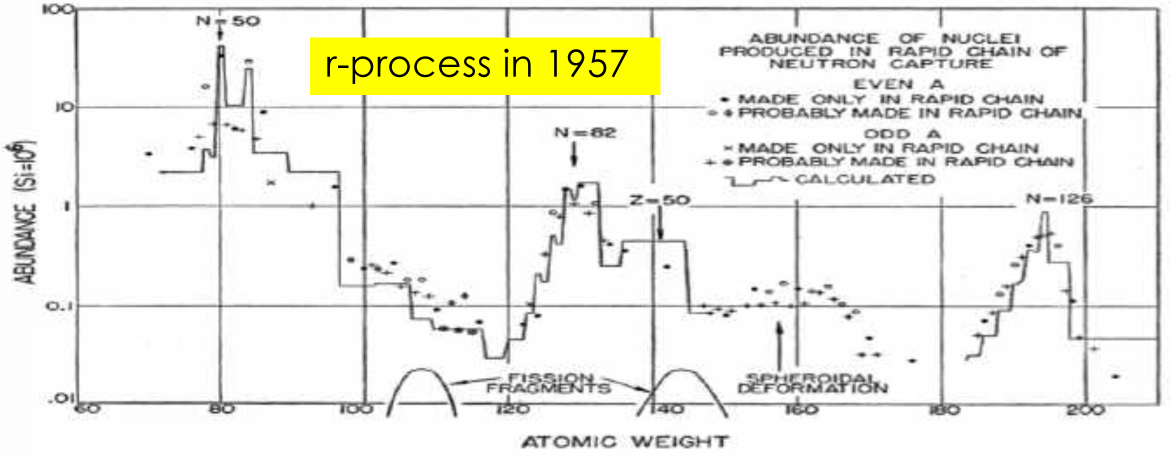
MODERN PHYSICS

LUME 29, NUMBER 4 OCTOBER, 1957

Synthesis of the Elements in Stars*

E. MARGARET BURBIDGE, G. R. BURBIDGE, WILLIAM A. FOWLER, AND F. HOYLE

Kellogg Radiation Laboratory, California Institute of Technology, and
Mount Wilson and Palomar Observatories, Carnegie Institution of Washington,
California Institute of Technology, Pasadena, California



r-process in 1957

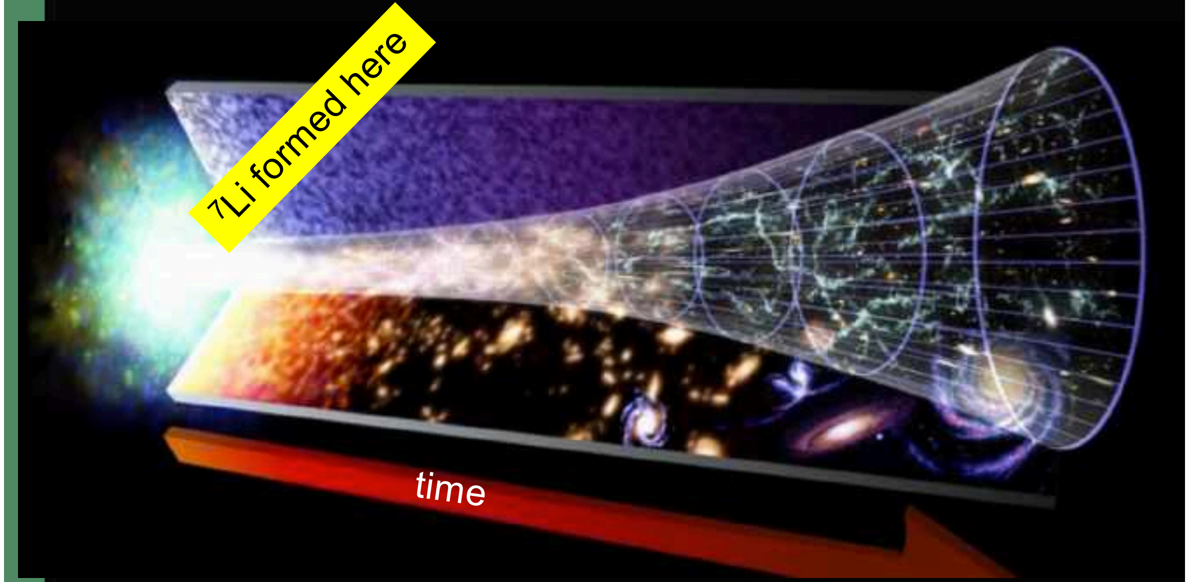
M Burbridge

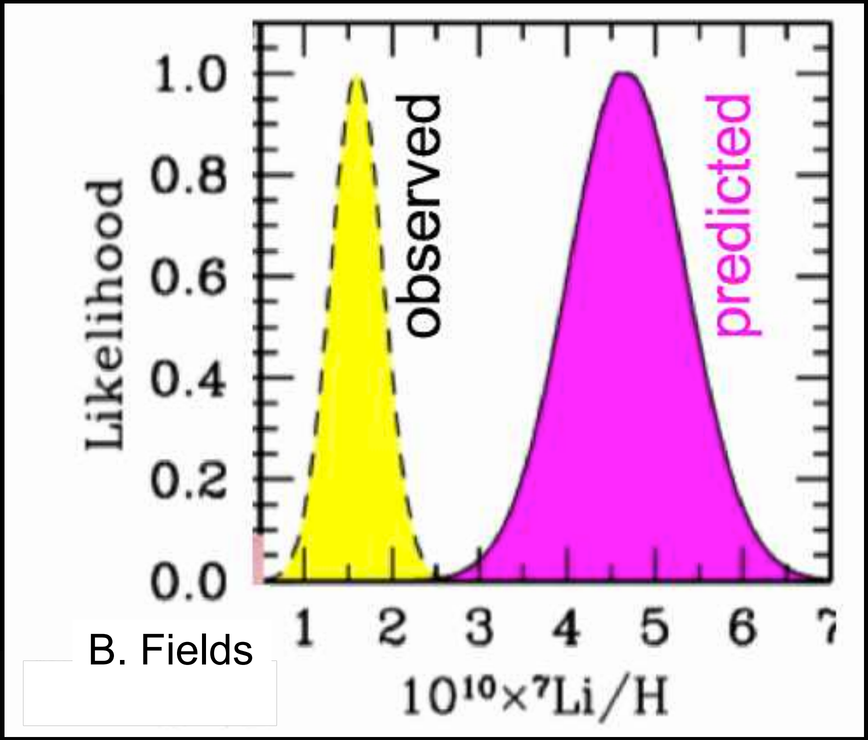
G Burbridge

W Fowler

F Hoyle

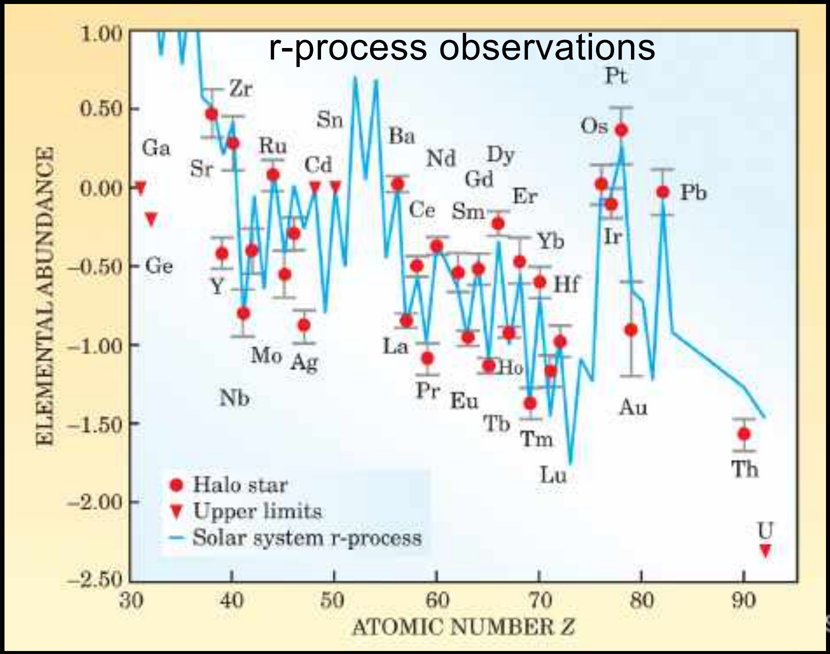
Open Nucleosynthesis Puzzles

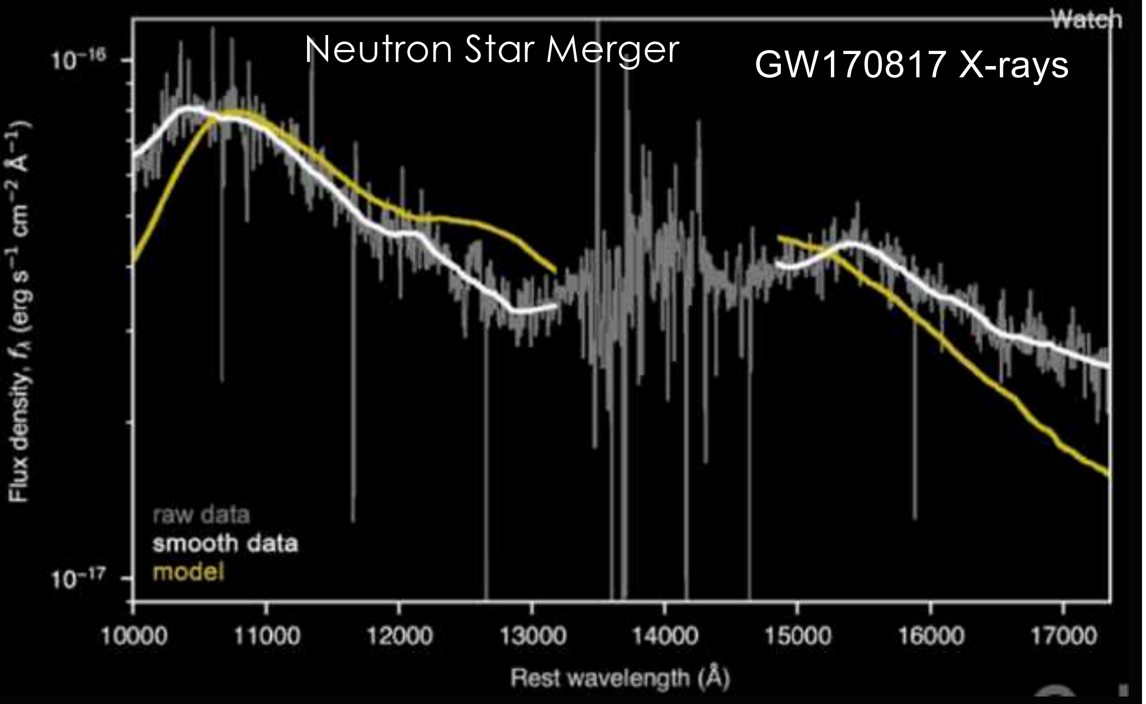




- ^{7}Li problem in Big Bang Nucleosynthesis

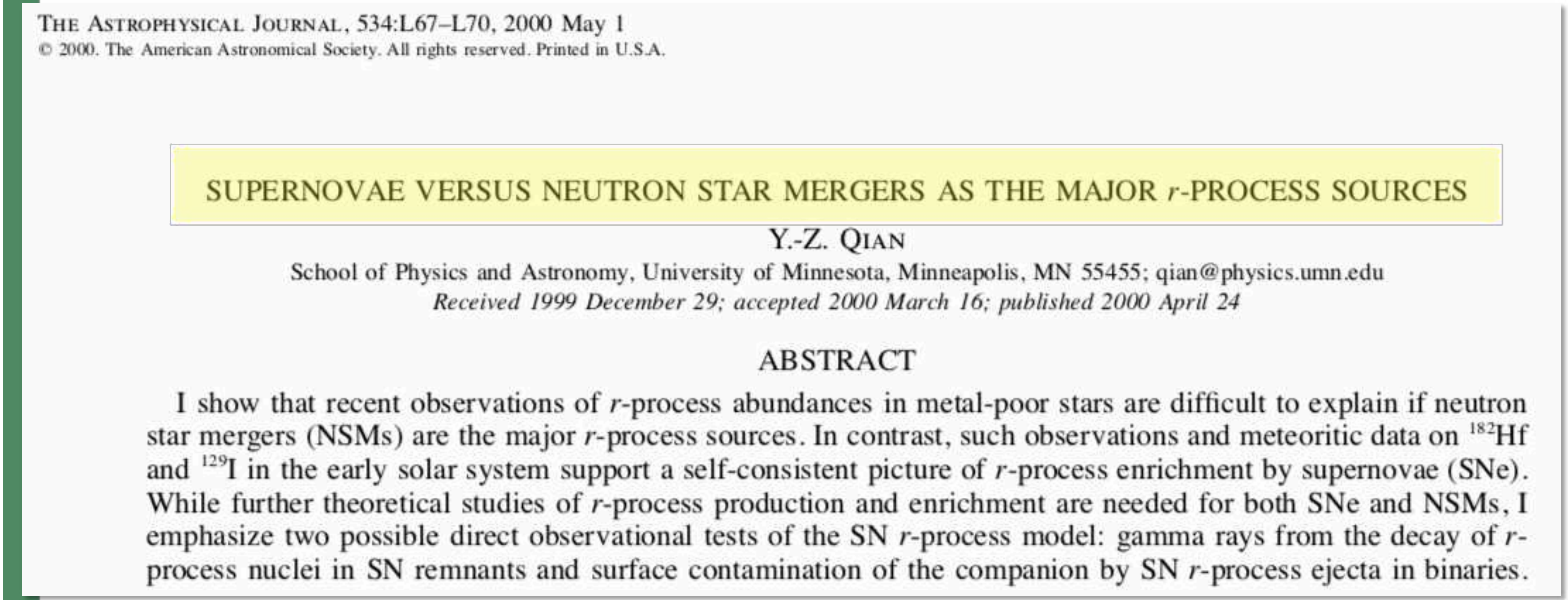
Open Nucleosynthesis Puzzles





- r-process in supernovae and neutron star mergers

Open Nucleosynthesis Puzzles



THE ASTROPHYSICAL JOURNAL, 534:L67–L70, 2000 May 1

SUPERNOVAE VERSUS NEUTRON STAR MERGERS AS THE MAJOR *r*-PROCESS SOURCES

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Received 1999 December 29; accepted 2000 March 16; published 2000 April 24

ABSTRACT

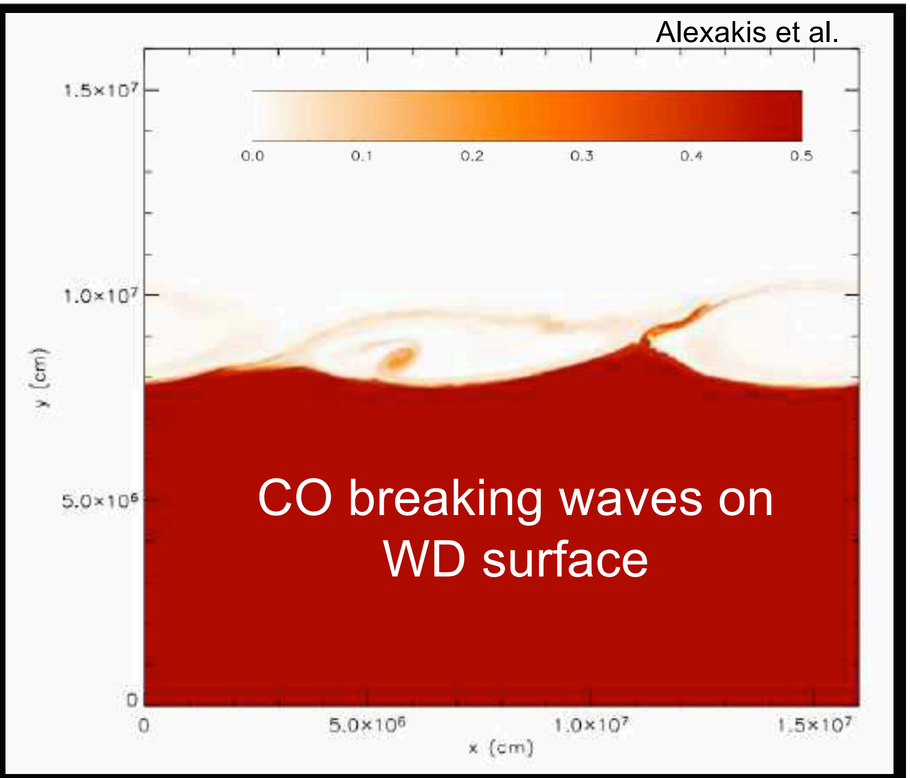
I show that recent observations of *r*-process abundances in metal-poor stars are difficult to explain if neutron star mergers (NSMs) are the major *r*-process sources. In contrast, such observations and meteoritic data on ^{182}Hf and ^{129}I in the early solar system support a self-consistent picture of *r*-process enrichment by supernovae (SNe). While further theoretical studies of *r*-process production and enrichment are needed for both SNe and NSMs, I emphasize two possible direct observational tests of the SN *r*-process model: gamma rays from the decay of *r*-process nuclei in SN remnants and surface contamination of the companion by SN *r*-process ejecta in binaries.

- r-process in supernovae and neutron star mergers

Open Nucleosynthesis Puzzles

mixing / flame on WD surface

Kercek & Hillebrandt

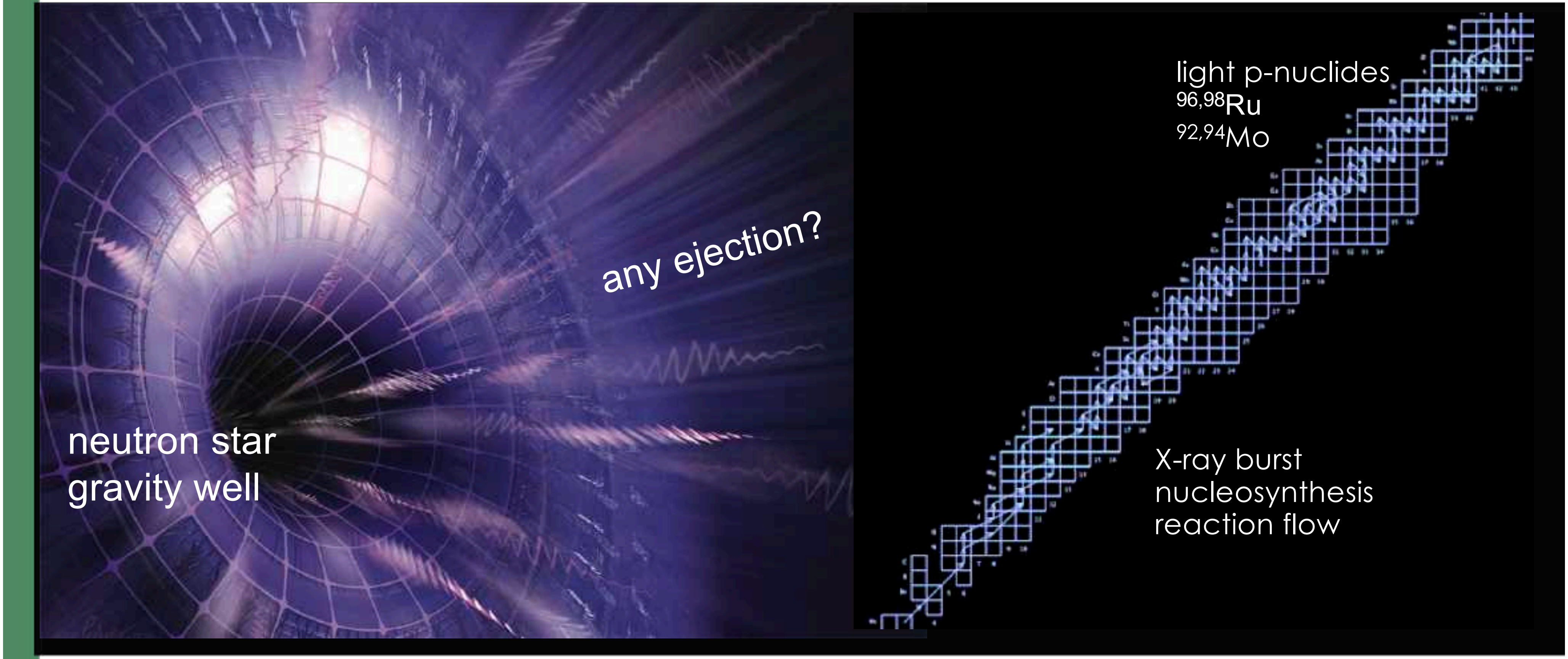


Alexakis et al.

CO breaking waves on WD surface

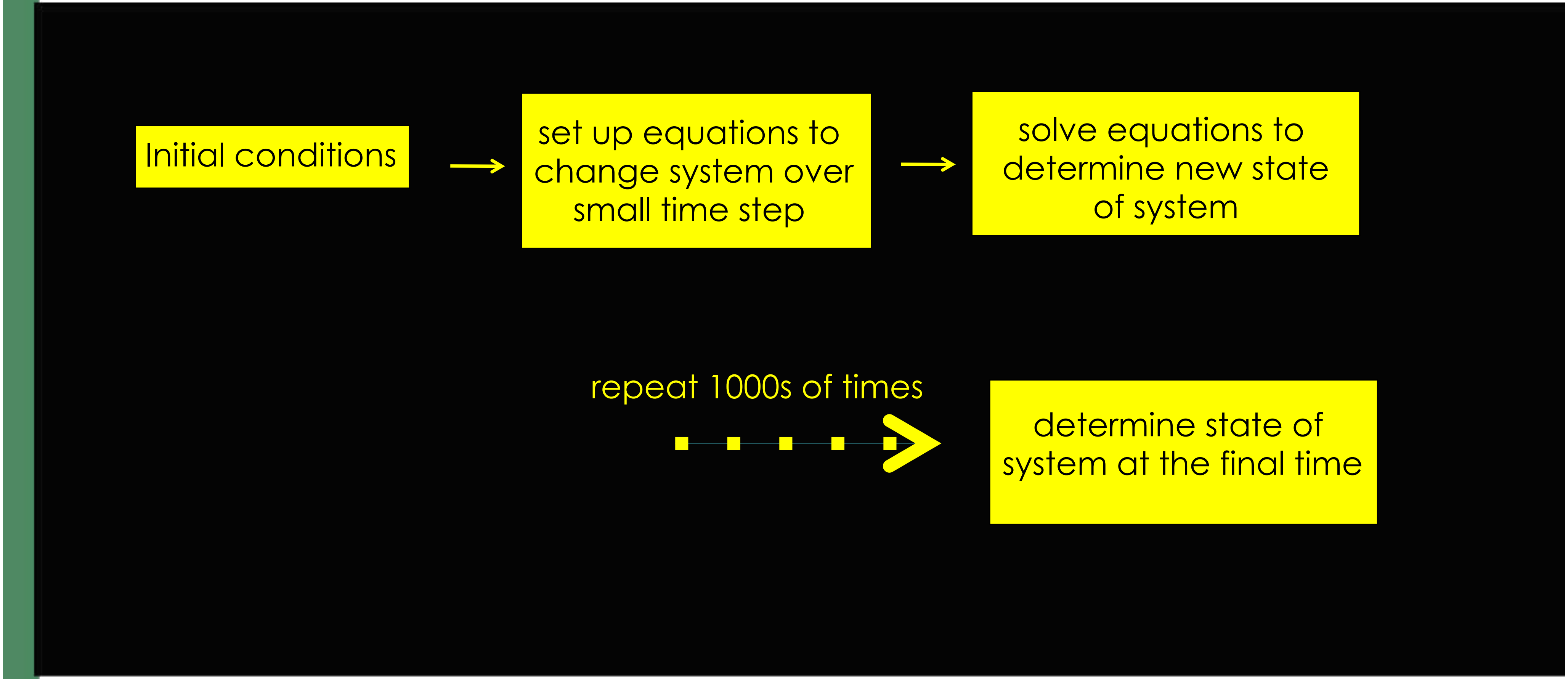
- What is the trigger for a nova explosion?

Open Nucleosynthesis Puzzles



- Can any material escape from an X-ray burst?

