

Parameter study of r-process lanthanide production and heating rates in kilonovae with SkyNet

arXiv:1508.03133

Jonas Lippuner

Luke Roberts

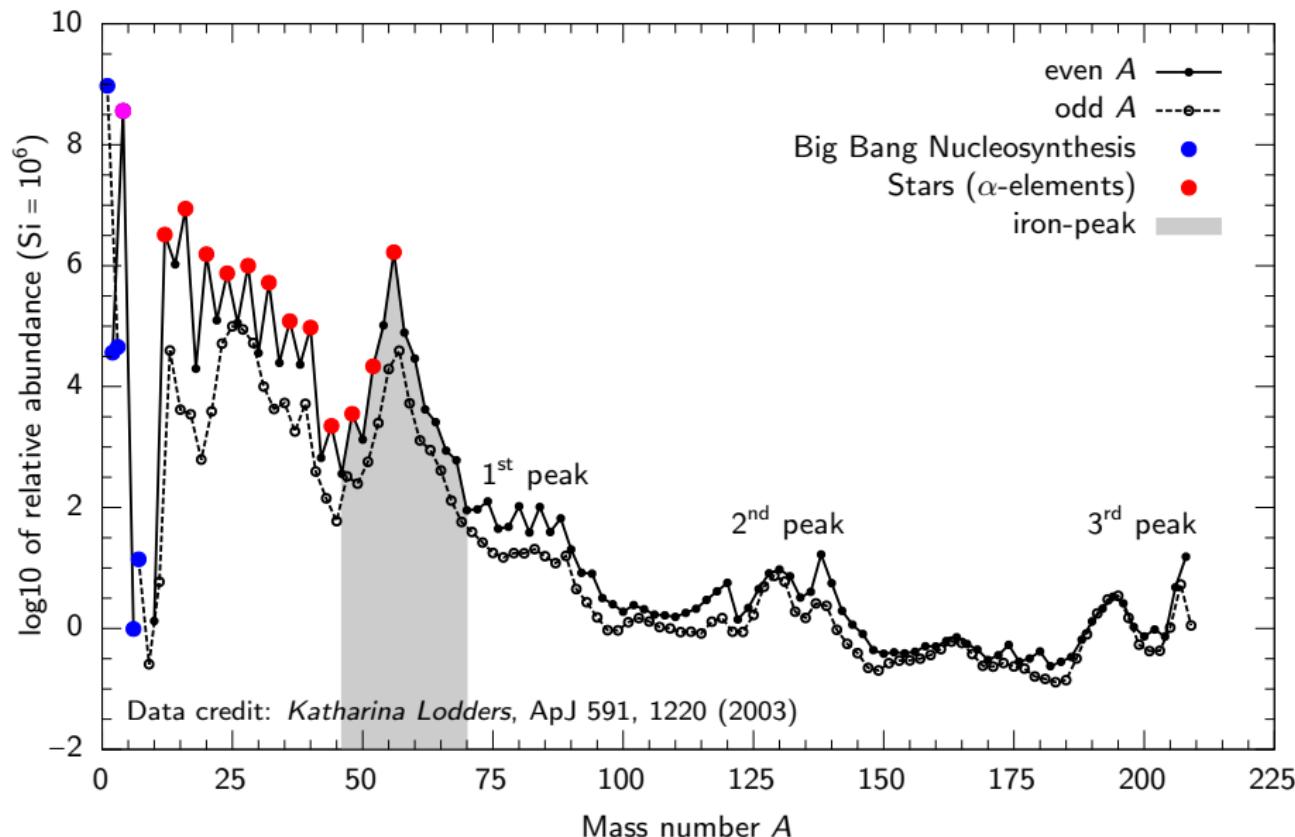
Caltech

MICRA 2015

Stockholm, August 17 – 21, 2105

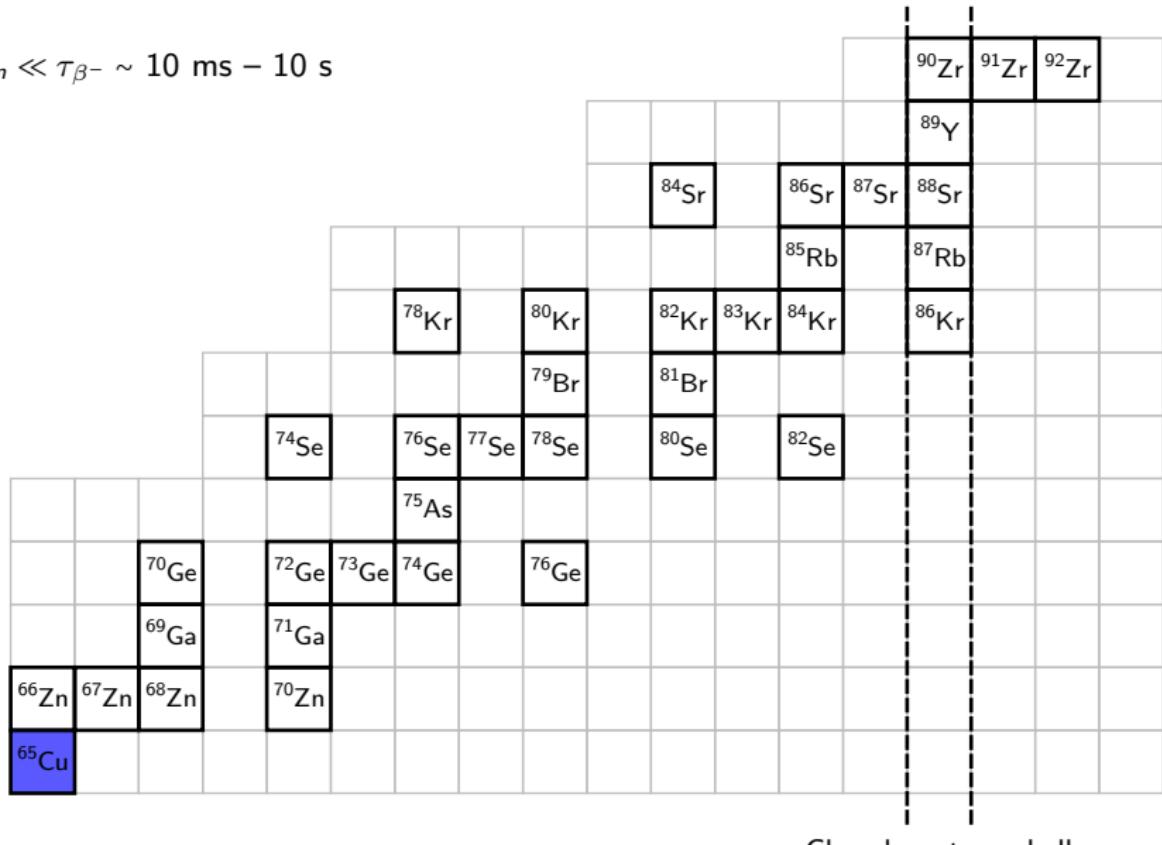
Solar System Abundances

Caltech



The r-process

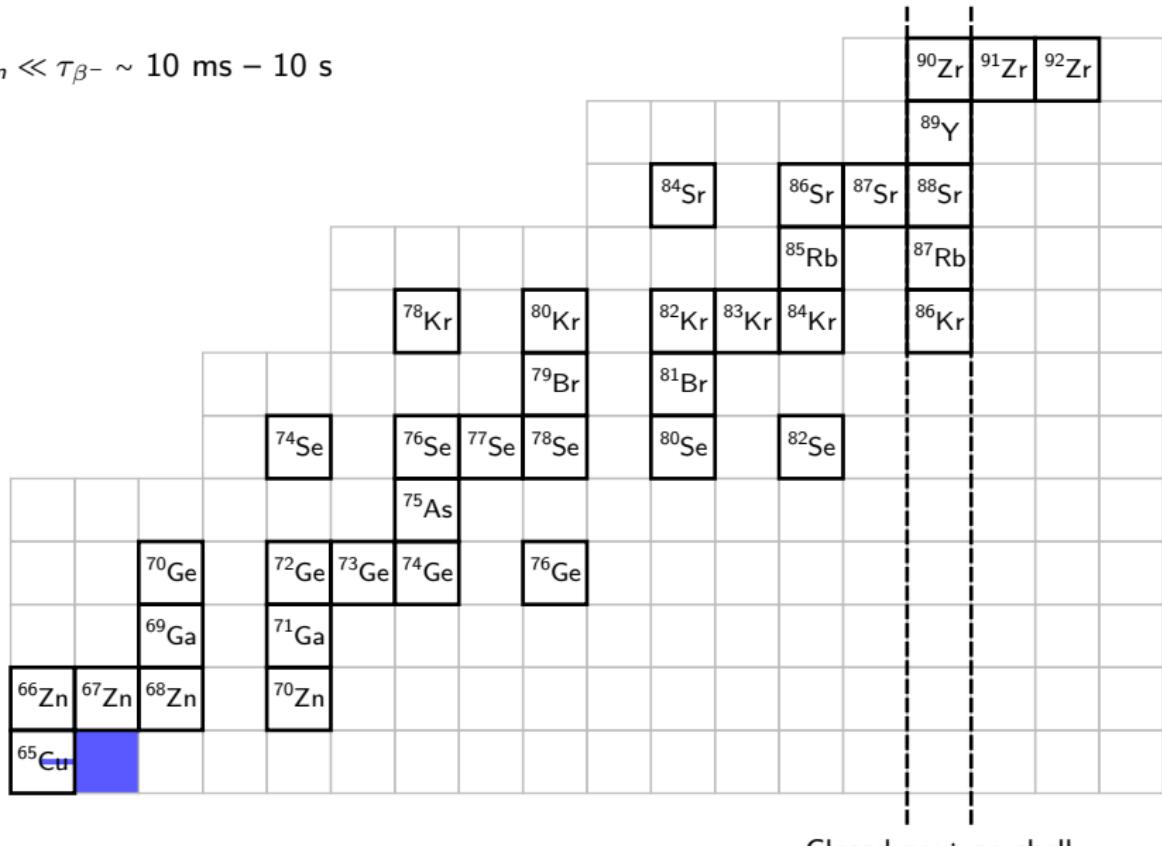
$\tau_n \ll \tau_{\beta^-} \sim 10 \text{ ms} - 10 \text{ s}$



