How to make elements in my computer

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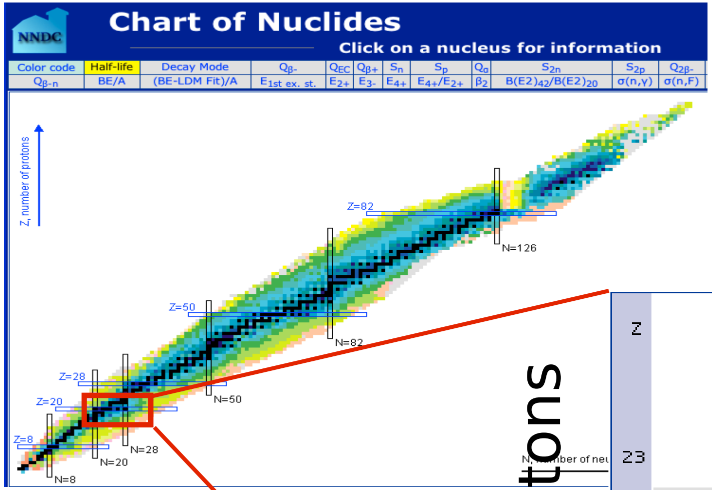
- @JINA-CEE (http://www.jinaweb.org/)

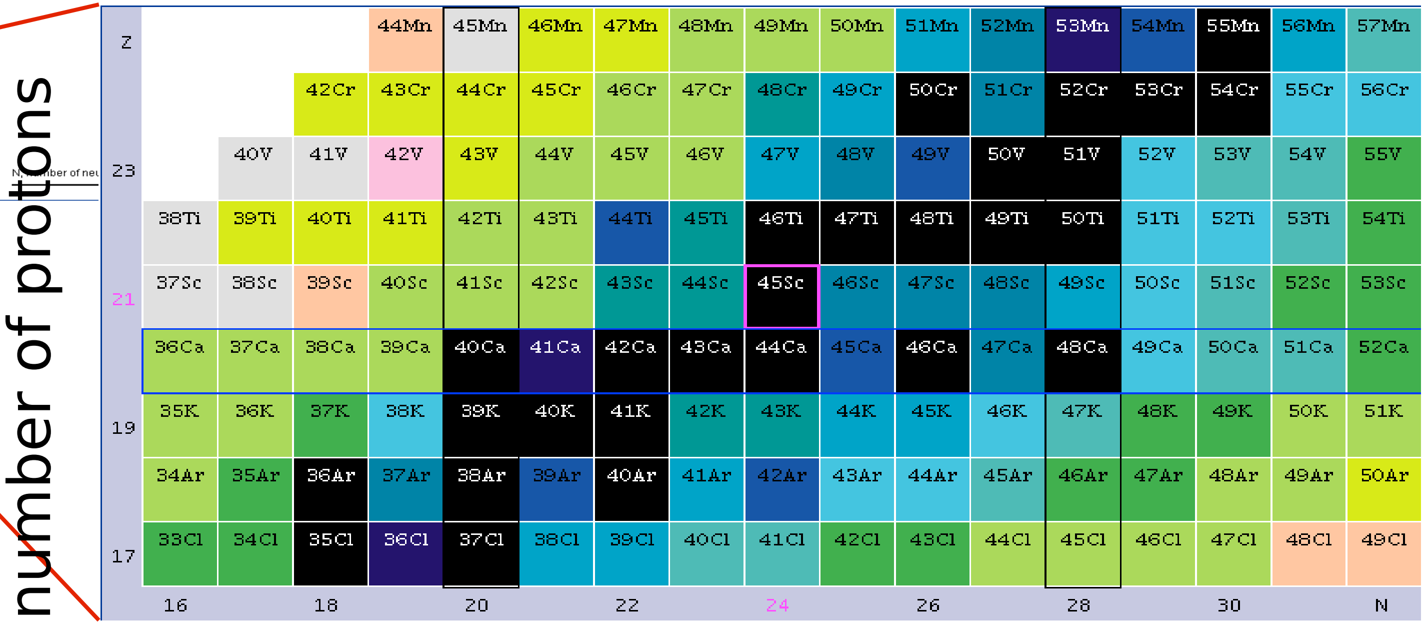
Outline

- The origin of elements and isotopes
- Stellar models and stellar nucleosynthesis: some context for a framework of computational experiments
- Impact studies of nuclear reaction rates from experiments: comparing examples requiring different approaches (Ne22+α and Fe59(n,γ))
- Making elements in stars: the example of with Ti and its isotopes, and many more for explosive nucleosynthesis.
- ...and another example for low-mass AGB stars.

What is the origin of the elements?

100+ elements
254 stable isotopes
<u>6000+</u> isotopes including all unstable species



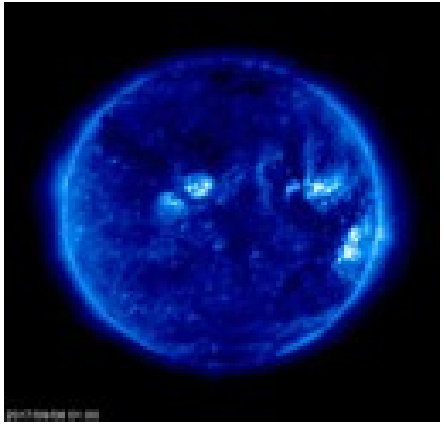


number of neutrons

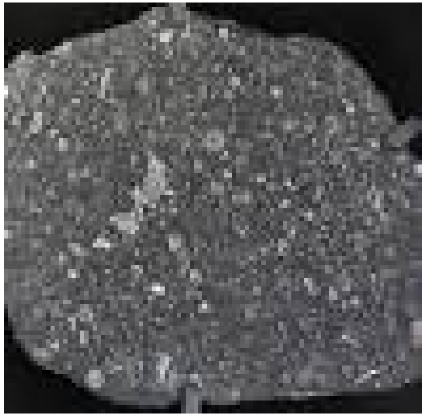
Stable elements are made of stable isotopes.
From many observations we may assume C12 ~ C and O16 ~ O, but for many other elements things are more complicated.

^{14}O 1.18 m β^+	^{15}O 2.04 m β^+	^{16}O 99.762 0.038 mb	^{17}O 0.038	^{18}O 0.2 0.00886 mb
^{13}N 9.96 m β^+	^{14}N 99.634 0.041 mb	^{15}N 0.366 0.0058 mb	^{16}N 7.13 s β^-	^{17}N 4.17 s β^-
^{12}C 98.89 0.0154 mb	^{13}C 1.11 0.021 mb	^{14}C 5.70 ka 0.00848 mb, β^-	^{15}C 2.45 s β^-	^{16}C 747.00 ms β^-

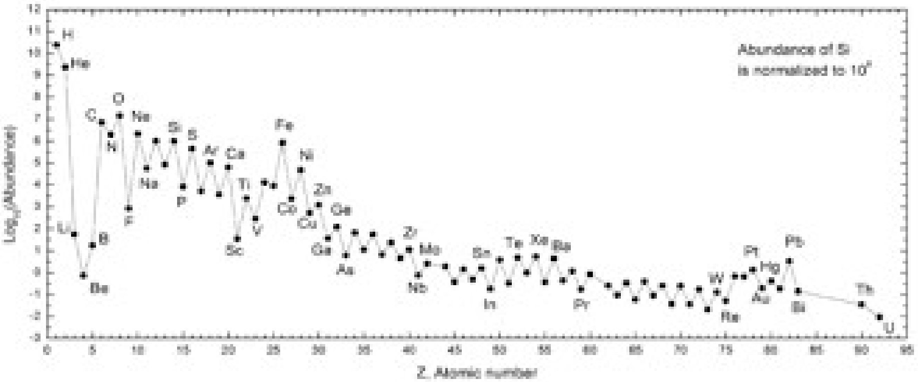
What is the origin of the elements... nearby?



Soho image
of the Sun
(Extreme ultraviolet Imaging Telescope)

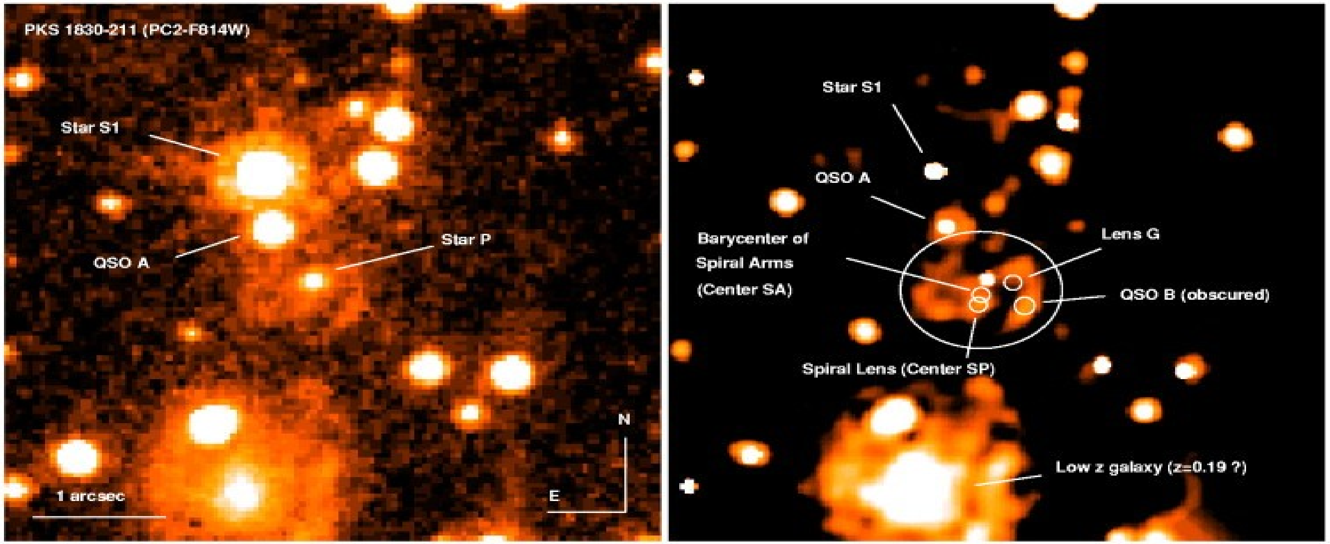


Allende
Meteorite
(1969)



Review: Lodders 2021 SSRv 217

...or really far away?



Quasar PKS 1830-211: Courbin+A&A 2002

Absorption line from a spiral galaxy between the quasar and us:
Quasar: redshift Z ~ 2.5
Galaxy Age/distance: z=0.89 corresponds to a look back time of 7.2 Gyr, yielding an age ≤ 6 Gyr
C, N, O, S observed from integrated lines (Muller et al. 2006 A&A)
Data in a GCE context: Pignatari+ 2015 ApJL and Kobayashi+ 2020 ApJ

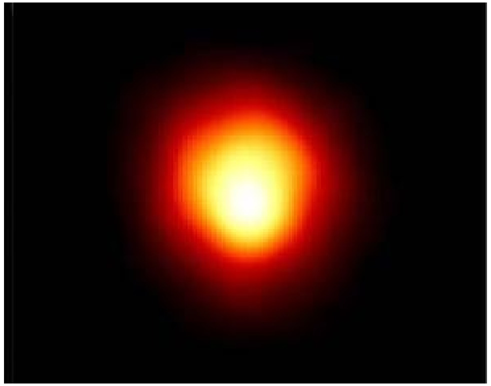
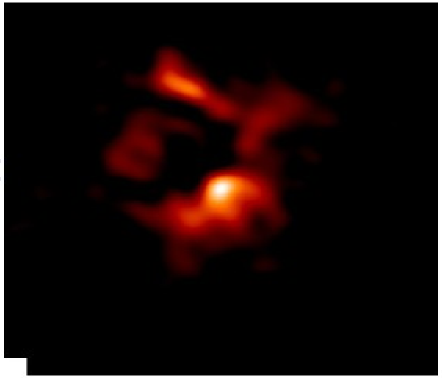


Image: A. Dupree/CFA/R. Gilliland/STScI/NASA/ESA

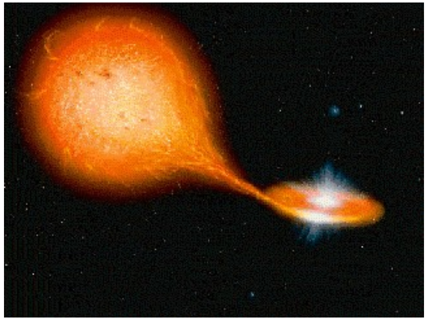
Betelgeuse (α-Ori):
~ 19 M_{sun}
~ 650 ly
~ 1180 R_{sun}

.....

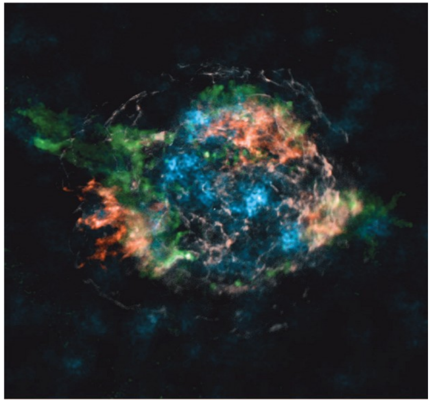
CWLeo
(IRC+10216)
~2-3 M_{sun}
~ 400 lyr
~ 250 R_{sun}



Tuthill et al. 2000, A&A, Keck Telescope

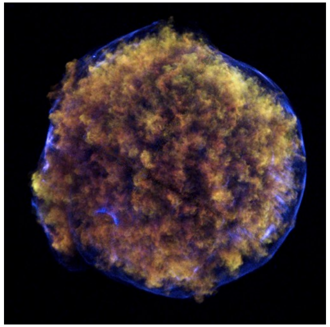


Artist conception of the WD and the binary system



CCSN: Cas A
~ 11000 lyr
~ 300 years ago

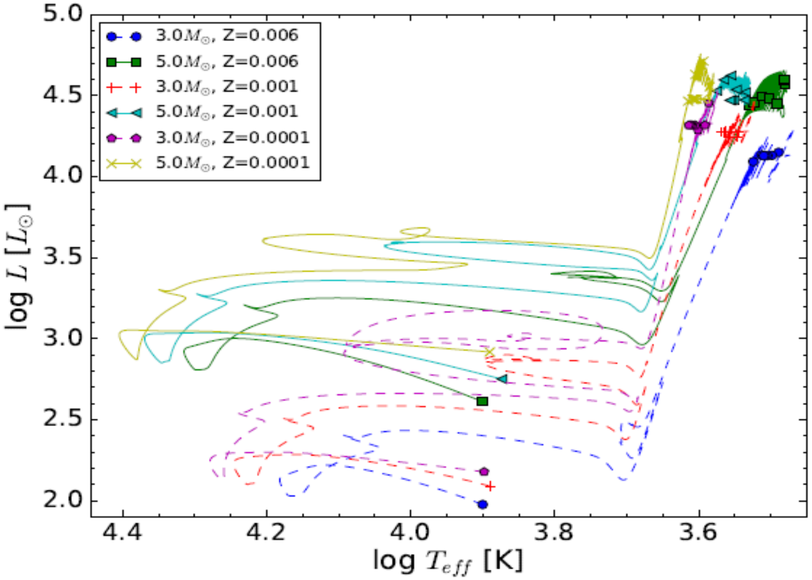
Grefenstette et al. 2014, Nature (NuSTAR data)