Basic Simulation Approach



Initial conditions →

set up equations to change system over small time step →

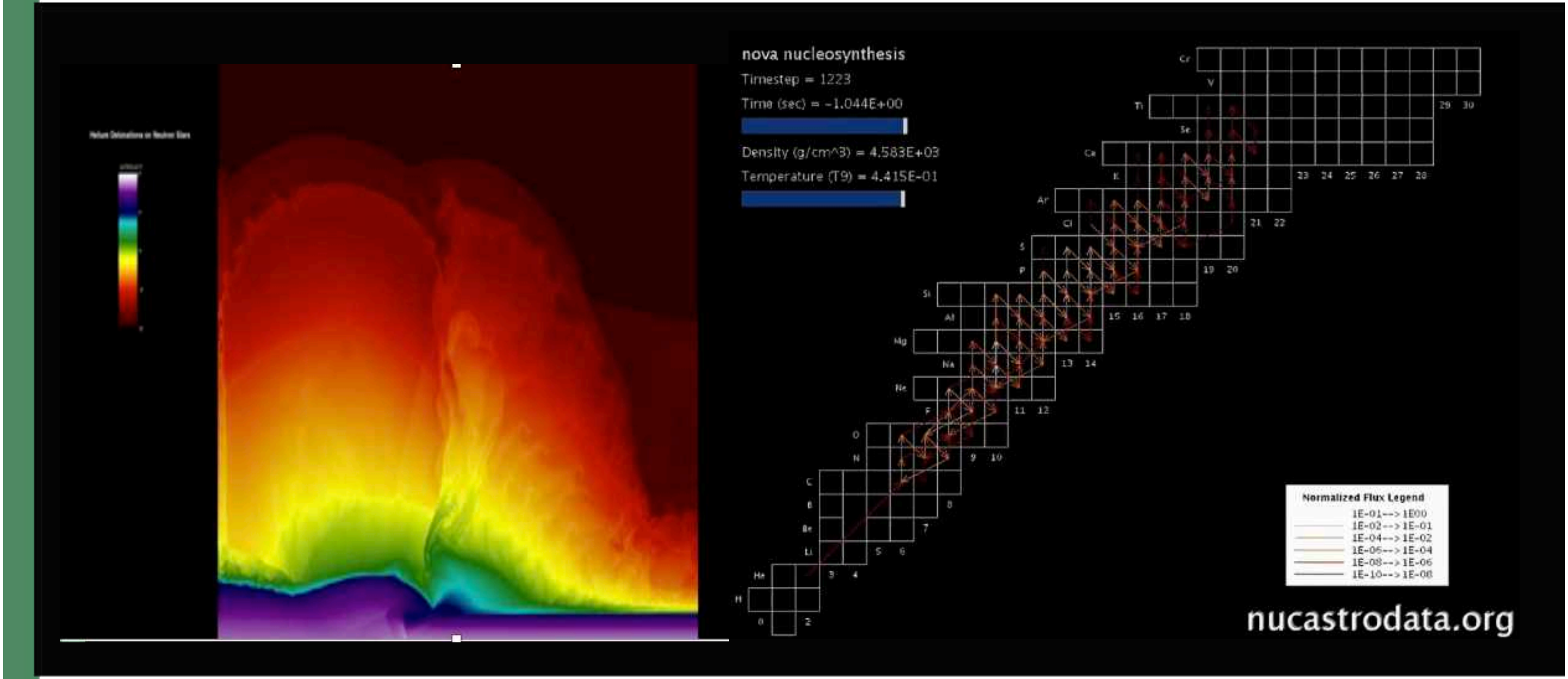
solve equations to determine new state of system

repeat 1000s of times

determine state of system at the final time

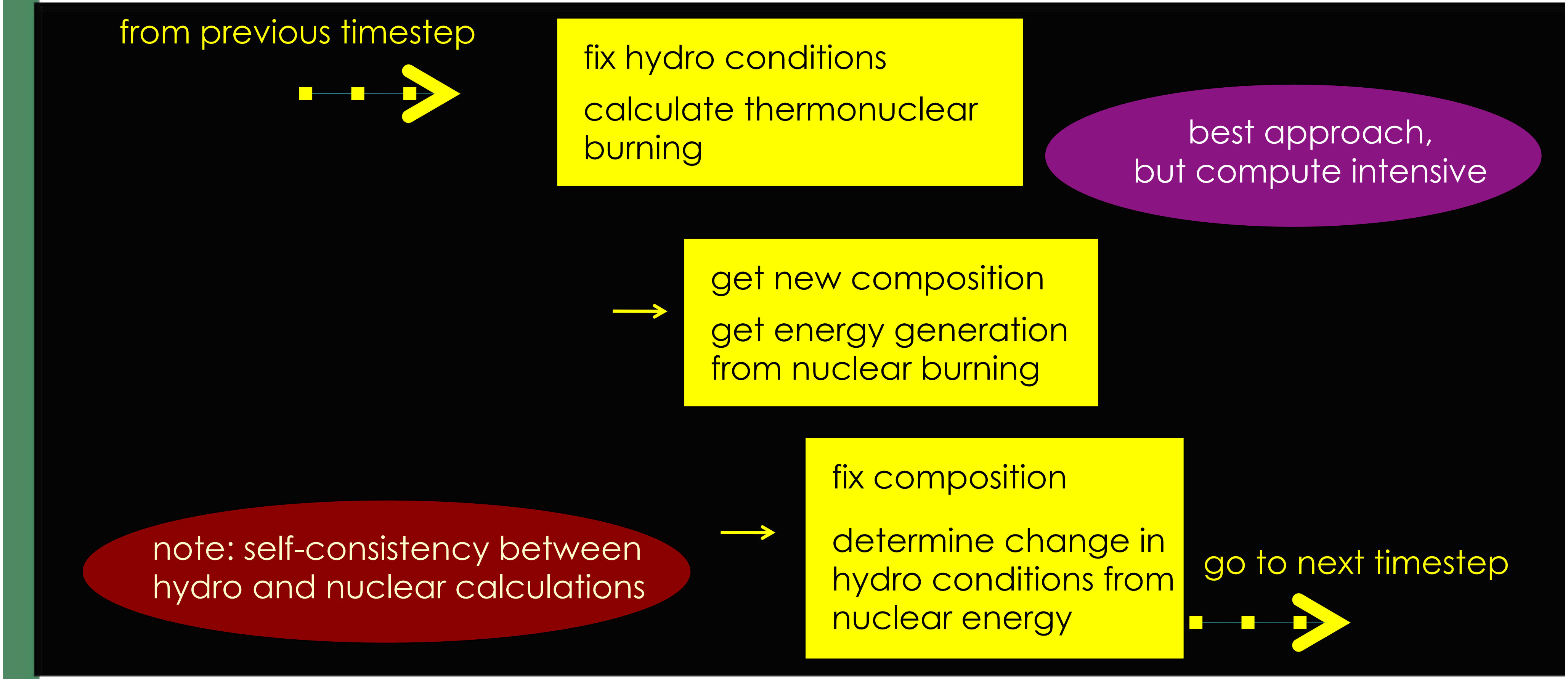
- time evolution of the system from initial to final conditions

Simulation Components



- hydrodynamics and thermonuclear burning

One Approach – Fully Coupled Simulations



from previous timestep

fix hydro conditions

calculate thermonuclear burning

best approach, but compute intensive

get new composition

get energy generation from nuclear burning

fix composition

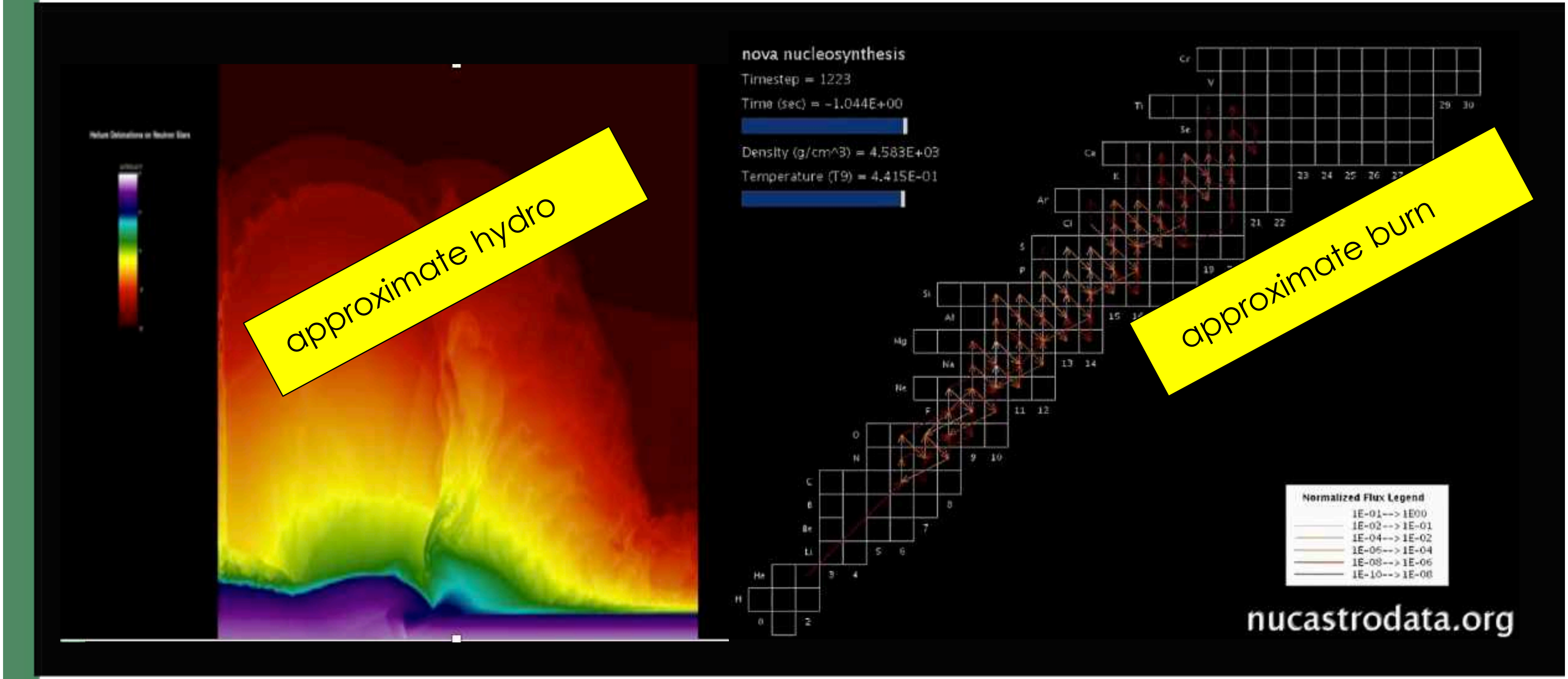
determine change in hydro conditions from nuclear energy

note: self-consistency between hydro and nuclear calculations

go to next timestep

- couple hydrodynamics and thermonuclear burning

Practical Simulations



approximate hydro

approximate burn

nova nucleosynthesis

Timestep = 1223

Time (sec) = -1.044E+00

Density (g/cm^3) = 4.583E+03

Temperature (T9) = 4.415E-01

- hydrodynamics and thermonuclear burning

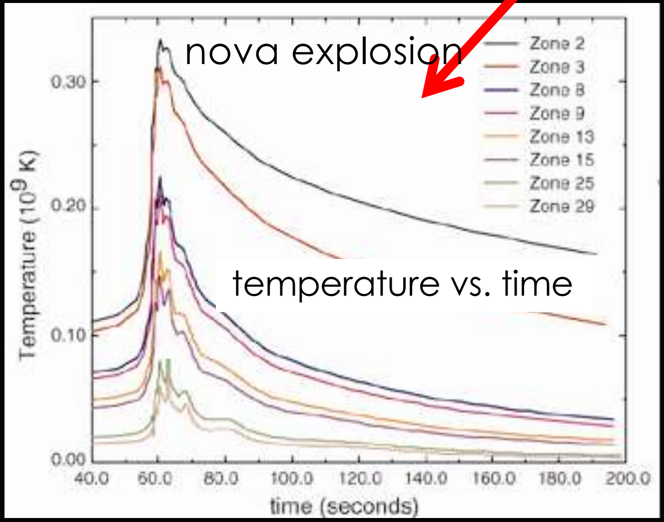
Post - Processing Nucleosynthesis Approach

from previous timestep

look up hydro conditions

calculate thermonuclear burning

approximate FAST approach



nova explosion

temperature vs. time

→ get new composition

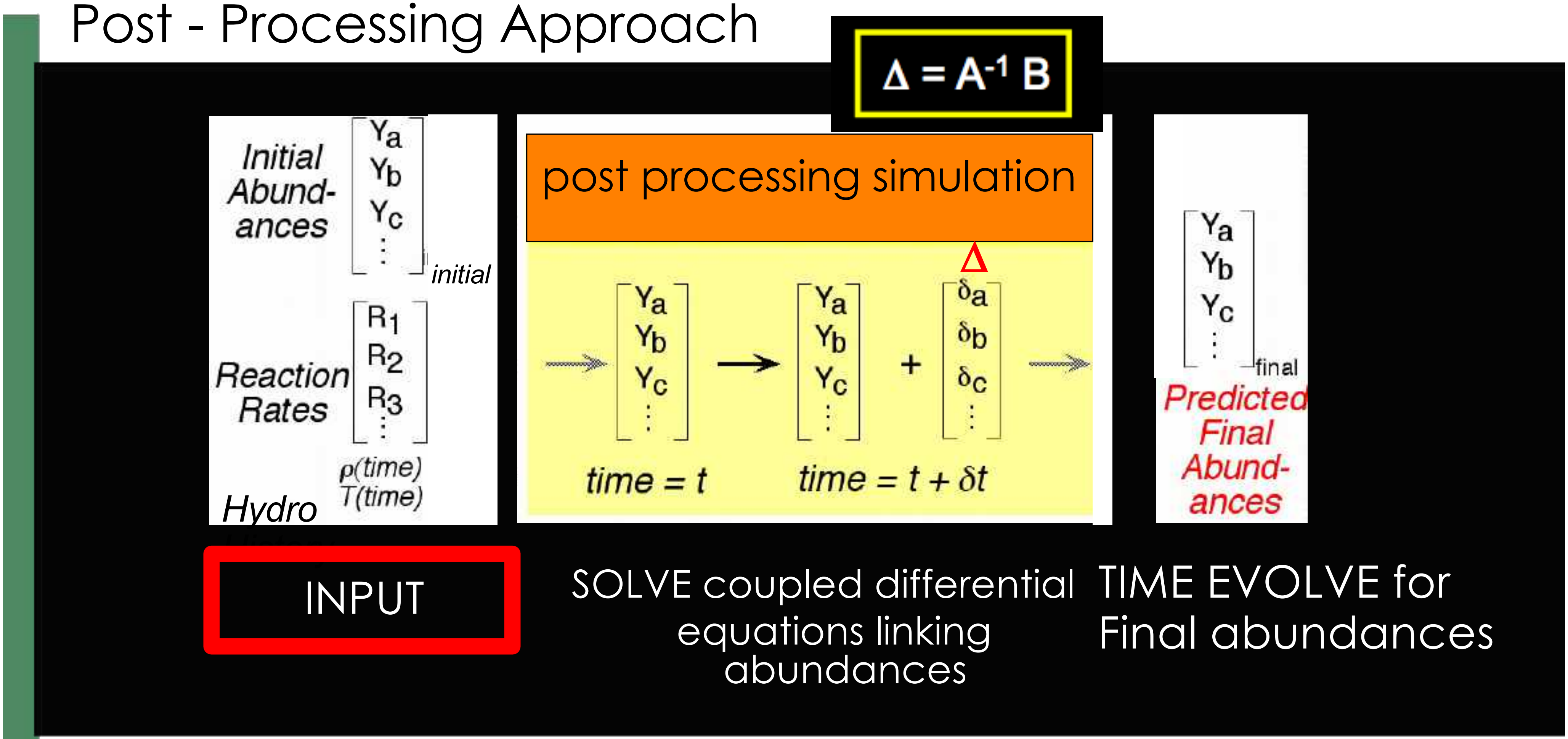
fix composition

→ go to next timestep

determine change in hydro conditions from nuclear energy

- determine thermonuclear burning over a *fixed* hydro profile

Post - Processing Approach



$\Delta = A^{-1} B$

post processing simulation

INPUT

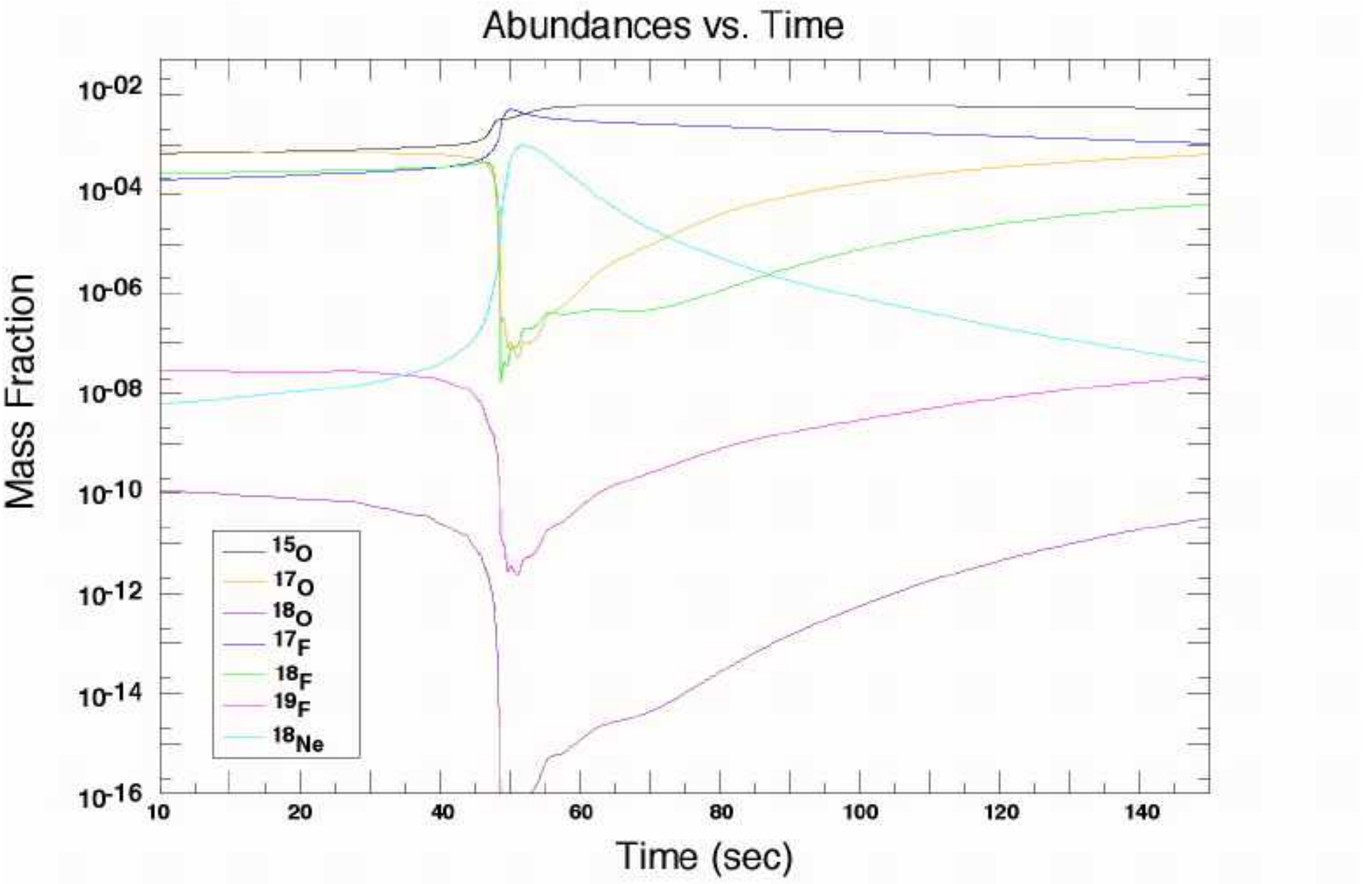
SOLVE coupled differential equations linking abundances

TIME EVOLVE for Final abundances

- time-evolving composition via thermonuclear burning

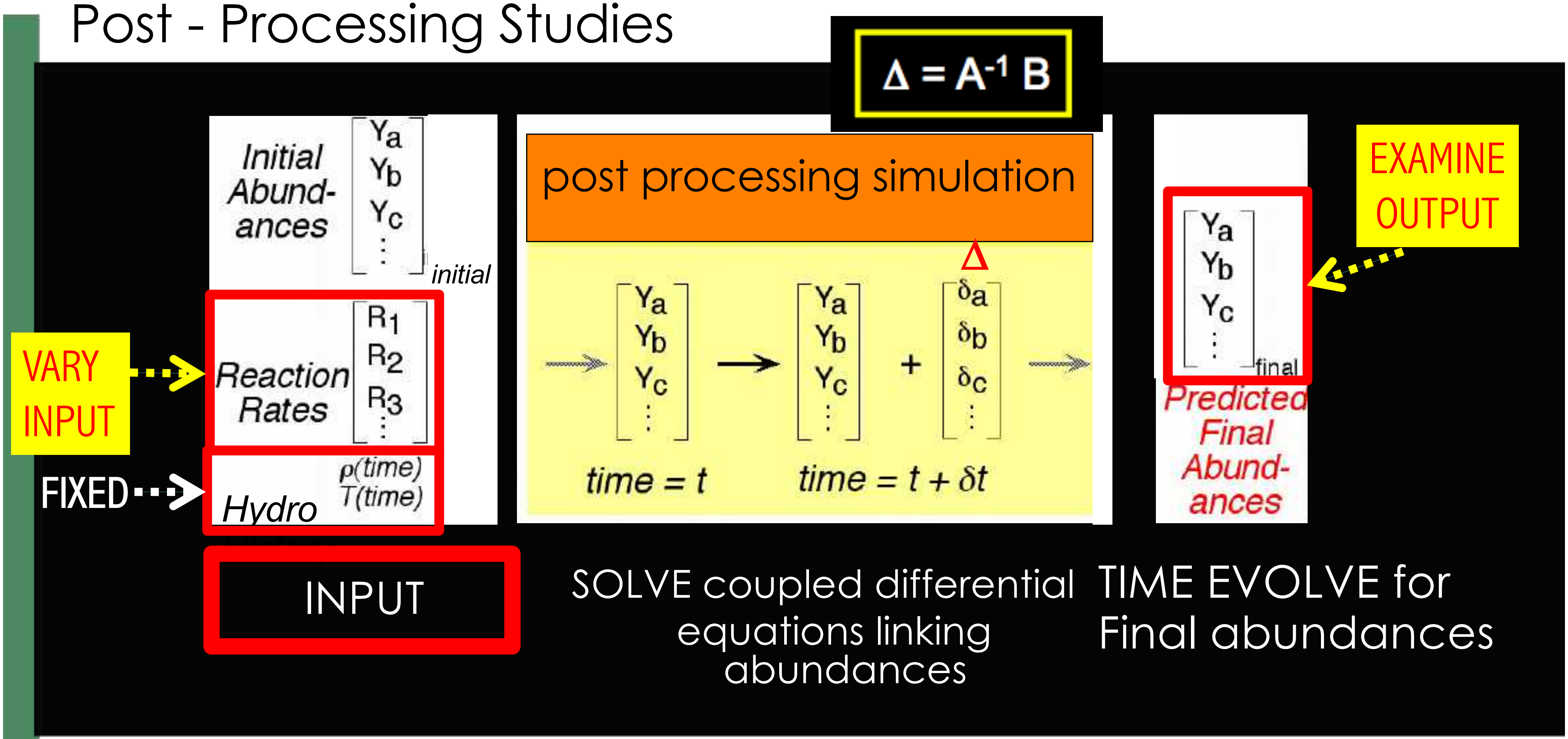
Post - Processing Approach

example: time evolution of abundances in nova outburst



Nova outburst on 1.25 Solar Mass White Dwarf

Post - Processing Studies



$\Delta = A^{-1} B$

Initial Abund- ances $\begin{bmatrix} Y_a \\ Y_b \\ Y_c \\ \vdots \end{bmatrix}_{initial}$

VARY INPUT

Reaction Rates $\begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ \vdots \end{bmatrix}$

FIXED

Hydro $\rho(time)$ $T(time)$

INPUT

post processing simulation

$$\begin{bmatrix} Y_a \\ Y_b \\ Y_c \\ \vdots \end{bmatrix} \longrightarrow \begin{bmatrix} Y_a \\ Y_b \\ Y_c \\ \vdots \end{bmatrix} + \overset{\Delta}{\begin{bmatrix} \delta_a \\ \delta_b \\ \delta_c \\ \vdots \end{bmatrix}}$$

time = t   time = t + δt

SOLVE coupled differential equations linking abundances

EXAMINE OUTPUT

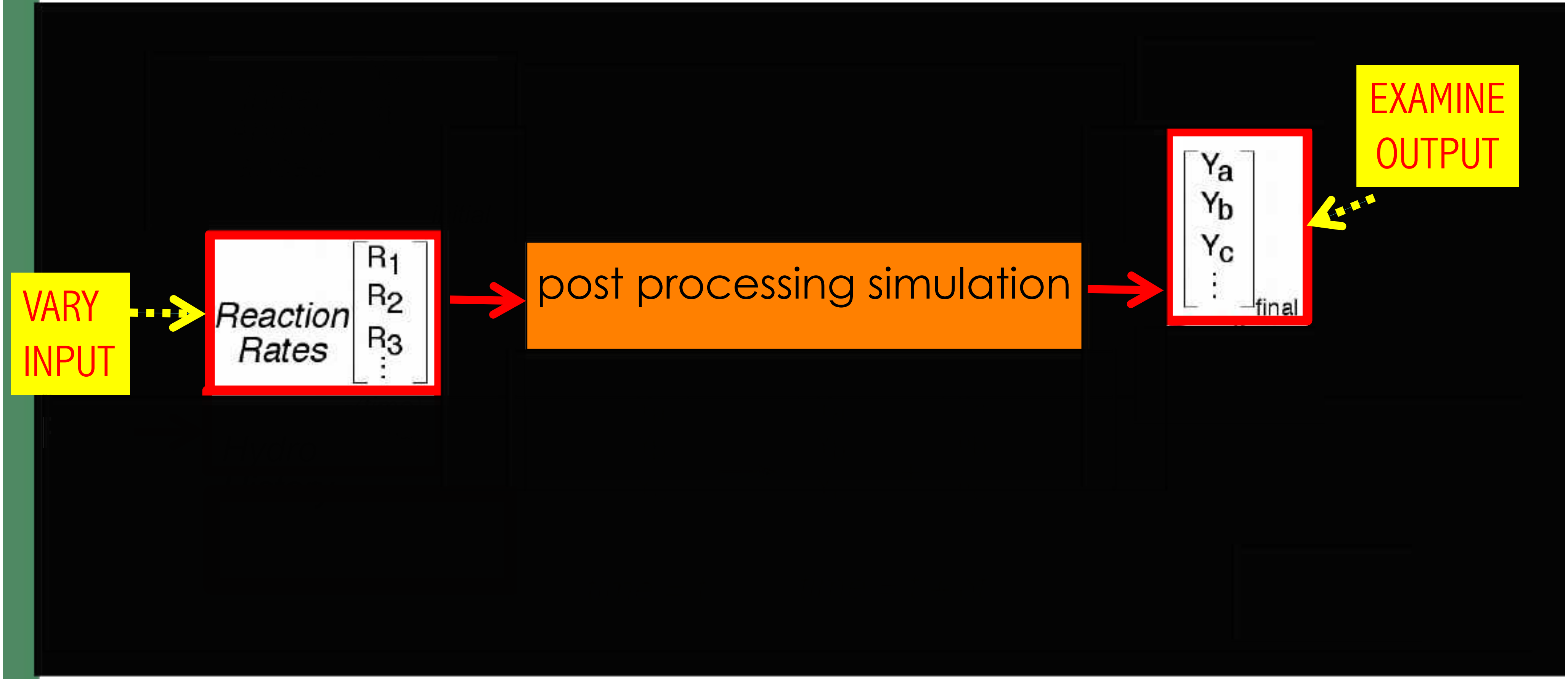
$\begin{bmatrix} Y_a \\ Y_b \\ Y_c \\ \vdots \end{bmatrix}_{final}$