Closed neutron shell

The r-process

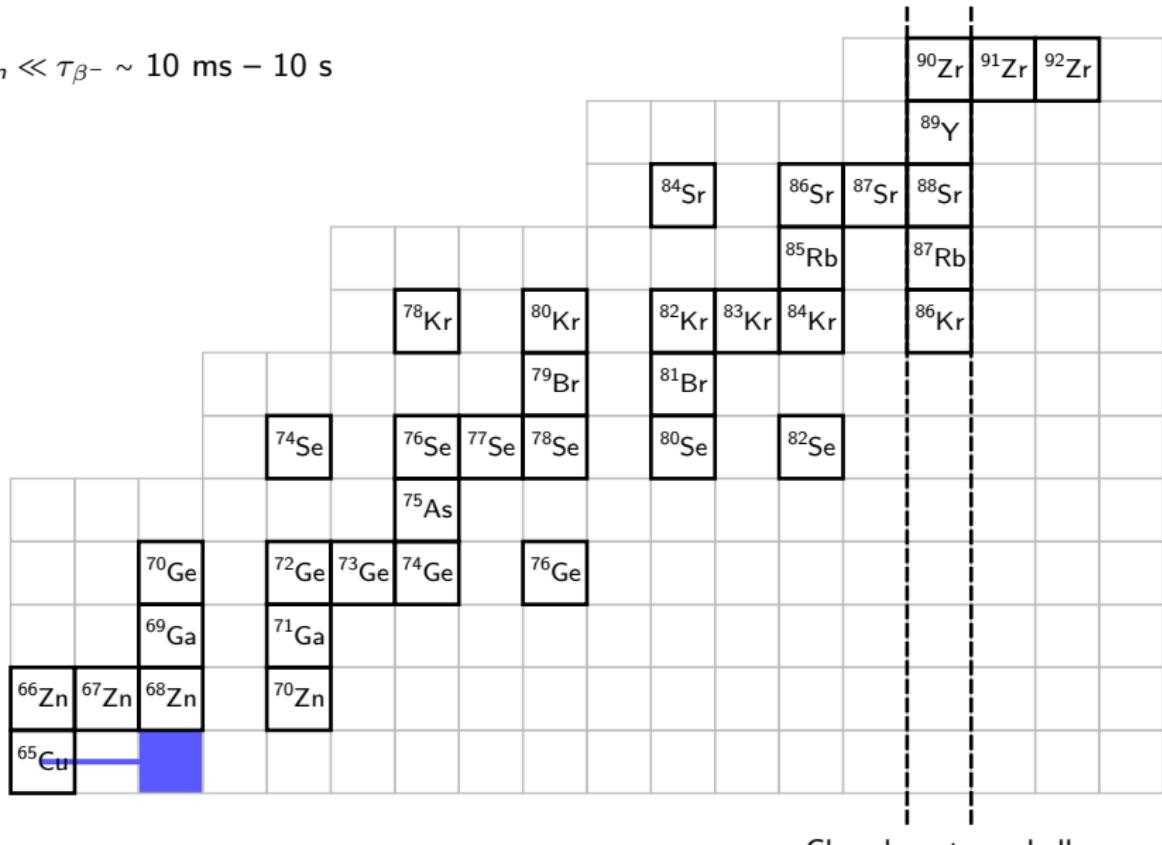
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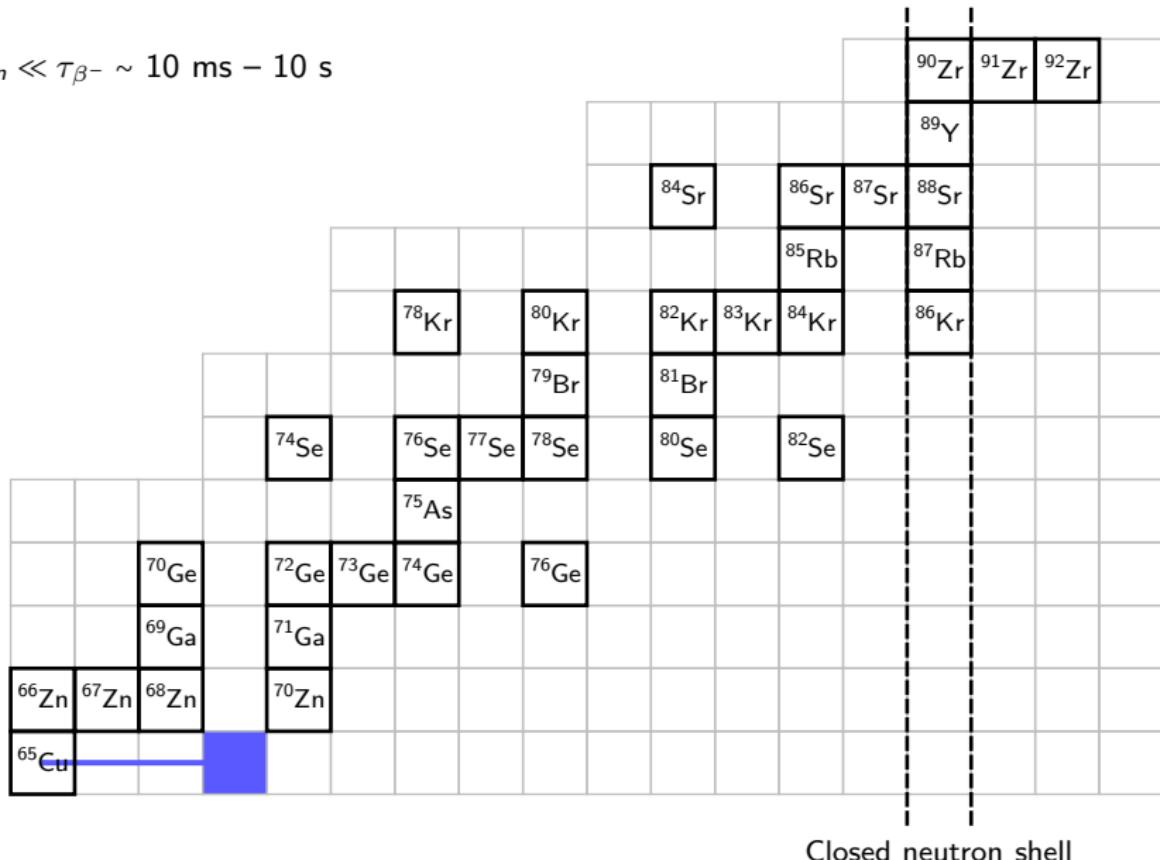
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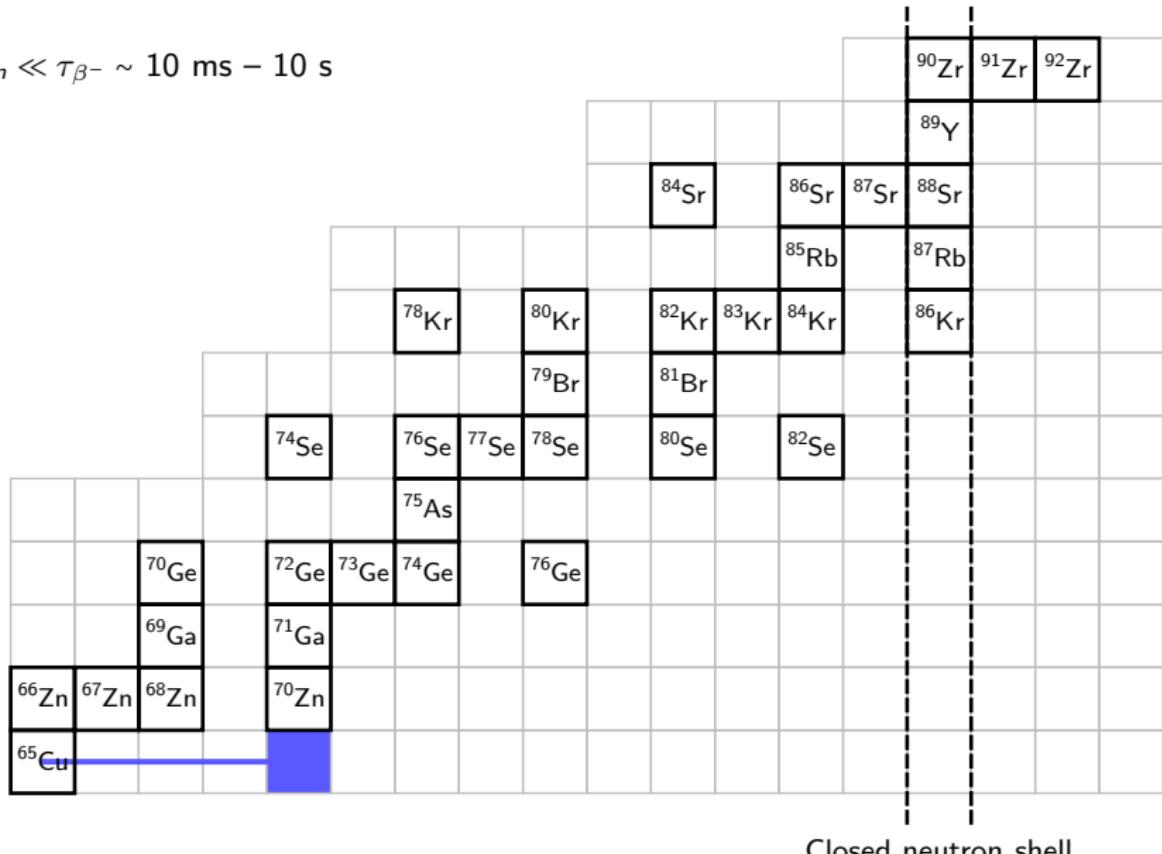
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$$\tau_n \ll \tau_{\beta^-} \sim 10 \text{ ms} - 10 \text{ s}$$



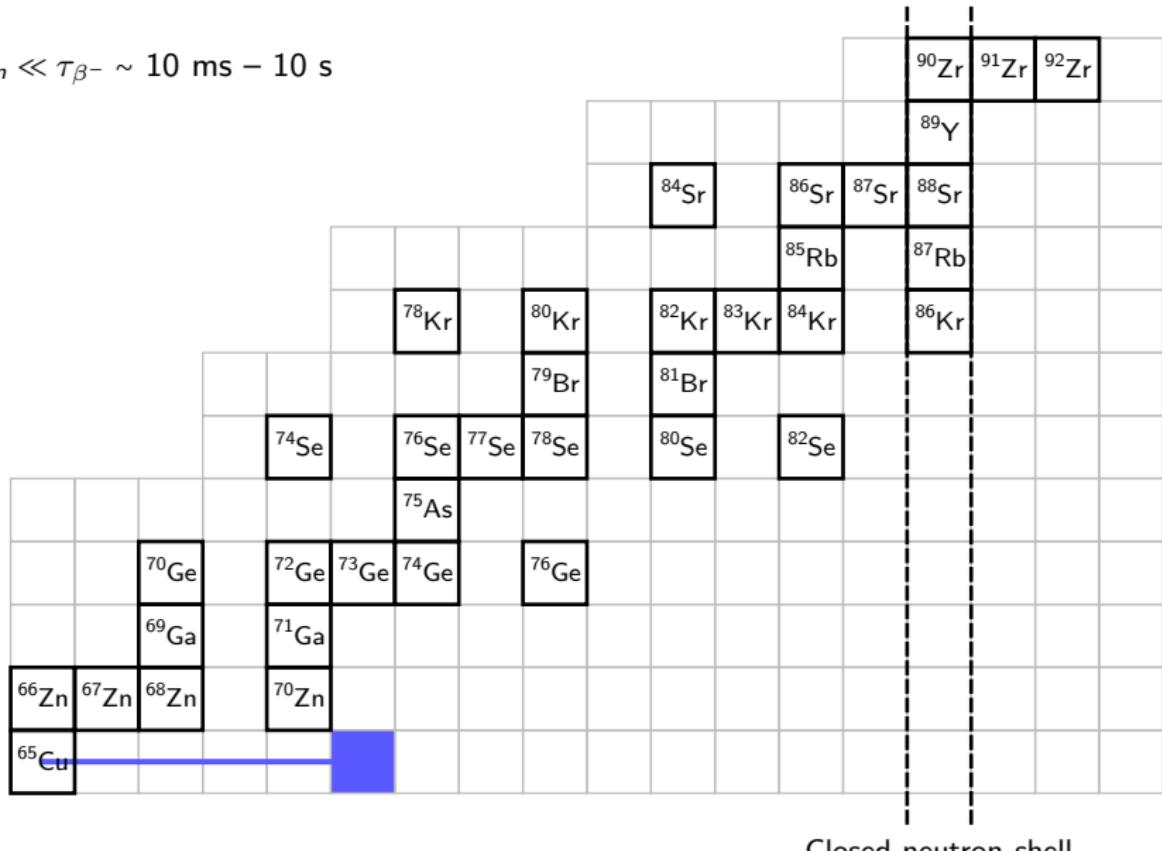
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The r-process

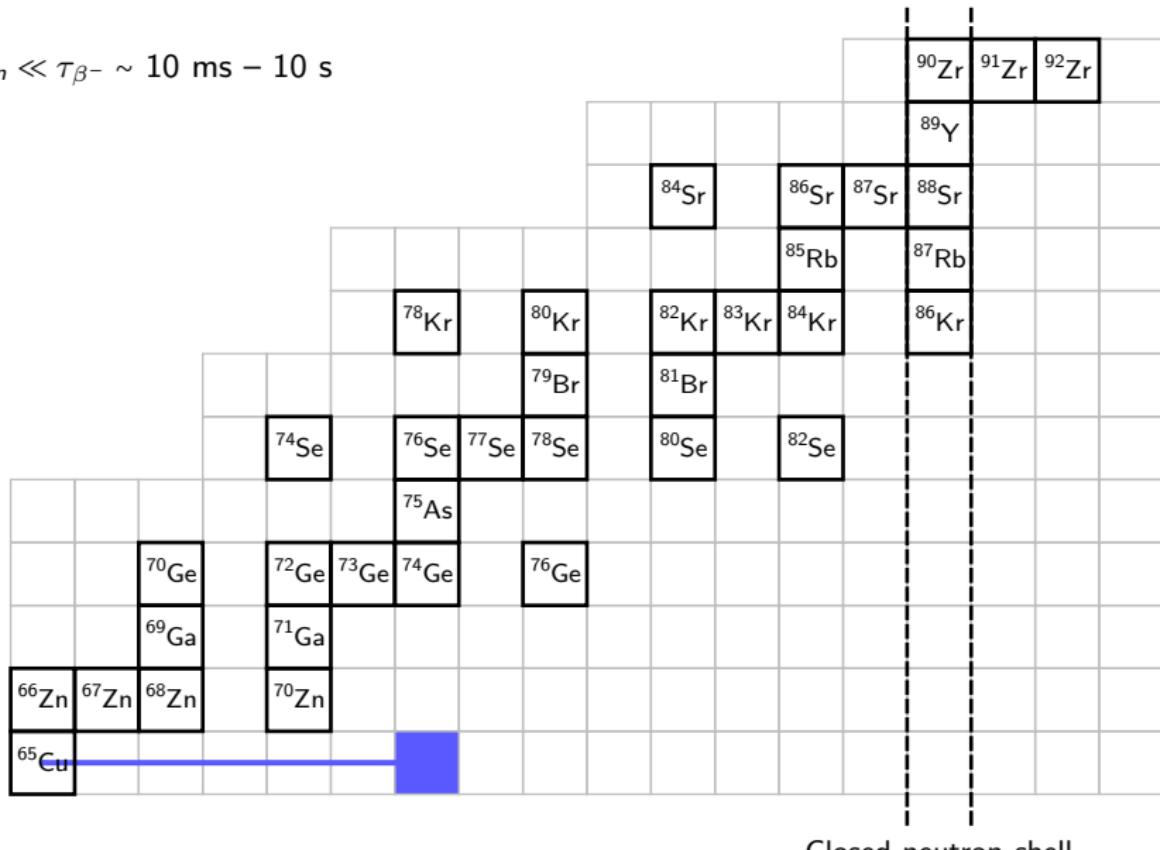
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Closed neutron shell