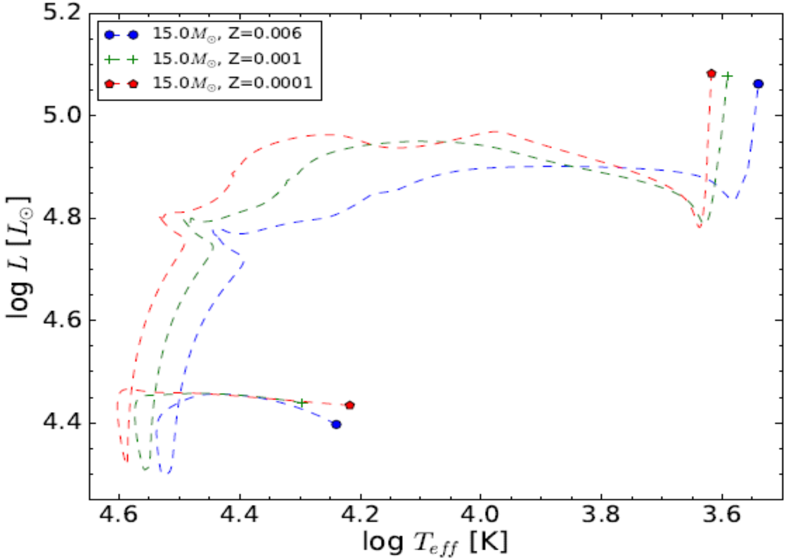


SNIa: Tycho’s supernova (B Cas)
~ 9000 lyr
~ observed in 1572

Chandra X-ray telescope +

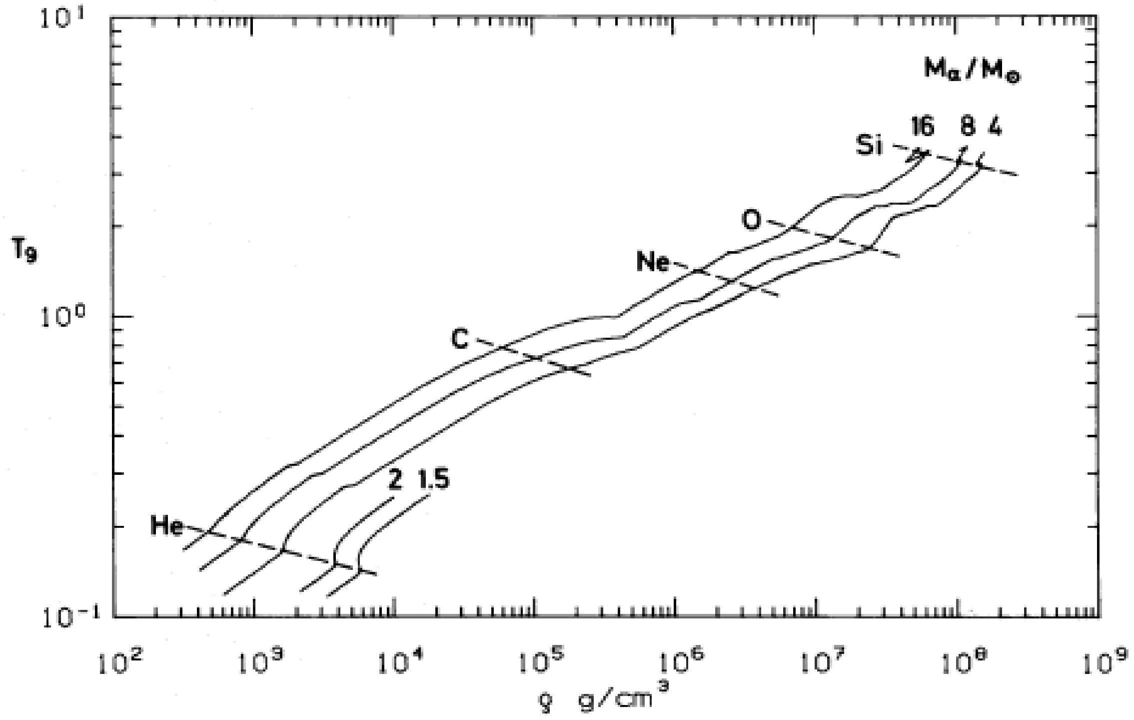
Structure evolution outside





Ritter, MP et al. 2018 MNRAS

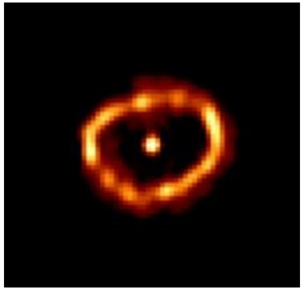
Structure evolution inside



Thielemann & Arnett 1985 ApJ

Binary stars and else: another zoo

Novae

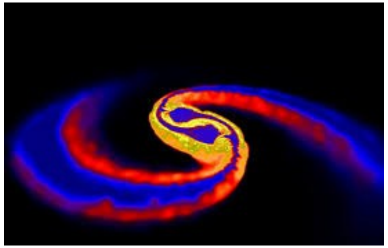


Nova Cygni 1992 (HST)

E ~ 10^{45} ergs
Mass ejected = 10^{-4} – 10^{-5} Msun
Nucl. contribution ~ C13, N15, O17

Jose & Hernanz 2007,
Casanova et al. 2011

NS-NS mergers

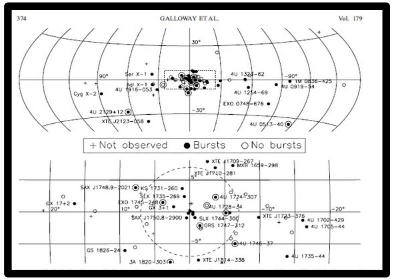


Neutron Star Mergers:
protons/neutrons ≤ 0.1

Source of gold?
Gravitational waves… LIGO

Cowan et al. 2021
Rev of Mod Phys

X-ray binaries



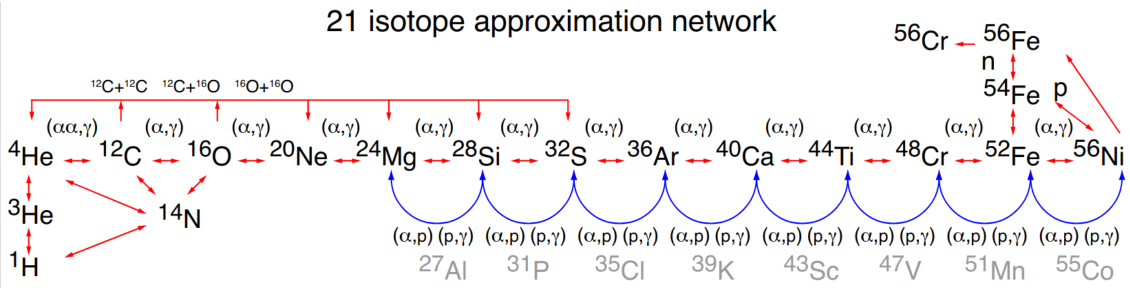
Galloway et al. 2008

E ~ 10^{39} ergs
Mass ejected = ?
Nucl. contribution ?
p nuclei ^{92,94}Mo and ^{96,98}Ru?

Schatz et al. 2001

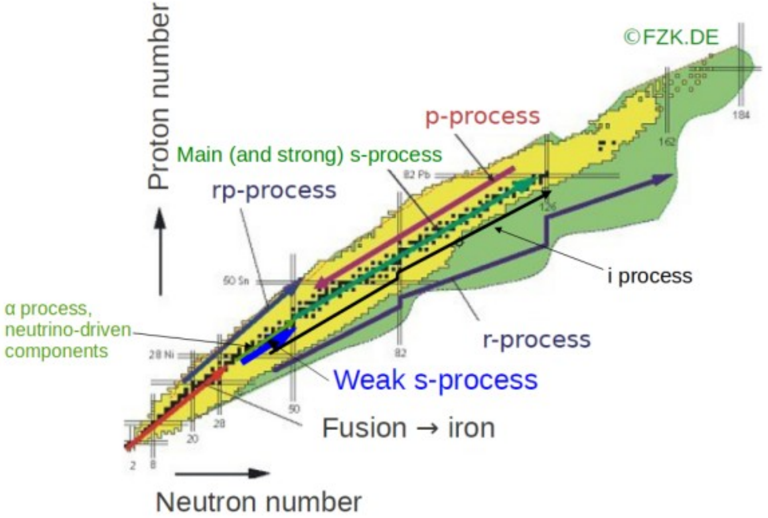
… and many more!

Isotopes for stars vs isotopes for (relevant) nucleosynthesis in stars



Source:
https://cococubed.com
Often default for MESA for massive stars (extension from Weaver+1978)

Full nucleosynthesis products:
It depends on the stellar conditions and the nucleosynthesis of interest.



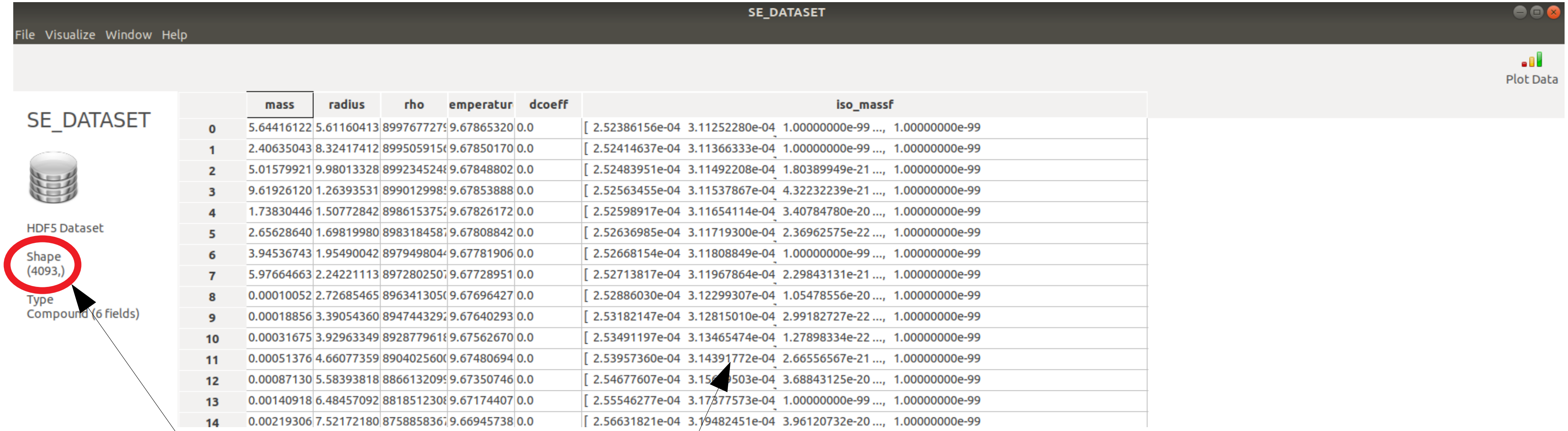
Labs for computational experiments in nucleosynthesis

Locally:
Some simple calculations (e.g., single trajectories);
Nuclear sensitivity studies (light configurations);
Vizualization.

Viper-HPC @Hull
ChETEC-INFRA
TNA event
24 November 2021

HPC:
Full stellar models;
Stellar yields sets for GCE;
Visualization.

Data in hdf5: looking at one file with, e.g., HDF compass ...



	mass	radius	rho	emperatur	dcoeff	iso_massf
0	5.64416122	5.61160413	8997677279	9.67865320	0.0	[2.52386156e-04 3.11252280e-04 1.00000000e-99 ..., 1.00000000e-99
1	2.40635043	8.32417412	8995059156	9.67850170	0.0	[2.52414637e-04 3.11366333e-04 1.00000000e-99 ..., 1.00000000e-99
2	5.01579921	9.98013328	8992345248	9.67848802	0.0	[2.52483951e-04 3.11492208e-04 1.80389949e-21 ..., 1.00000000e-99
3	9.61926120	1.26393531	8990129985	9.67853888	0.0	[2.52563455e-04 3.11537867e-04 4.32232239e-21 ..., 1.00000000e-99
4	1.73830446	1.50772842	8986153752	9.67826172	0.0	[2.52598917e-04 3.11654114e-04 3.40784780e-20 ..., 1.00000000e-99
5	2.65628640	1.69819980	8983184587	9.67808842	0.0	[2.52636985e-04 3.11719300e-04 2.36962575e-22 ..., 1.00000000e-99
6	3.94536743	1.95490042	8979498044	9.67781906	0.0	[2.52668154e-04 3.11808849e-04 1.00000000e-99 ..., 1.00000000e-99
7	5.97664663	2.24221113	8972802507	9.67728951	0.0	[2.52713817e-04 3.11967864e-04 2.29843131e-21 ..., 1.00000000e-99
8	0.00010052	2.72685465	8963413050	9.67696427	0.0	[2.52886030e-04 3.12299307e-04 1.05478556e-20 ..., 1.00000000e-99
9	0.00018856	3.39054360	8947443292	9.67640293	0.0	[2.53182147e-04 3.12815010e-04 2.99182727e-22 ..., 1.00000000e-99
10	0.00031675	3.92963349	8928779618	9.67562670	0.0	[2.53491197e-04 3.13465474e-04 1.27898334e-22 ..., 1.00000000e-99
11	0.00051376	4.66077359	8904025600	9.67480694	0.0	[2.53957360e-04 3.14391772e-04 2.66556567e-21 ..., 1.00000000e-99
12	0.00087130	5.58393818	8866132099	9.67350746	0.0	[2.54677607e-04 3.15[illegible]9503e-04 3.68843125e-20 ..., 1.00000000e-99
13	0.00140918	6.48457092	8818512308	9.67174407	0.0	[2.55546277e-04 3.17377573e-04 1.00000000e-99 ..., 1.00000000e-99
14	0.00219306	7.52172180	8758858367	9.66945738	0.0	[2.56631821e-04 3.19482451e-04 3.96120732e-20 ..., 1.00000000e-99

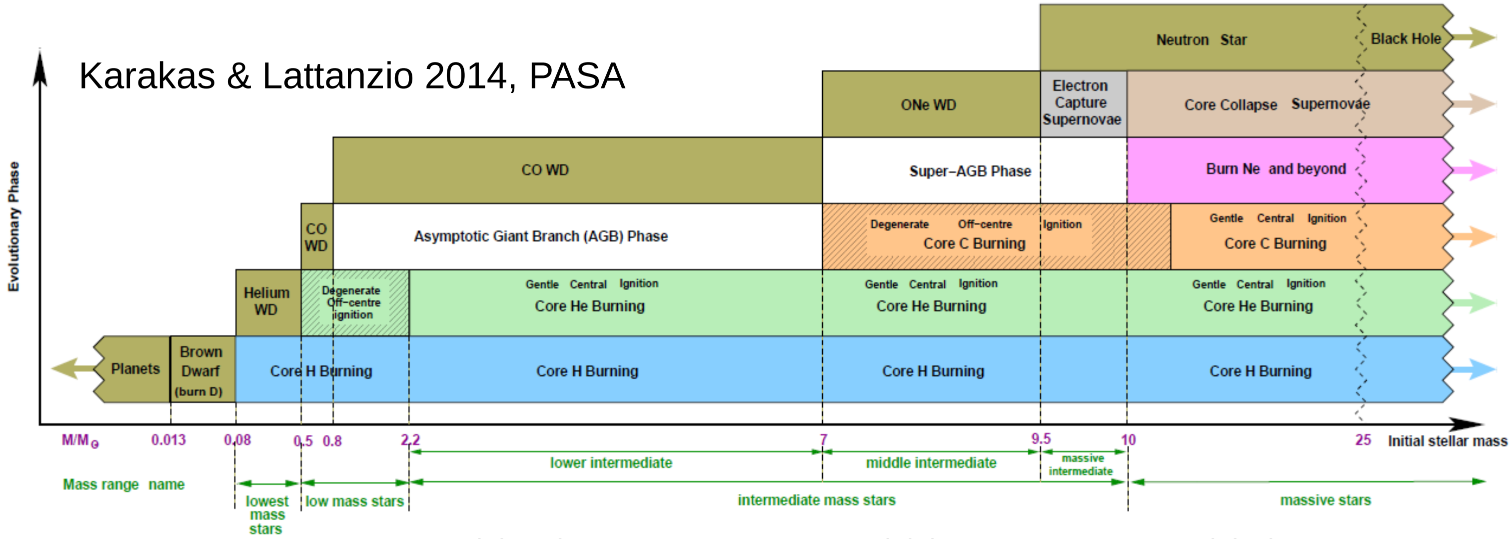
data: [4093 rows x (5 x 1 dp + 1 x 5134 dp)] x **1 evolution step**

Example: 1D stellar model (CCSN progenitor)

What data am I looking at? What do I need them for?