Predicted Final Abund- ances

TIME EVOLVE for Final abundances

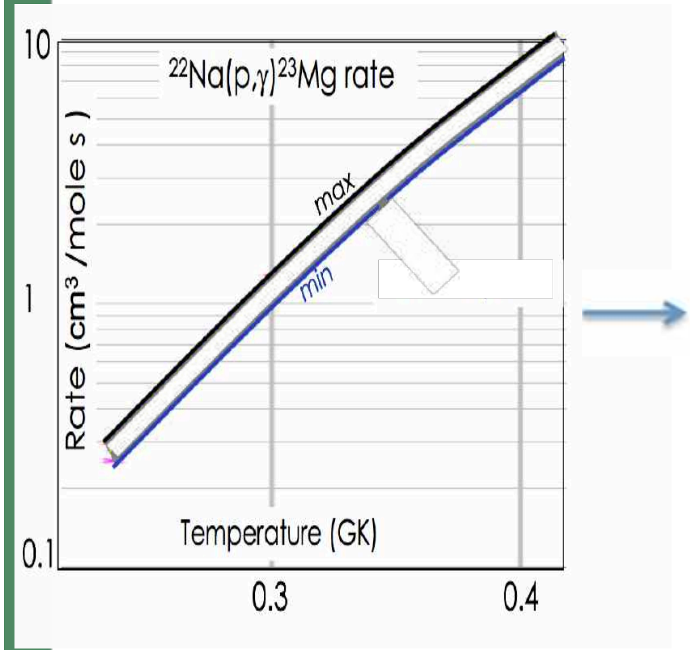
- variation of input nuclear physics is the key approach

Post - Processing Studies

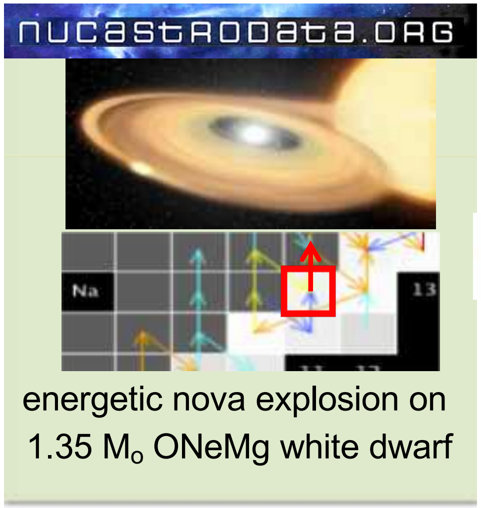


- variation of input nuclear physics is the key approach

Post - Processing Studies

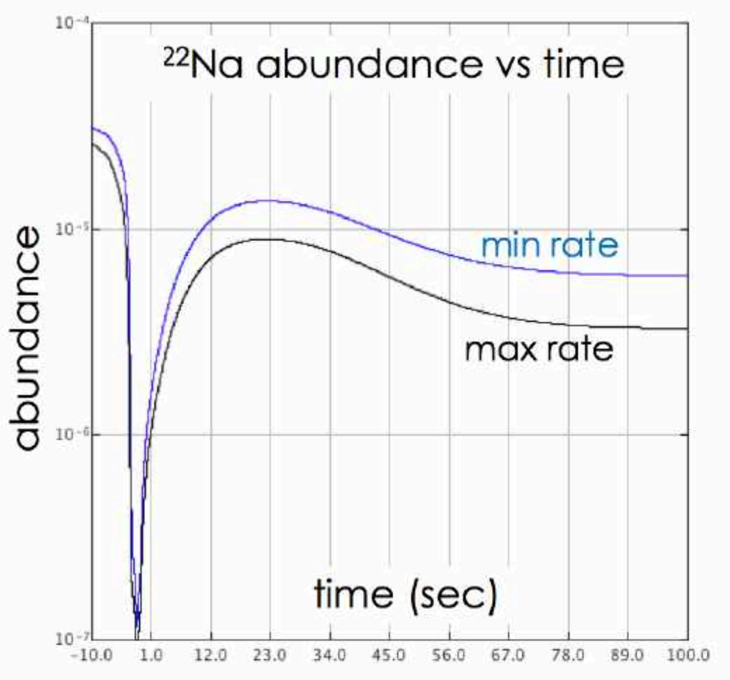


two different inputs for
same reaction rate



energetic nova explosion on
1.35 M_o ONeMg white dwarf

SIMULATION

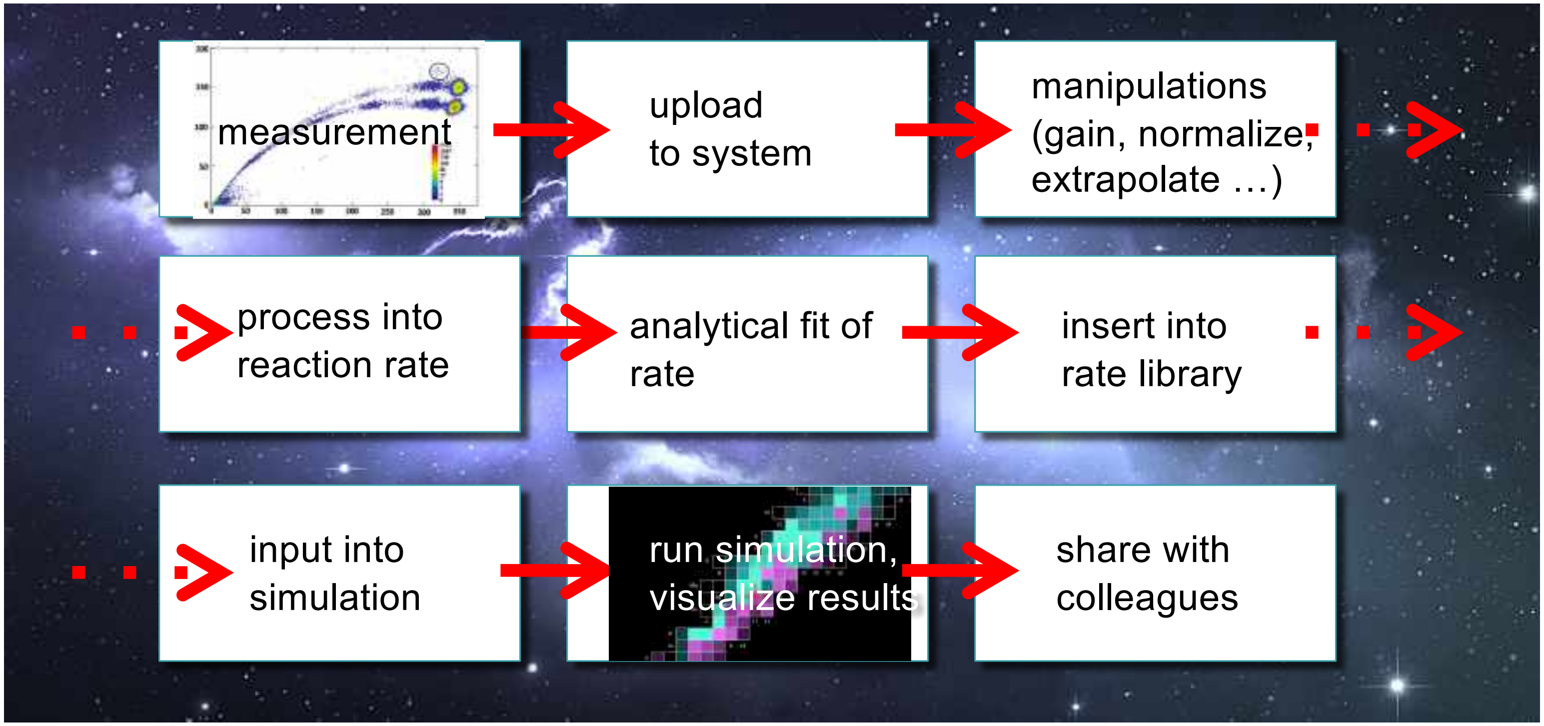


two different abundance vs time
predictions

- variation of input nuclear physics is the key approach

Online Software System

Nuclear Astro Data Pipeline



measurement

upload to system

manipulations (gain, normalize, extrapolate …)

process into reaction rate

analytical fit of rate

insert into rate library

input into simulation

run simulation, visualize results

share with colleagues

- nucleosynthesis studies with point-and-click interface

unique cloud computing system

platform independent

automated sensitivity studies

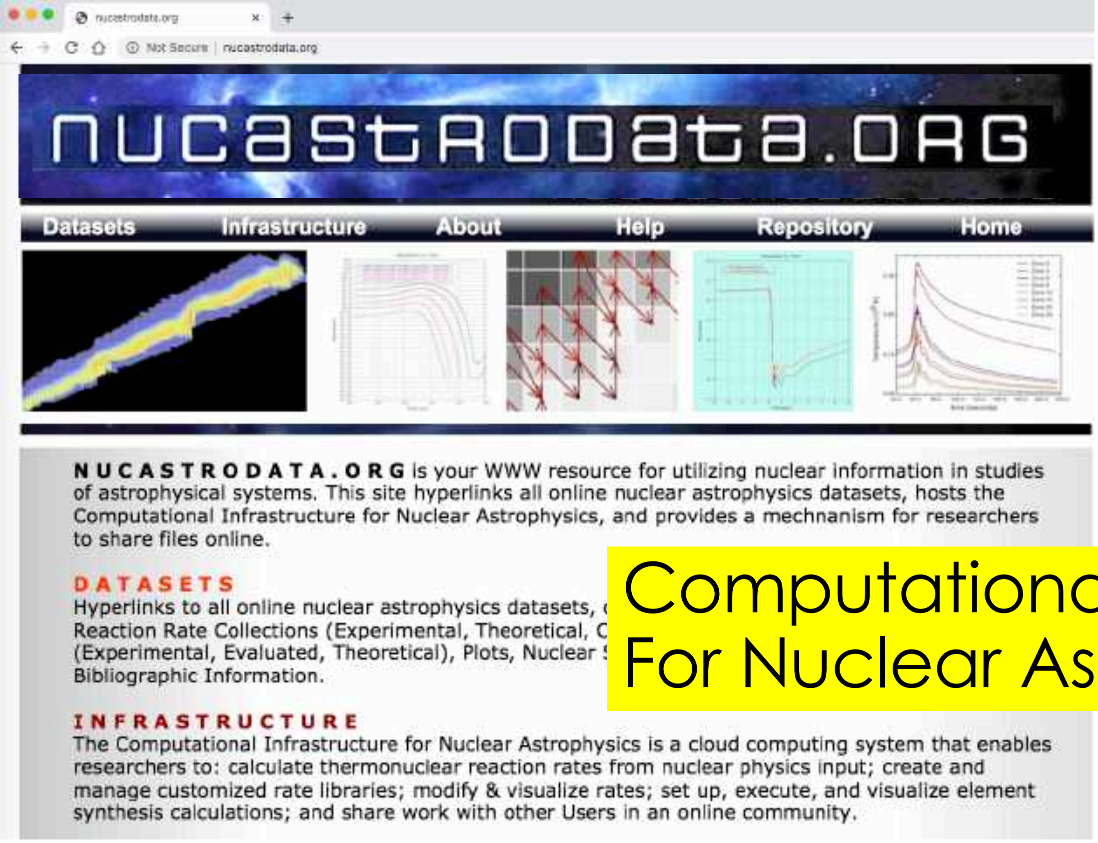
help files available

174 institutes In 39 countries

free to use

10GB free storage

Online Software System



NUCASTRODATA.ORG is your WWW resource for utilizing nuclear information in studies of astrophysical systems. This site hyperlinks all online nuclear astrophysics datasets, hosts the Computational Infrastructure for Nuclear Astrophysics, and provides a mechnanism for researchers to share files online.

DATASETS

Hyperlinks to all online nuclear astrophysics datasets,
Reaction Rate Collections (Experimental, Theoretical,
(Experimental, Evaluated, Theoretical), Plots, Nuclear
Bibliographic Information.

INFRASTRUCTURE

The Computational Infrastructure for Nuclear Astrophysics is a cloud computing system that enables researchers to: calculate thermonuclear reaction rates from nuclear physics input; create and manage customized rate libraries; modify & visualize rates; set up, execute, and visualize element synthesis calculations; and share work with other Users in an online community.

Computational Infrastructure
For Nuclear Astrophysics CINA

Software Developer:
Eric Lingerfelt, Pandia Software LLC
pandiasoftware.com

- register for the system at nucastrodata.org

Thermonuclear Burn Formalism

create isotope **j** by the reaction $k + l \longrightarrow j + i$

change in abundance **j** ~ abundance of k • abundance of l • interaction rate

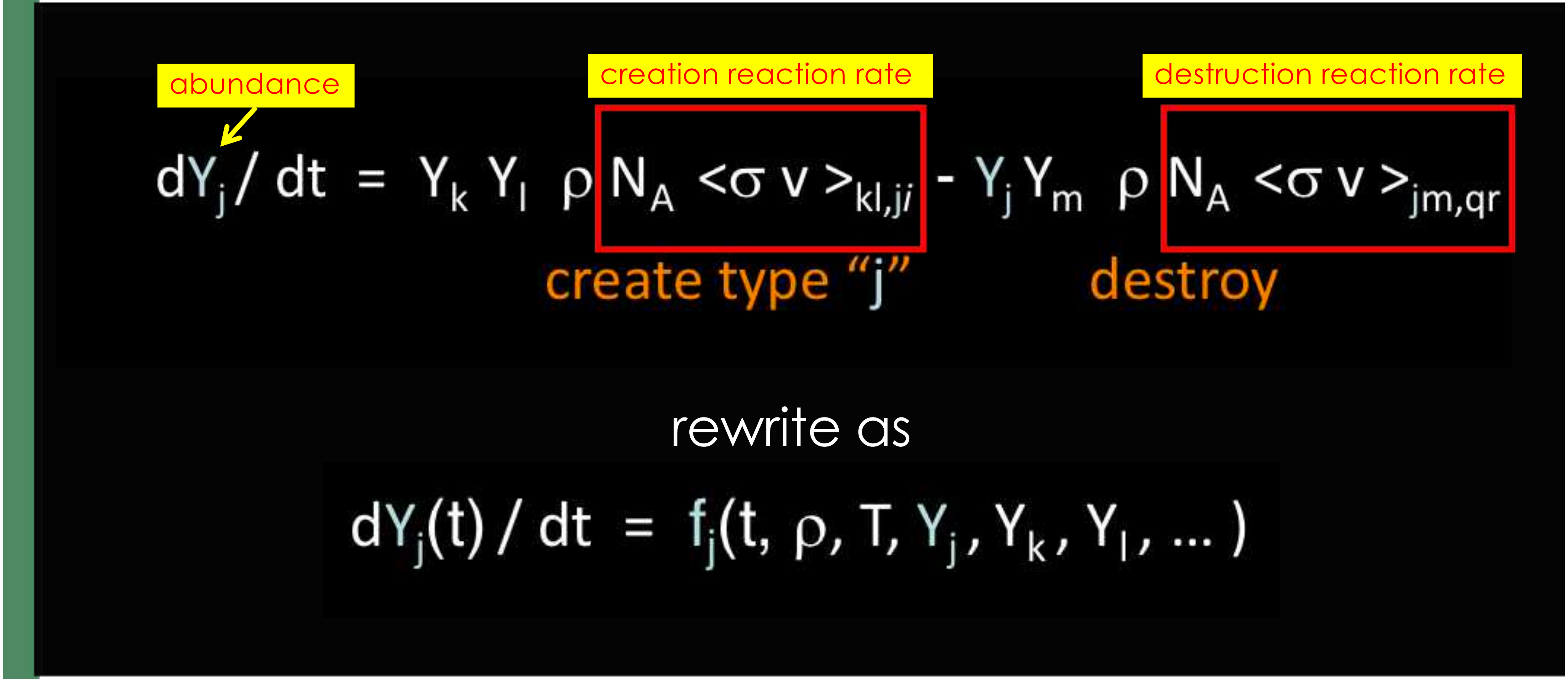
abundance

reaction rate

$$dY_j / dt = Y_k \, Y_l \, \rho \, \boxed{N_A \, <\sigma \, v>_{kl,ji}}$$

- write the time evolution equation for any abundance

Thermonuclear Burn Formalism



abundance

creation reaction rate

destruction reaction rate

$$dY_j / dt = Y_k Y_l \rho \boxed{N_A \langle \sigma v \rangle_{kl,ji}} - Y_j Y_m \rho \boxed{N_A \langle \sigma v \rangle_{jm,qr}}$$

create type “j”

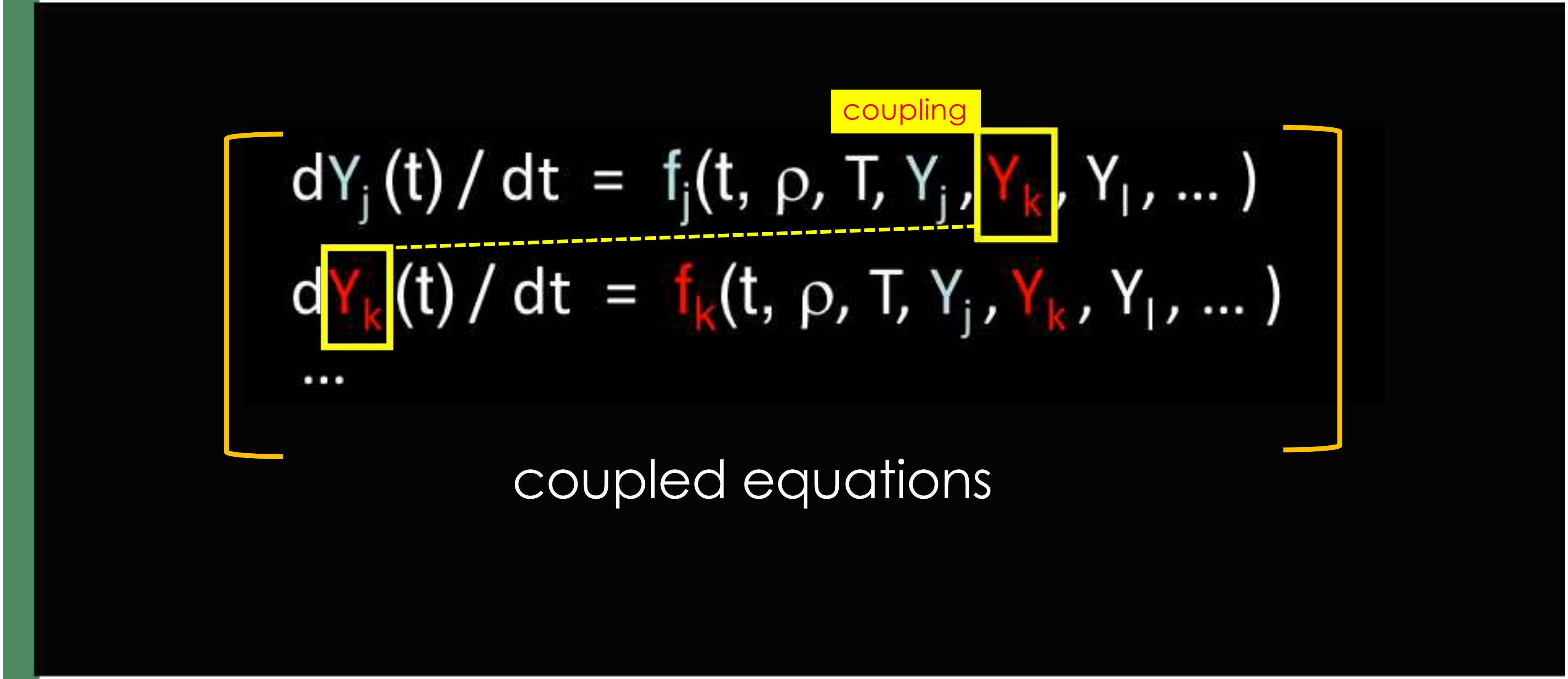
destroy

rewrite as

$$dY_j(t) / dt = f_j(t, \rho, T, Y_j, Y_k, Y_l, \ldots)$$

- write the time evolution equation for any abundance

Thermonuclear Burn Formalism



$$\left[\begin{array}{l} dY_j(t) / dt = f_j(t, \rho, T, Y_j, \boxed{Y_k}, Y_l, \ldots) \\ d\boxed{Y_k}(t) / dt = f_k(t, \rho, T, Y_j, Y_k, Y_l, \ldots) \\ \ldots \end{array}\right]$$

coupled equations

- write the coupled time evolution equation for **ALL** abundances

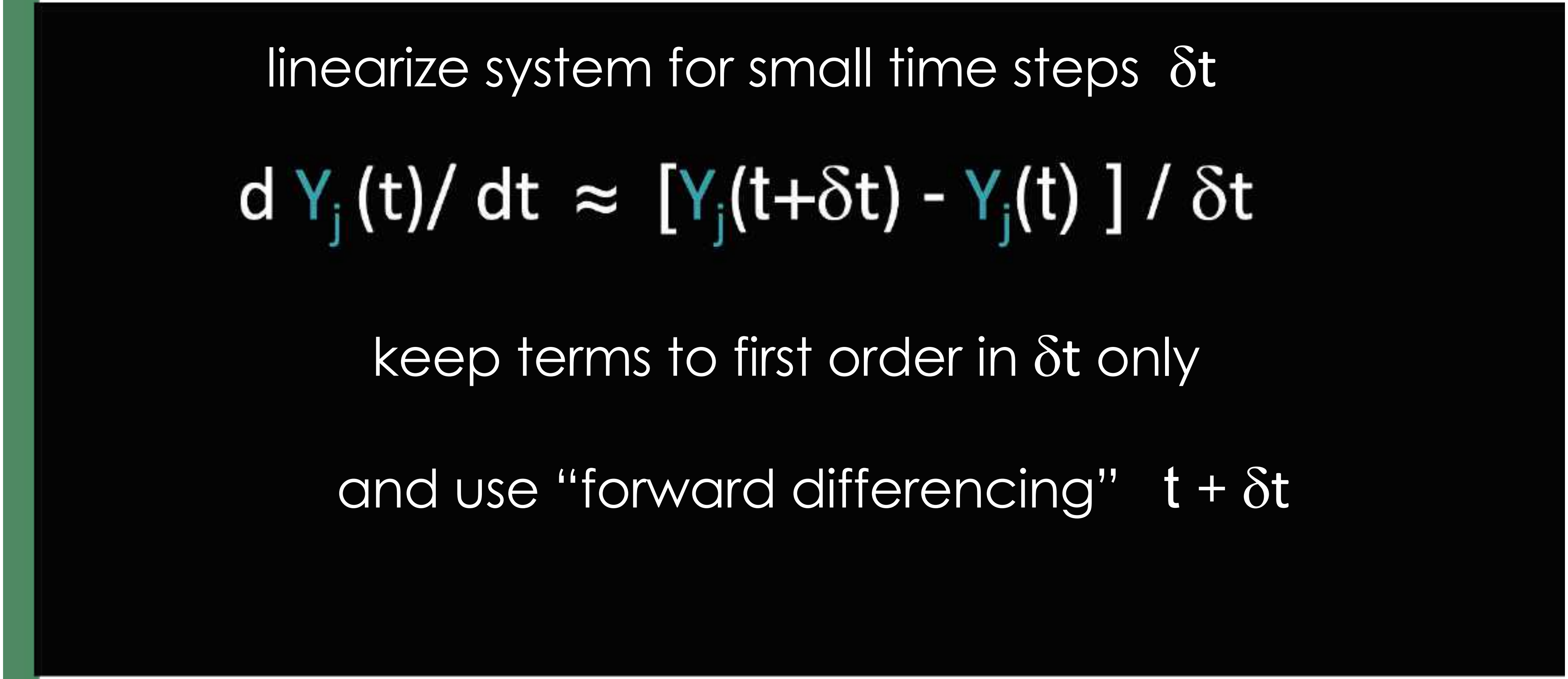
Thermonuclear Burn Formalism

$$\left[\begin{array}{l} dY_j(t)/dt = f_j(t, \rho, T, Y_j, Y_k, Y_l, \ldots) \\ dY_k(t)/dt = f_k(t, \rho, T, Y_j, Y_k, Y_l, \ldots) \\ \ldots \end{array}\right]$$

"reaction network"