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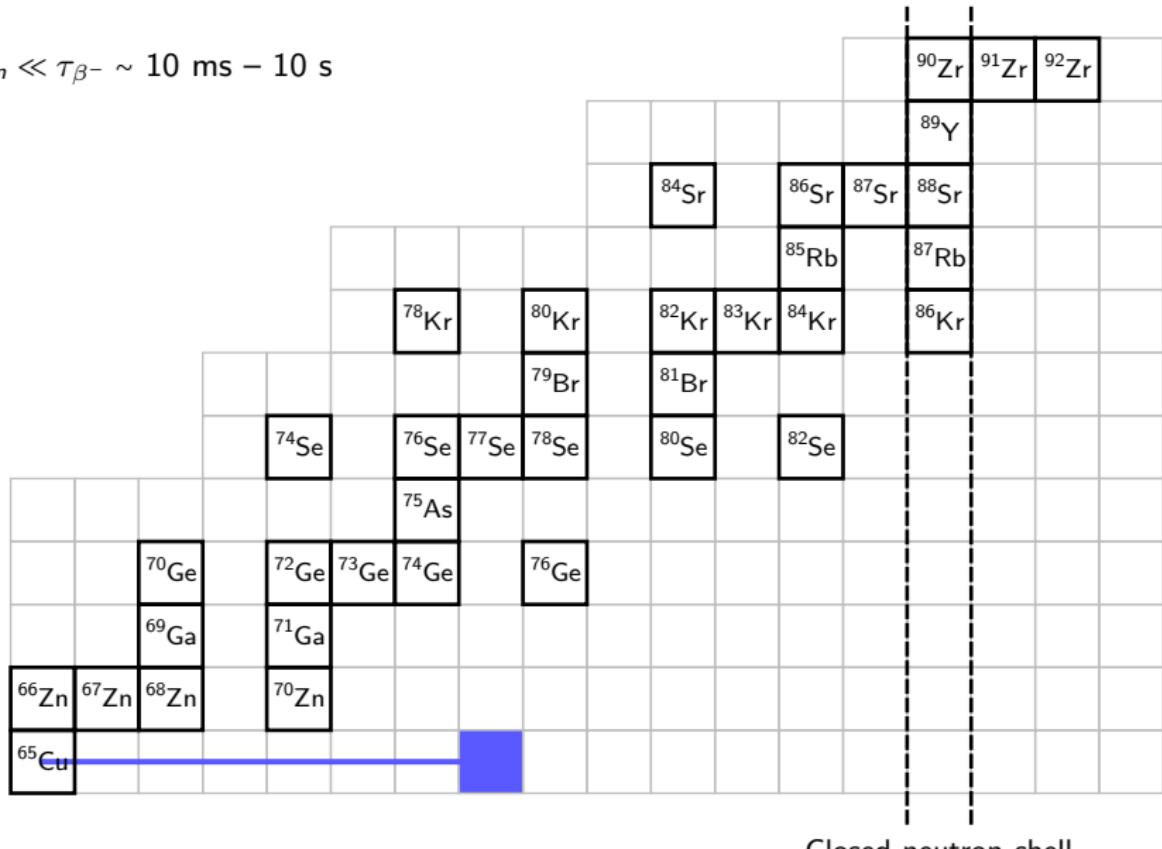
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Closed neutron shell

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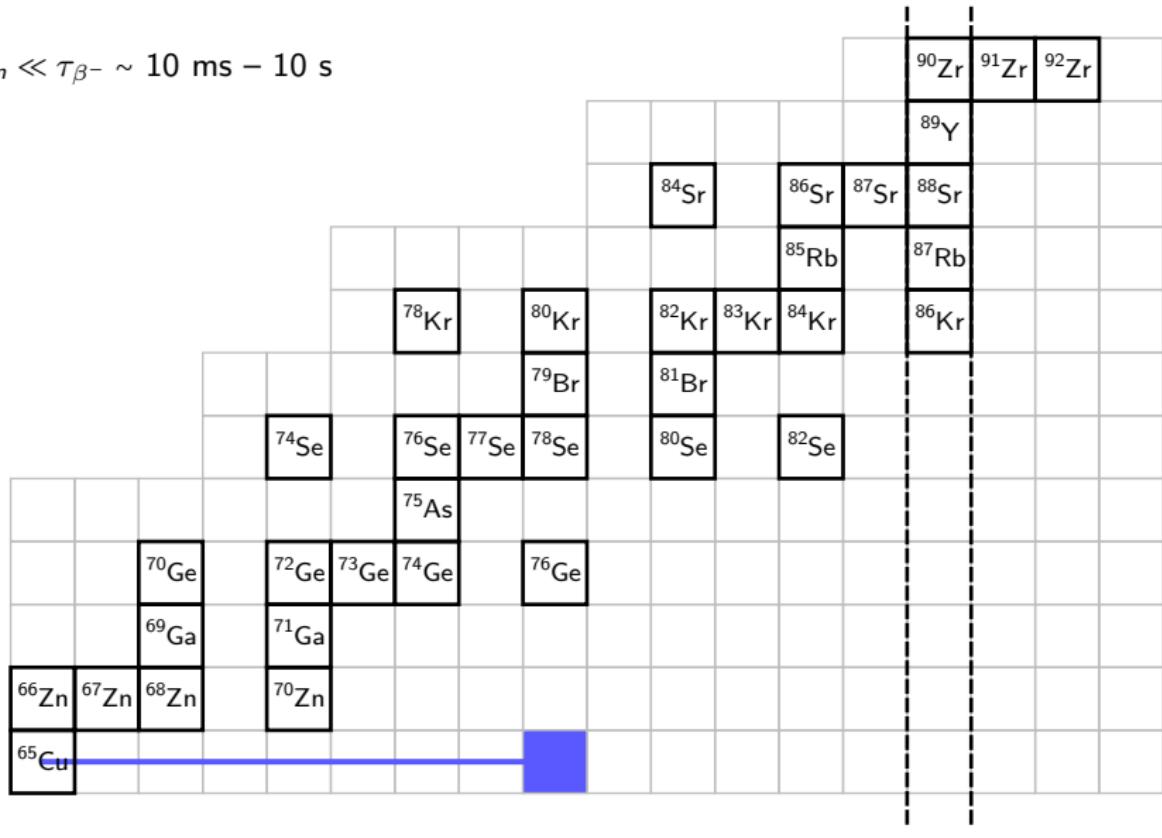
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Closed neutron shell

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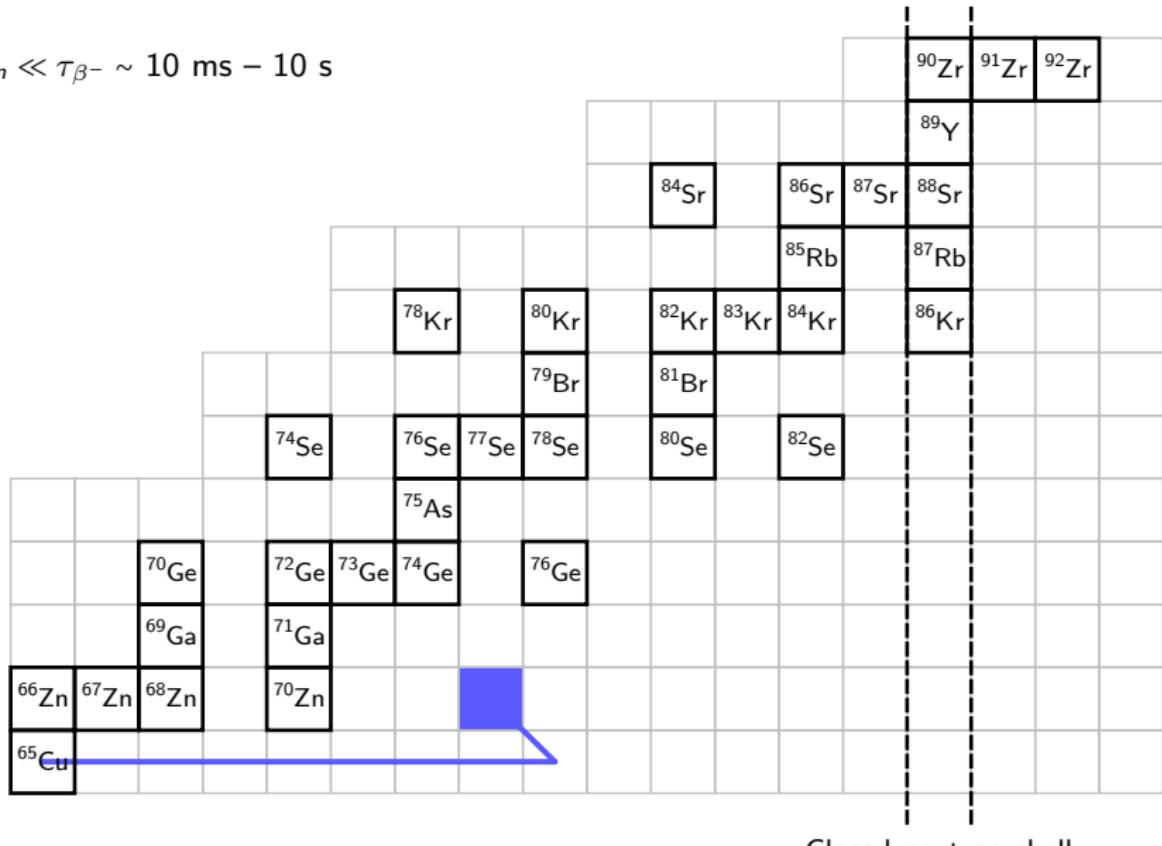
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Closed neutron shell