THINK PLAN DO

Stellar evolution: from low-mass star to massive stars



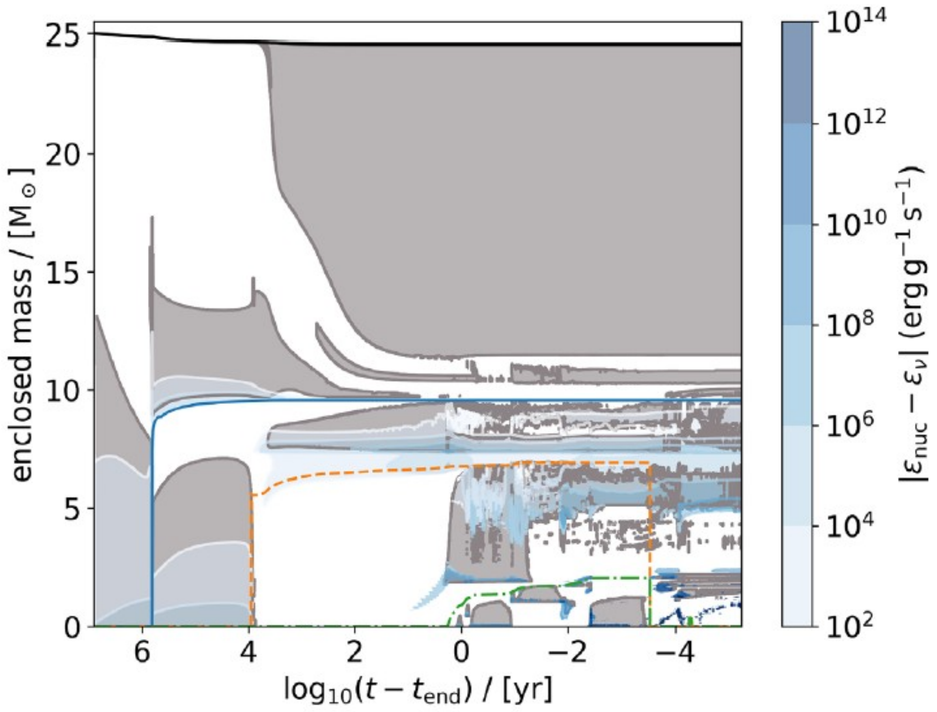
~30-50K steps

>200K steps

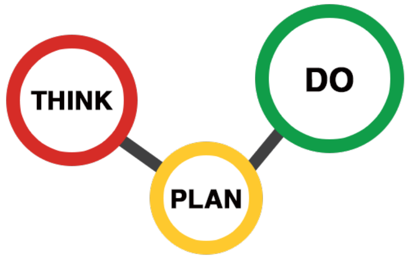
~20-25K steps

Steps for 1D stellar progenitors?

What data am I looking at? What do I need them for?



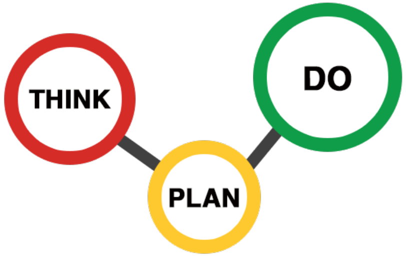
Kippenhahn diagram:
M = 25M_{sun} Z=0.02, Ritter et al. 2018 MNRAS

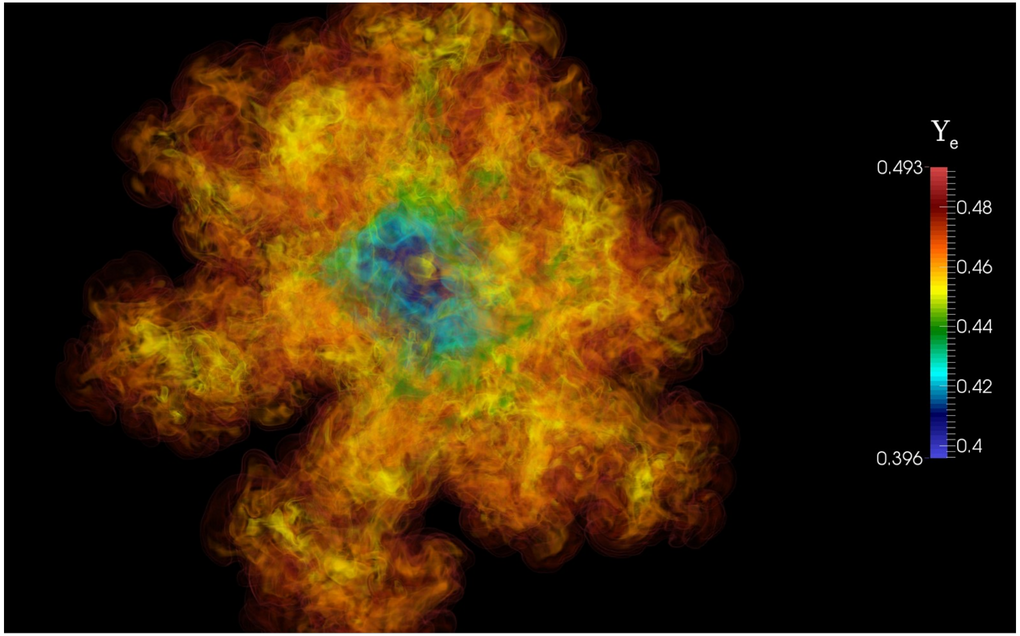


1D stellar model
about 20000 evolution steps

How many evolution steps I need to print out?
In this case from Ritter et al. 2018, 1/10 steps were printed

What data am I looking at? What do I need them for?





ECSN model, Jones et al. 2019 A&A

Hydrodynamics simulations:
2D: 10^3-10^5 trajectories
3D: > 10^6 trajectories

How many evolution steps I need to print out?
In this case (Jones et al. 2019), only the last step was printed.

Additional things to consider (data maintenance and visualization)

- Reproducibility of the results:
  - Long term data storage
  - Visualization:
    - Can you make the same plots after 3 year ?
    - Can you reproduce the same plots made 3 year ago?
- data accessibility to collaborators

Impact studies for nuclear reaction rates from experiments

- Simple approach*: stellar simulations are the same, excepting for 1 or more nuclear reaction rates, changed within uncertainties.
- A nuclear reaction rate uncertainty will have a specific impact on the stellar abundance products. The main questions to define priority and strategy are:
  - Is the simulation framework representative of what stars are doing?
  - Is this reaction more important than other rates?
  - Is there an observable or a kind of diagnostic that I can compare my simulations with?

* More complex approaches do exist, e.g., making use of MC techniques, see e.g., Iliaids+ 2011, Bertolli+ 2013, Nishimura+ 2017, Densisenkov+ 2018, Goriely+ 2021

Example: The s-process in massive stars

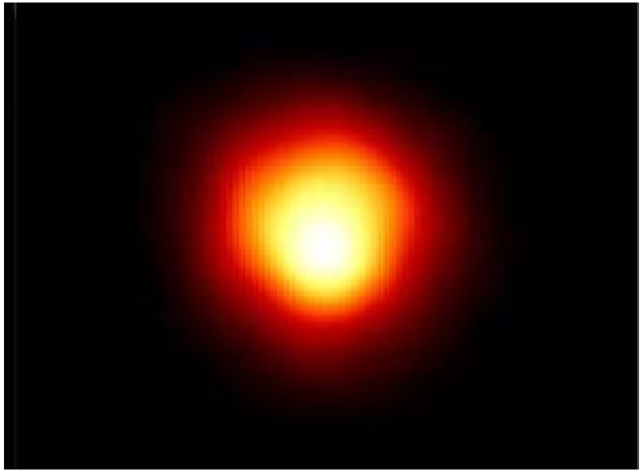


Image: A. Dupree/CFA/R. Gilliland/STScI/NASA/ESA

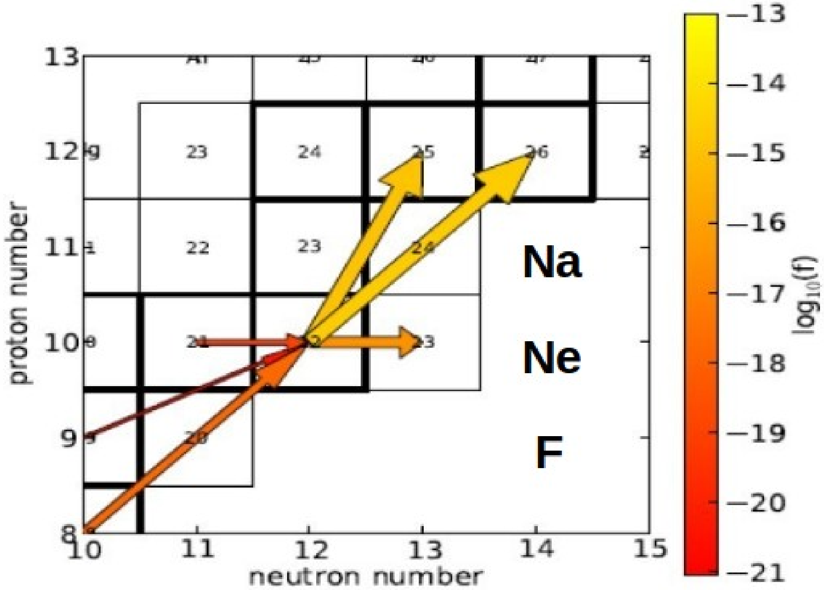
Betelgeuse (α-Ori):

~ 19 M_{sun}

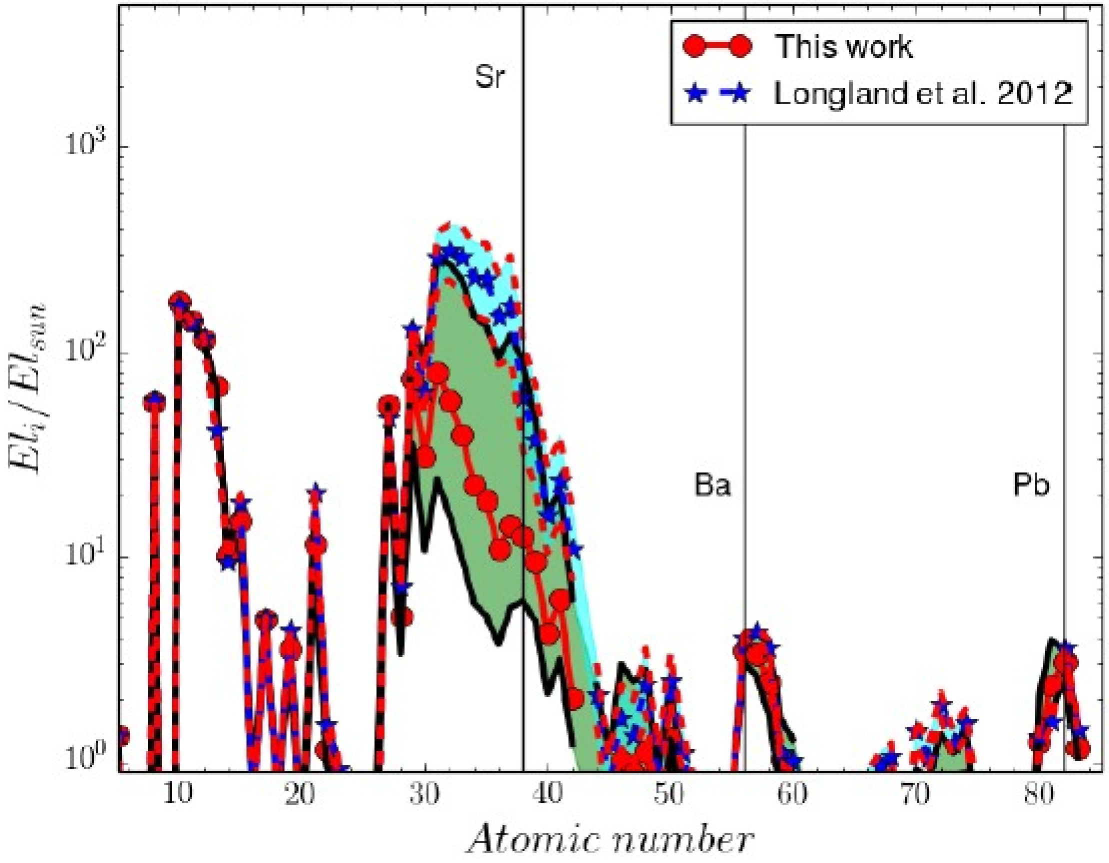
~ 650 ly

~ 1180 R_{sun}

$^{22}Ne(\alpha,n)^{25}Mg$ & $^{22}Ne(\alpha,\gamma)^{26}Mg$



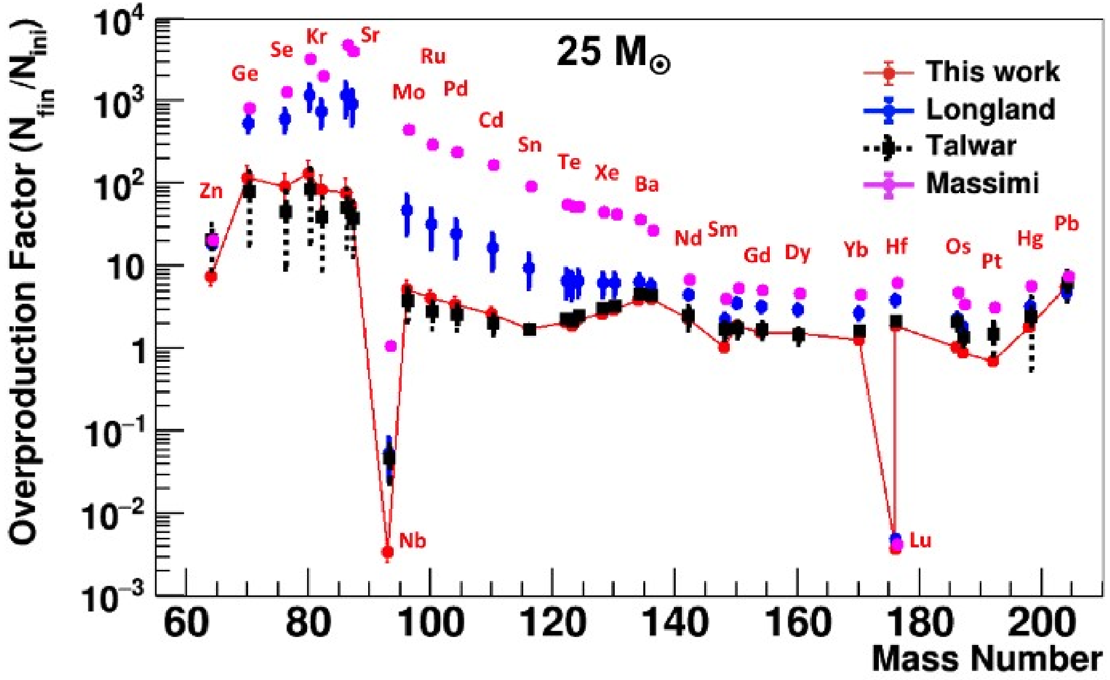
Production of fresh neutrons



Plot published in Talwar et al. 2016 Phys Rev C 93

- Trajectory for s-process extracted from a 1D massive star model (e.g., Hirschi+ 2008)

- different combinations of the $^{22}Ne+\alpha$ rates are tested (10)