- write the coupled time evolution equation for **ALL** abundances

Thermonuclear Burn Formalism



linearize system for small time steps δt

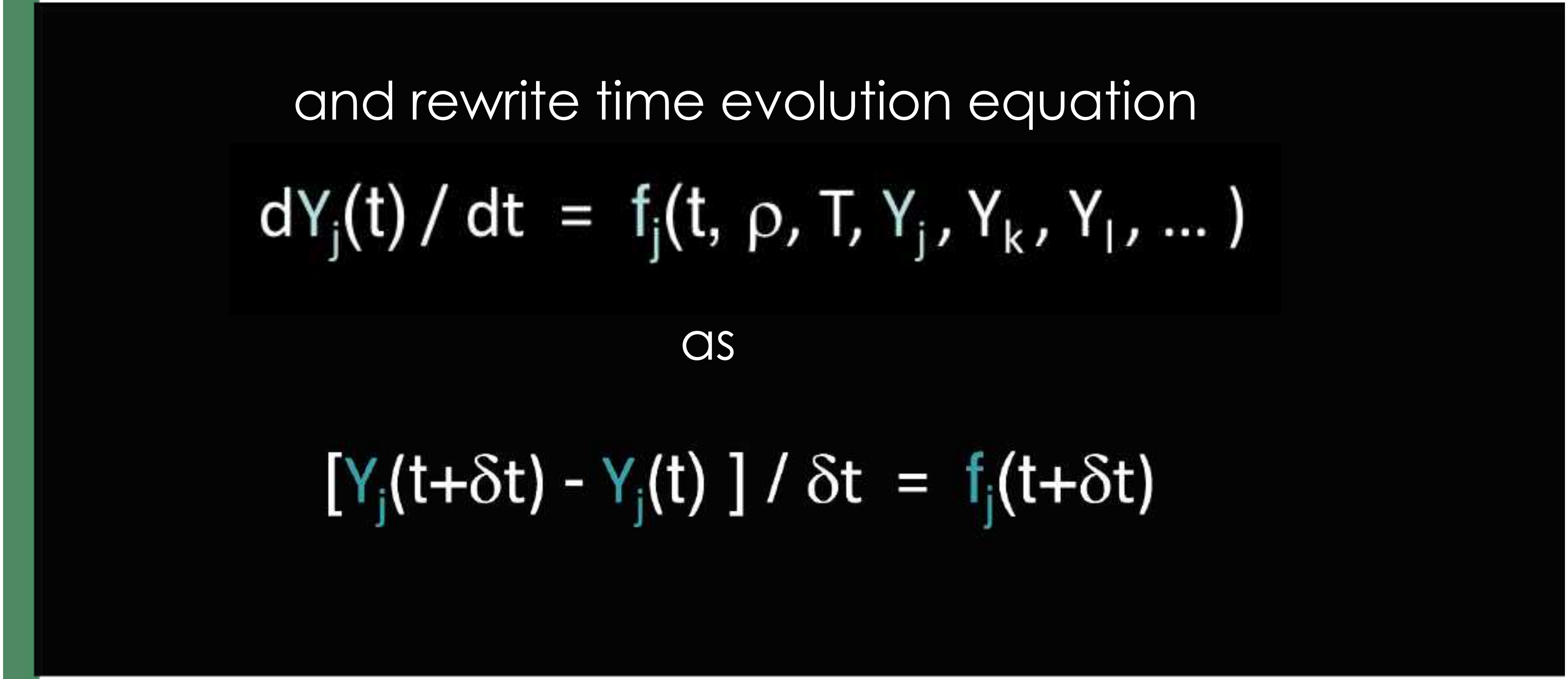
$$d\, Y_j(t)/\, dt \approx [Y_j(t+\delta t) - Y_j(t)\,] \,/\, \delta t$$

keep terms to first order in δt only

and use “forward differencing” $t + \delta t$

- linearize system with implicit approach for small time steps

Thermonuclear Burn Formalism



and rewrite time evolution equation

$$dY_j(t) / dt = f_j(t, \rho, T, Y_j, Y_k, Y_l, \ldots)$$

as

$$[Y_j(t+\delta t) - Y_j(t)] / \delta t = f_j(t+\delta t)$$

- linearize system with “forward differencing” for small time steps

Thermonuclear Burn Formalism

then rewrite

$$[Y_j(t+\delta t) - Y_j(t)] / \delta t = f_j(t+\delta t)$$

as

$$\Delta_j / \delta t = f_j(t+\delta t) \quad \text{with} \quad \Delta_j = Y_j(t+\delta t) - Y_j(t)$$

- linearize system with “forward differencing” for small time steps

Thermonuclear Burn Formalism

then rewrite the reaction network as

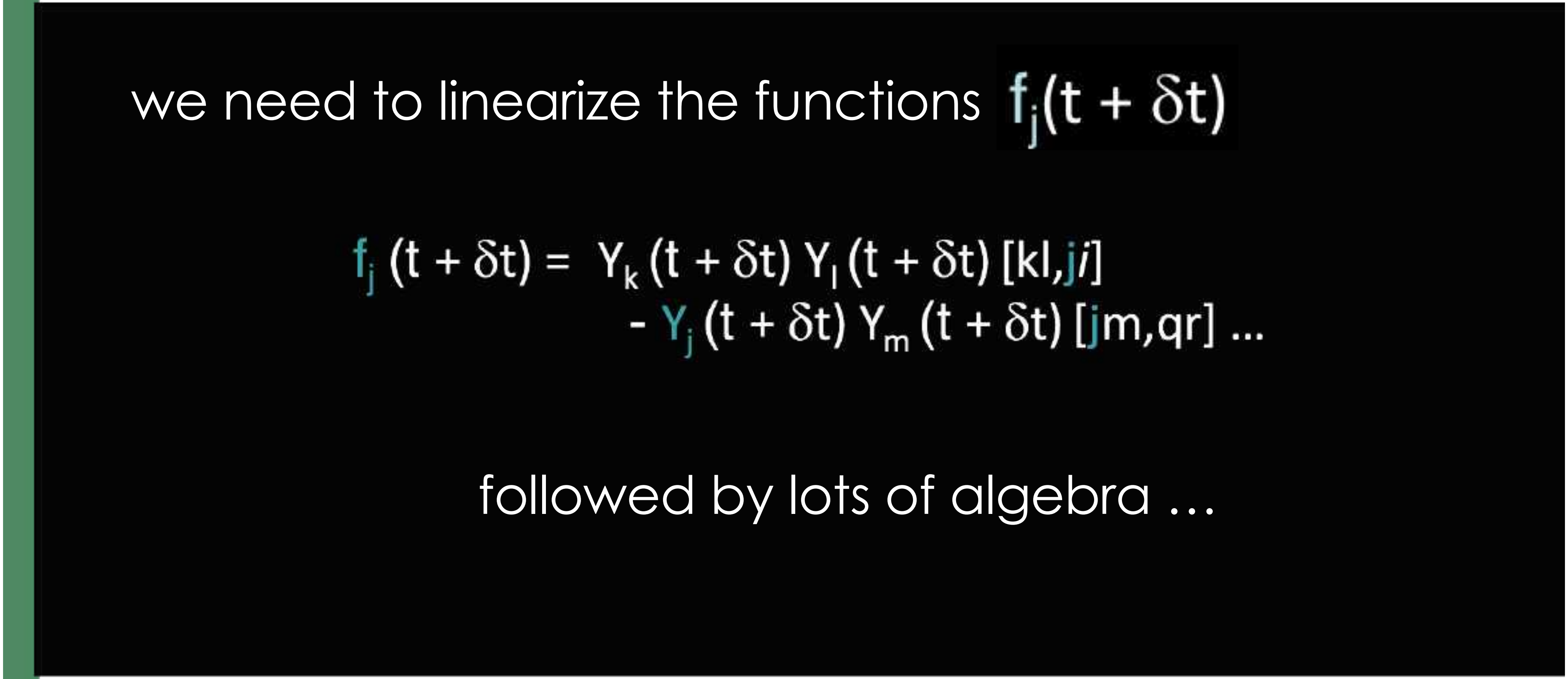
$$\left[\begin{array}{l} \Delta_j = f_j(t + \delta t)\ \delta t \\ \Delta_k = f_k(t + \delta t)\ \delta t \\ \ldots \end{array}\right]$$

and solve
for small
differences
at each
time step

$$\Delta = \left[\begin{array}{c} \Delta_j \\ \Delta_k \\ \ldots \end{array}\right]$$

- linearize system with “forward differencing” for small time steps

Thermonuclear Burn Formalism



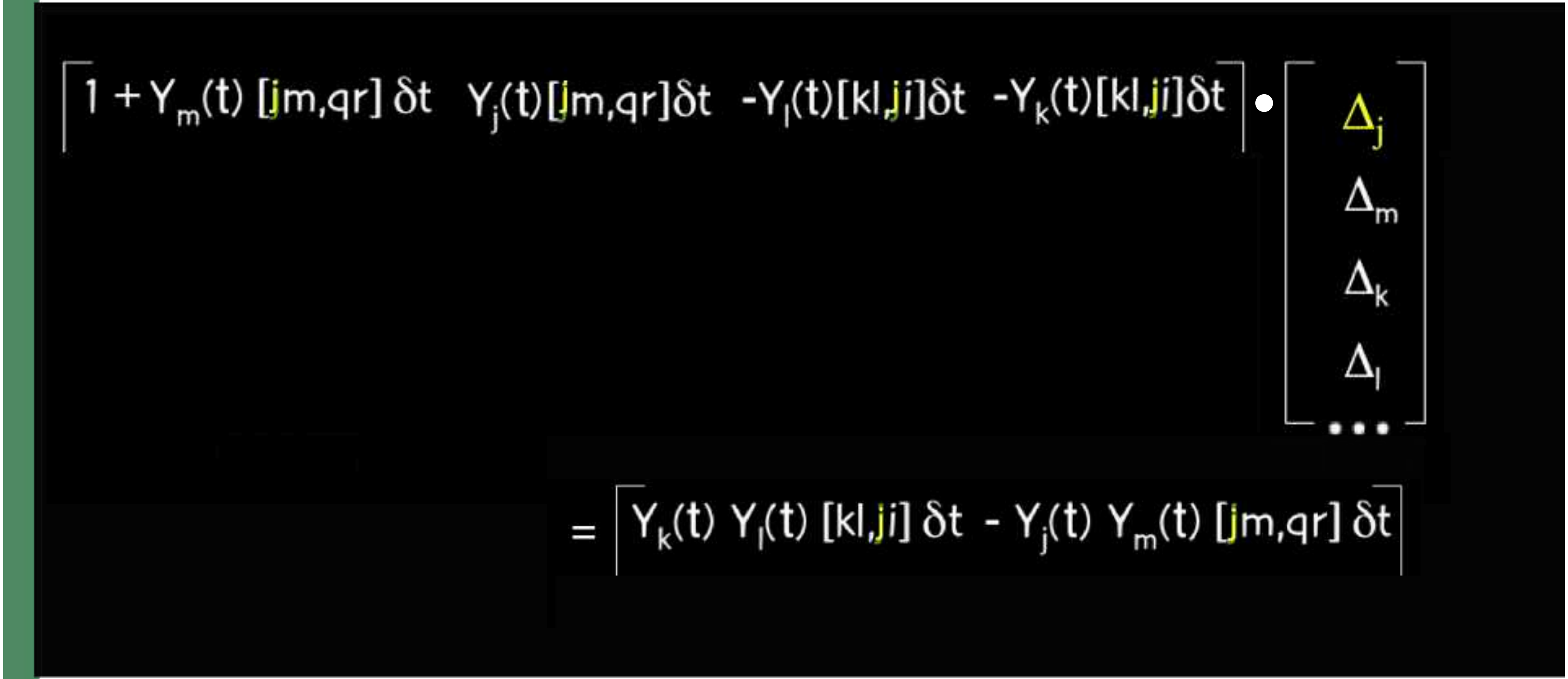
we need to linearize the functions $f_j(t + \delta t)$

$$f_j\,(t + \delta t) = Y_k\,(t + \delta t)\,Y_l\,(t + \delta t)\,[kl,ji] - Y_j\,(t + \delta t)\,Y_m\,(t + \delta t)\,[jm,qr] \ldots$$

followed by lots of algebra …

- linearize system with “forward differencing” for small time steps

Thermonuclear Burn Formalism

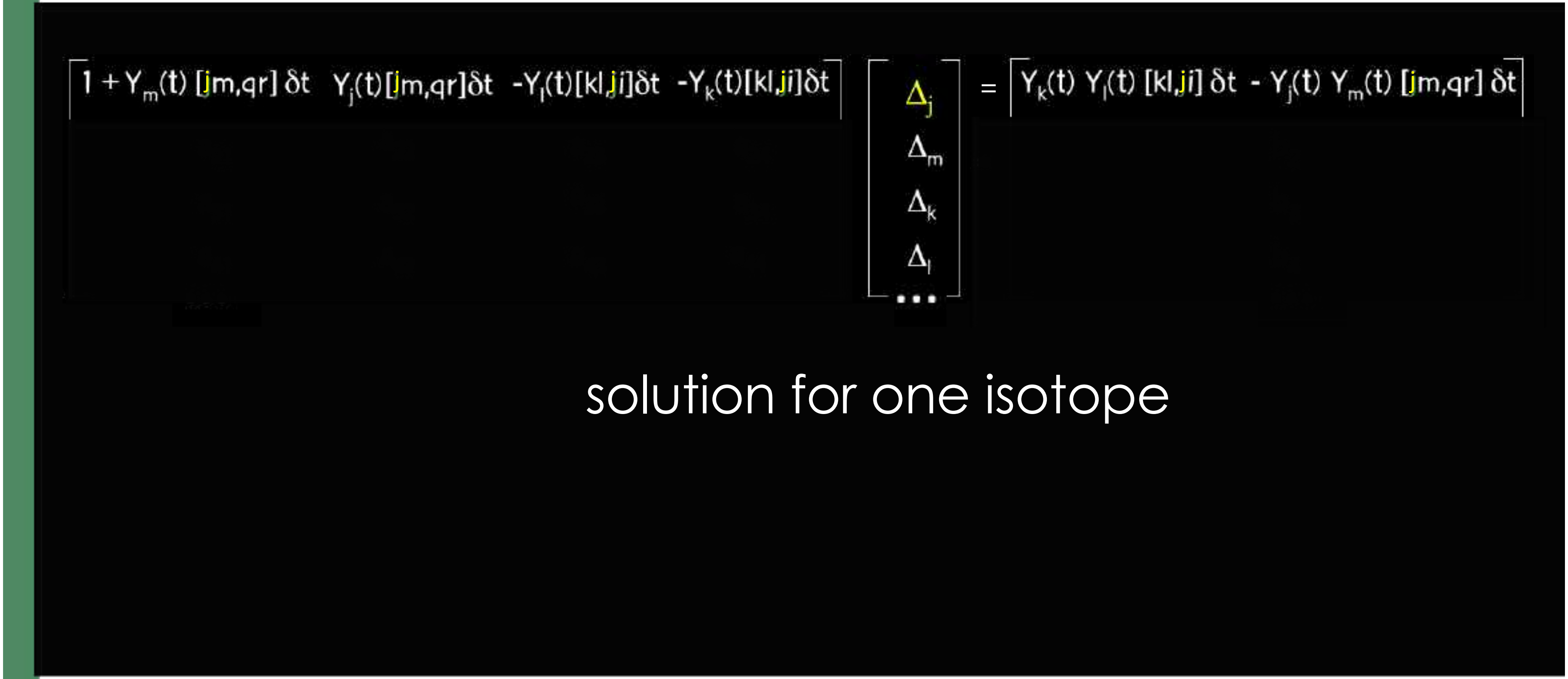


$$\begin{bmatrix} 1 + Y_m(t)\,[jm,qr]\,\delta t & Y_j(t)[jm,qr]\delta t & -Y_l(t)[kl,ji]\delta t & -Y_k(t)[kl,ji]\delta t \end{bmatrix} \bullet \begin{bmatrix} \Delta_j \\ \Delta_m \\ \Delta_k \\ \Delta_l \\ \cdots \end{bmatrix}$$

$$= \begin{bmatrix} Y_k(t)\; Y_l(t)\;[kl,ji]\;\delta t \; - \; Y_j(t)\; Y_m(t)\;[jm,qr]\;\delta t \end{bmatrix}$$

- after linearization, the solution for one isotope is …

Thermonuclear Burn Formalism

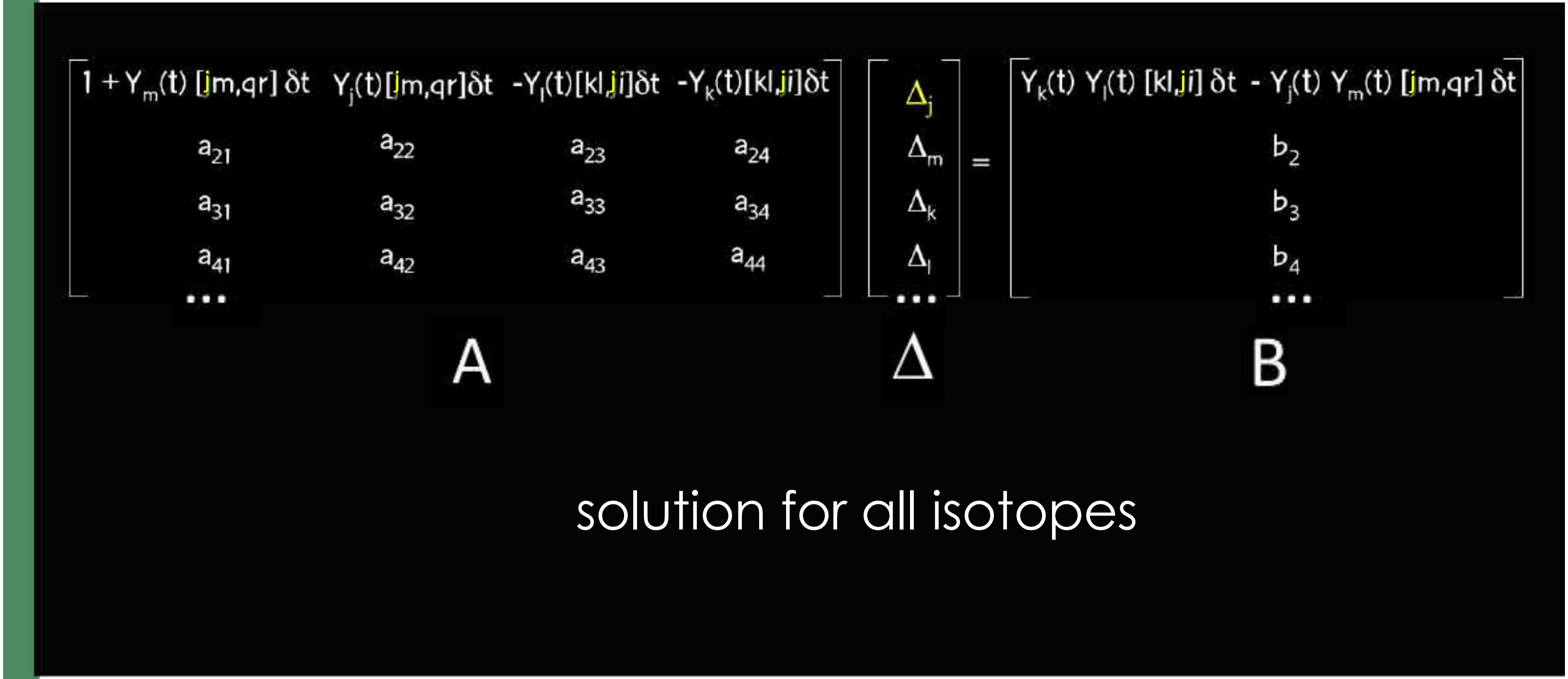


$$\begin{bmatrix} 1 + Y_m(t)\,[jm,qr]\,\delta t & Y_j(t)[jm,qr]\delta t & -Y_l(t)[kl,ji]\delta t & -Y_k(t)[kl,ji]\delta t \end{bmatrix} \begin{bmatrix} \Delta_j \\ \Delta_m \\ \Delta_k \\ \Delta_l \\ \cdots \end{bmatrix} = \begin{bmatrix} Y_k(t)\, Y_l(t)\, [kl,ji]\, \delta t \; - \; Y_j(t)\, Y_m(t)\, [jm,qr]\, \delta t \end{bmatrix}$$

solution for one isotope

- the solution for one isotope

Thermonuclear Burn Formalism



$$\underbrace{\begin{bmatrix} 1 + Y_m(t)\,[jm,qr]\,\delta t & Y_j(t)[jm,qr]\delta t & -Y_l(t)[kl,ji]\delta t & -Y_k(t)[kl,ji]\delta t \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \\ \cdots & & & \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} \Delta_j \\ \Delta_m \\ \Delta_k \\ \Delta_l \\ \cdots \end{bmatrix}}_{\Delta} = \underbrace{\begin{bmatrix} Y_k(t)\,Y_l(t)\,[kl,ji]\,\delta t - Y_j(t)\,Y_m(t)\,[jm,qr]\,\delta t \\ b_2 \\ b_3 \\ b_4 \\ \cdots \end{bmatrix}}_{B}$$

solution for all isotopes

- the solution for all isotopes

Thermonuclear Burn Formalism

$$\underbrace{\begin{bmatrix} 1+Y_m(t)\,[jm,qr]\,\delta t & Y_j(t)[jm,qr]\delta t & -Y_l(t)[kl,ji]\delta t & -Y_k(t)[kl,ji]\delta t \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \\ \cdots & & & \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} \Delta_j \\ \Delta_m \\ \Delta_k \\ \Delta_l \\ \cdots \end{bmatrix}}_{\Delta} = \underbrace{\begin{bmatrix} Y_k(t)\,Y_l(t)\,[kl,ji]\,\delta t - Y_j(t)\,Y_m(t)\,[jm,qr]\,\delta t \\ b_2 \\ b_3 \\ b_4 \\ \cdots \end{bmatrix}}_{B}$$

rewrite in matrix notation

solve at each time step

$$A \bullet \Delta = B \longrightarrow \boxed{\Delta = A^{-1} B}$$

- the solution for all isotopes

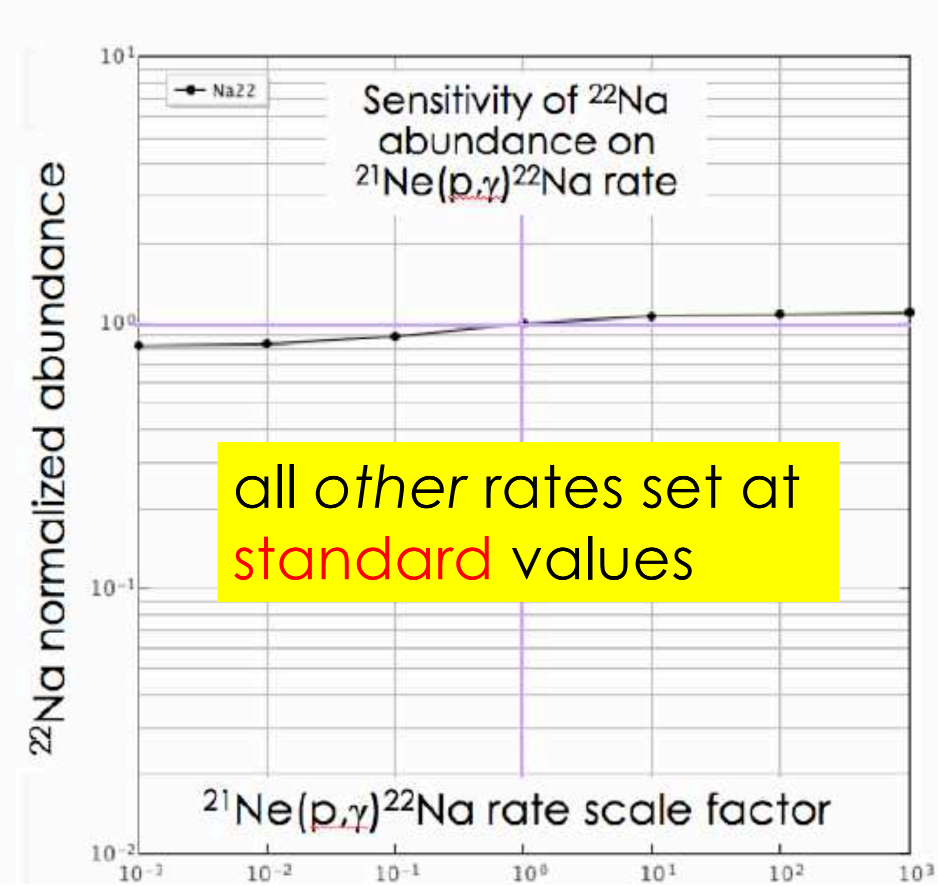
Thermonuclear Burn Formalism

$$\begin{array}{c|ccccccc|}
 & Y_1 & Y_2 & Y_3 & \cdots & Y_i & \cdots & Y_N \\
\hline
Y_1 & a_{11} & a_{12} & a_{13} & \cdots & a_{1i} & \cdots & a_{1N} \\
Y_2 & a_{21} & a_{22} & a_{23} & \cdots & a_{2i} & \cdots & a_{2N} \\
Y_3 & a_{31} & a_{32} & a_{33} & \cdots & a_{3i} & \cdots & a_{3N} \\
\cdots & \cdots & & & & & & \\
Y_J & a_{J1} & a_{J2} & a_{J3} & \cdots & \boxed{a_{Ji}} & \cdots & a_{JN} \\
\cdots & \cdots & & & & & & \\
Y_N & a_{N1} & a_{N2} & a_{N3} & \cdots & a_{Ni} & \cdots & a_{NN}
\end{array}$$