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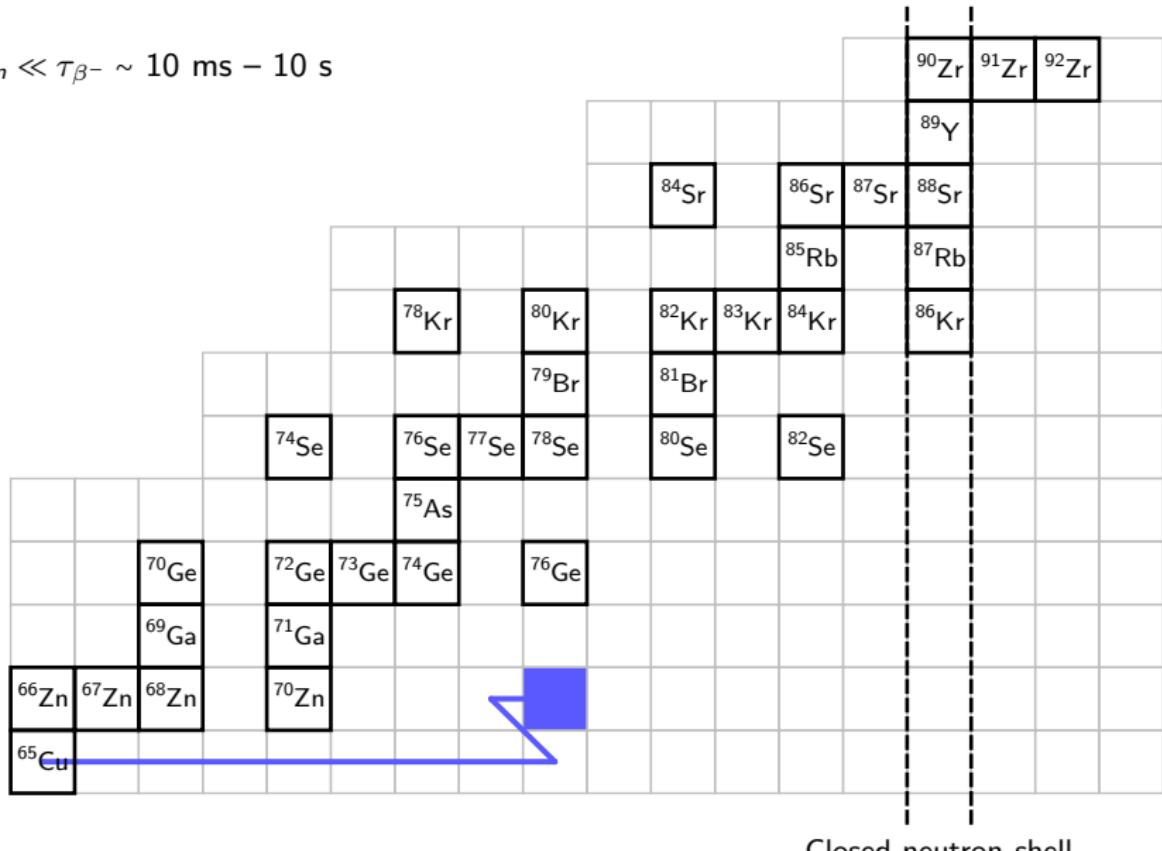
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Closed neutron shell

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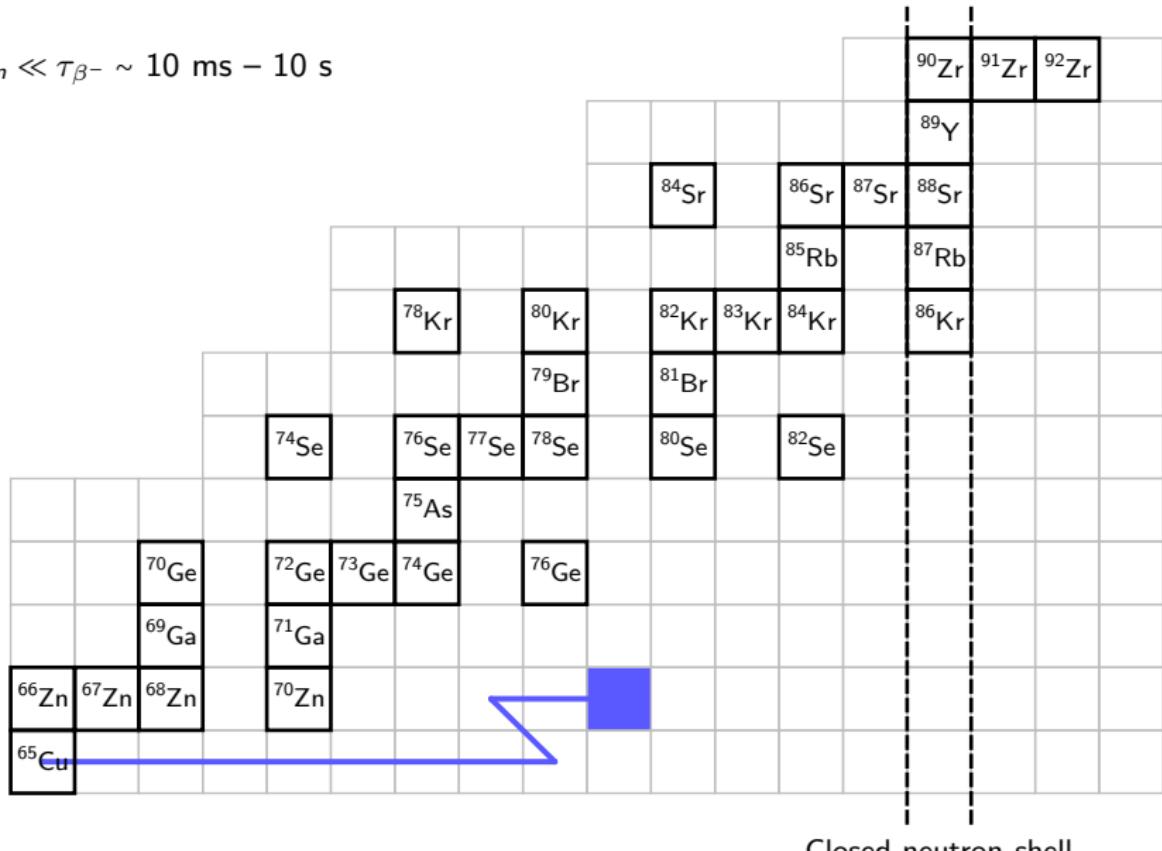
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Closed neutron shell

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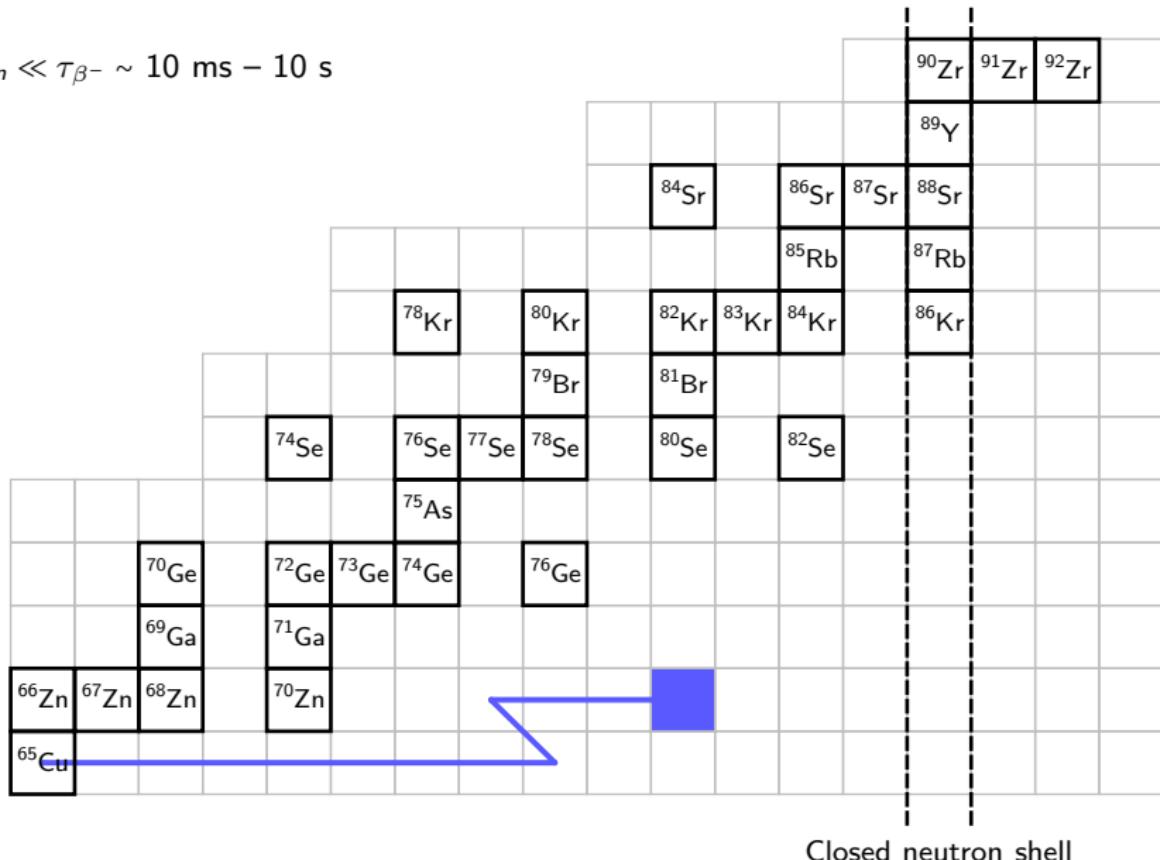
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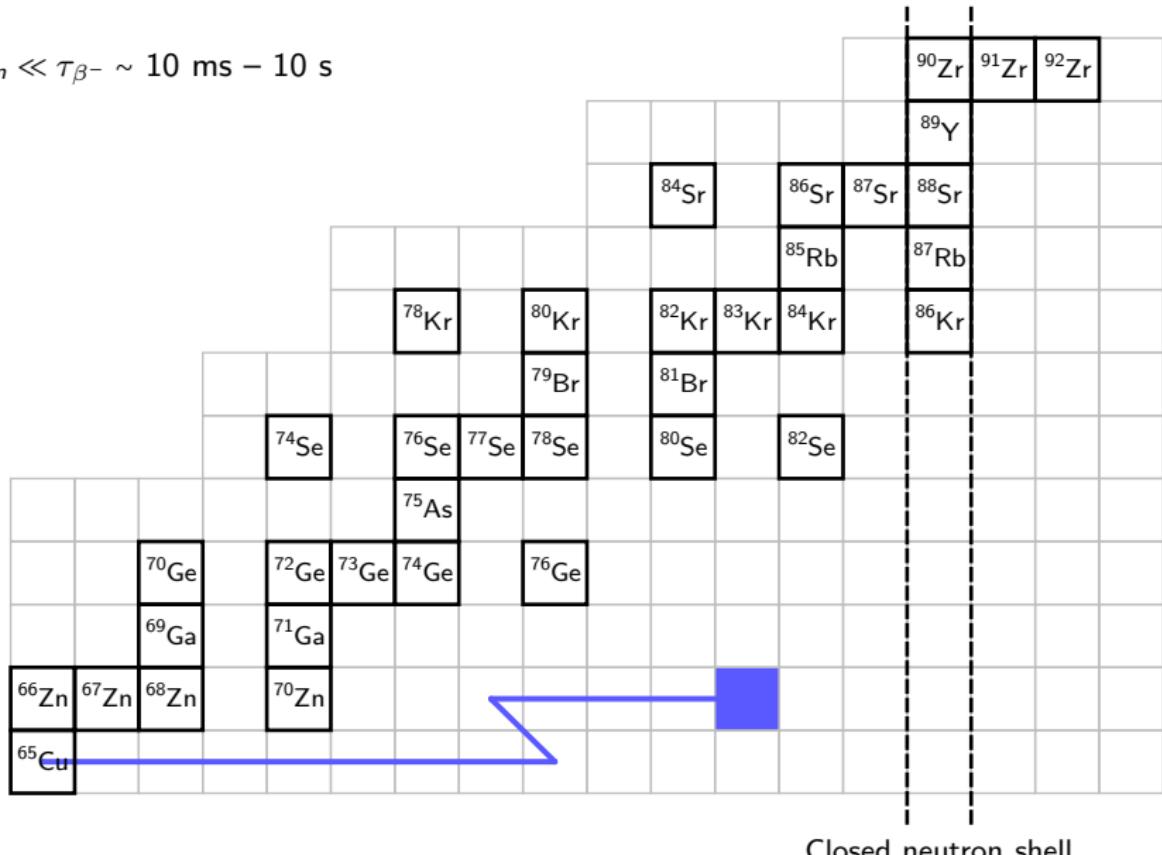
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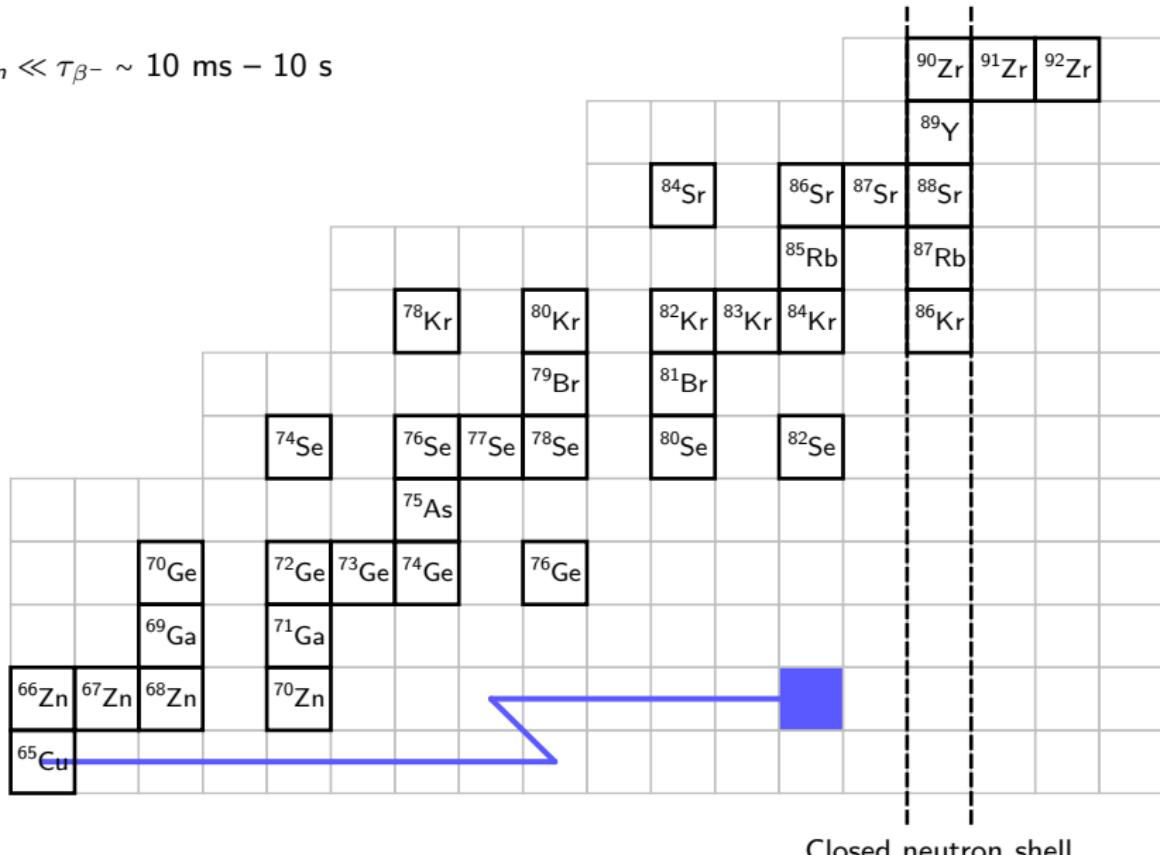
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Closed neutron shell