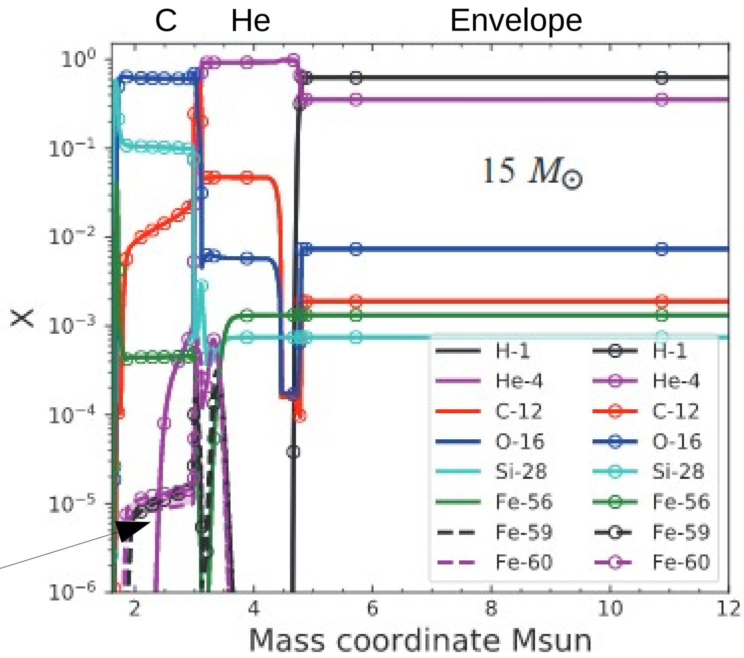


Plot published in Ota+ 2021, Phys Rev C 104

- Full model (25Msun, Z=0.02, Ritter+ 2018)

- Impact of different ^{22}Ne+α rates are tested (13)

Impact of the ^{59}Fe(n,γ)^{60}Fe: Yan+ MP, ML, 2021 ApJ 919

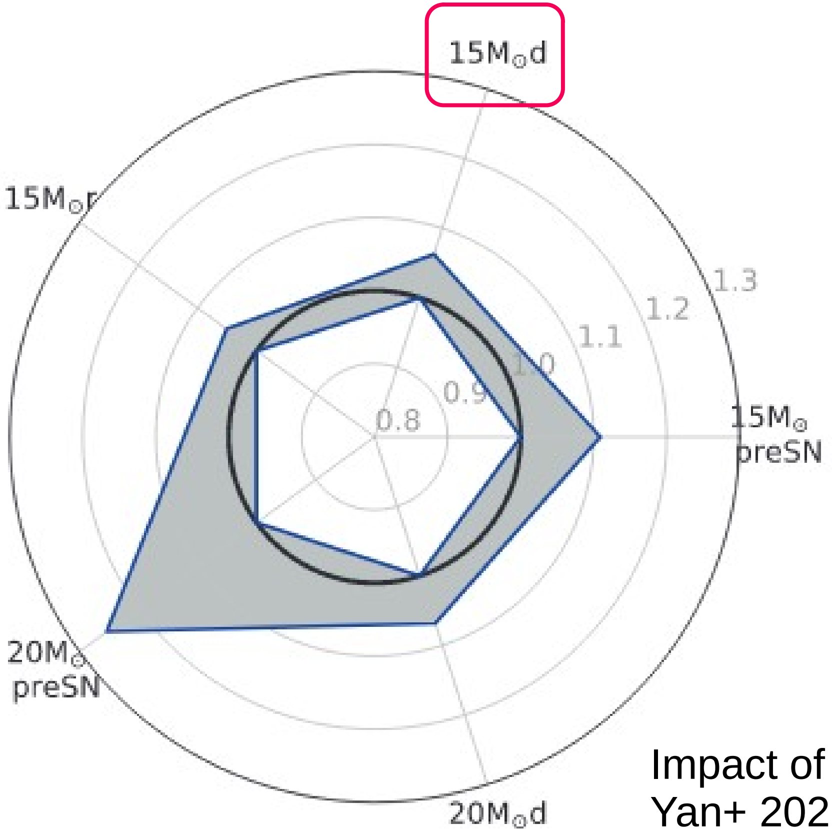


^{59}Ni 75.99 ka 87 mb, β^+	^{60}Ni 26.223 30 mb	^{61}Ni 1.14 82 mb	^{62}Ni 3.634 22.3 mb	^{63}Ni 100.11 a 31 mb, β^-
^{58}Co 70.86 d β^+	^{59}Co 100 38 mb	^{60}Co 5.27 a β^-	^{61}Co 1.65 h β^-	^{62}Co 1.50 m β^-
^{57}Fe 2.119 40 mb	^{58}Fe 0.282 12.1 mb	^{59}Fe 44.50 d β^-	^{60}Fe 1.50 Ma β^-	^{61}Fe 5.98 m β^-
^{56}Mn 2.58 h β^-	^{57}Mn 1.42 m β^-	^{58}Mn 3.00 s β^-	^{59}Mn 4.59 s β^-	^{60}Mn 51.00 s β^-
^{55}Cr 3.50 m β^-	^{56}Cr 5.94 m β^-	^{57}Cr 21.10 s β^-	^{58}Cr 7.00 s β^-	^{59}Cr 460.00 ms β^-

2 supernova models shown here.
Total of 9 complete CCSN models made for the study

Fe60 in CCSNe:
e.g., Timmes+ 1995, Limongi+2006, Tur+ 2010, Jones+ 2019

Variation of the ^{60}Fe produced, tested in 5 different models using 3 $^{59}Fe(n,\gamma)^{60}Fe$ rates.



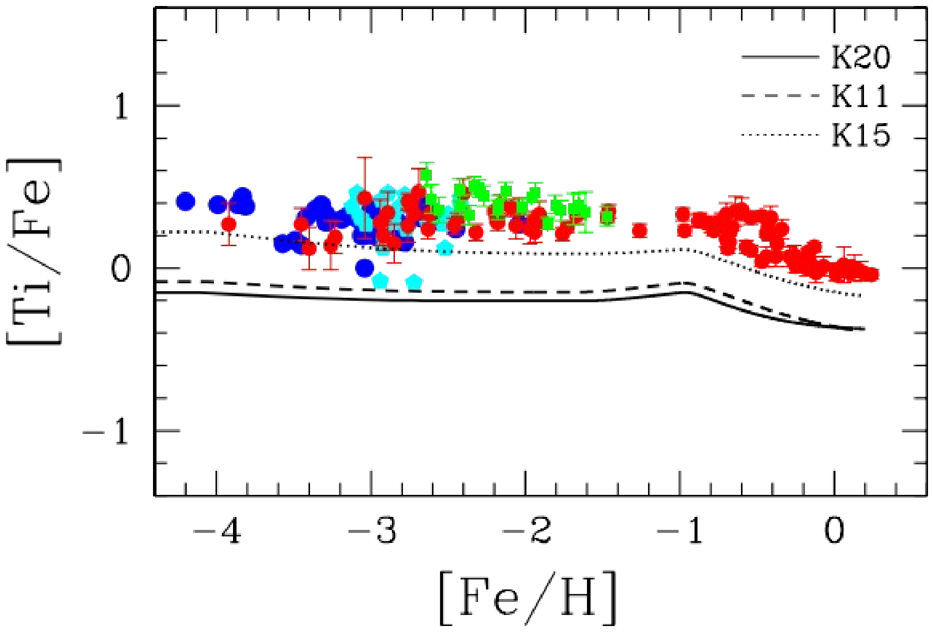
Impact of the new Fe59(n,γ)Fe60 on Fe60 yields:
Yan+ 2021, ApJ 919

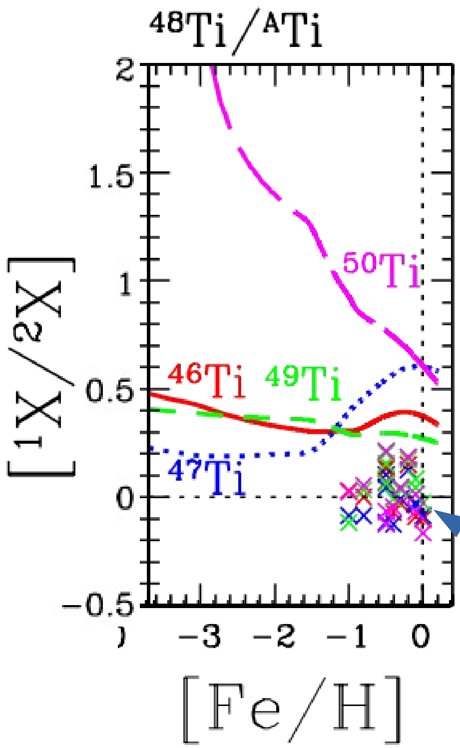
Production of elements and their isotopes in explosive conditions.

The example of Ti (Z=22)

^{45}V 547.00 ms	^{46}V 423.00 ms	^{47}V 32.60 m	^{48}V 15.97 d	^{49}V 329.05 d	^{50}V 0.25	^{51}V 99.75	^{52}V 3.74 m
^{44}Ti 59.99 a	^{45}Ti 3.08 h	^{46}Ti 8.25	^{47}Ti 7.44	^{48}Ti 73.72	^{49}Ti 5.41	^{50}Ti 5.18	^{51}Ti 5.76 m
^{43}Sc 3.89 h	^{44}Sc 3.97 h	^{45}Sc 100	^{46}Sc 83.79 d	^{47}Sc 3.35 d	^{48}Sc 1.82 d	^{49}Sc 57.20 m	^{50}Sc 1.71 m

Ti in summary (today..)

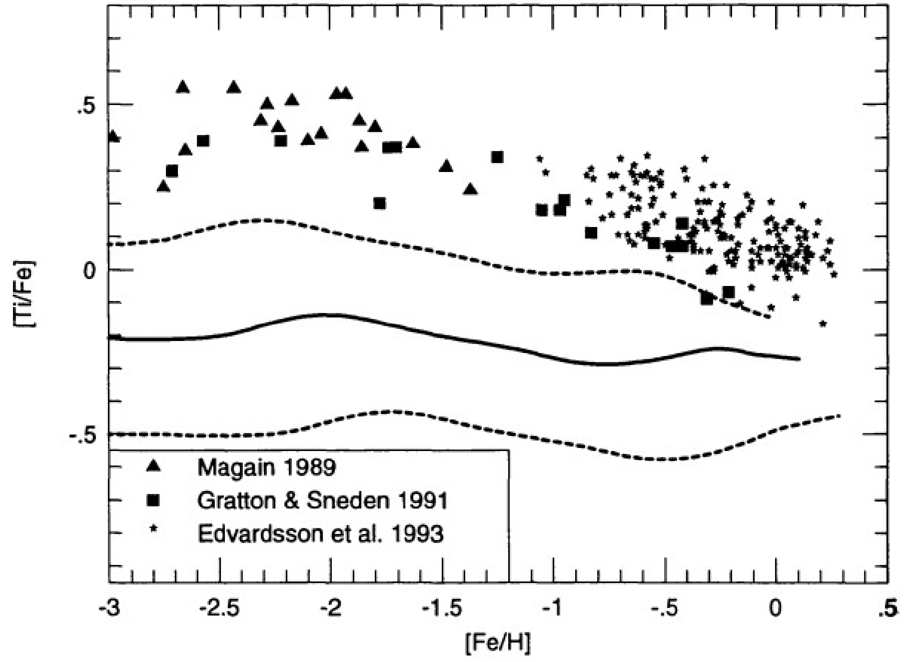


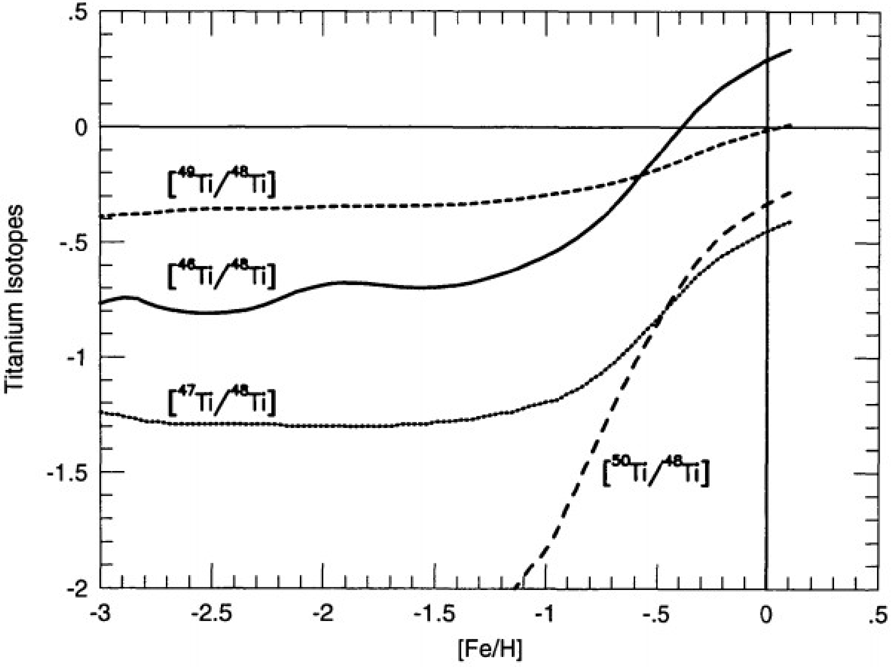


Chavez & Lambert 2009

Kobayashi+ 2020 ApJ

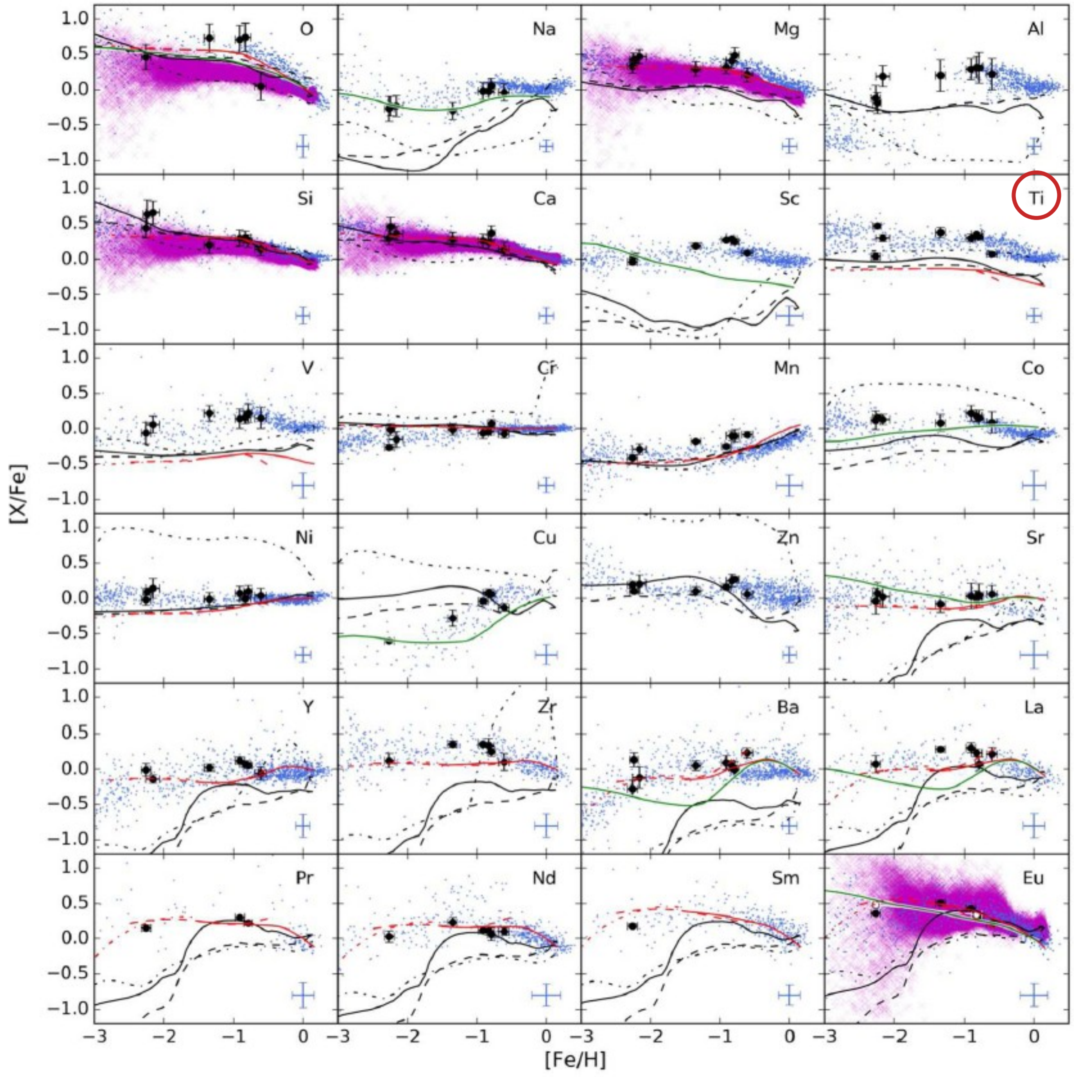
.. and back in 1995





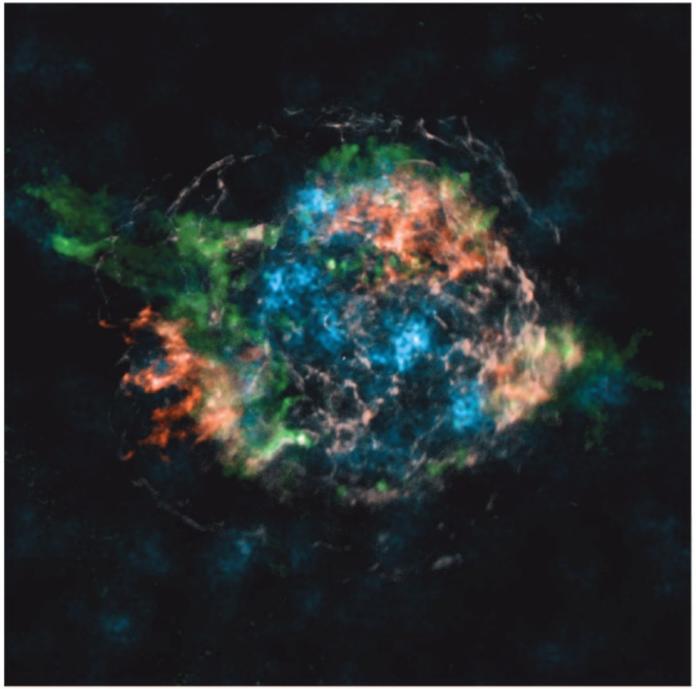
Timmes+ 1995 ApJS

Comparing results from 3 different GCE codes: OMEGA (Cote+ 2017), GeTOOL (Hughes+ 2008) and by Bisterzo+ 2014.
The problem does not go away. Mishenina+ 2017, MNRAS