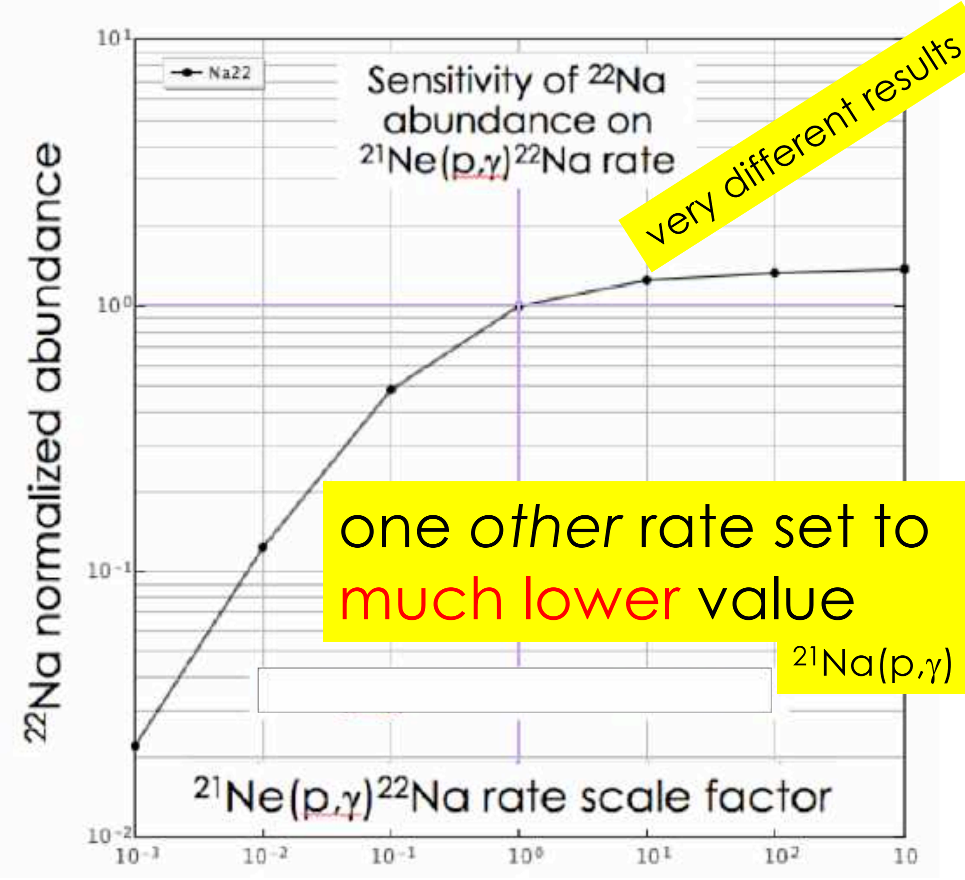
a_{ji} is only non-zero if Yi and Yj are coupled

- the “A” matrix contains all the connections between isotopes

Common Simulation Problems – Reference Data



all *other* rates set at standard values



very different results

one *other* rate set to much lower value

^{21}Na(p,γ)

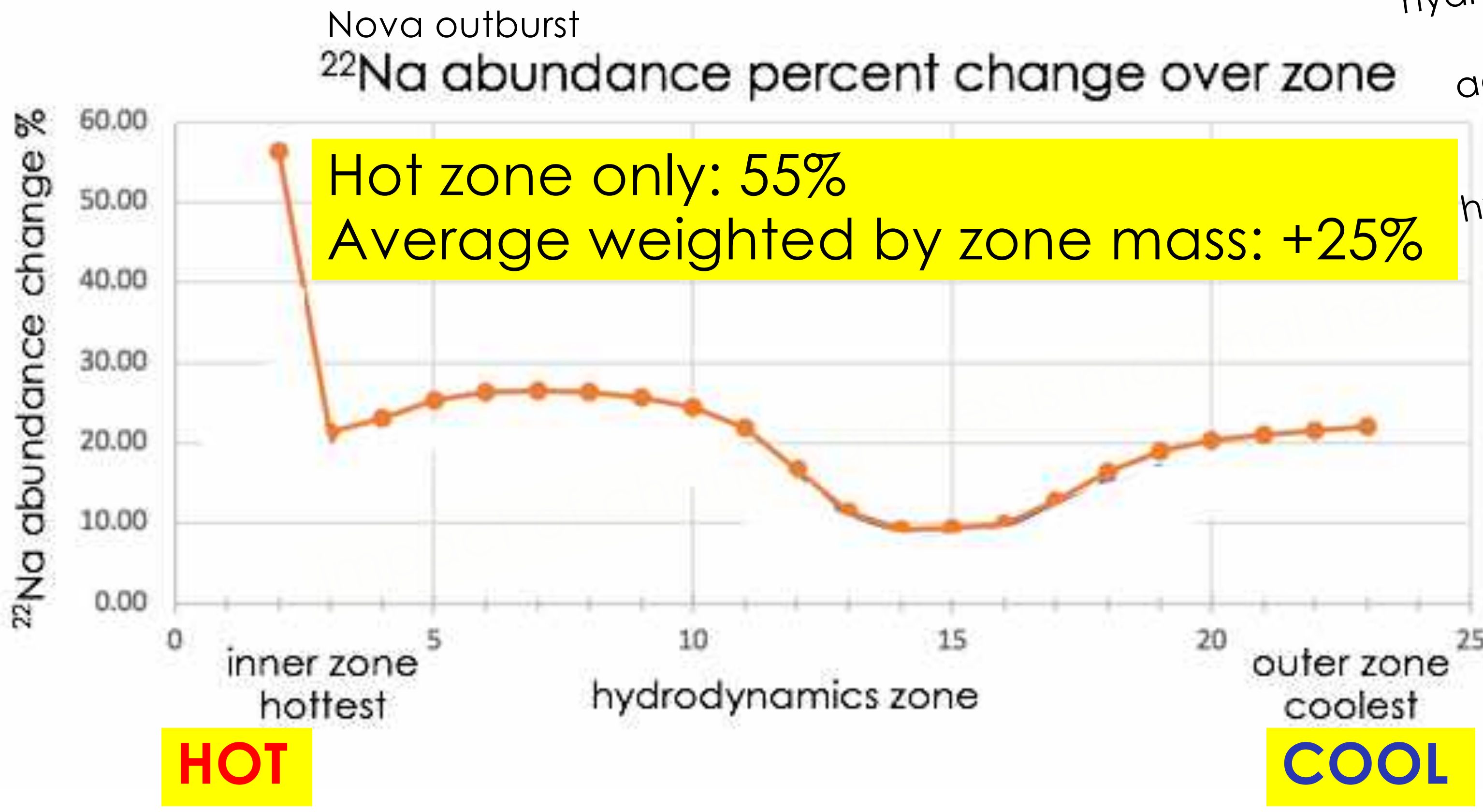
- reference data for sensitivity studies

Common Simulation Problems – Zone Issues

impact of changing rates is maximal here

- some impact studies only consider the hottest zone

Common Simulation Problems – Zone Issues



Hot zone only: 55%
Average weighted by zone mass: +25%

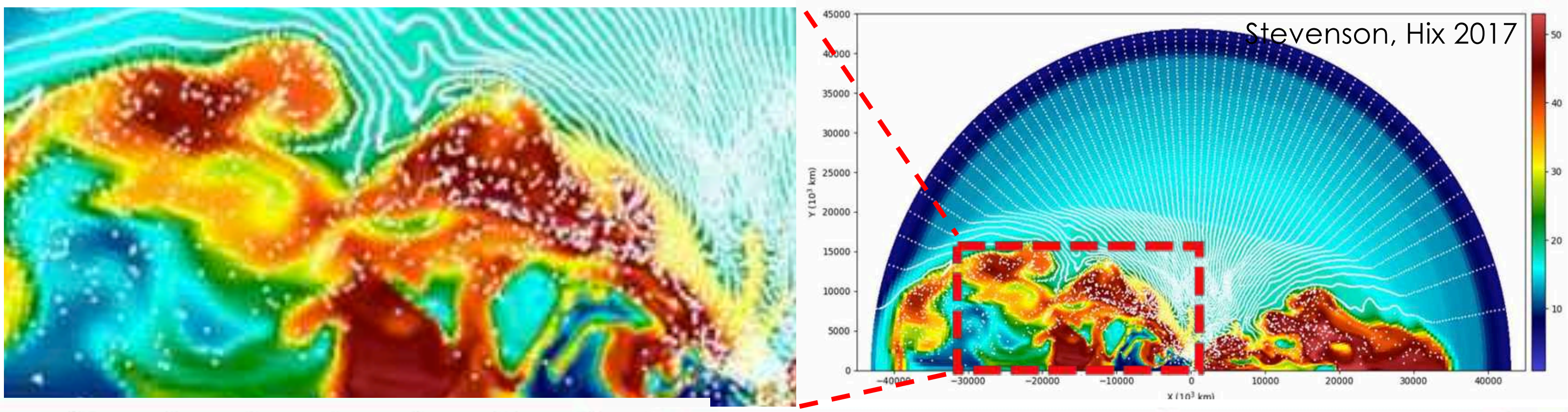
HOT

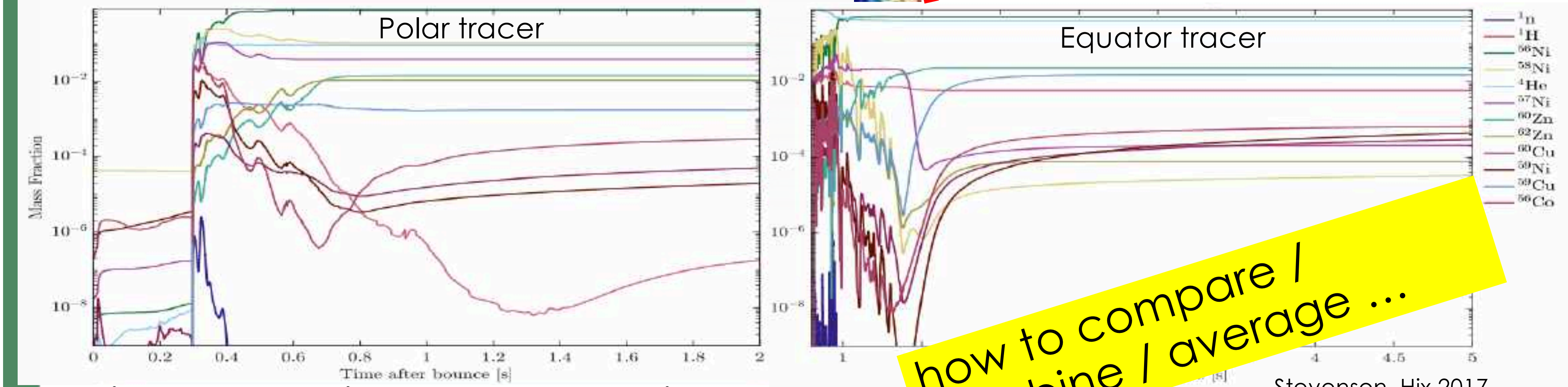
COOL

- some impact studies only consider the hottest zone

Common Simulation Problems – Tracer Particles

Core Collapse
Supernova
2D simulation
12 solar mass



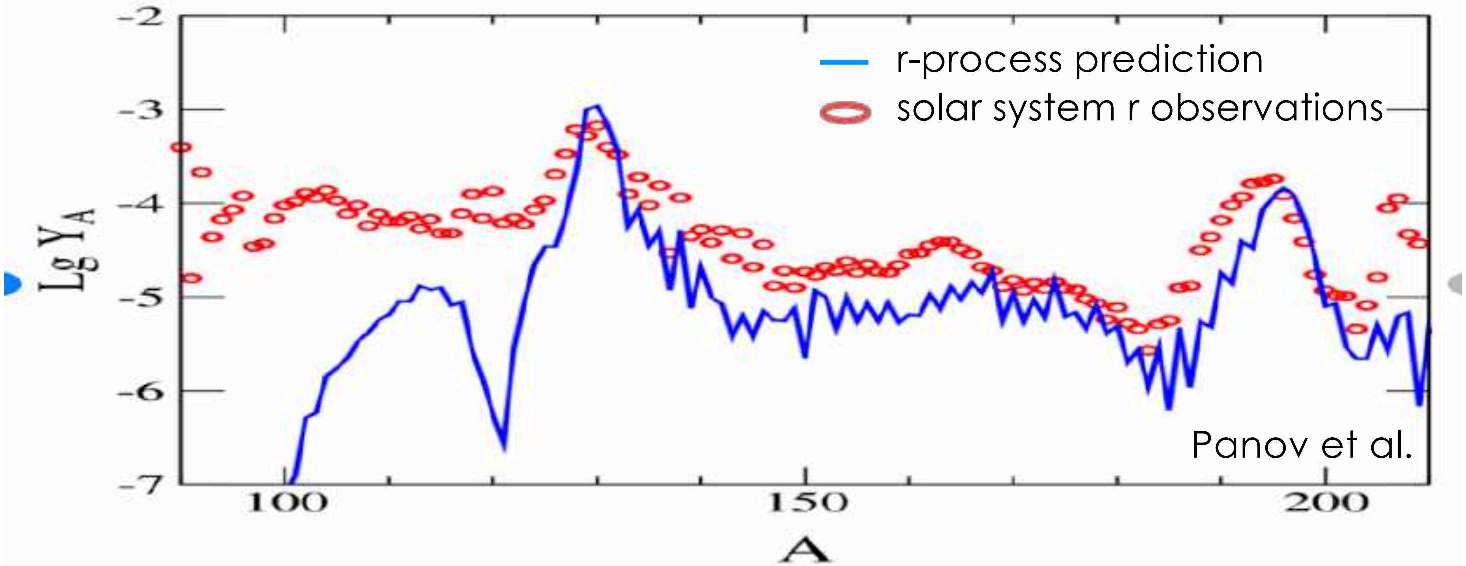


Stevenson, Hix 2017

how to compare / combine / average …

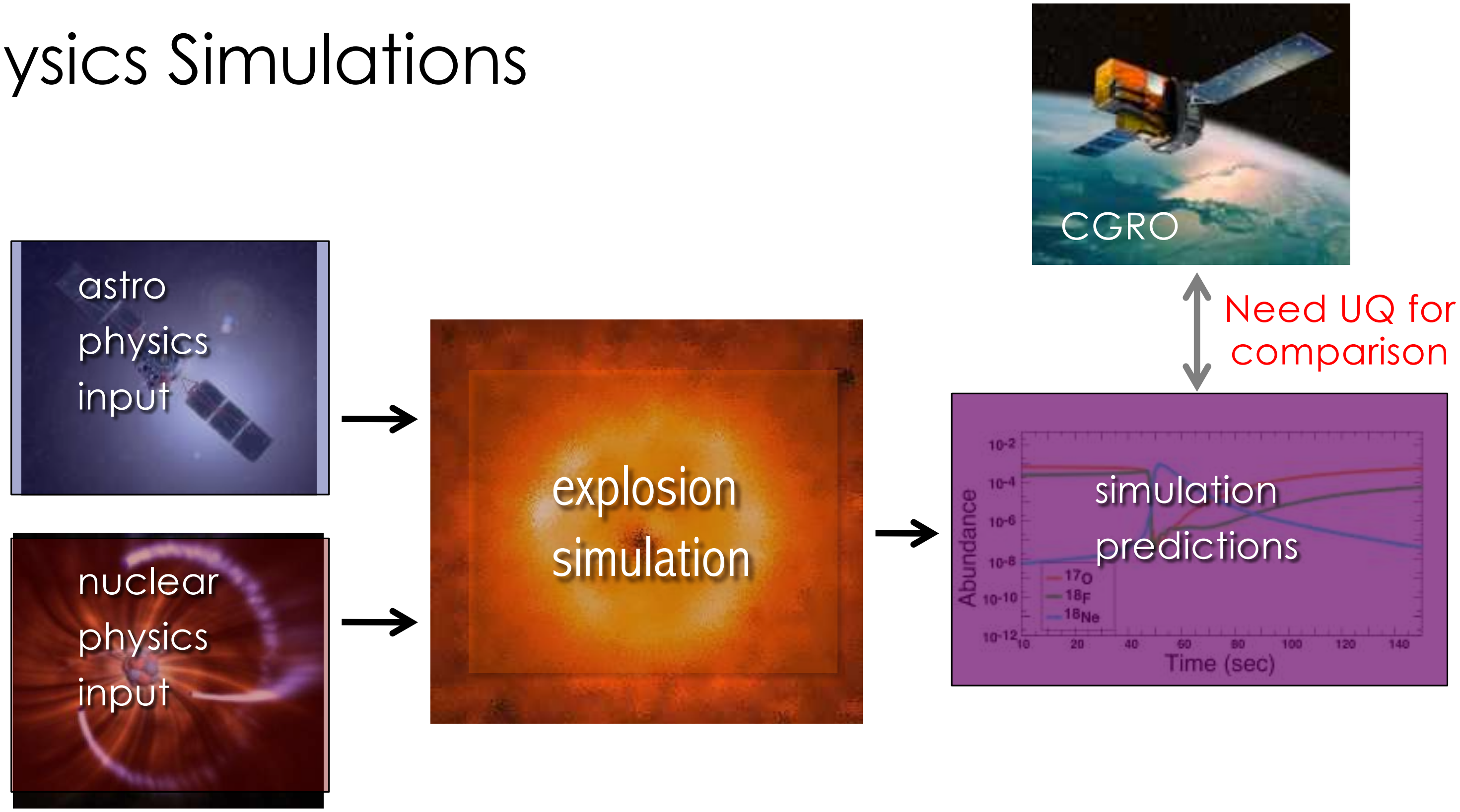
- interpretating tracer particle results

Common Simulation Problems – Other Issues



- predictions with no uncertainties
- no direct comparison to observations
- insufficient number of tracked isotopes
- cross section (rate) over inappropriate energy (temp) range

Astrophysics Simulations


CGRO

astro physics input

nuclear physics input

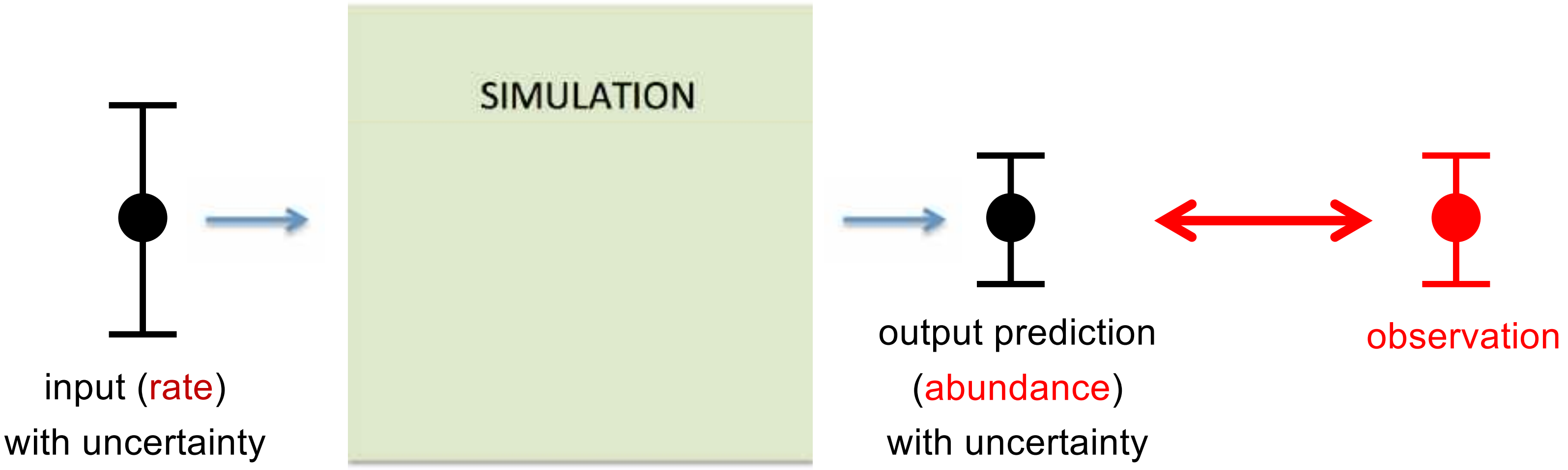
explosion simulation

simulation predictions

Need UQ for comparison

- a simplified flowchart of these studies looks like this
- improving the simulation requires quantitative comparisons with observations …
- this requires uncertainty quantification UQ in the predictions … usually not given

General Approach



input (rate)
with uncertainty

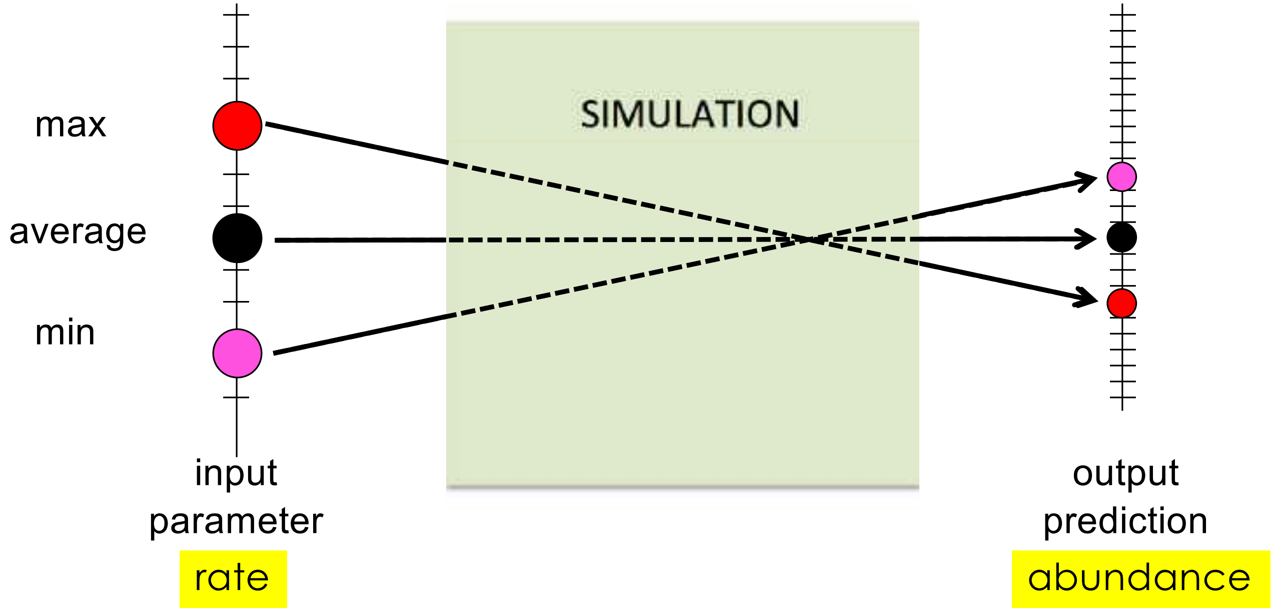
output prediction
(abundance)
with uncertainty

observation

- approach:
  - assess uncertainties of input nuclear reaction rates
  - propagate uncertainties through astro simulation
  - analyze predictions to determine their uncertainties
  - quantitatively compare predictions with observations

Min-Max UQ Approach

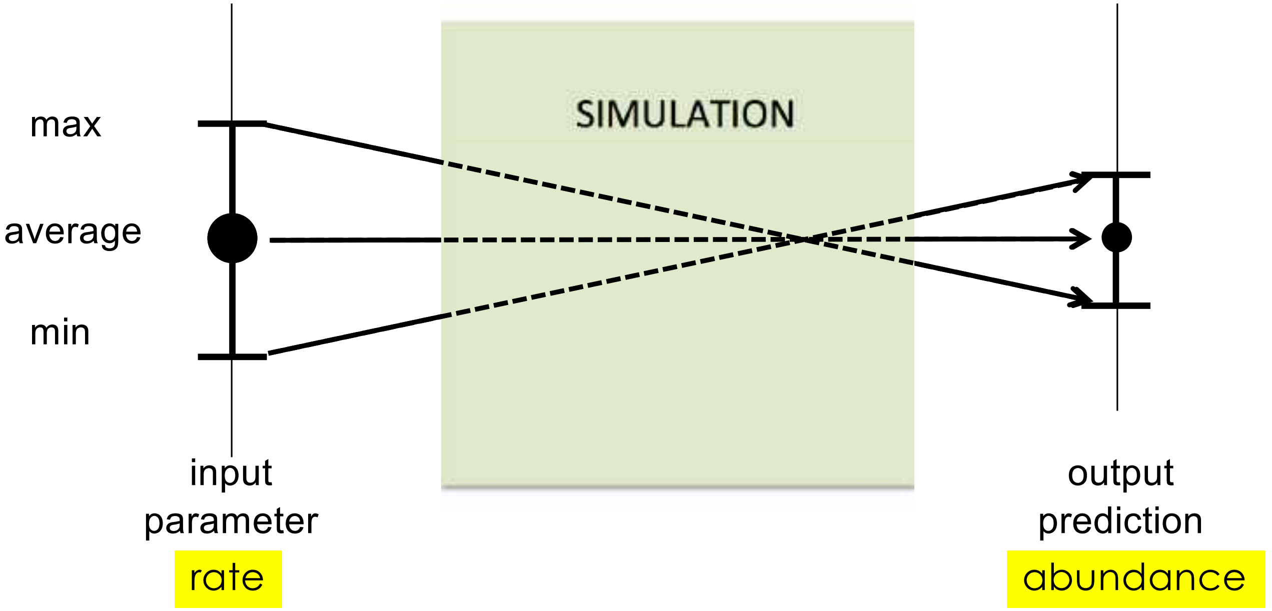
qualitative concept



- quick and simple uncertainty quantification
- vary a simulation input parameter between **minimum** and **maximum** values
- **range** of simulation prediction values gives its **uncertainty**