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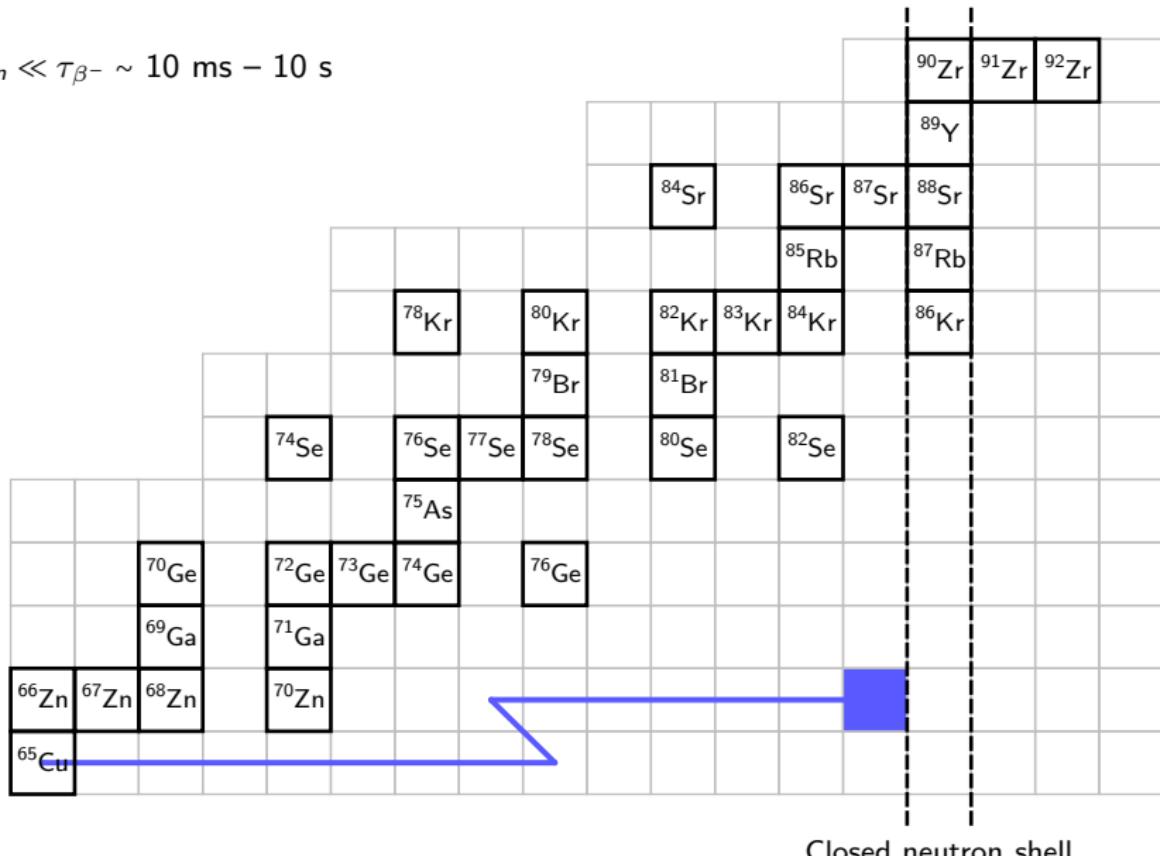
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Closed neutron shell

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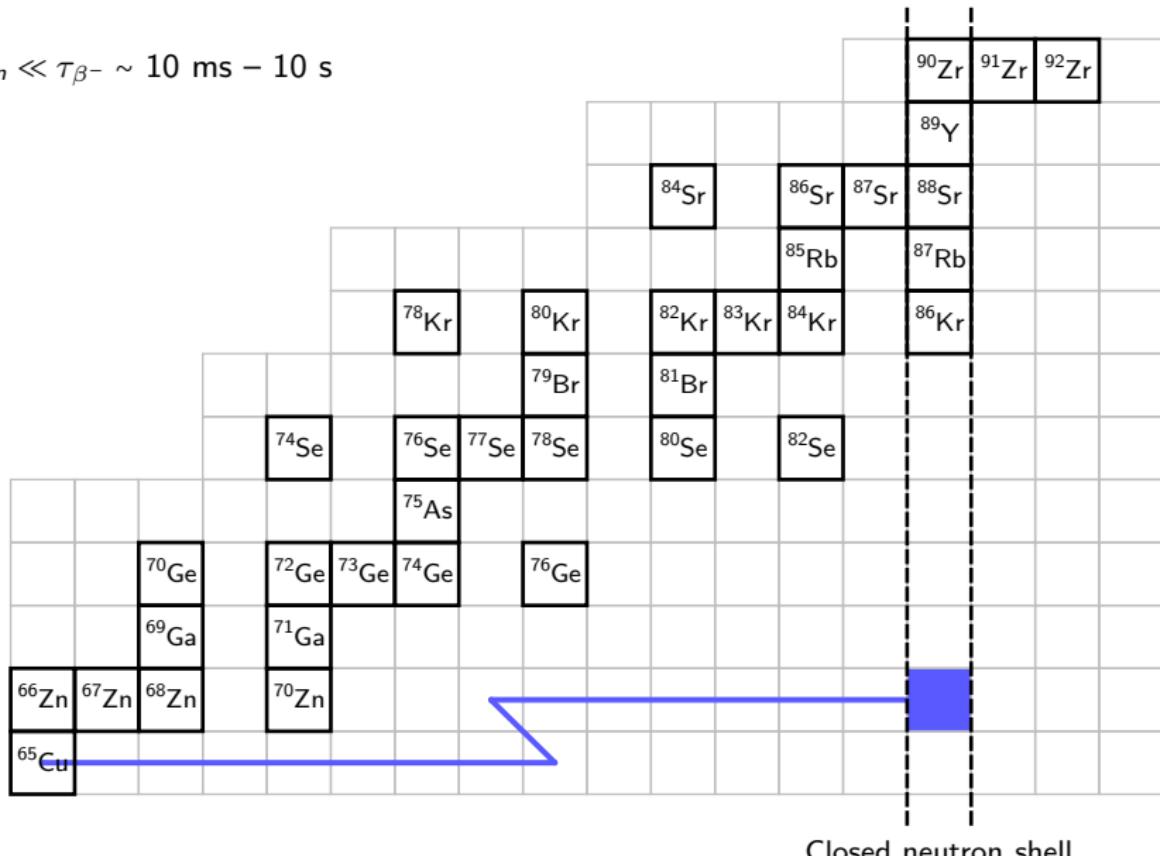
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Closed neutron shell

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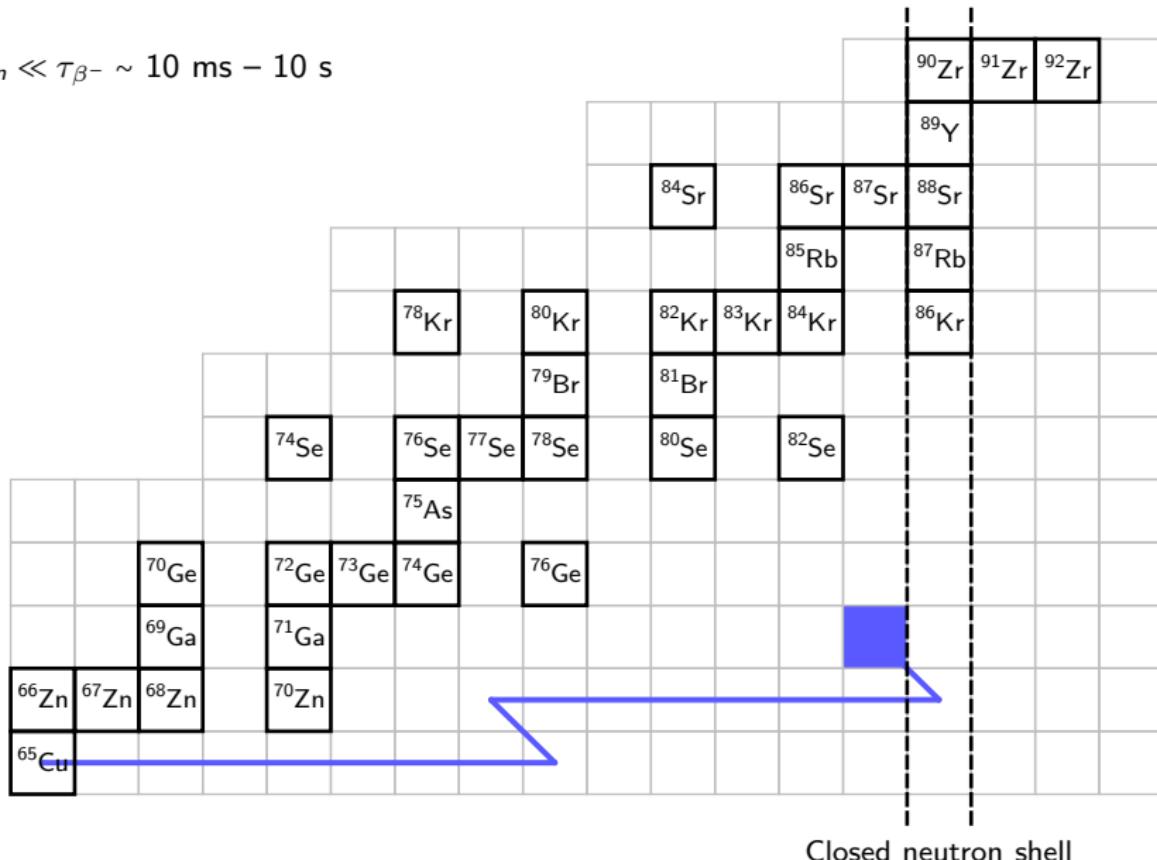
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Closed neutron shell