Ti in summary: there is also Ti44

CCSN remnant



Grefenstette+ 2014, Nature
(NuSTAR data)

Cas A
11000 ly
~ 300 years ago

Red shows Fe
Blue is Ti
Green is Si

Ti44 production in CCSNe -
Some references:
Chieffi & Limongi 2017 ApJ
Wongwathanarat+ 2017 ApJ
Magkotsios+ 2010 ApJS

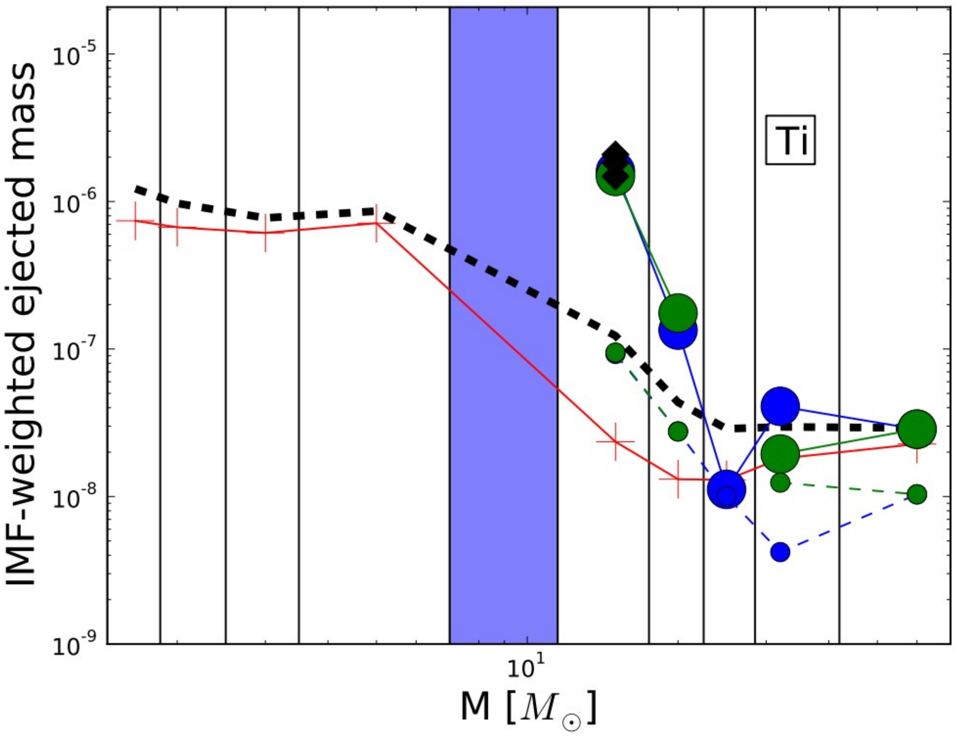
A&A 450, 1037–1050 (2006)
DOI: 10.1051/0004-6361:20054626

Astronomy & Astrophysics

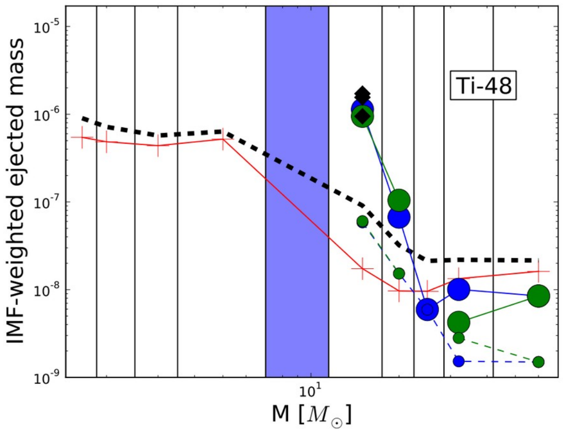
Are ^{44}Ti-producing supernovae exceptional?★

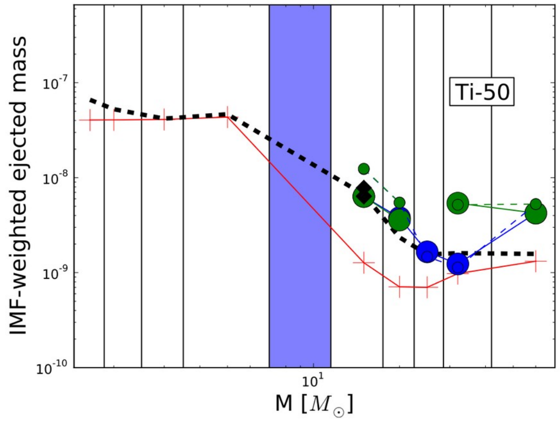
L.-S. The[1], D. D. Clayton[1], R. Diehl[2], D. H. Hartmann[1], A. F. Iyudin[2,3], M. D. Leising[1], B. S. Meyer[1], Y. Motizuki[4], and V. Schönfelder[2]

What stars make Ti? CCSNe



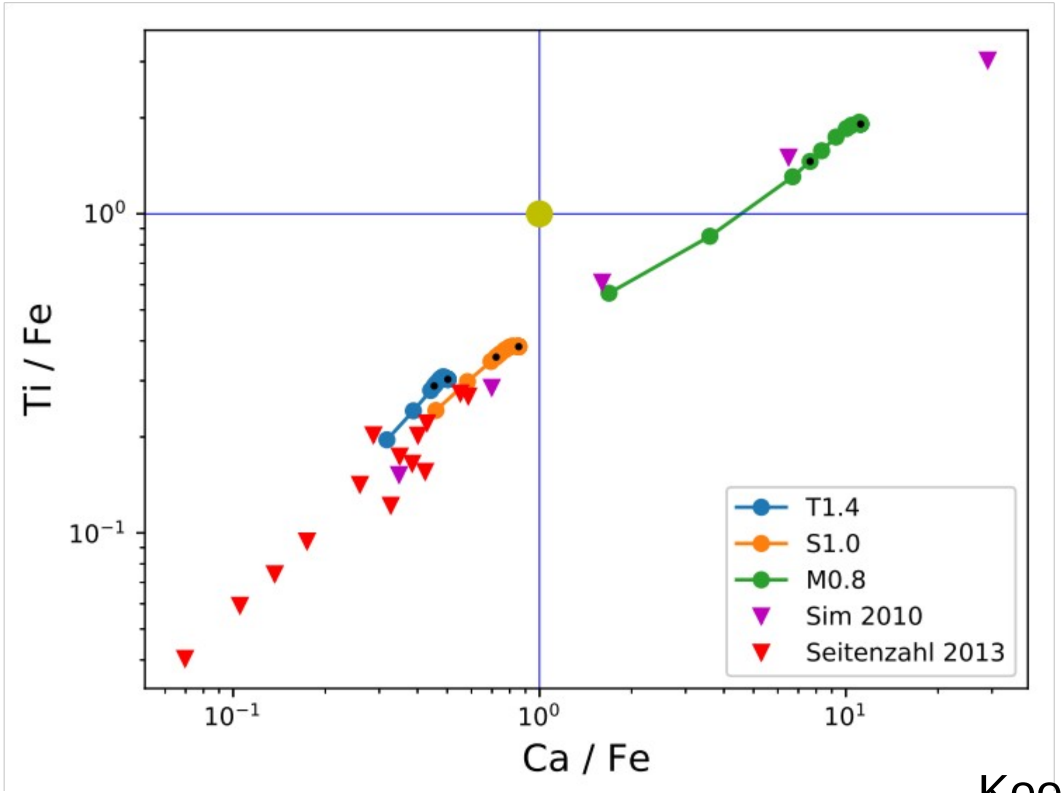
Ti ≈ Ti48





Pignatari+ 2016, ApJS

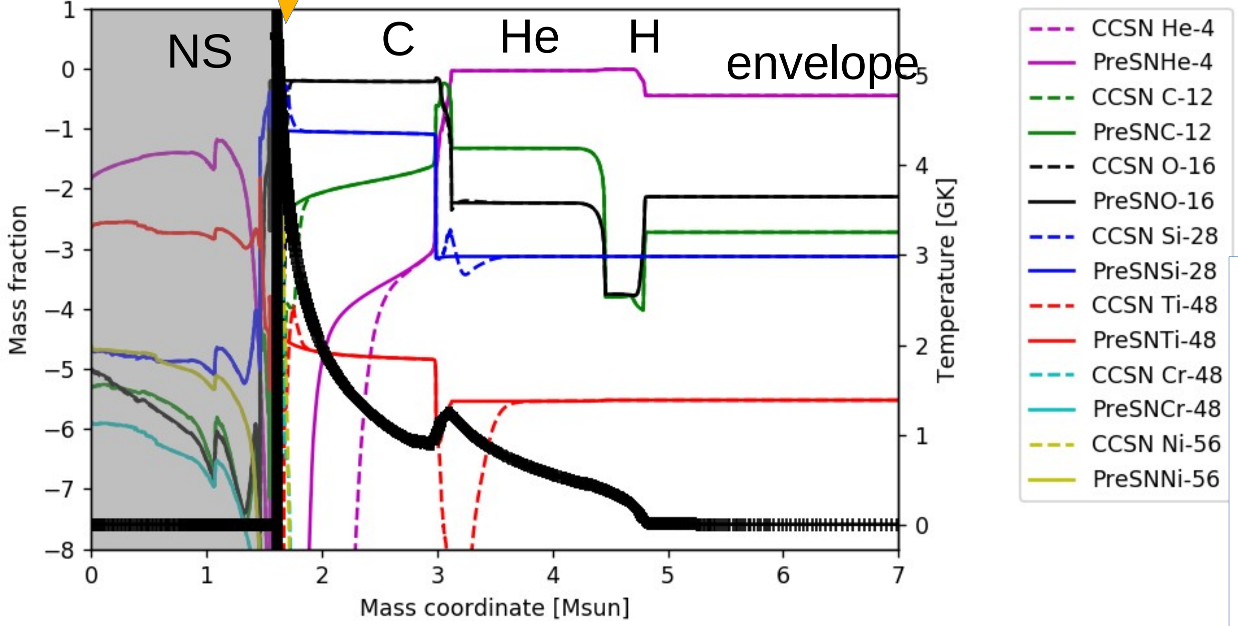
What stars make Ti? SNIa

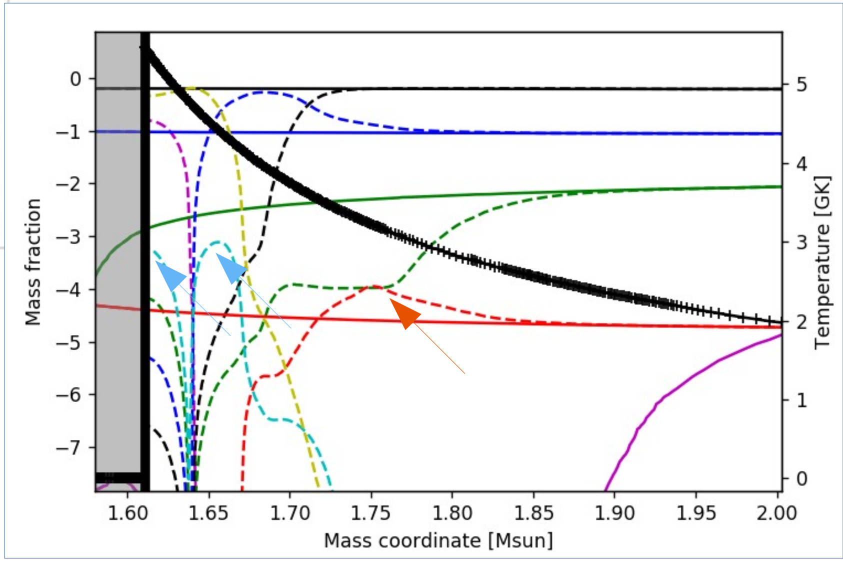


Keegans et al. 2022, in prep.

CCSNe: Ti~Ti48

O-, Si-..