Min-Max UQ Approach

qualitative concept



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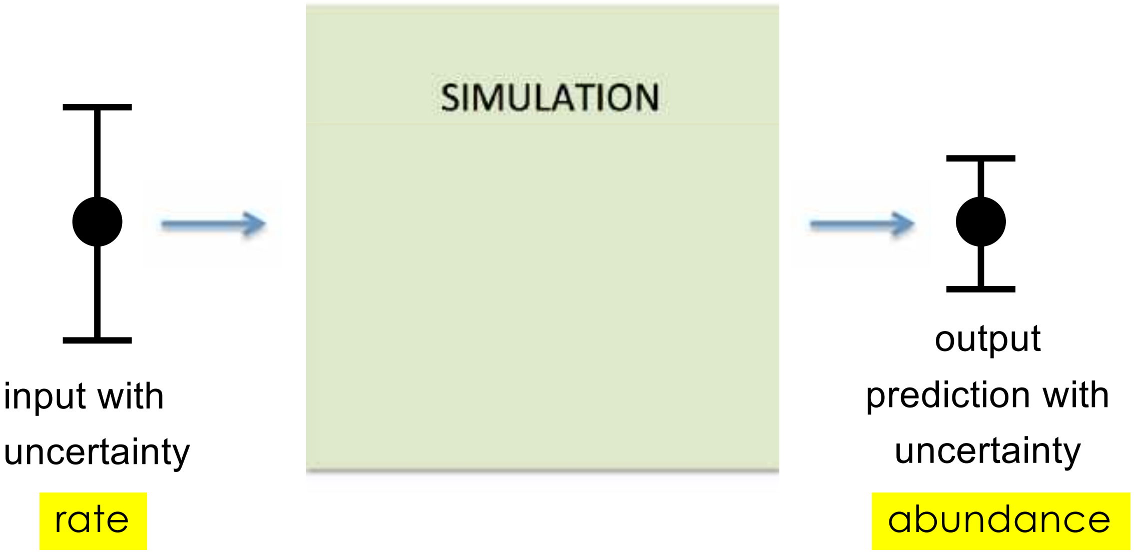
Min-Max UQ Approach

qualitative concept



SIMULATION

input with uncertainty

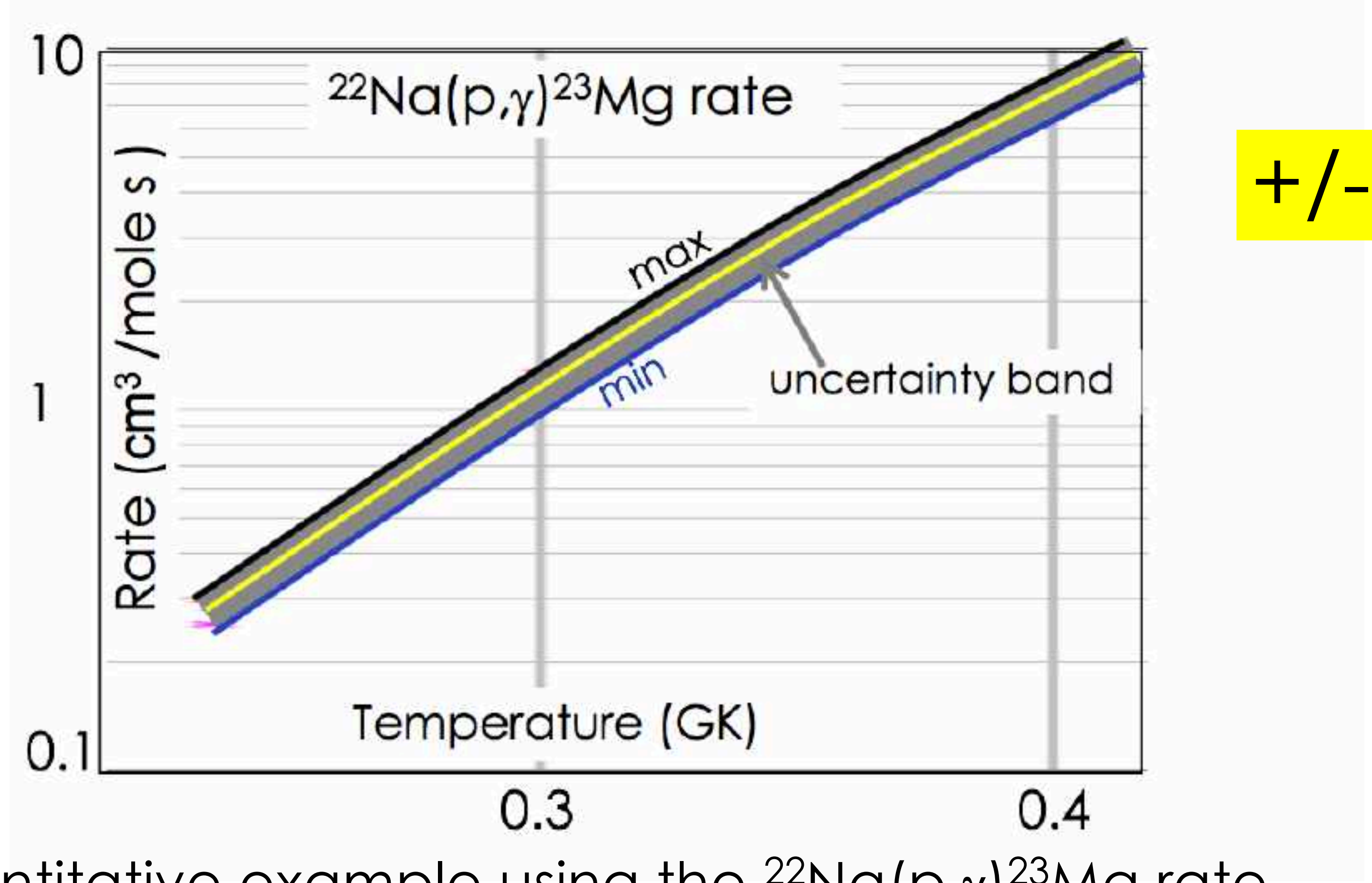
rate

output prediction with uncertainty

abundance

- quick and simple uncertainty quantification
- vary a simulation input parameter between **minimum** and **maximum** values
- **range** of simulation prediction values gives its **uncertainty**

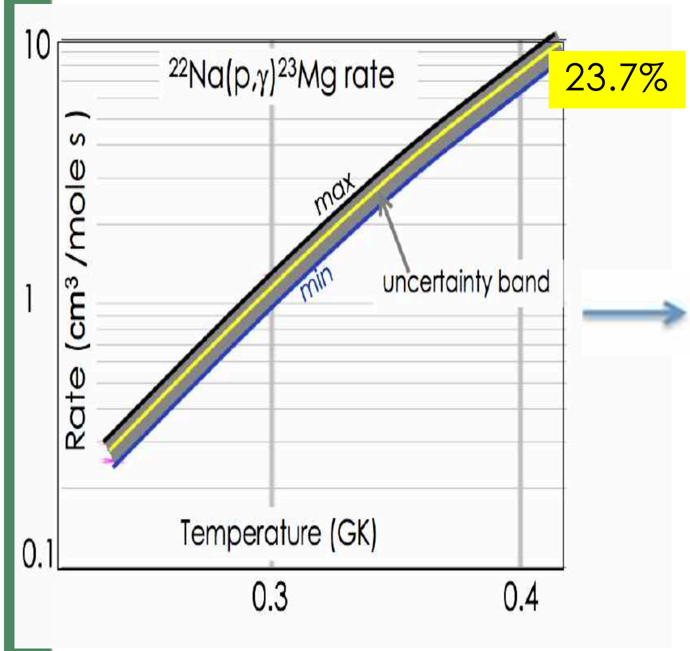
Min-Max UQ Approach



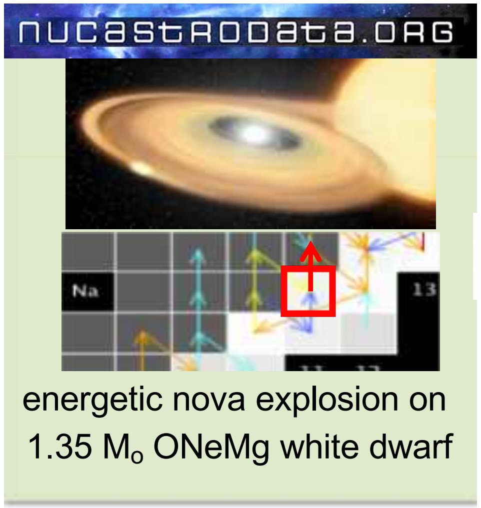
+/-23.7%

- Quantitative example using the ^{22}Na(p,γ)^{23}Mg rate

Post - Processing Studies

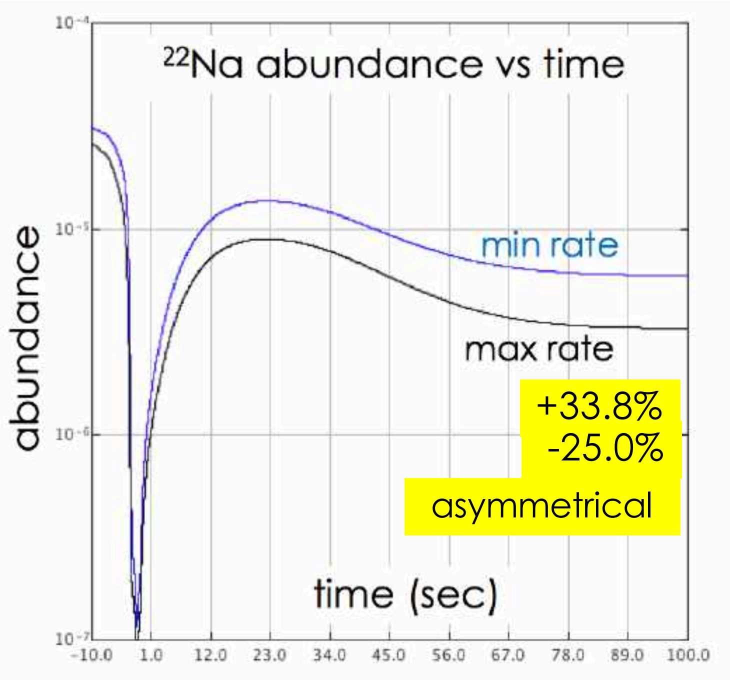


two different inputs for same reaction rate



energetic nova explosion on $1.35\ M_o$ ONeMg white dwarf

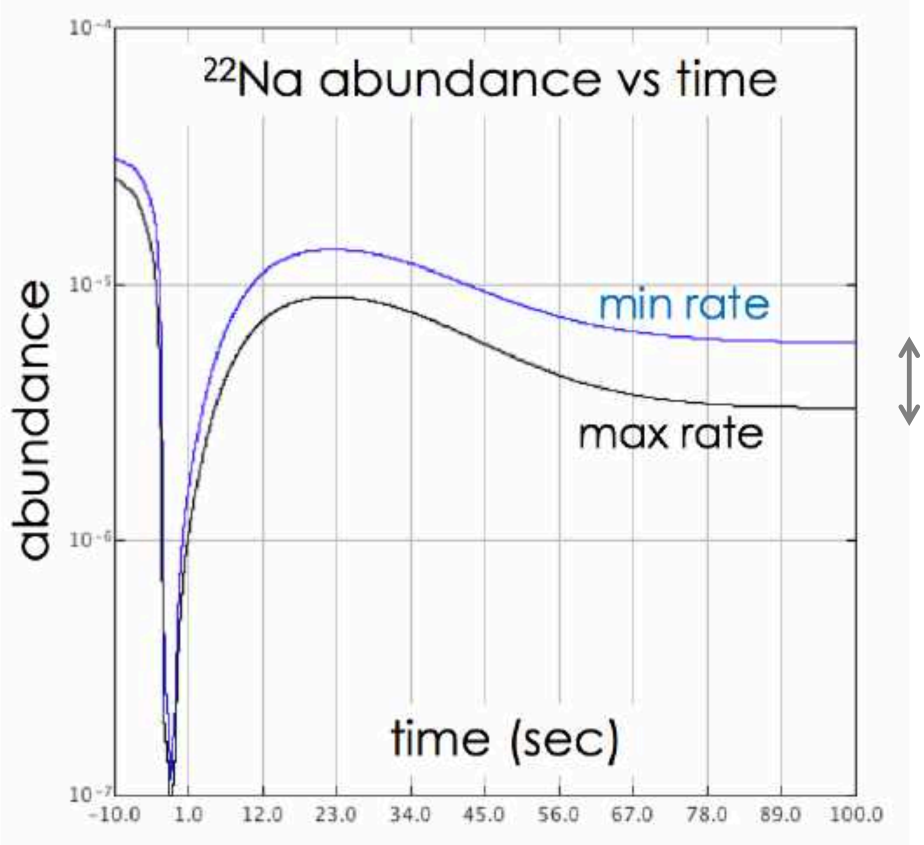
SIMULATION



two different abundance vs time predictions

- Quantitative example using the ^{22}Na(p,γ)^{23}Mg rate

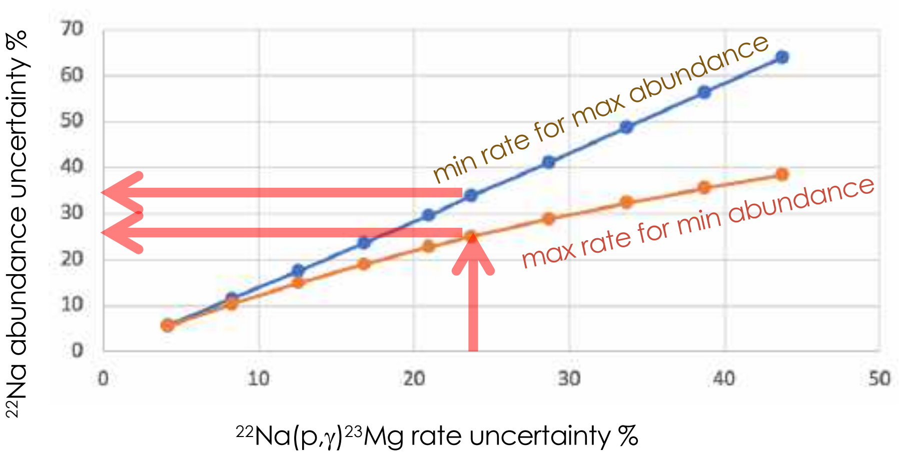
Min-Max UQ Approach



abundance
prediction
(output)
uncertainty

- what is dependence on input reaction rate uncertainties ?

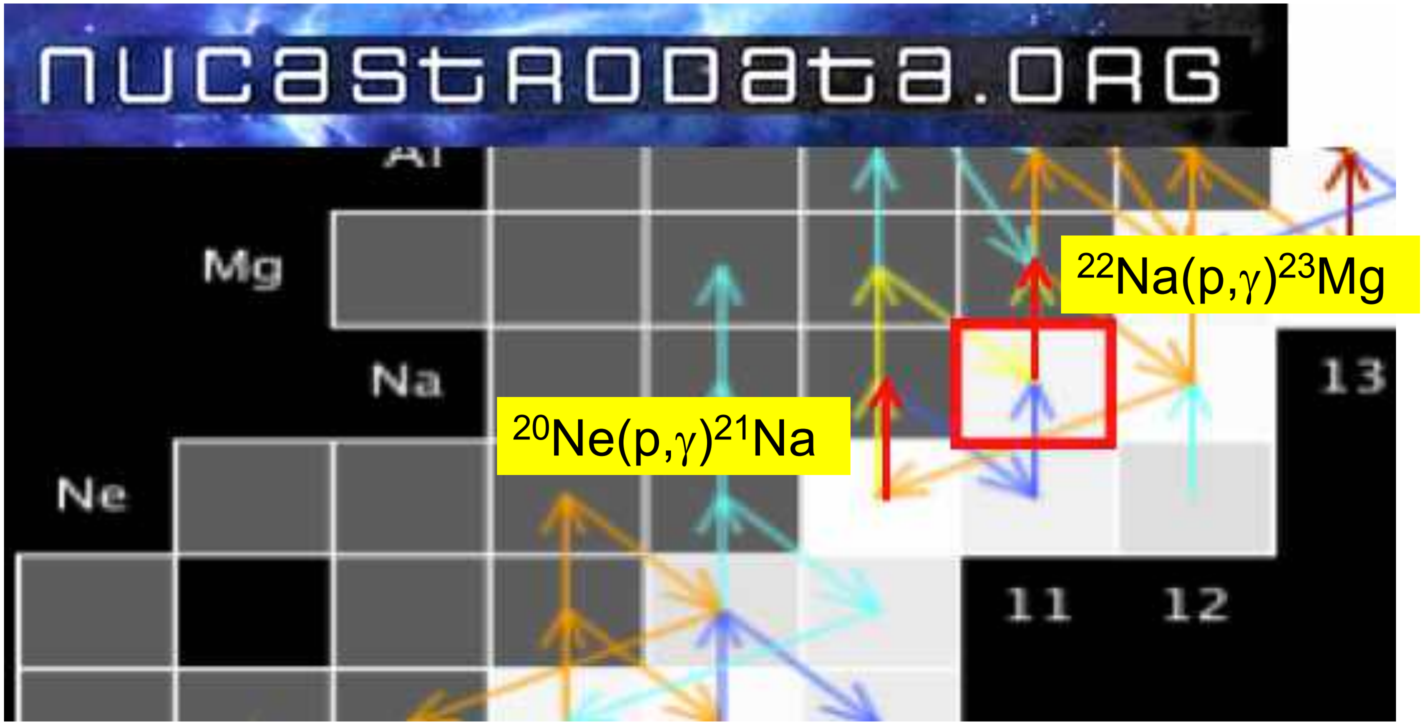
Min-Max UQ Approach


^{22}Na abundance uncertainty vs. ^{22}Na(p,γ)^{23}Mg rate uncertainty

^{22}Na(p,γ)^{23}Mg rate Uncertainty %	^{22}Na Abundance Prediction Uncertainty %
4.2	+5.75 / -5.43
8.3	+11.2 / -10.3
12.6	+17.6 /-14.9
16.8	+ 23.6/ -19.0
21.0	+ 29.7/ -22.7
→ 23.7	+ 33.8 / -25.0
28.7	+ 41.1 / -28.8
33.7	+ 48.7 / -32.4
38.7	+ 56.3 / -35.6
43.7	+ 64.1 / -38.5

- abundance prediction (output) uncertainty **scales with rate (input) uncertainty**
- therefore important to have **accurate assessments of input rate uncertainties**

Min-Max UQ Approach

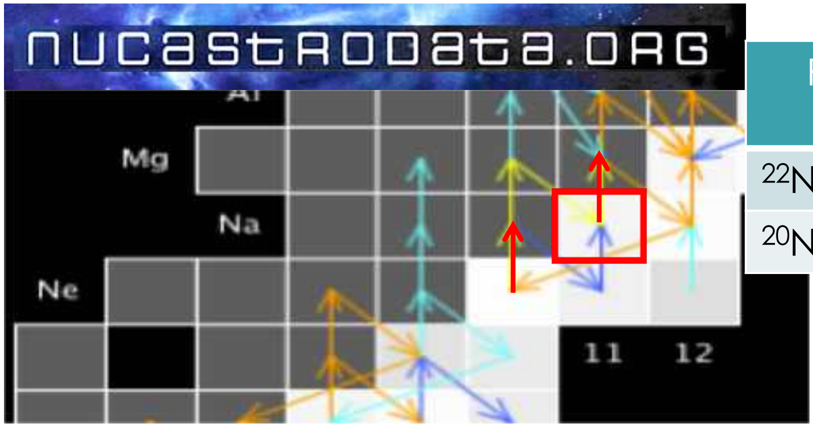


$^{22}Na(p,\gamma)^{23}Mg$

$^{20}Ne(p,\gamma)^{21}Na$

- how to handle variation of multiple rate inputs?

Min-Max UQ Approach



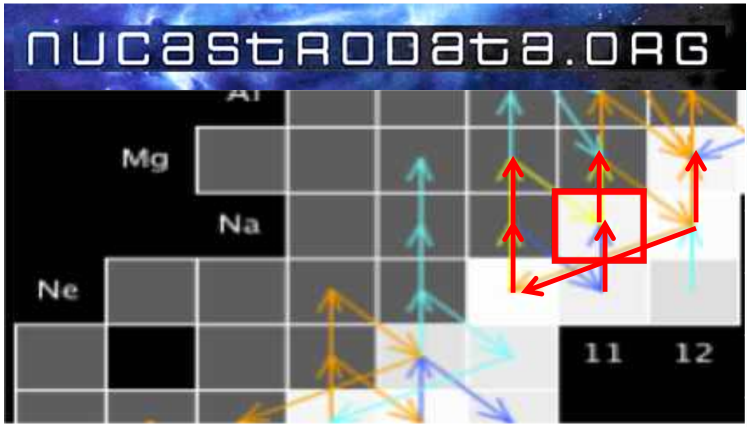
Reaction	Rate Uncertainty %	22Na Abundance Prediction Uncertainty %
^{22}Na(p,γ)^{23}Mg	23.7	+ 33.8 / -25.0
^{20}Ne(p,γ)^{21}Na	22.8	+5.8 / -5.7

2 reactions varied independently

Add in quadrature:
+ 34.2 % / -25.6%

- vary **other** inputs **individually** and compare predicted output uncertainties
- add individual "partial" uncertainties **in quadrature** to get "total" uncertainty
- assumes **no correlation** between inputs

Min-Max UQ Approach



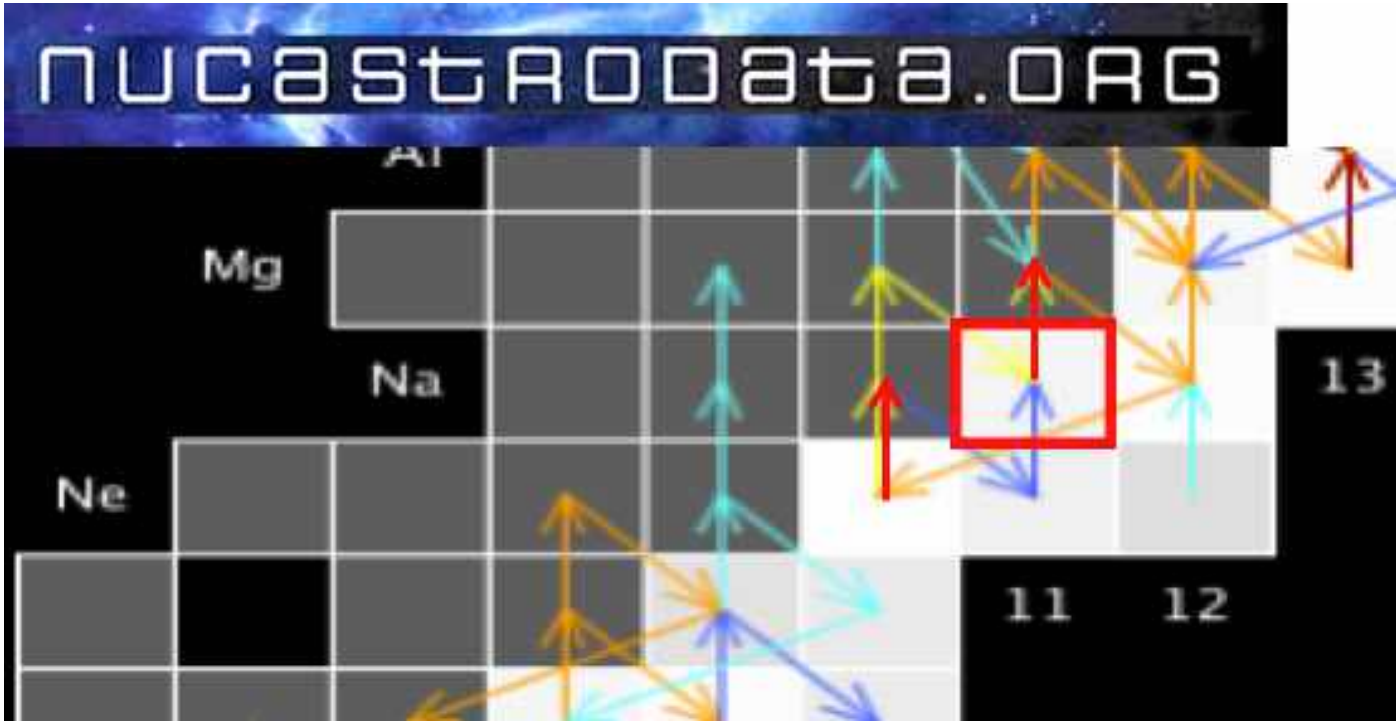
Reaction	Rate Uncertainty %	22Na Abundance Prediction Uncertainty %
^{22}Na(p,γ)^{23}Mg	23.7	+ 33.8 / -25.0
^{20}Ne(p,γ)^{21}Na	22.8	+5.8 / -5.7
^{23}Na(p,α)^{20}Ne	18.7	+/- 2.9
^{23}Na(p,γ)^{24}Mg	34.2	+4.5 / -4.6
^{21}Na(p,γ)^{22}Mg	22.9	+2.2 / -1.9
^{21}Ne(p,γ)^{22}Na	21.8	+0.72 / -0.83

6 reactions varied independently

Add in quadrature: + 34.8% / -26.2%

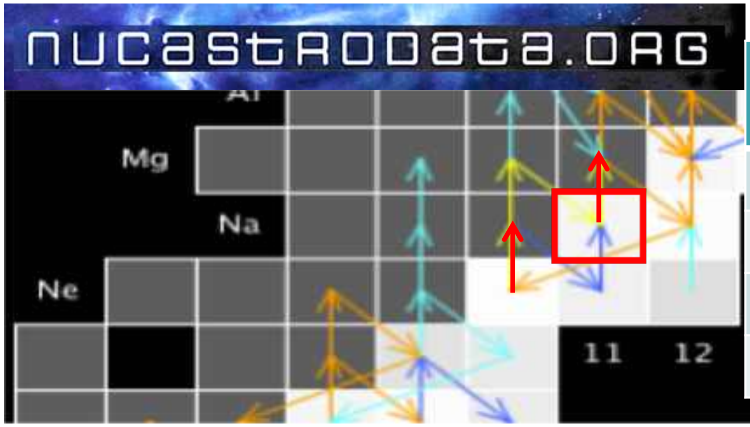
- vary **other** inputs **individually** and compare predicted output uncertainties
- add individual “partial” uncertainties **in quadrature** to get “total” uncertainty
- assumes **no correlation** between inputs

Min-Max UQ Approach



- what about correlations between two input rates?