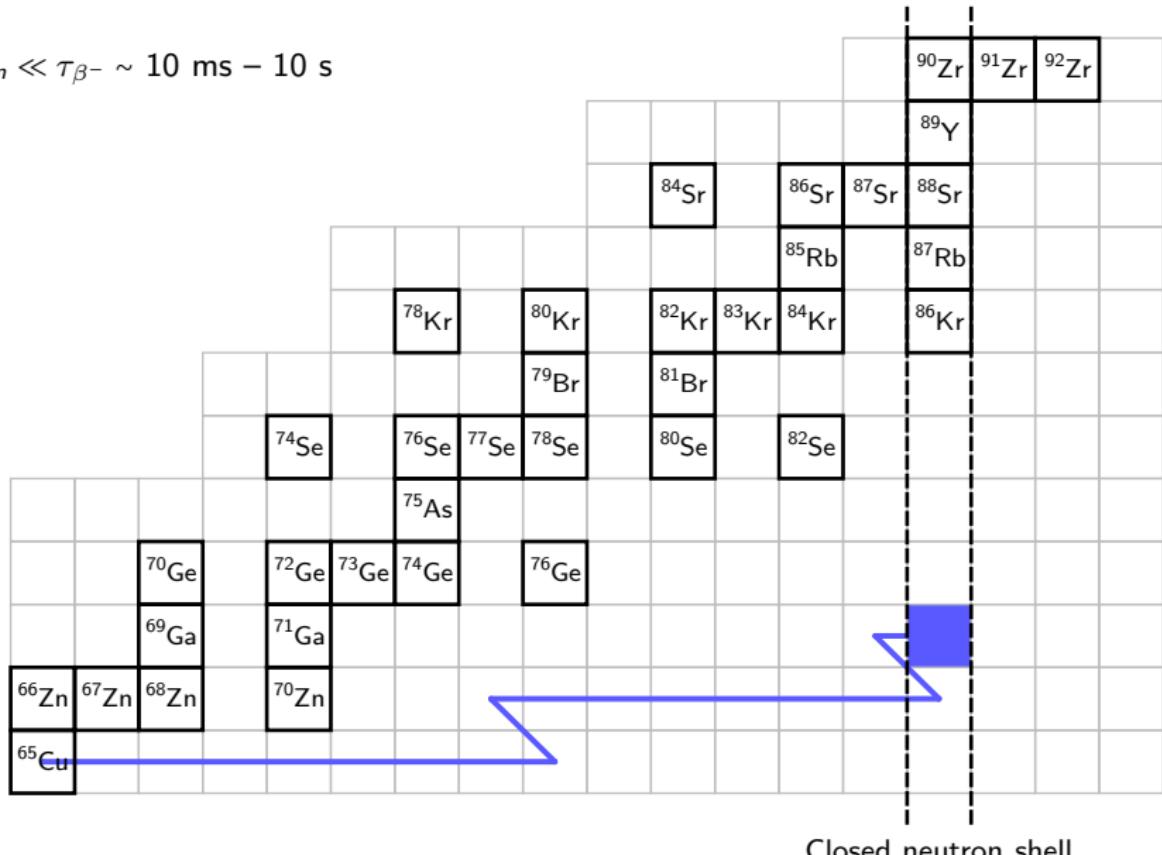
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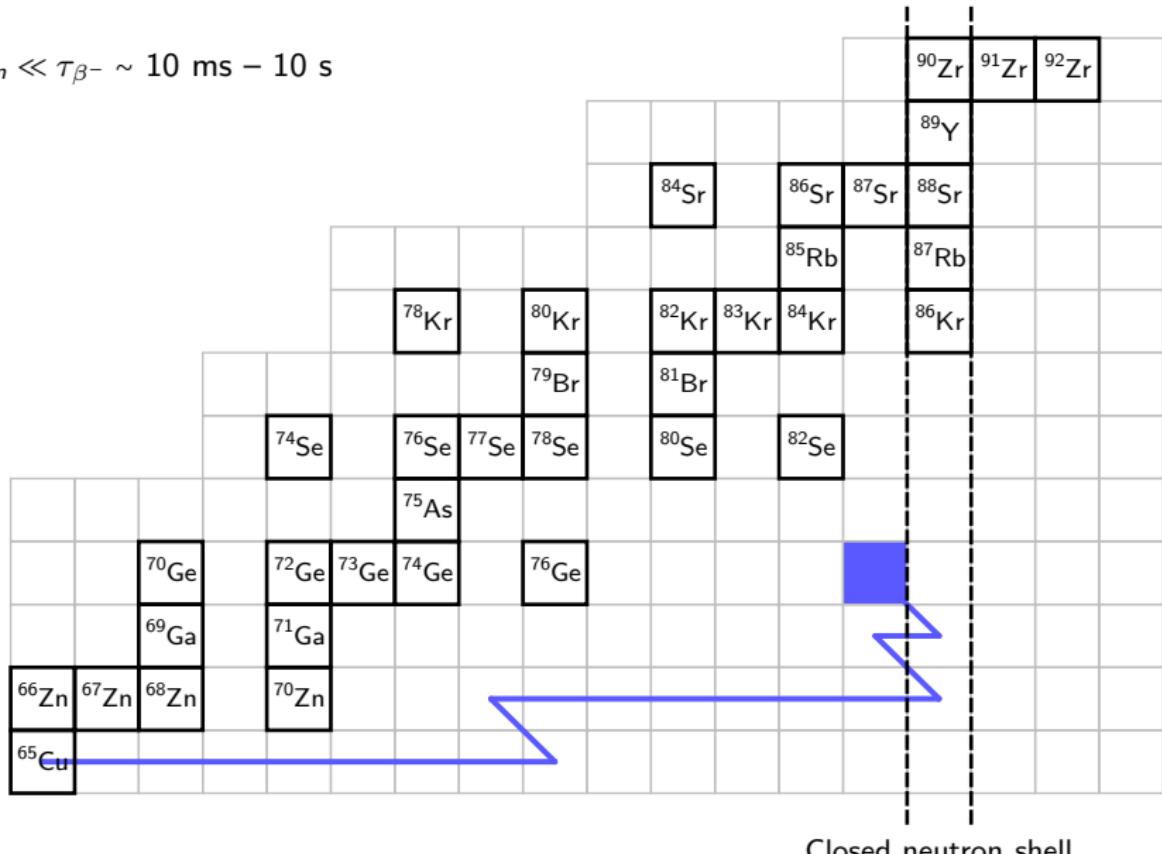
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Closed neutron shell

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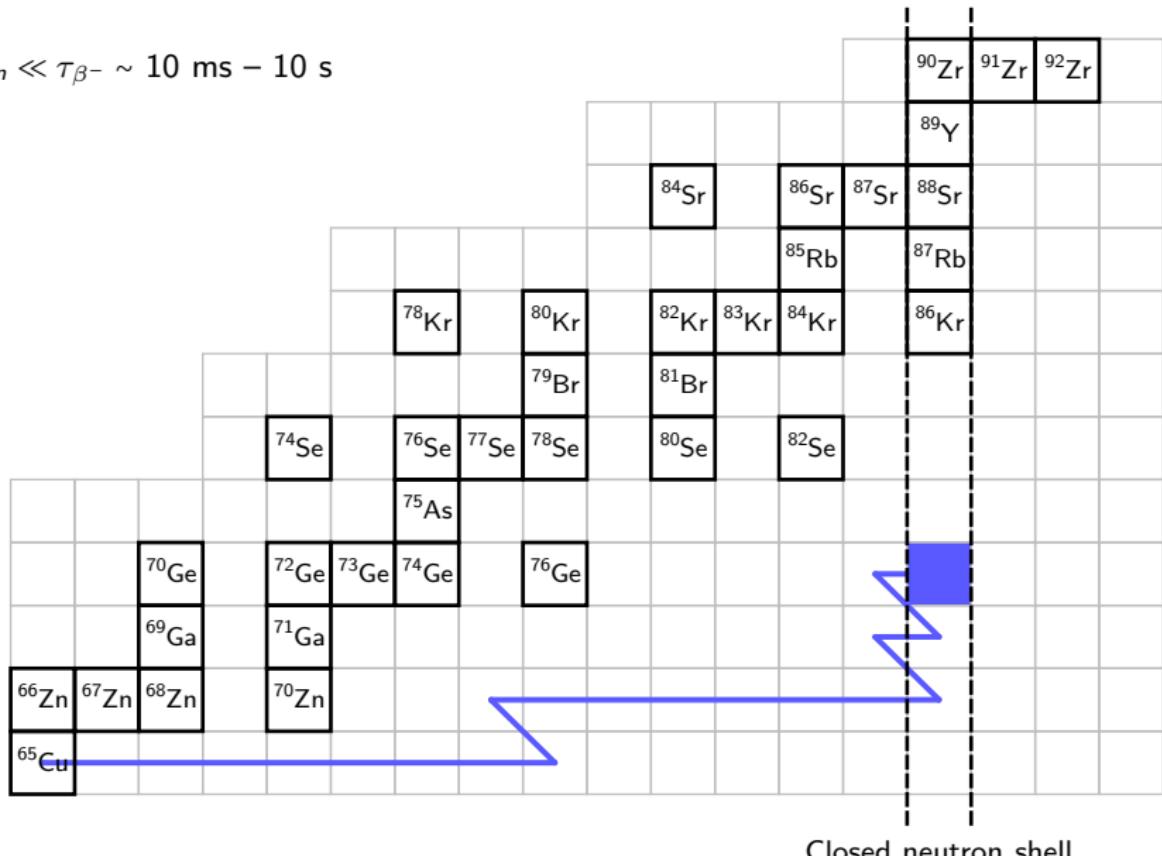
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Closed neutron shell

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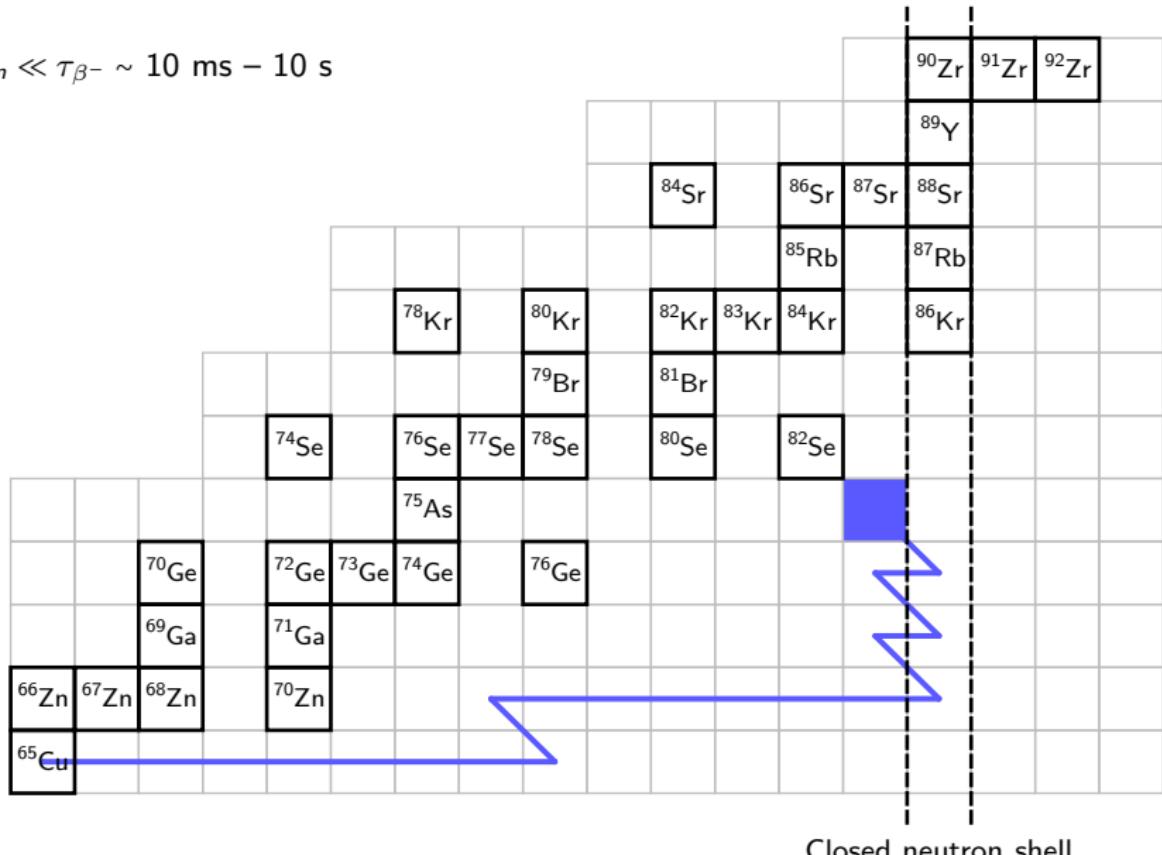
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Closed neutron shell