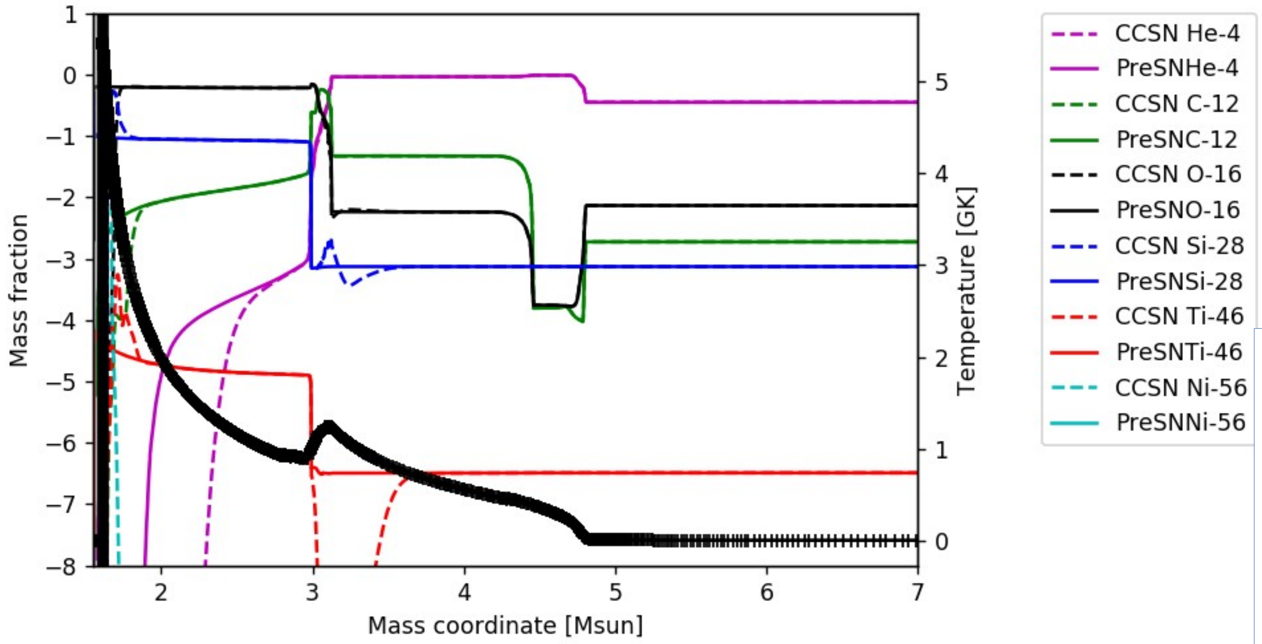




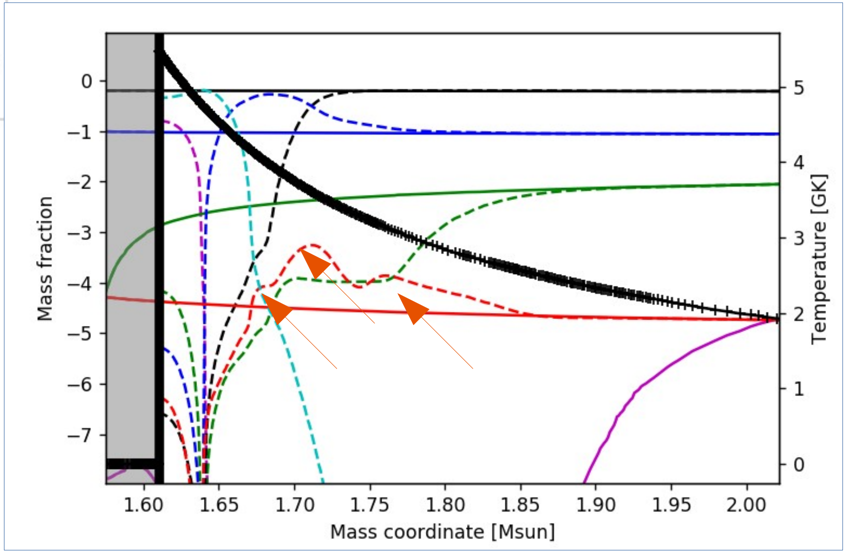
M=15Msun, Z=0.02

Ritter+ 2018 MNRAS

Ti48 vs Ti46

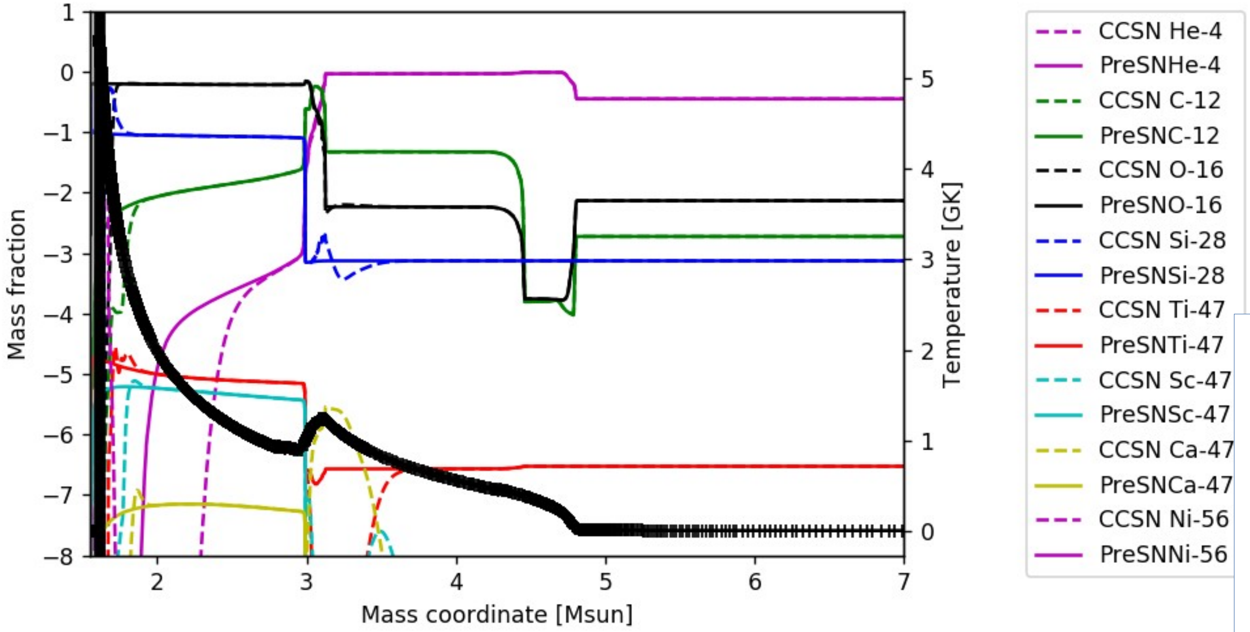


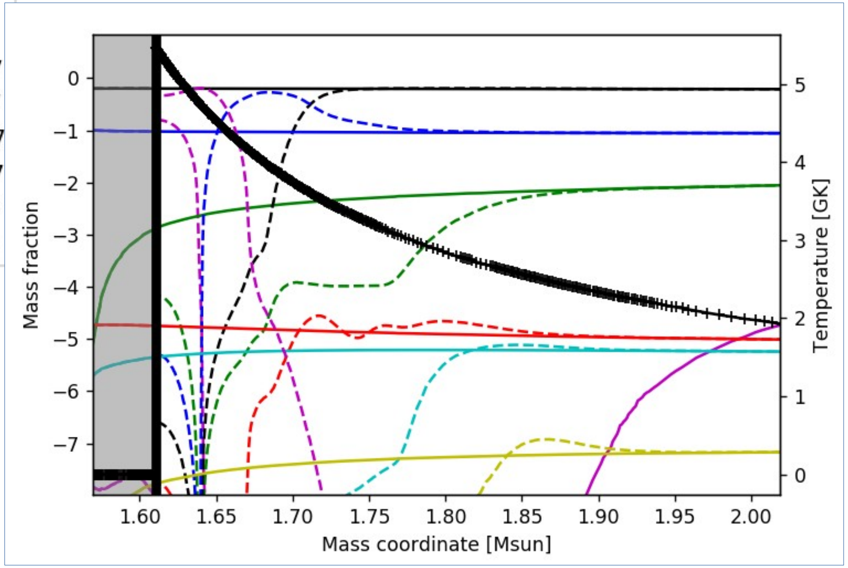
Can we select single stellar trajectories to study the production of Ti46/Ti48 in CCSNe?



M=15Msun, Z=0.02
Ritter+ 2018 MNRAS

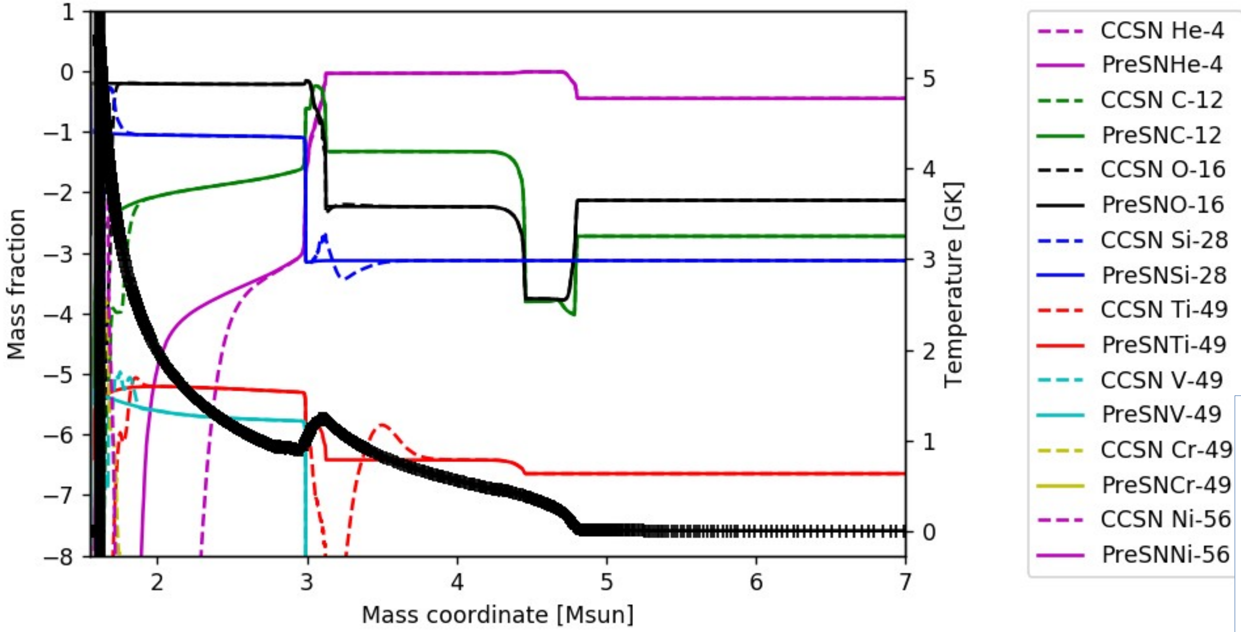
Ti48 vs Ti47

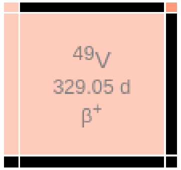




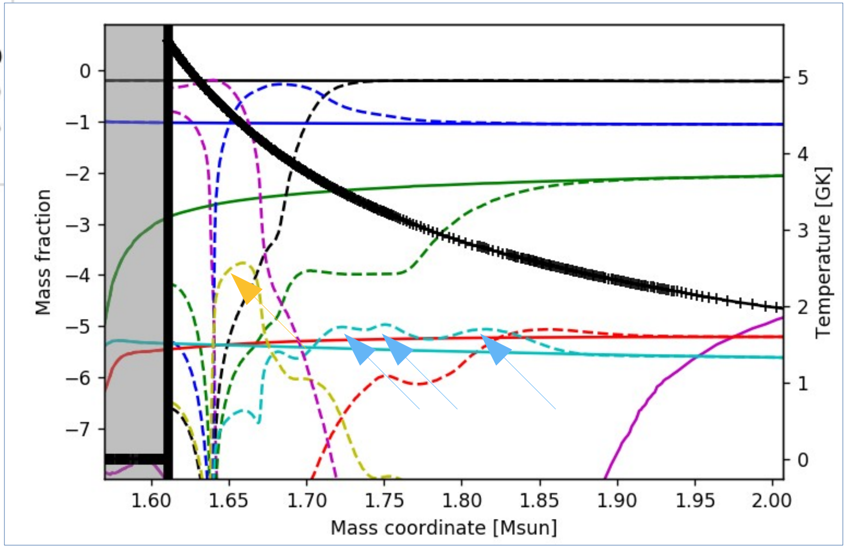
M=15Msun, Z=0.02
Ritter+ 2018 MNRAS

Ti48 vs Ti49



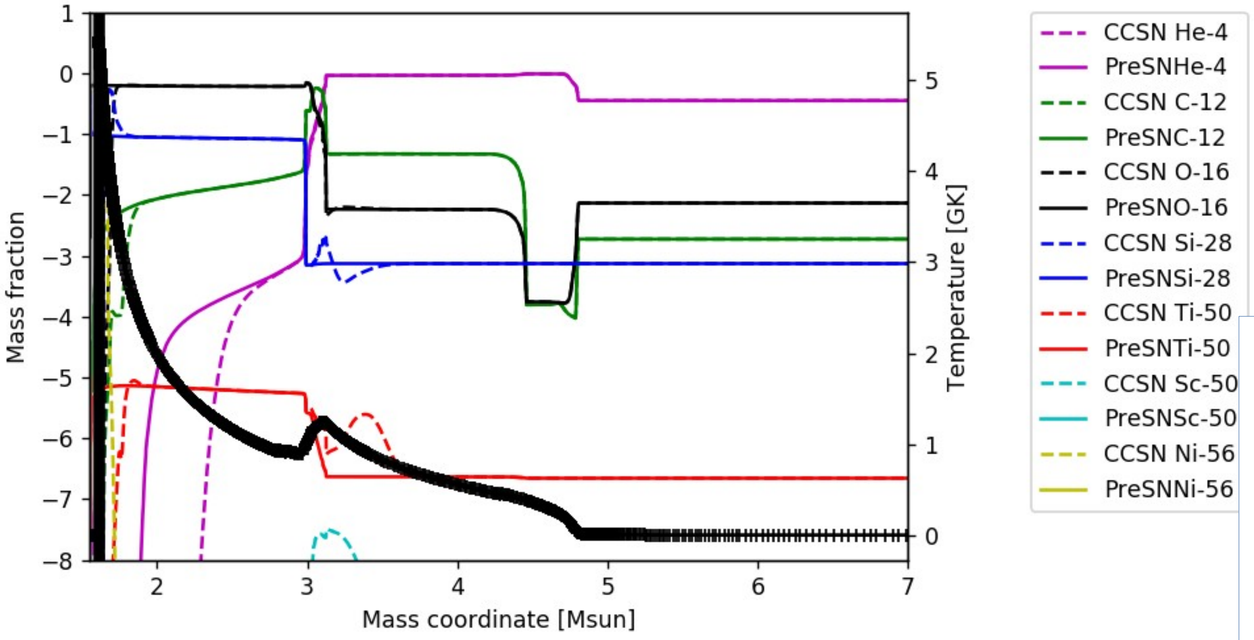


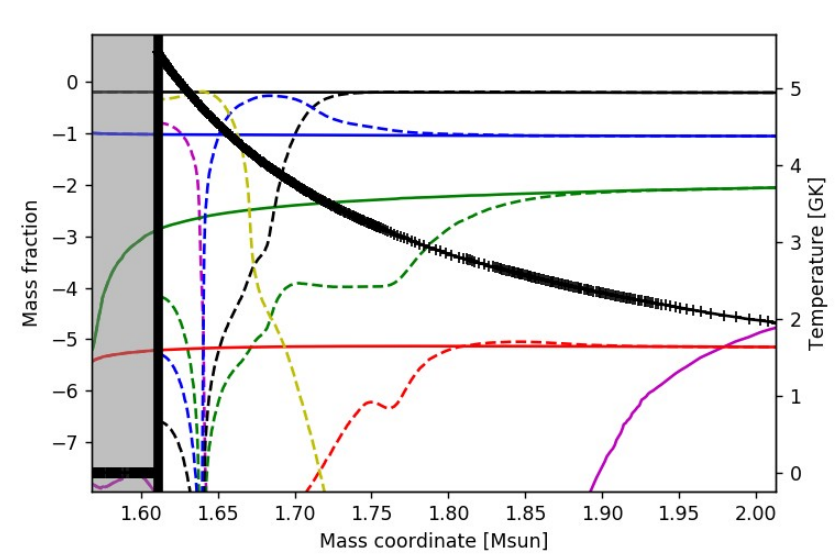
...another interesting radiactive isotope: V49