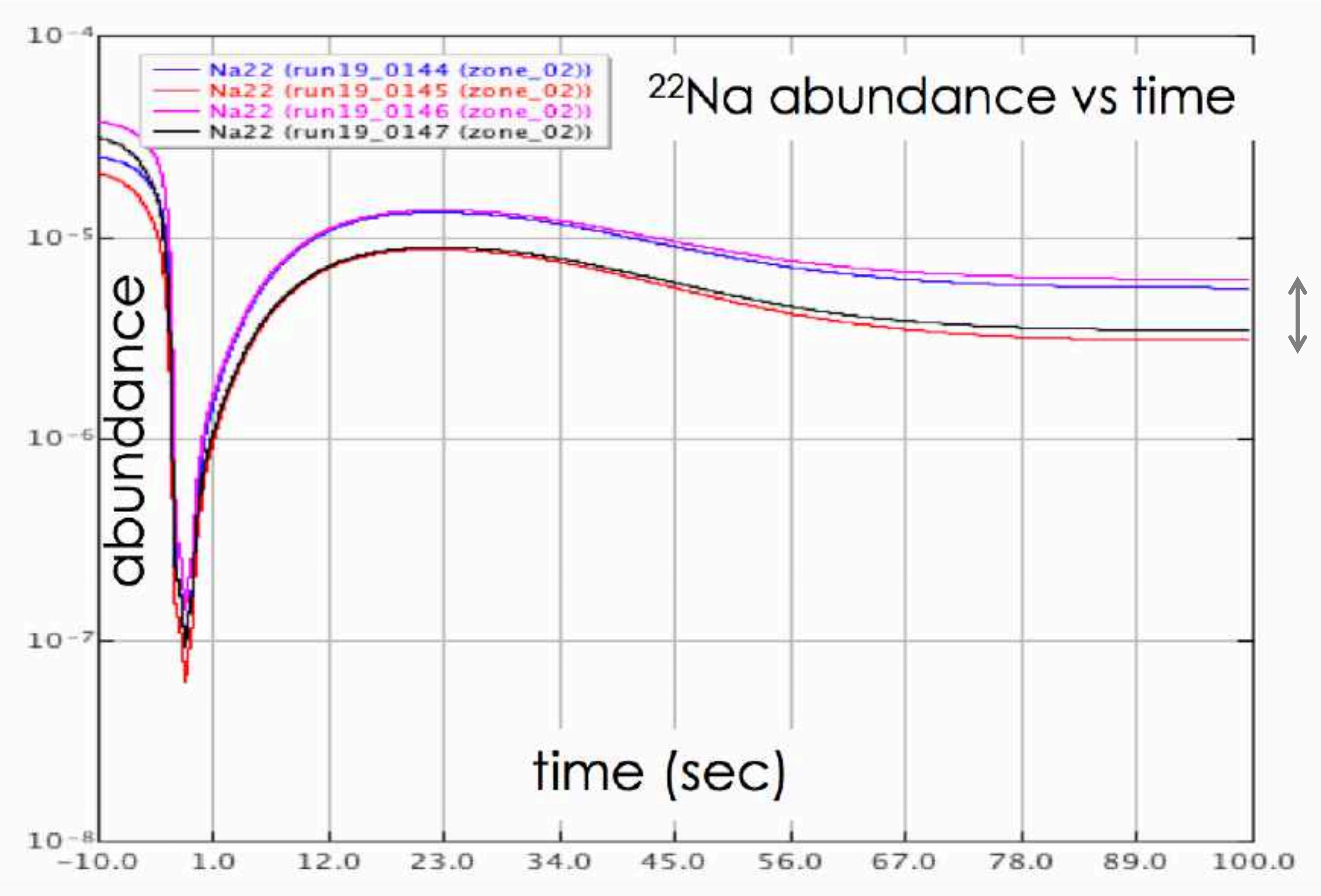
Min-Max UQ Approach and Correlations



rate 1 value (% change)	rate 2 value (% change)	^{22}Na Abundance Prediction Uncertainty %
- 23.7 (min)	- 22.8 (min)	
+23.7 (max)	- 22.8 (min)	
- 23,7 (min)	+22.8 (max)	
+23.7 (max)	+22.8 (max)	

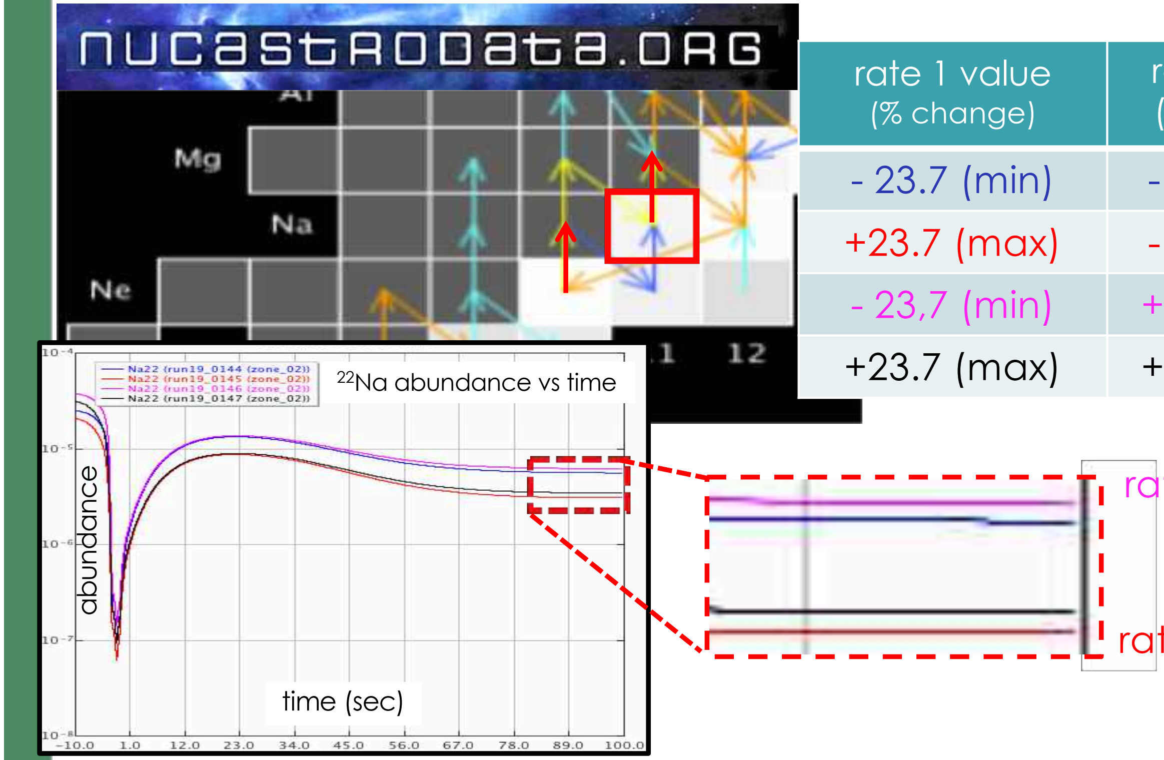
- consider **all combinations** of multiple reaction variations between min and max values
- compare prediction output uncertainties
- "brute force" exploration of input correlations

Min-Max UQ Approach



abundance
prediction
uncertainty

Min-Max UQ Approach



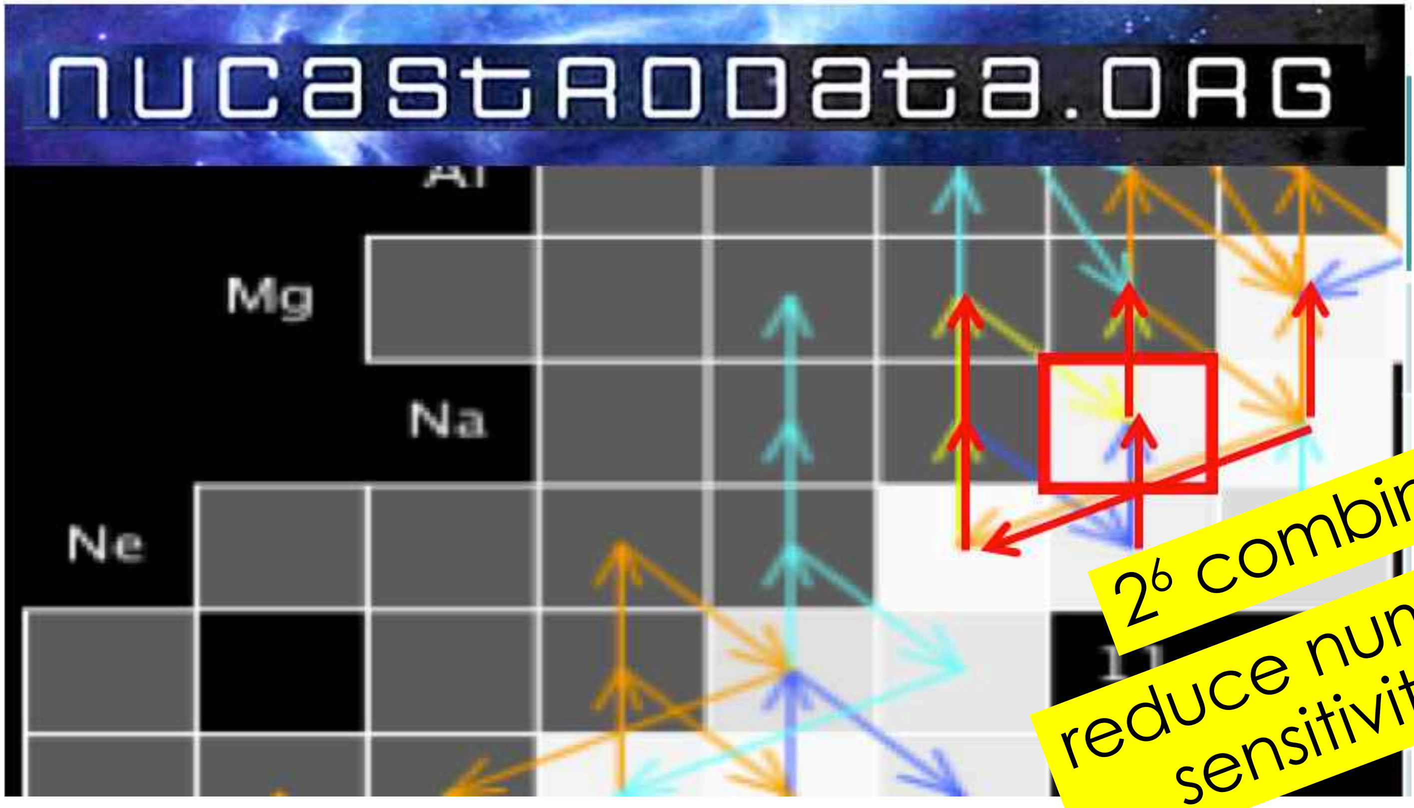
rate 1 value (% change)	rate 2 value (% change)	^{22}Na Abundance Prediction Uncertainty %
- 23.7 (min)	- 22.8 (min)	26.7
+23.7 (max)	- 22.8 (min)	-29.5
- 23,7 (min)	+22.8 (max)	40.7
+23.7 (max)	+22.8 (max)	-20.1

2 reactions varied together in all min-max combinations: + 40.7% / -29.5%

- consider **all combinations** of multiple reaction variations between min and max values
- compare prediction output uncertainties
- **“brute-force”** exploration of input correlations

Rate 1 gives dominant contribution with an anti-correlation with abundance

Min-Max UQ Approach

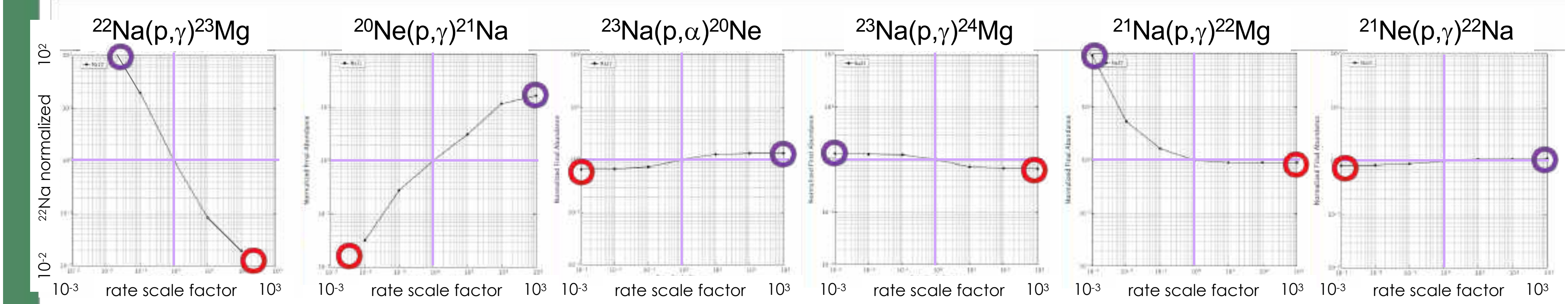


2^6 combinations!

reduce number using sensitivity studies

- what about correlations between six input rates?

Guiding Min-Max UQ with Sensitivity Studies



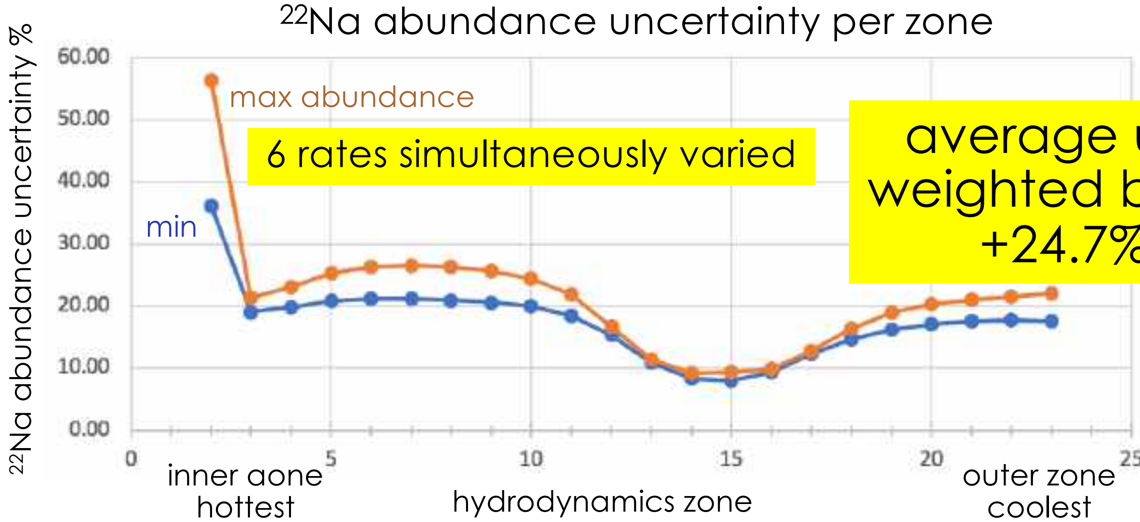
Obtain ^{22}Na **min** abundance with
max of ^{22}Na(p,γ)^{23}Mg
min of ^{20}Ne(p,γ)^{21}Na
min of ^{23}Na(p,α)^{20}Ne
max of ^{23}Na(p,γ)^{24}Mg
max of ^{21}Na(p,γ)^{22}Mg
min of ^{21}Ne(p,γ)^{22}Na

Obtain ^{22}Na **max** abundance with
min of ^{22}Na(p,γ)^{23}Mg
max of ^{20}Ne(p,γ)^{21}Na
max of ^{23}Na(p,α)^{20}Ne
min of ^{23}Na(p,γ)^{24}Mg
min of ^{21}Na(p,γ)^{22}Mg
max of ^{21}Ne(p,γ)^{22}Na

- simultaneous variation of multiple input parameters
- variations **guided** by sensitivity studies
- **quicker exploration** of input correlations than brute force approach

6 rates simultaneously varied gives ^{22}Na uncertainty of +56.3% / -36.2%

Min-Max rate UQ with multi-zone hydrodynamics

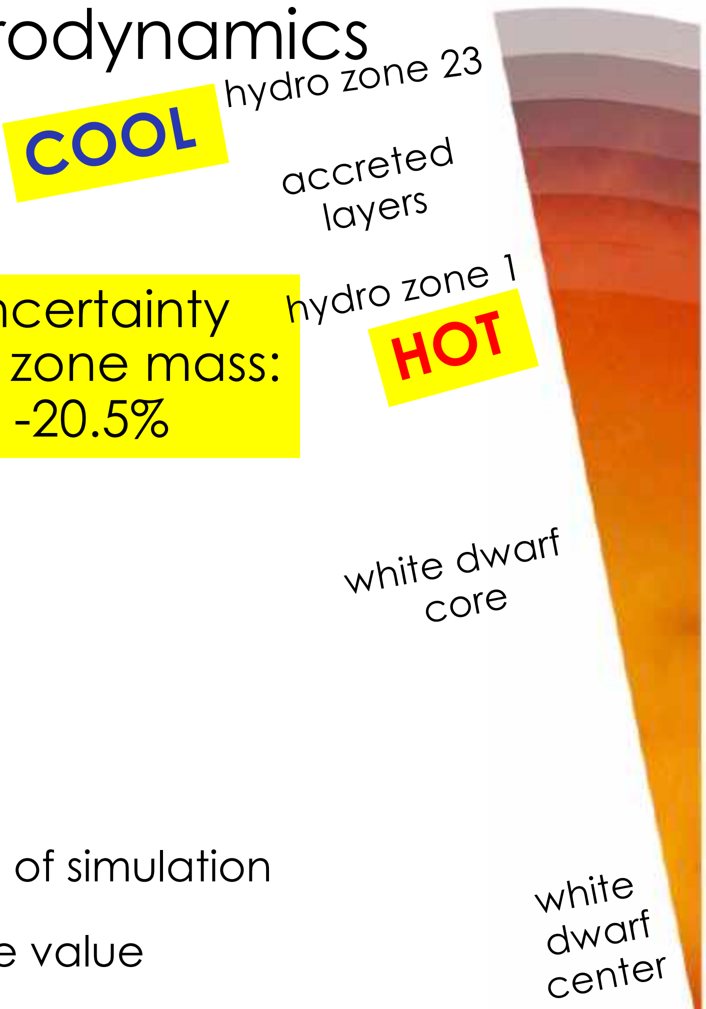


6 rates simultaneously varied

average uncertainty weighted by zone mass: +24.7% / -20.5%

HOT

COOL



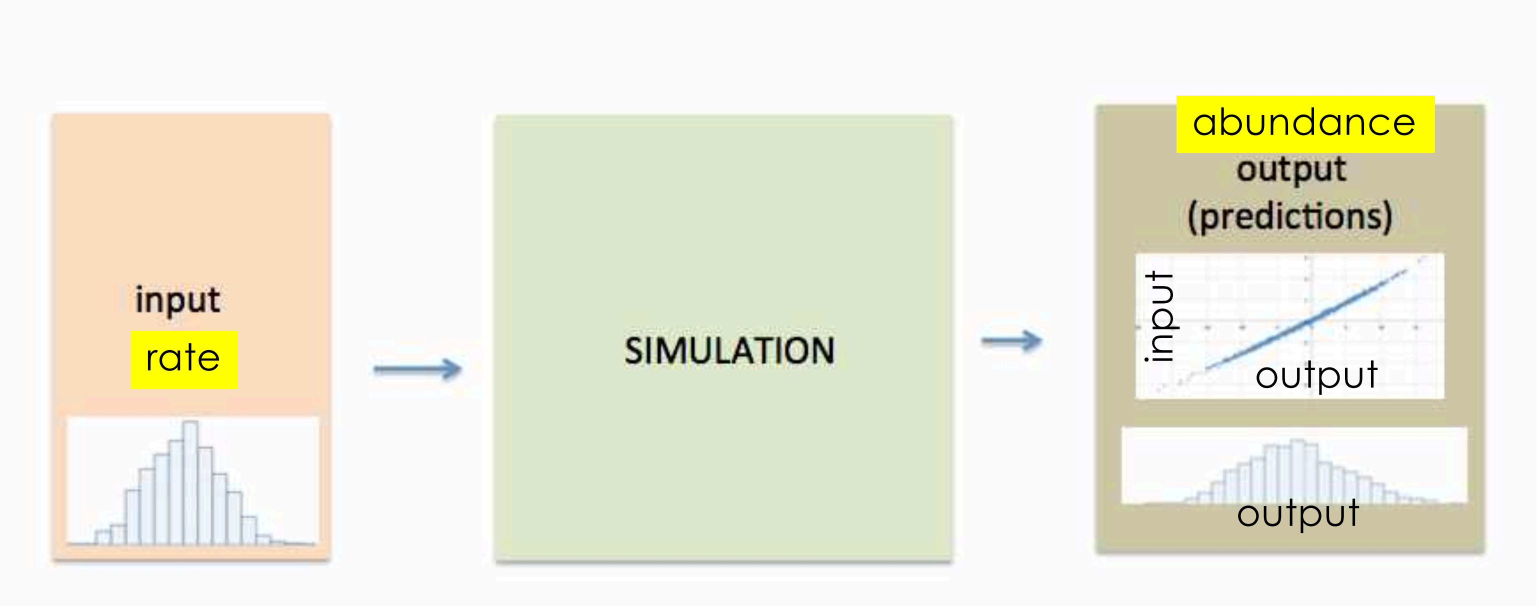
- repeat above analysis over multiple hydrodynamic zones of simulation
- can weight uncertainties by zone mass to get an average value
- enables **more realistic** exploration of impact of extrema of rate uncertainty variations

Multiple UQ Approaches

Approach	^{22}Na Abundance Prediction Uncertainty %
min-max dominant reaction	+33.8 / -25.0
min-max 2 dominant reactions	+34.2 / -25.6
min-max 6 dominant reactions	+34.8 /-26.2
min-max correlated 2 reactions	+ 40.7/ -29.5
min-max correlated 6 reactions	+ 56.3/ -36.2
averaging over multizone hydro	+ 24.7 / -20.5

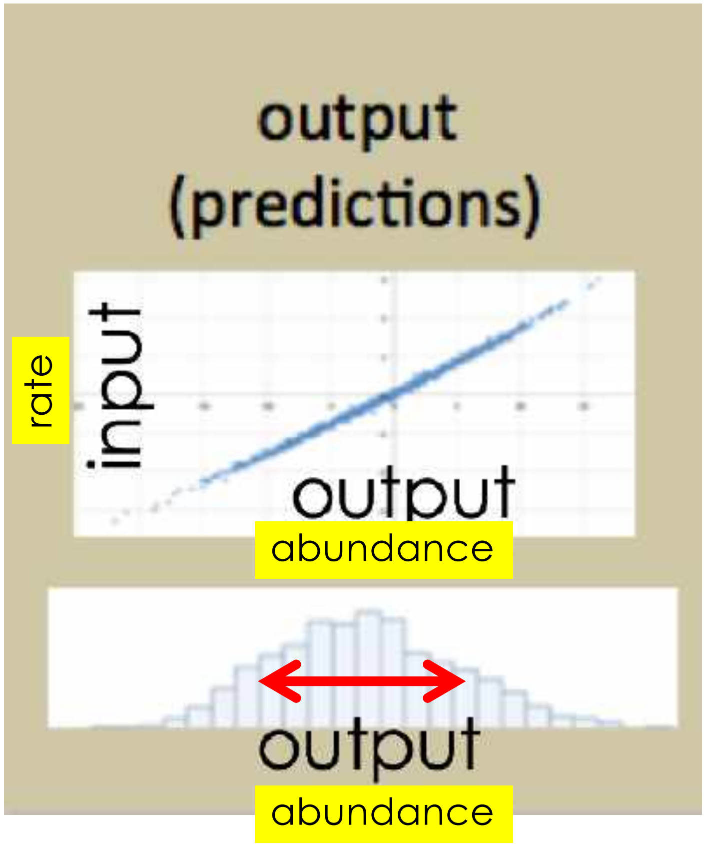
- different uncertainty estimates with different approaches

Monte Carlo Approaches



- simultaneous variation of **all** inputs within uncertainty
- **robust method** of propagating input uncertainties through simulations
- input correlations included
- works best for *small* variations of inputs