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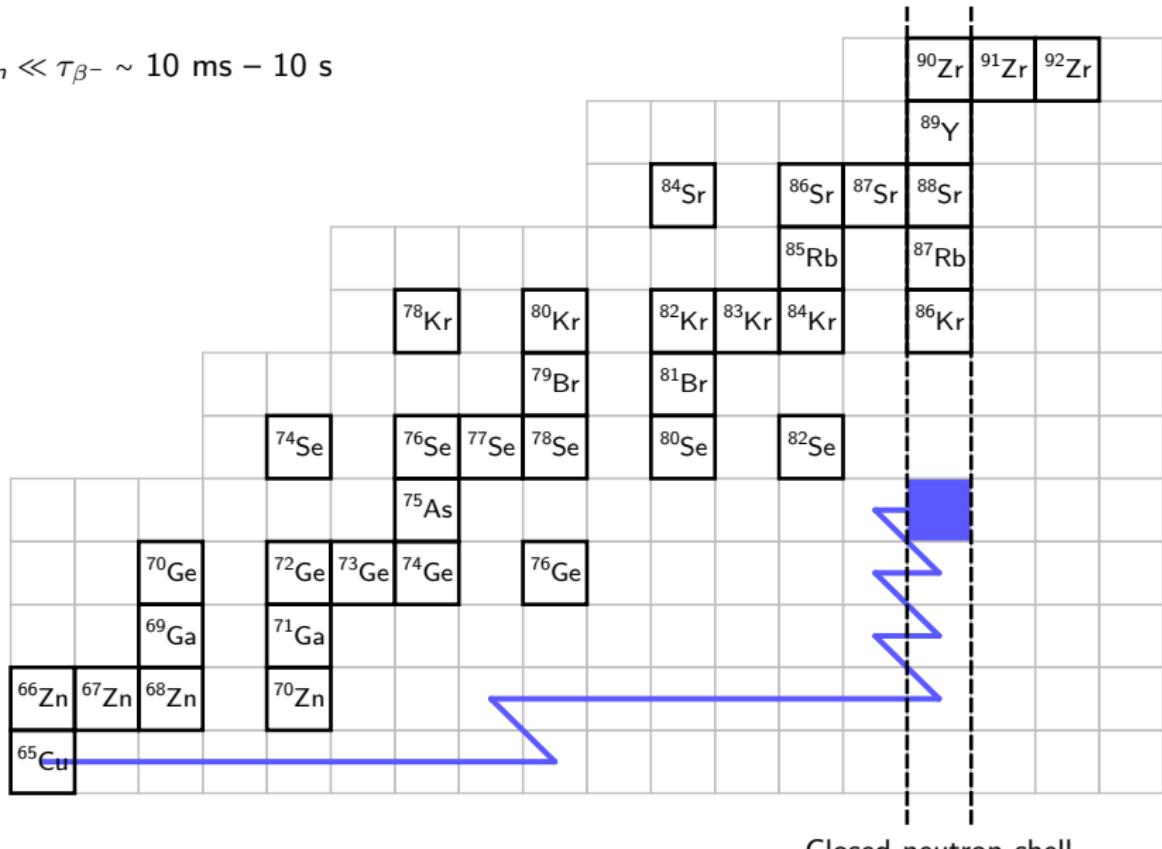
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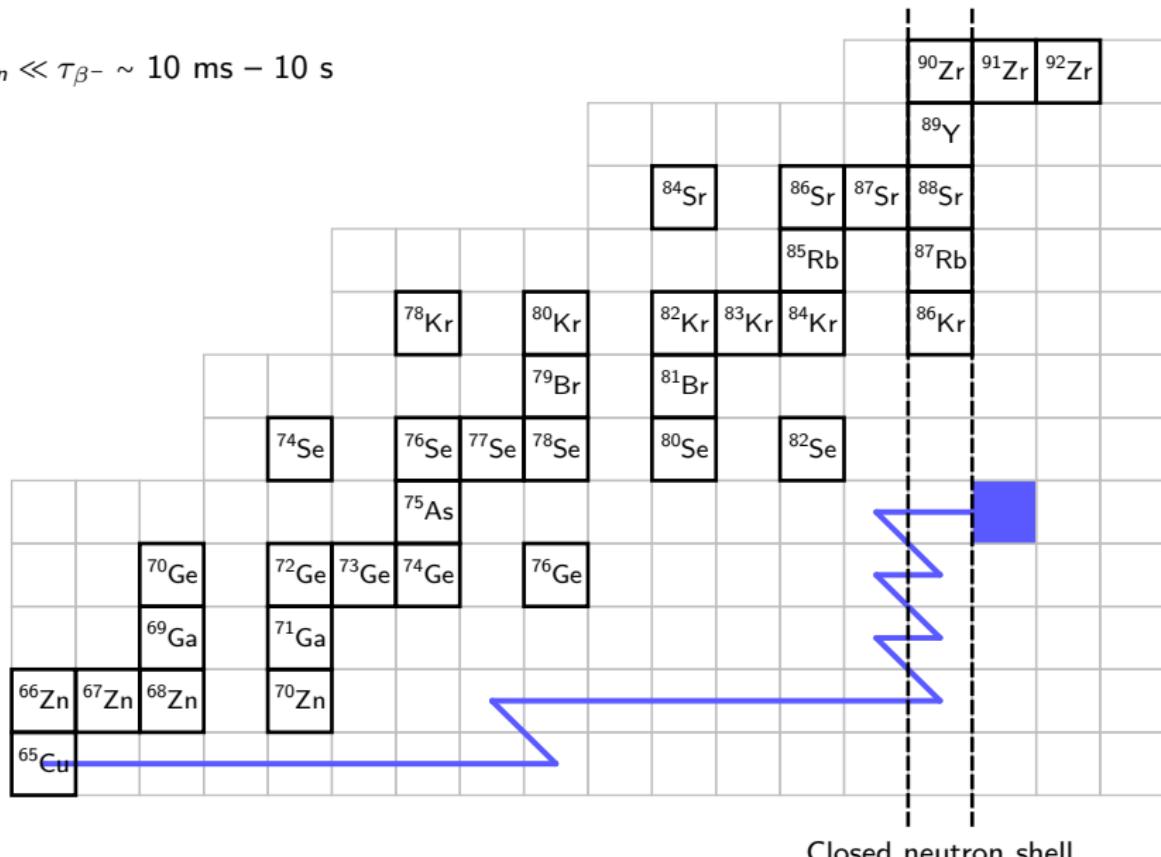
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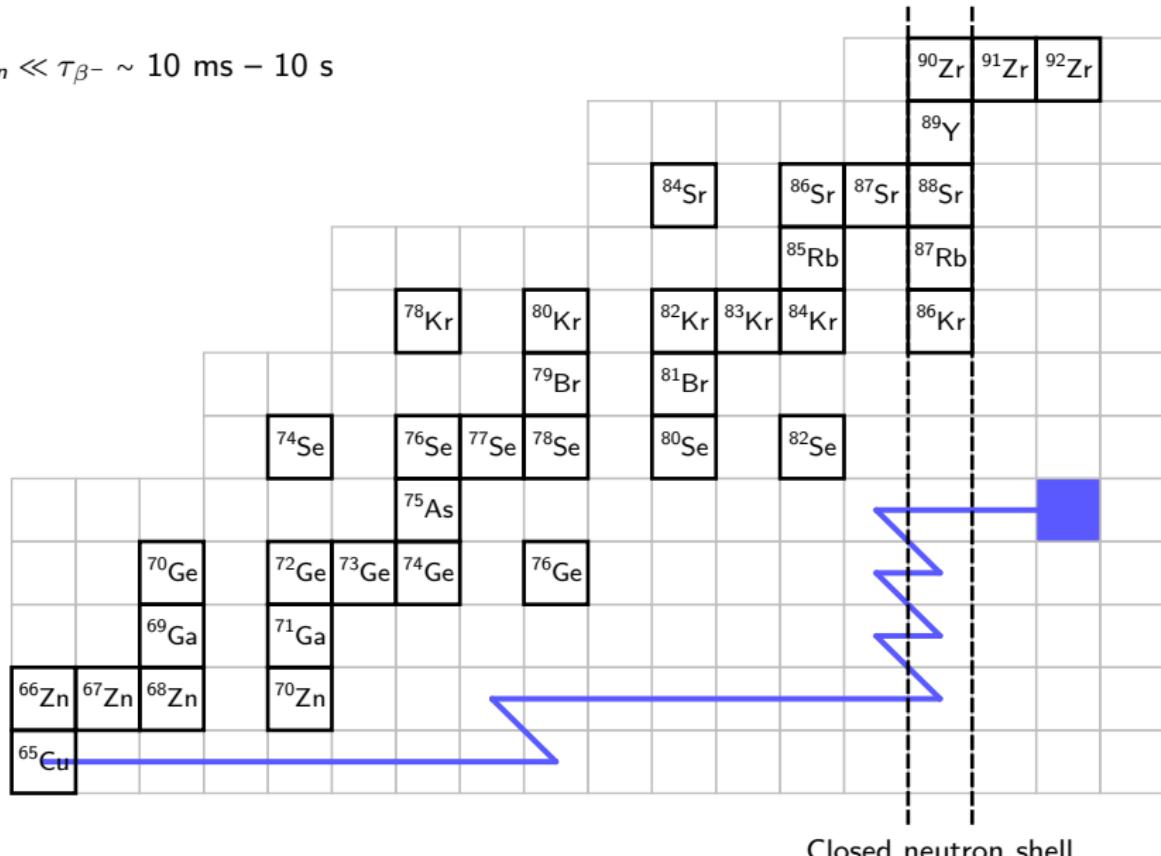
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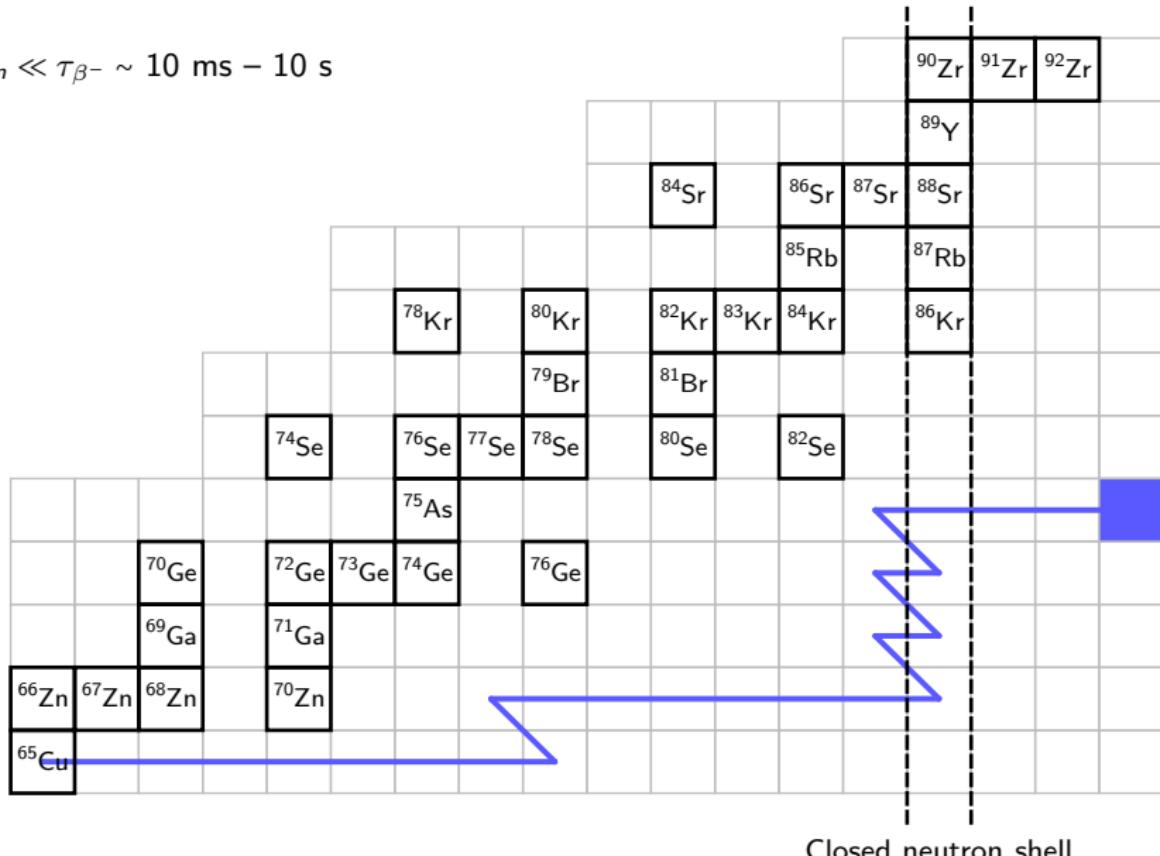
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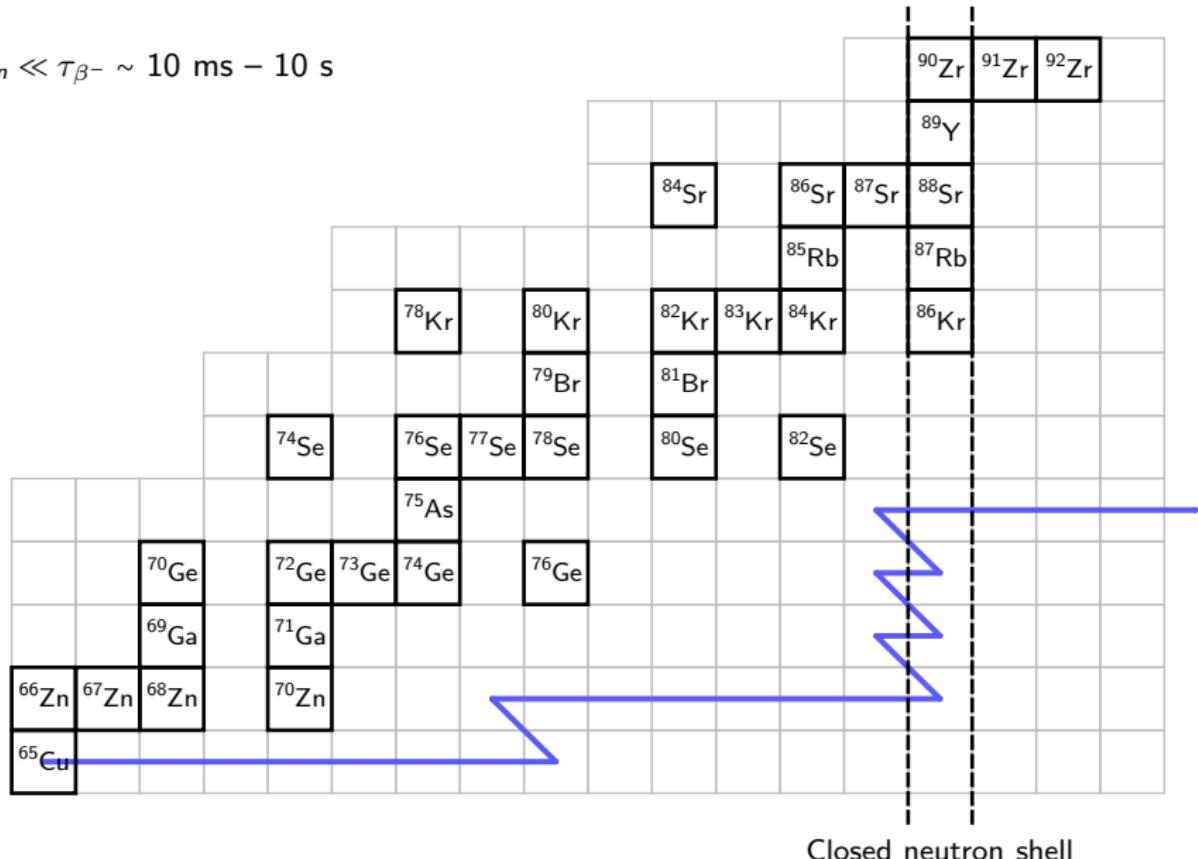
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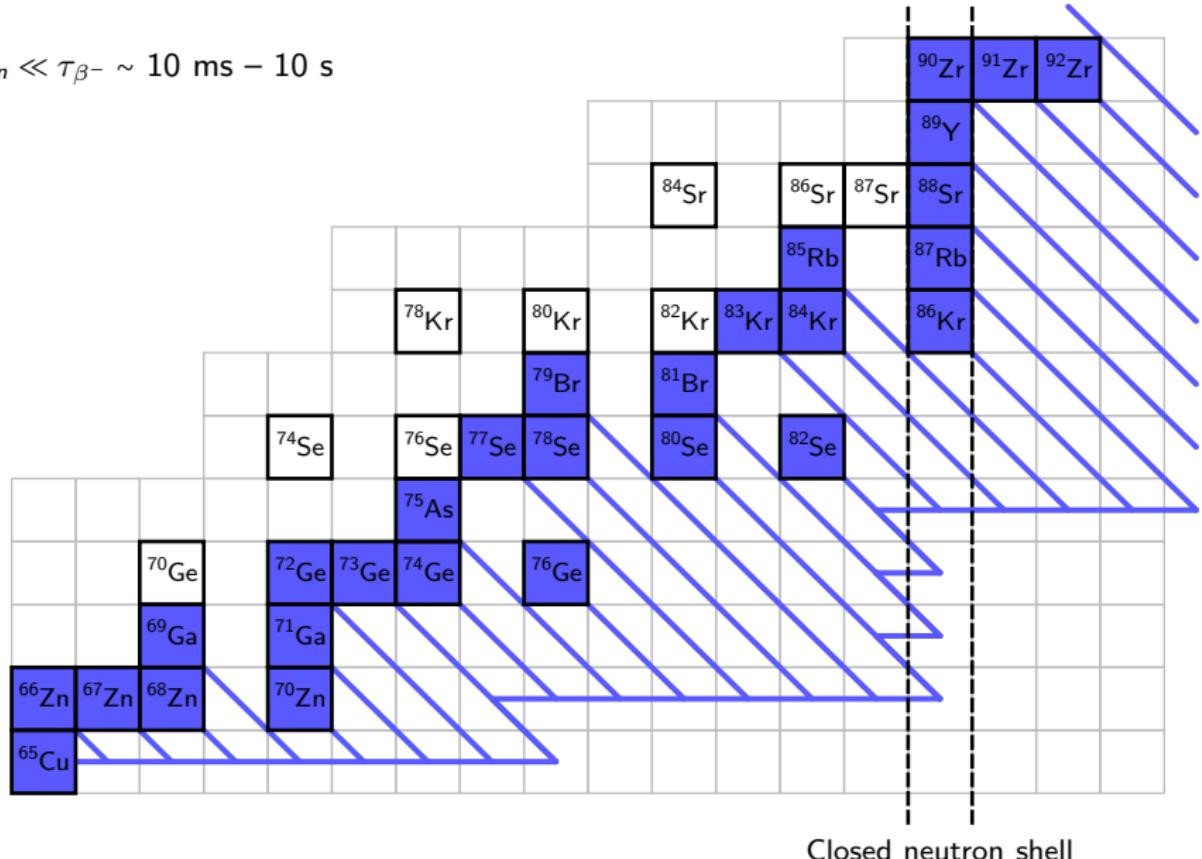
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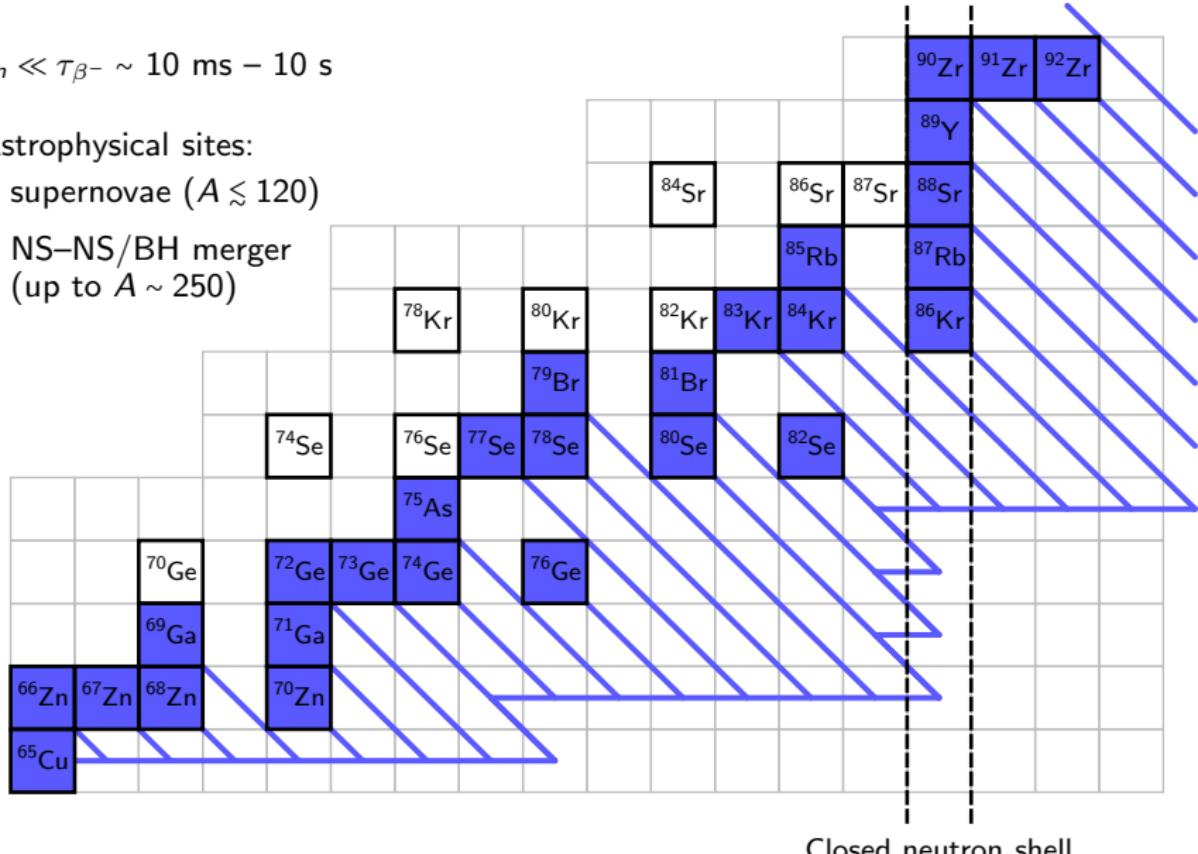
The r-process