M=15Msun, Z=0.02
Ritter+ 2018 MNRAS

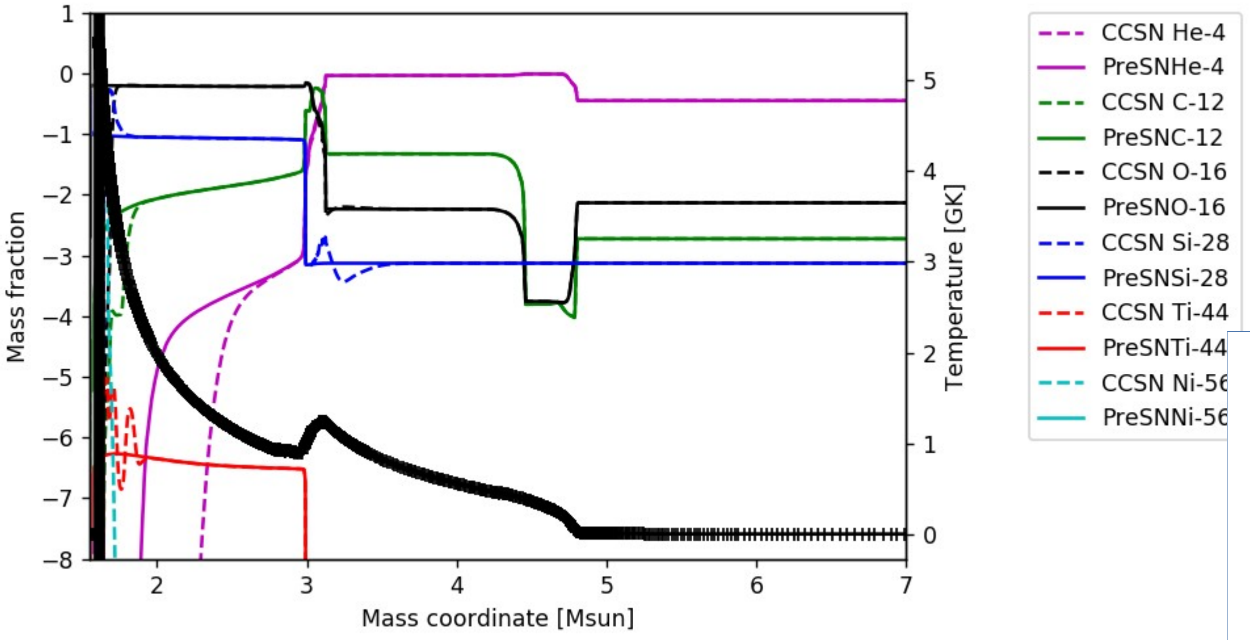
Ti48 vs Ti50

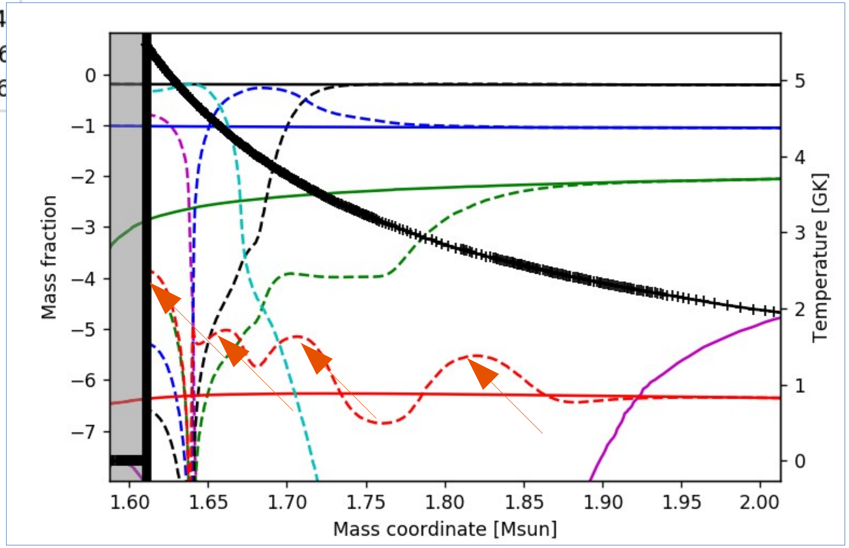




M=15Msun, Z=0.02
Ritter+ 2018 MNRAS

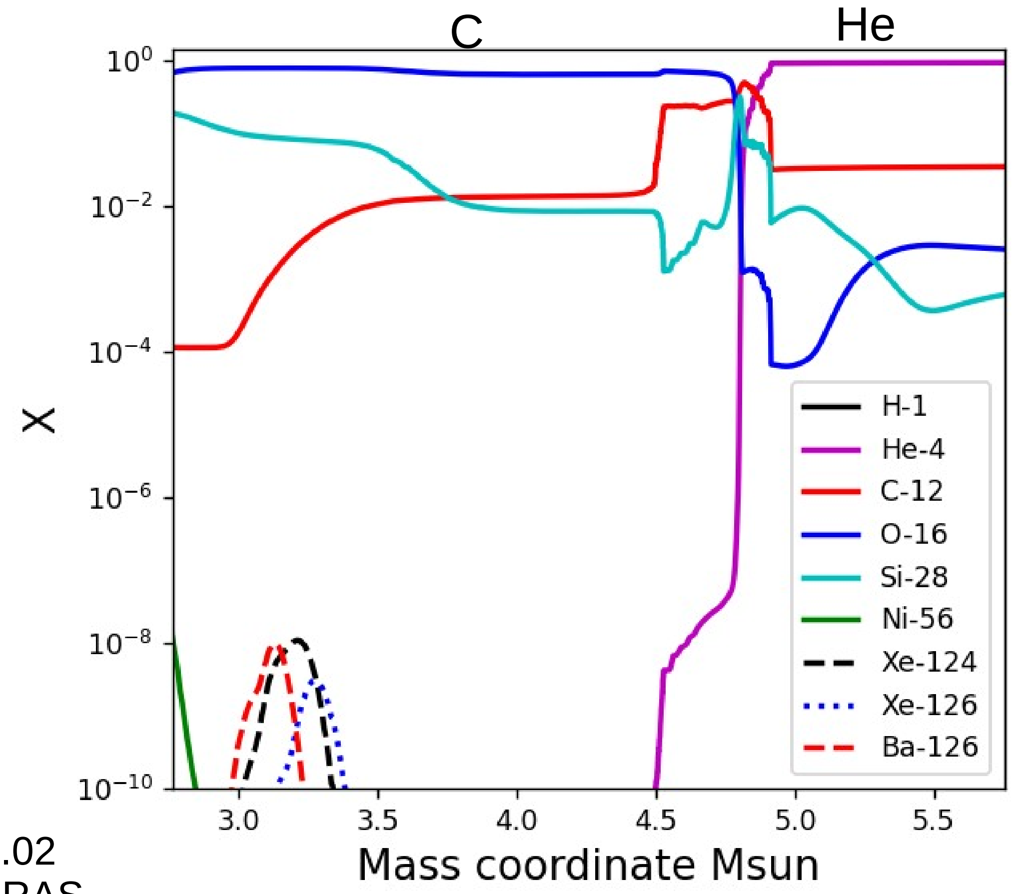
… and Ti44





M=15Msun, Z=0.02
Ritter+ 2018 MNRAS

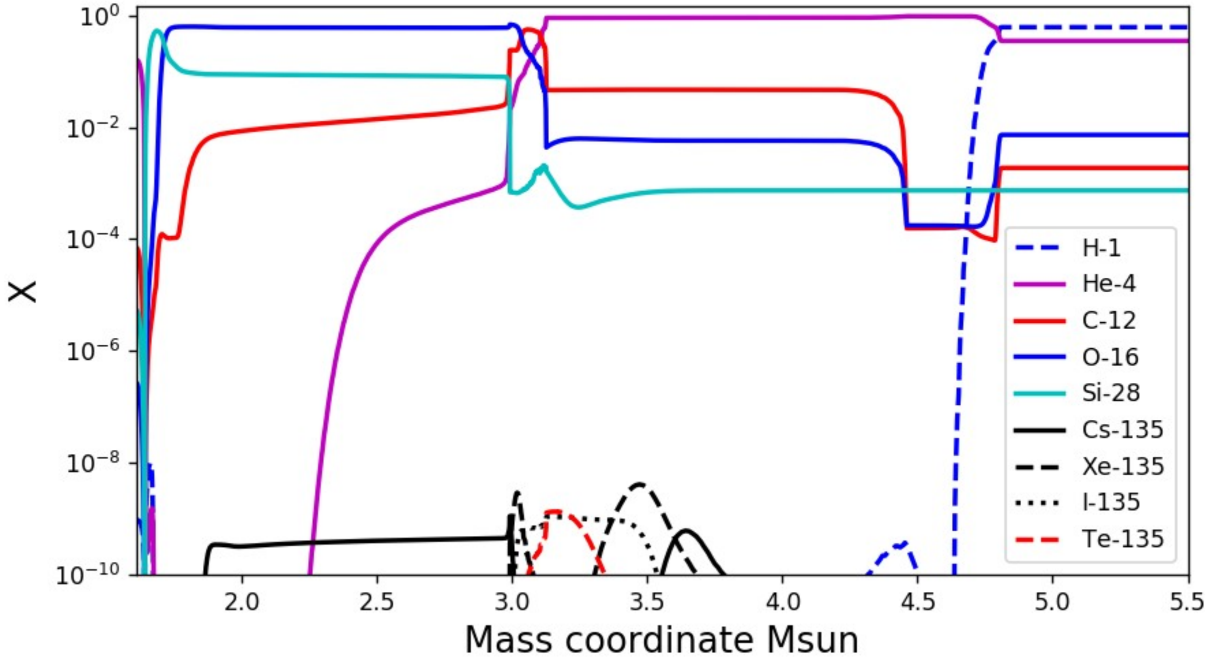
Other examples: ^{124}Xe and ^{126}Xe production by the γ-process



The γ-process in CCSNe:
- Arnould & Goriely 2003 Phys Rep
- Rauscher+ 2013 RPP
- Pignatari+ 2016 IJMPE

M=20Msun, Z=0.02
Ritter+ 2018 MNRAS

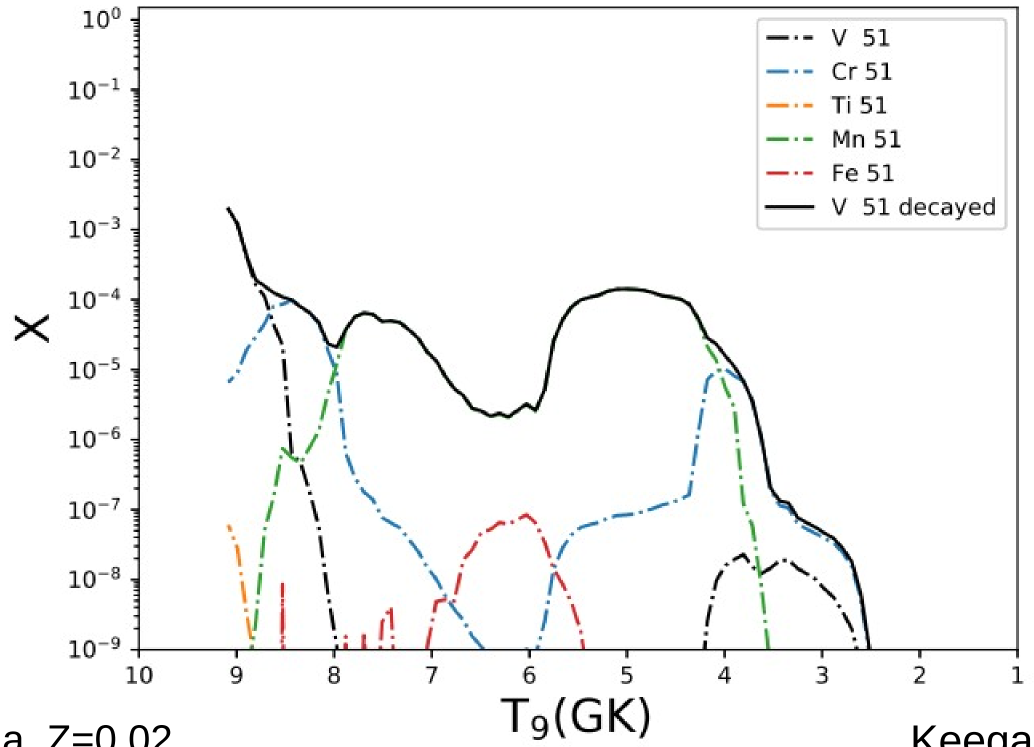
Neutron burst driven by the ^{22}Ne(α,n) in explosive He-burning: ^{135}Cs



The n-process in CCSNe:
- Blake & Schramm 1976 ApJ
- Meyer+ 2000 ApJ
- Pignatari+ 2018 GeCoA

M=15Msun, Z=0.02
Ritter+2018 MNRAS
MESA progenitor
Fryer+12 explosion

Production of V in SNIa: ^{51}V

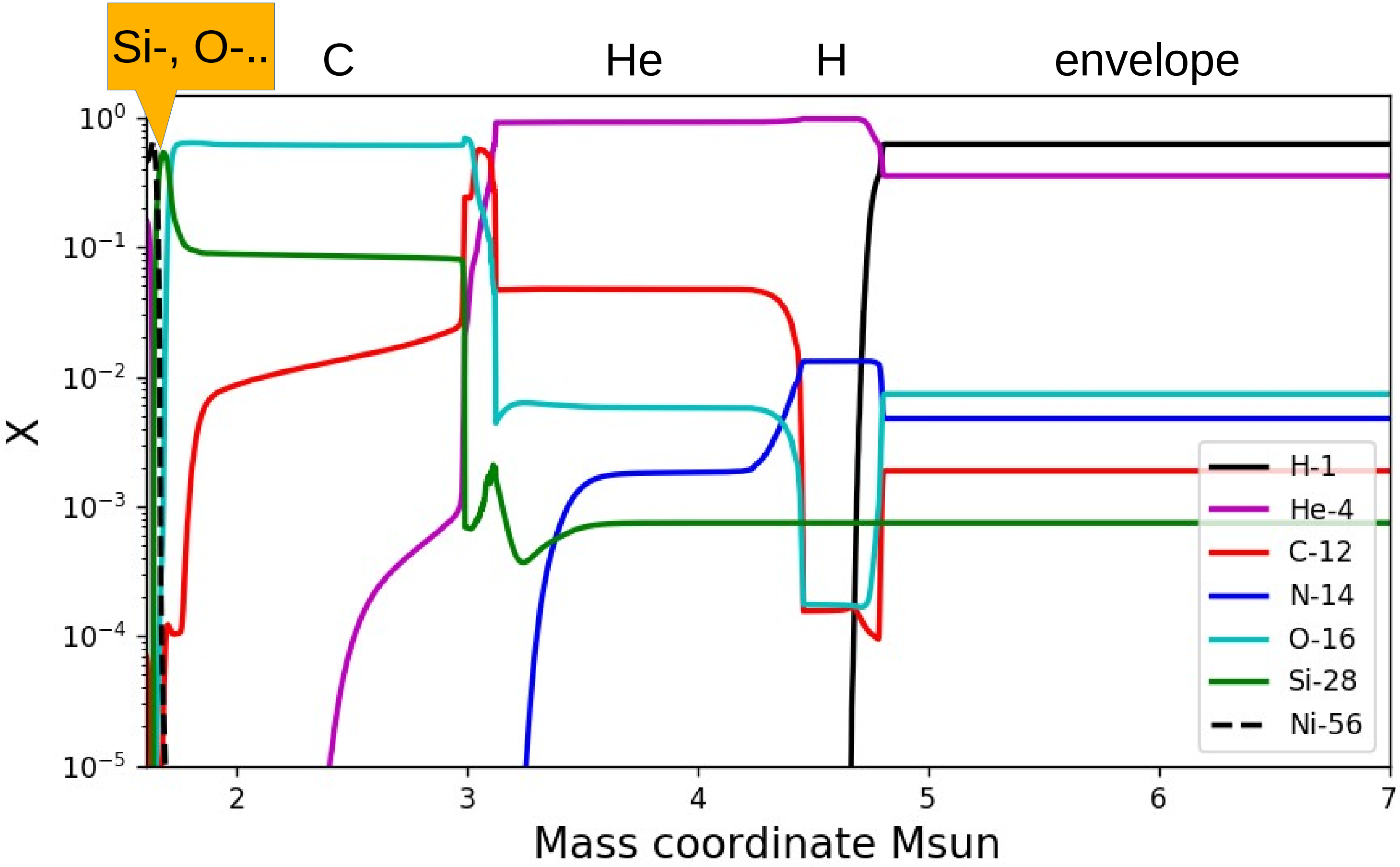


SNIa nucleosynthesis:
- Thielemann & Nomoto 1986
- Timmes+ 2003 ApJ
- Hillebrandt+ 2013 FrPhy

SD, Ch mass SN Type Ia, Z=0.02
Model by Townsley+ 2016 ApJS
Yields by Keegans+ 2022 in prep.