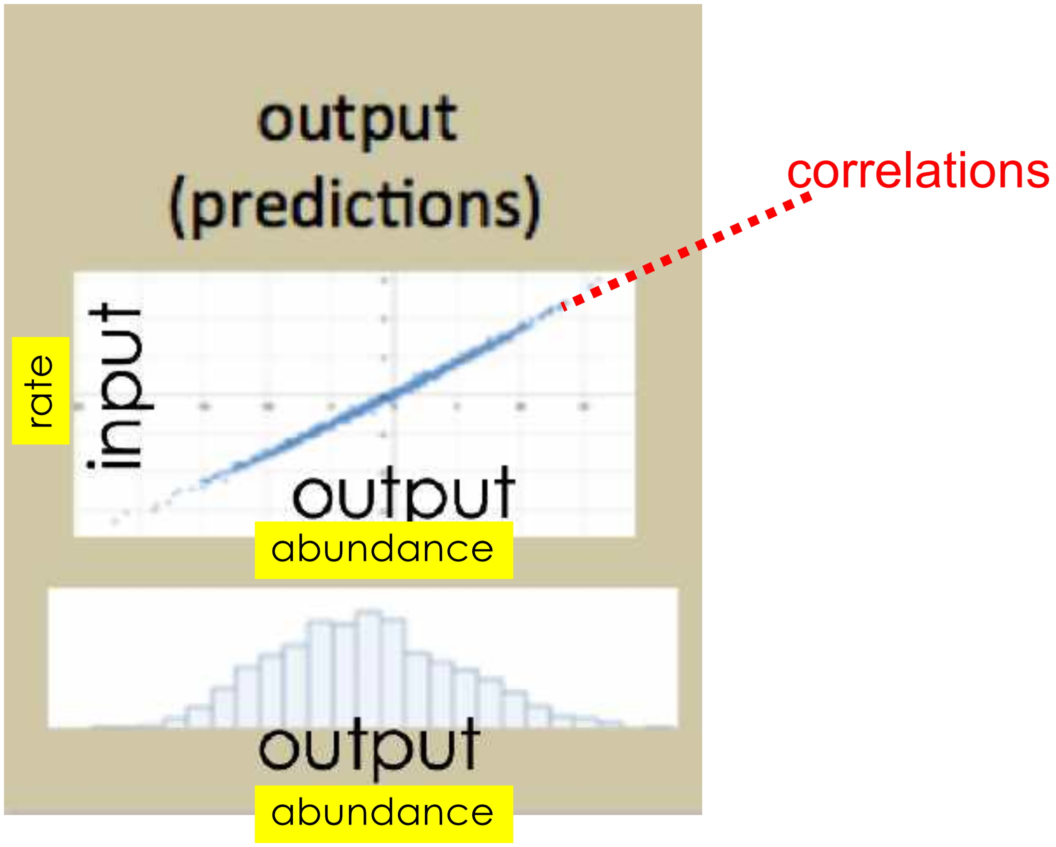
Monte Carlo Approaches



abundance
prediction
uncertainty

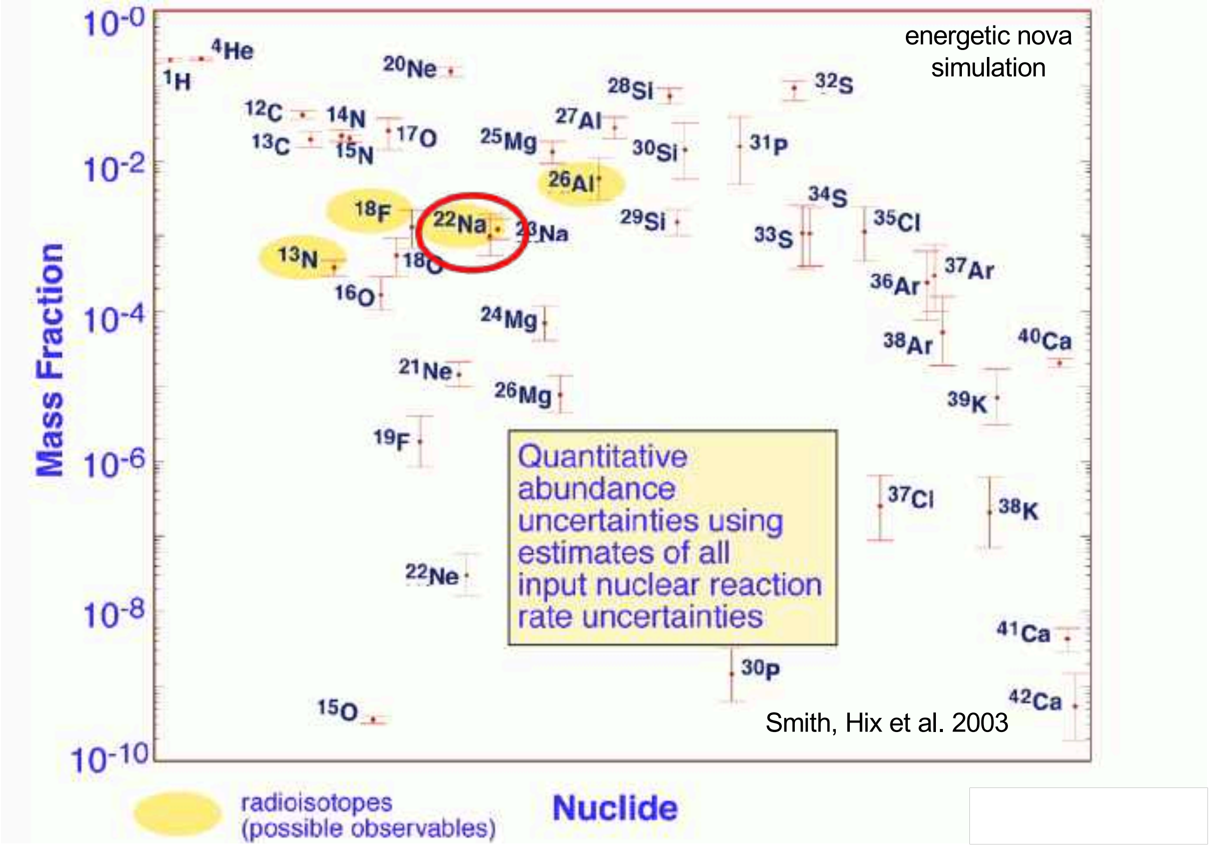
- obtain prediction (output) uncertainties

Monte Carlo Approaches



- obtain rate - abundance (input-output) correlations

Monte Carlo Approaches



energetic nova simulation

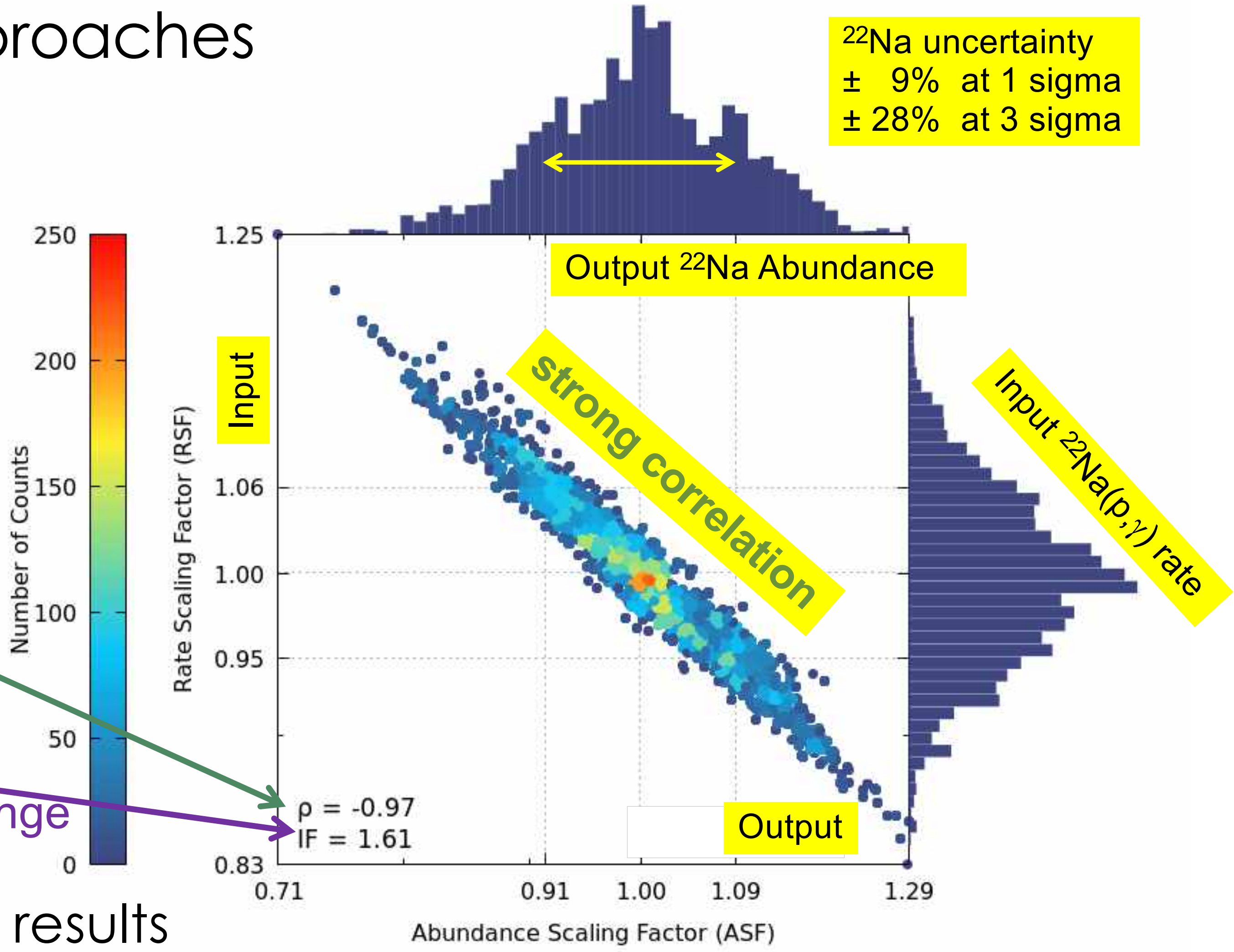
Quantitative abundance uncertainties using estimates of all input nuclear reaction rate uncertainties

Smith, Hix et al. 2003

- Quantitative example for Monte Carlo simulation of a nova

Monte Carlo Approaches

New Monte Carlo Results
Larry Zhang 2020
10000 runs
^{22}Na abundance vs.
^{22}Na(p,γ) rate variation



^{22}Na uncertainty
± 9% at 1 sigma
± 28% at 3 sigma

Output ^{22}Na Abundance

Input

strong correlation

Input ^{22}Na(p,γ) rate

Output

correlation coefficient

Impact factor :
output change / input change

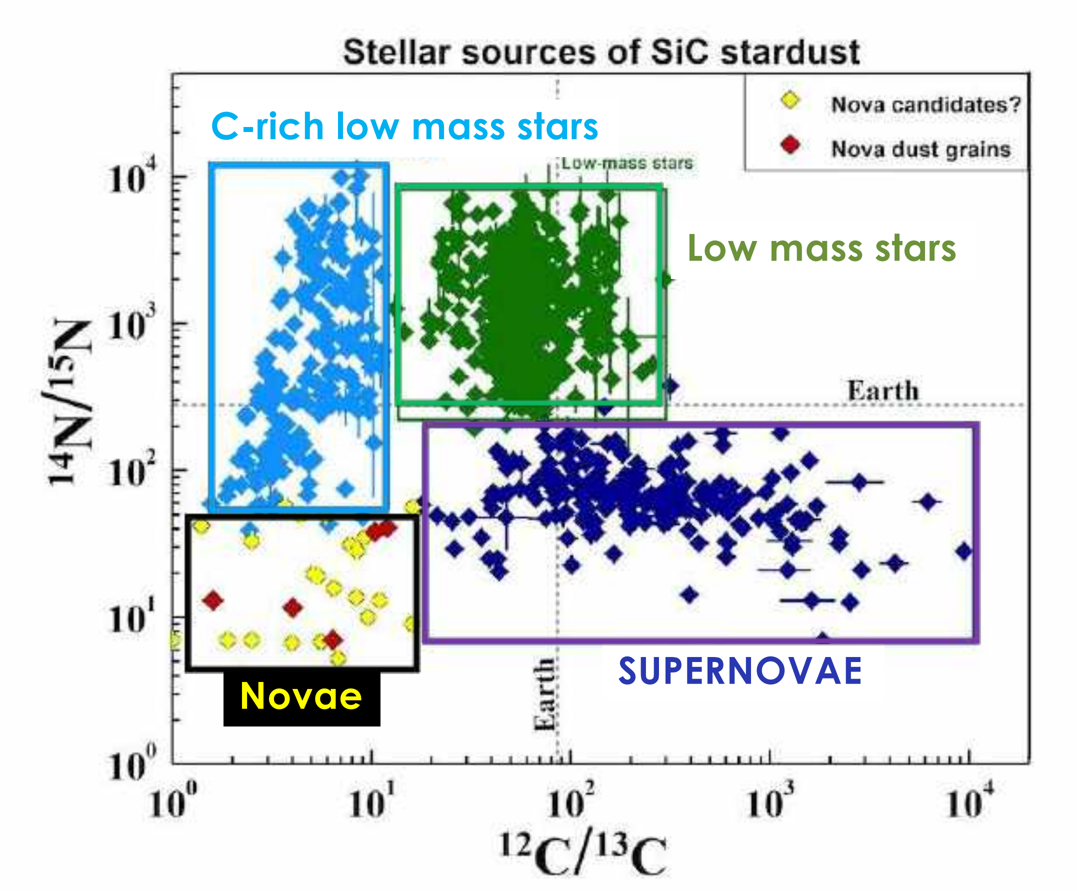
- New Monte Carlo results

Multiple Approaches

Approach	^{22}Na Abundance Prediction Uncertainty %
min-max dominant reaction	+33.8 / -25.0
min-max 2 dominant reactions	+34.2 / -25.6
min-max 6 dominant reactions	+34.8 /-26.2
min-max correlated 2 reactions	+ 40.7/ -29.5
min-max correlated 6 reactions	+ 56.3/ -36.2
averaging over multizone hydro	+ 24.7 / -20.5
Monte Carlo (3 sigma)	+ 28% / -28%

- because there are no "standards" yet, best to quote uncertainties from multiple approaches

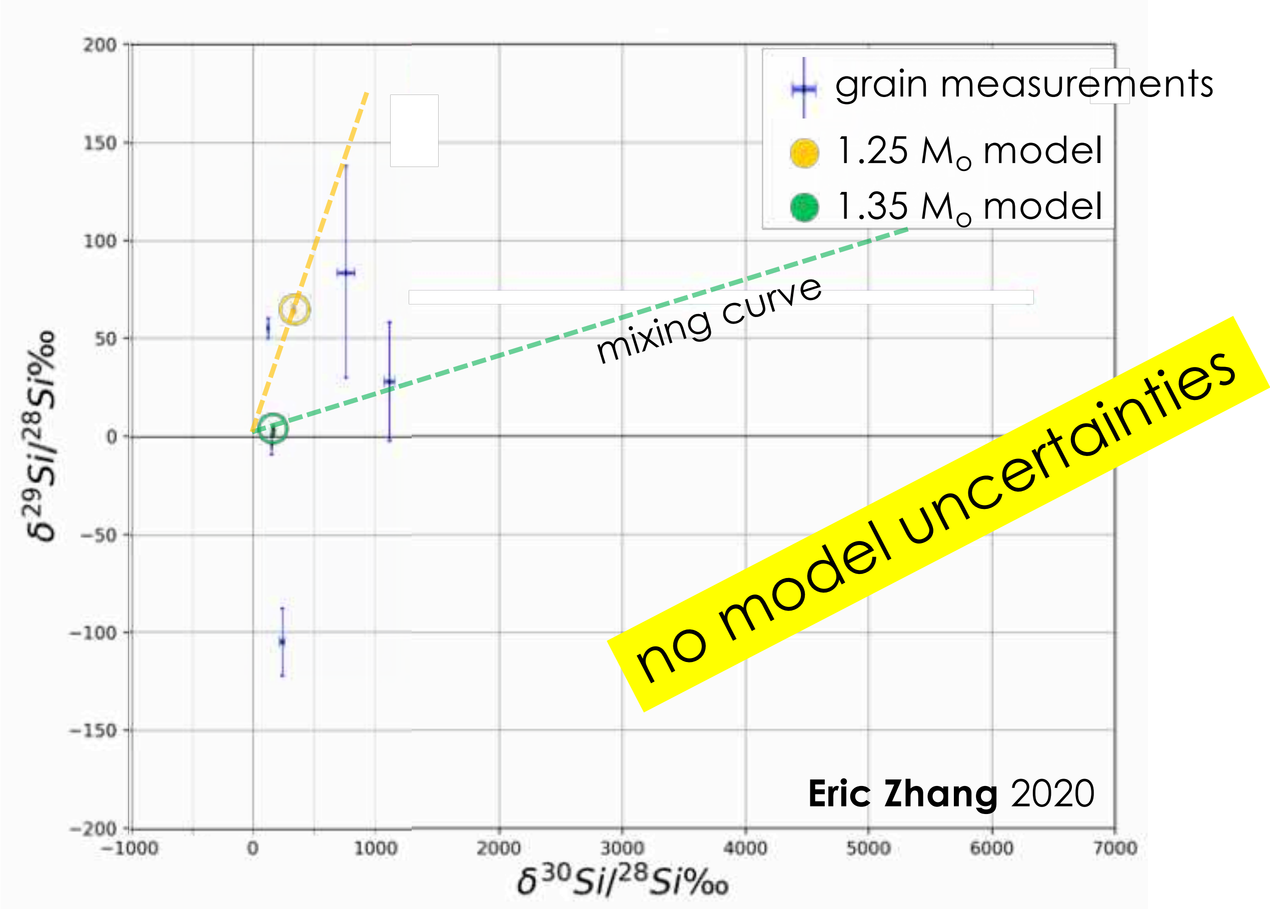
Nucleosynthesis UQ for Meteoritics



Abundance Ratios from Meteorite Grains

- comparisons of theory and observation requires uncertainties

Nucleosynthesis UQ for Meteoritics



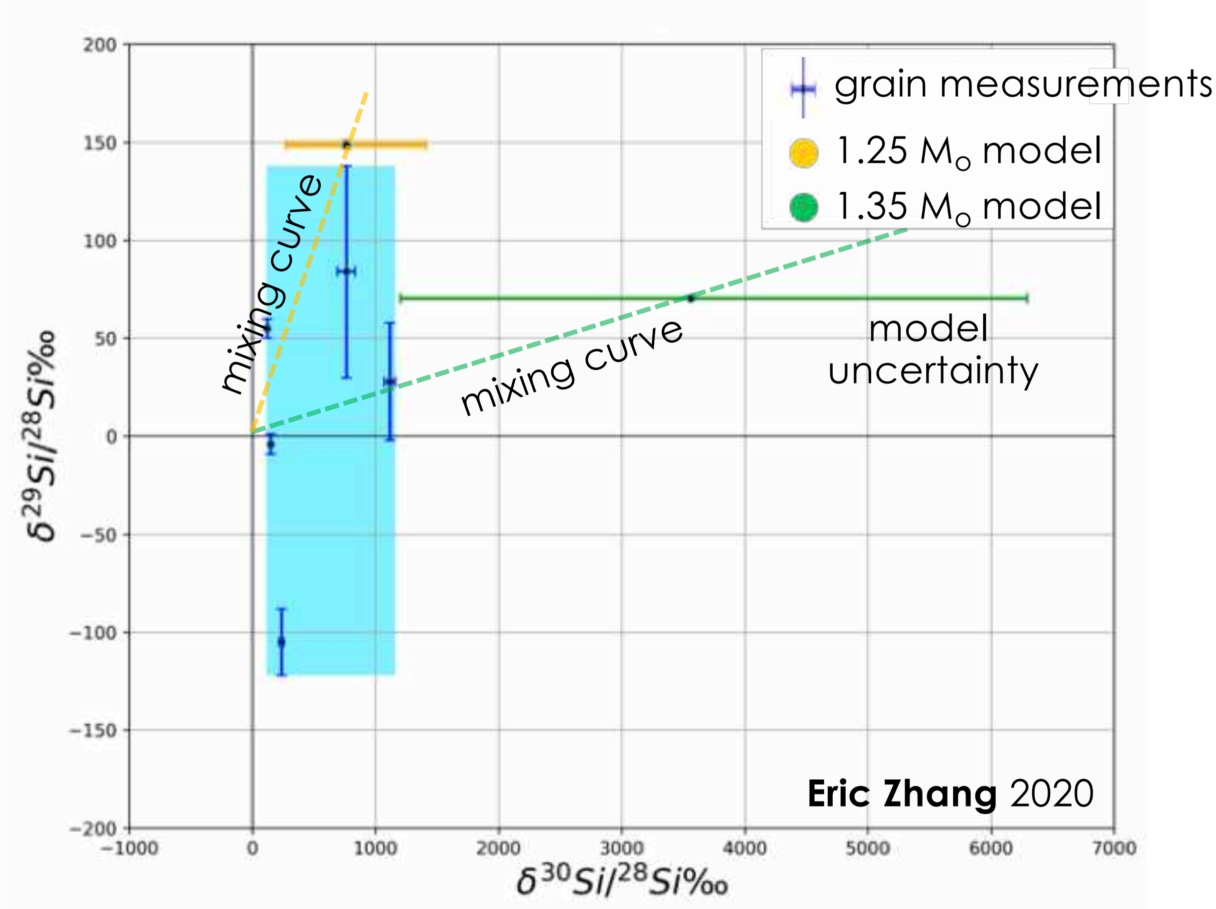
no model uncertainties

Eric Zhang 2020

Abundance Ratios from Meteorite Grains

- comparisons of theory and observation requires uncertainties

Nucleosynthesis UQ for Meteoritics

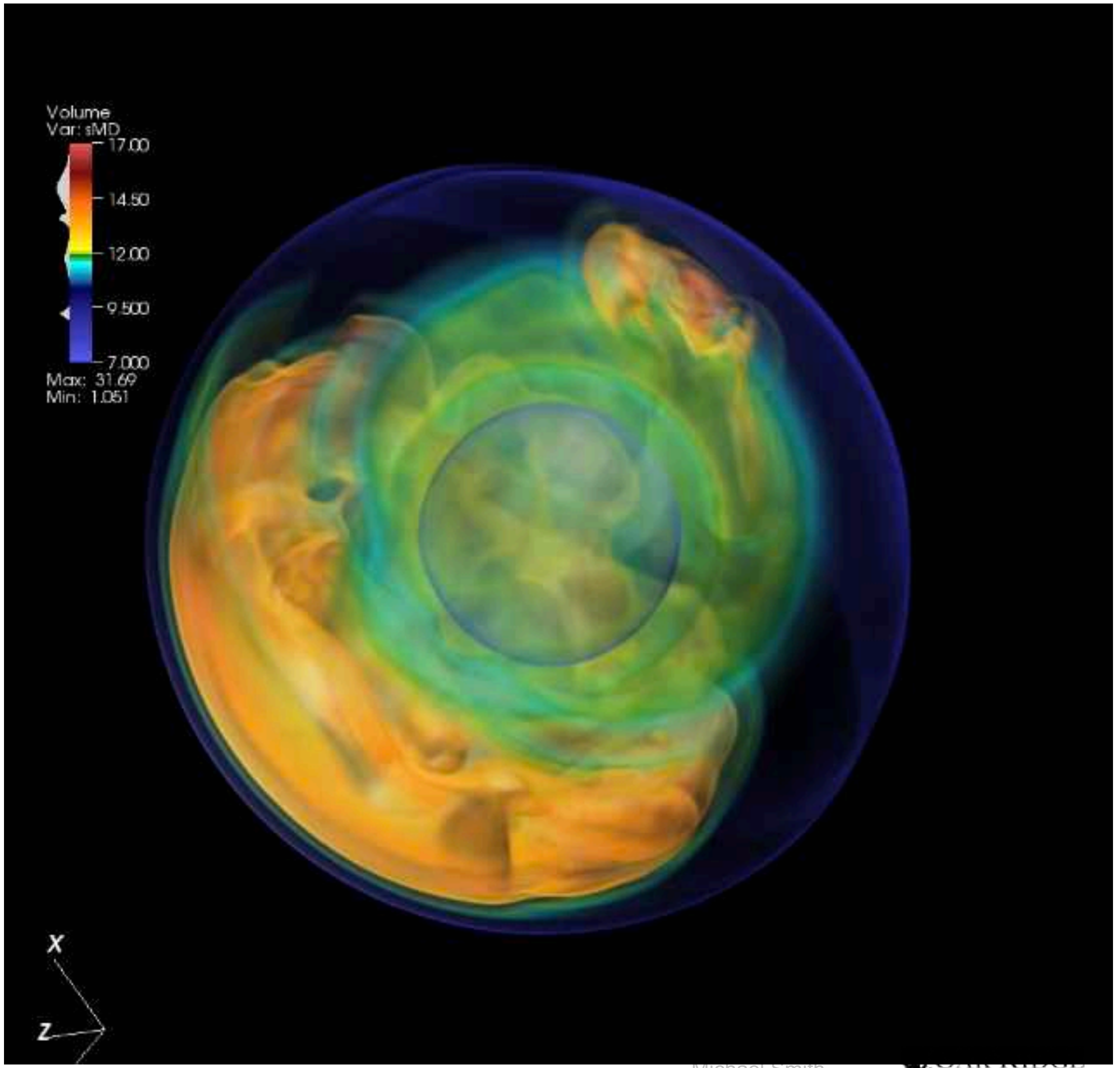


Abundance Ratios from Meteorite Grains

- comparisons of theory and observation requires uncertainties

Future Trends

- Couple full hydro with full nucleosynthesis
- Improved MC simulations
- Improved UQ
  - Bayesian approaches
  - ML approaches
- Better handling of tracer particles



Hix et al.

Summary

- Nucleosynthesis is a fascinating research area with many unsolved puzzles
- Nucleosynthesis studies can guide future experiments, interpret past experiments, connect observations to astrophysical sites, and more

Summary

- Uncertainty Quantification is an important (undeveloped) aspect of this work
- The Computational Infrastructure for Nuclear Astrophysics enables you to quickly explore many important nucleosynthesis puzzles