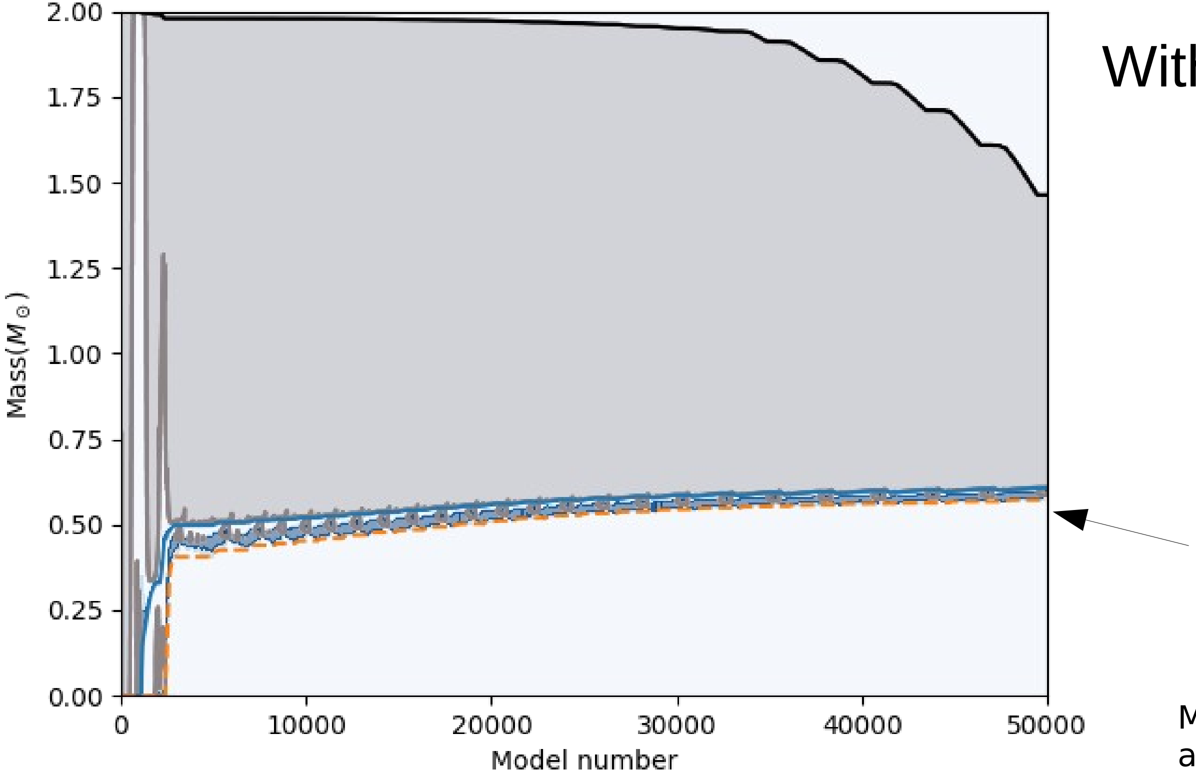
Keegans 2021, PhD thesis

Before studying the production of the elements in your laptop, you need to know where to look. :)



M=15Msun, Z=0.02
Ritter+2018 MNRAS
MESA progenitor
Fryer+12 explosion

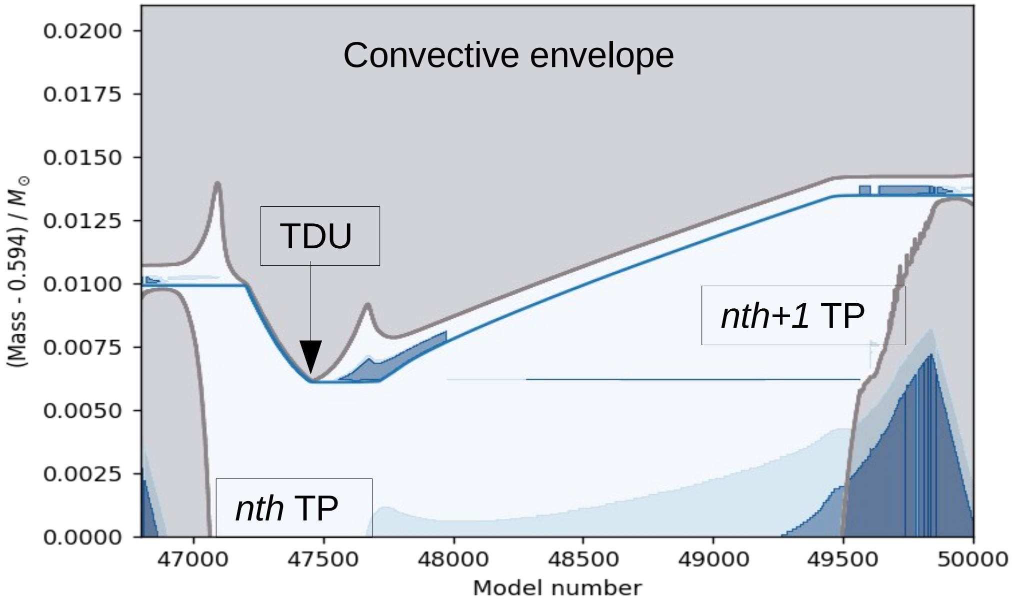
A good example: AGB stars



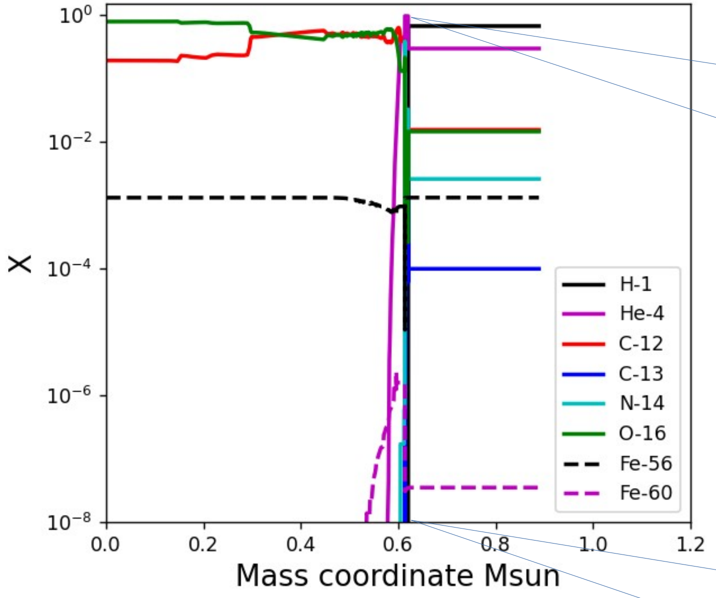
Without zooming...

M=2Msun, from MS to AGB
astrolab, @UVIC
Set1ext, Ritter+2018 MNRAS.
data.nugridstars.org

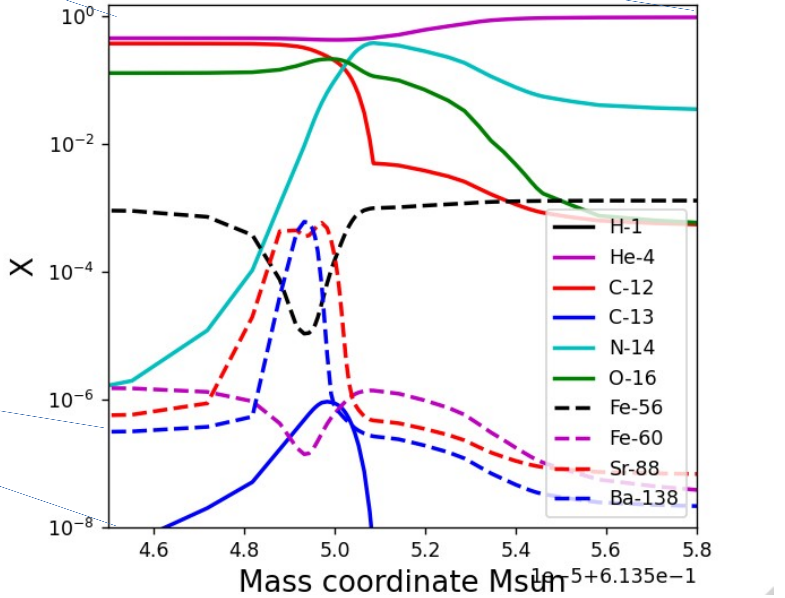
Zooming in the stellar structure: the Third Dredge-Up (TDU)



M=2Msun, TDU event
astrolab, @UVIC
Set1ext, Ritter+2018 MNRAS.
data.nugridstars.org



M=2Msun
Ritter+2018 MNRAS.
data.nugridstars.org

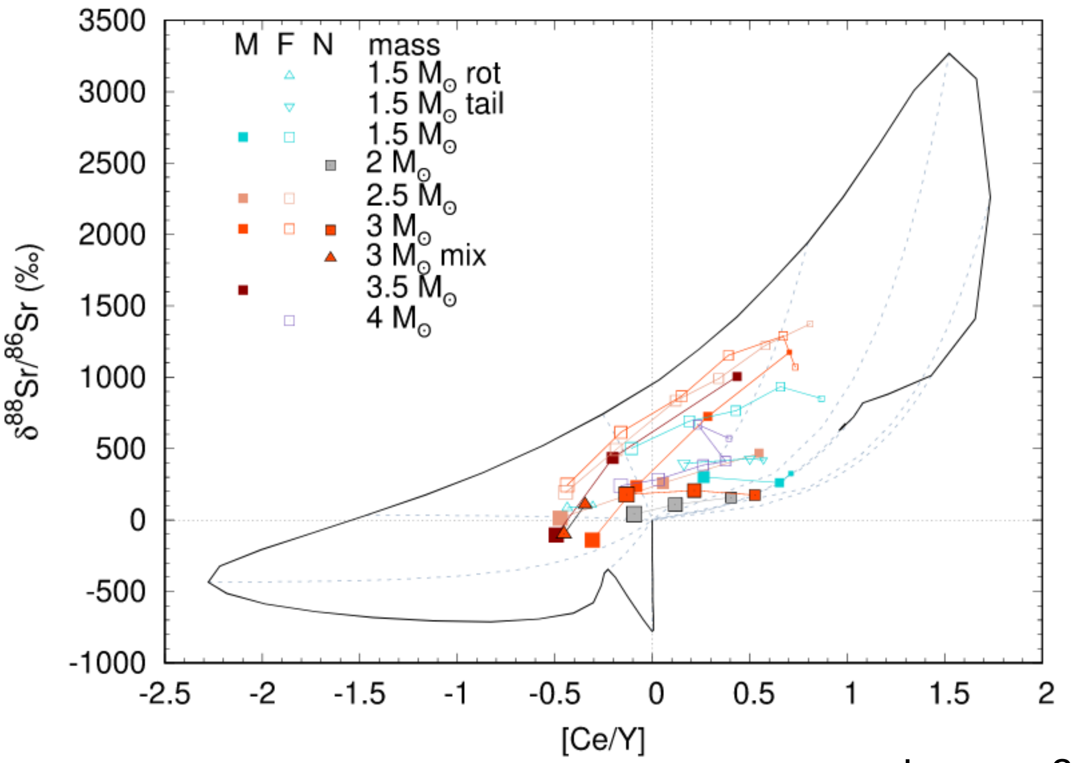


<u>What is(are) the physics mechanism(s) driving the formation of the 13C-pocket?</u>

Straniero+ 1995, Herwig+ 1997, Cristallo+2001, Denissenkov&Tout 2003, Lugaro+ 2003, Goriely&Siess 2004, Busso+2007, Straniero+ 2009, Cristallo+ 2009…. Not clear yet.

$^{12}C(p,\gamma)^{13}N(\beta+)^{13}C(\alpha,n)^{16}O$
$\sim 10^{7}$ n/cm^{3}
~ 95% of the all neutron exposure

Some of the abundance signatures are defined by basic properties: simplified models can be used (but carefully!)



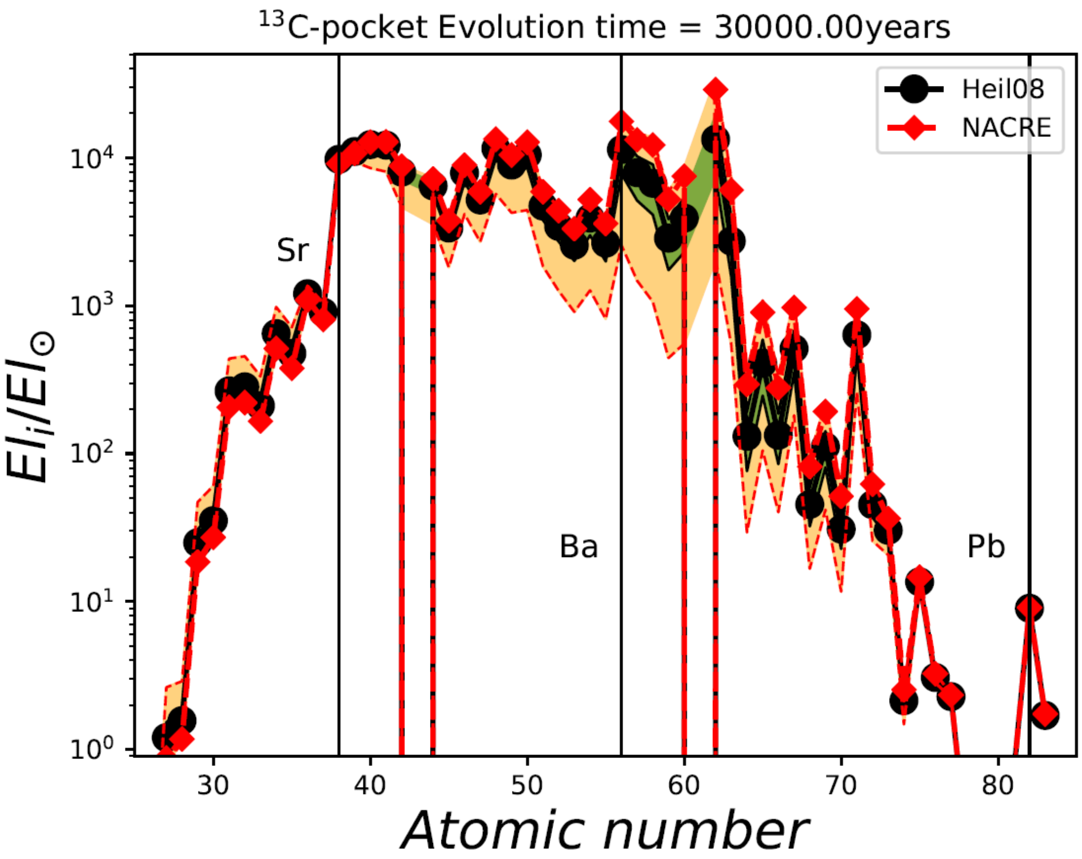
Lugaro+2020 ApJ 898

Simple impact study for the reaction $^{13}C(\alpha,n)^{16}O$

Analysis within the context of an international collaboration: ChETEC (http://www.chetec.eu/)

Relevance: main neutron source for the s-process in low-mass stars

This impact study can be quickly done in a laptop.



However, see Ciani+ 2021 PRL

Conclusions

- Making the elements in your computer or in your laptop: the simulation and visualization setup needs to be defined to study the problem in the right way.
- Impact of nuclear reaction rates on nucleosynthesis:
  - Approximations and simplifications can be made, but often full models are needed.
  - Examples: ^{22}Ne+α and of ^{59}Fe(n,γ)^{60}Fe impact.
- Producing abundances in stars:
  - The complexity of stellar sources often does not allow to get something useful from simple approaches. See the example of Ti and other products of explosive nucleosynthesis in CCSNe and SNIa.
  - But in certain cases we can! See an example from AGB stars and the impact of the ^{13}C(α,n)^{16}O.
- **ChETEC-INFRA: production of a public stellar library for nuclear sensitivity and uncertainty studies with specific guidelines: in progress.**
  The can-do and the cannot-do will be provided.

www.irenaweb.org

IReNA

www.jinaweb.org

JINA-CEE

NUGRID

www.nugridstars.org

CHETEC INFRA

www.chetec-infra.eu

Thanks!

...

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IReNA is a National Science Foundation AccelNet Network of Networks