$$\tau_n \ll \tau_{\beta^-} \sim 10 \text{ ms} - 10 \text{ s}$$

Astrophysical sites:

supernovae ($A \lesssim 120$)

NS–NS/BH merger
(up to $A \sim 250$)



Closed neutron shell

- ▶ Radioactively powered transient after r-process nucleosynthesis
- ▶ Triple coincidence: Gravitational wave signal, short GRB, kilonova
- ▶ Possibly observed after GRB060614 and GRB130603B
- ▶ Observational signature:
 - ▶ Heating rate → luminosity
 - ▶ Amount of lanthanides and actinides → opacity

Lanthanides (between 2nd and 3rd peak) and actinides (beyond 3rd peak) have open f-shells → very high line opacities

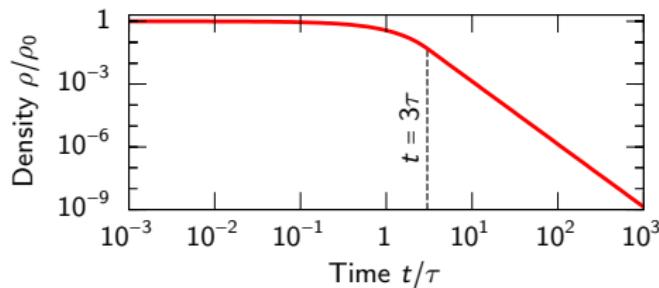
	lanthanide-free	lanthanide-rich
opacity	$\sim 0.1 \text{ cm}^2 \text{ g}^{-1}$	$\sim 10 \text{ cm}^2 \text{ g}^{-1}$
luminosity	bright	dim
timescale	$\sim \text{day}$	$\sim \text{week}$
band	blue / optical	red / infrared

Parameters

$0.01 \leq Y_e \leq 0.50$	initial electron fraction
$1 \text{ } k_B \text{ baryon}^{-1} \leq s \leq 100 \text{ } k_B \text{ baryon}^{-1}$	initial specific entropy
$0.1 \text{ ms} \leq \tau \leq 500 \text{ ms}$	expansion time scale

Density profile

$$\rho(t, \tau) = \begin{cases} \rho_0 e^{-t/\tau} & t \leq 3\tau \\ \rho_0 \left(\frac{3\tau}{te}\right)^3 & t \geq 3\tau \end{cases}$$



Initial conditions

- ▶ Choose initial temperature $T_0 = 6 \text{ GK}$
- ▶ Find ρ_0 by solving for NSE at T_0 and Y_e that produces specified s



- ▶ General-purpose nuclear reaction network
- ▶ ~8000 isotopes, ~110,000 nuclear reactions
- ▶ Evolves temperature and entropy based on nuclear reactions
- ▶ Input: $\rho(t)$, initial composition, initial entropy or temperature
- ▶ Open source (soon)

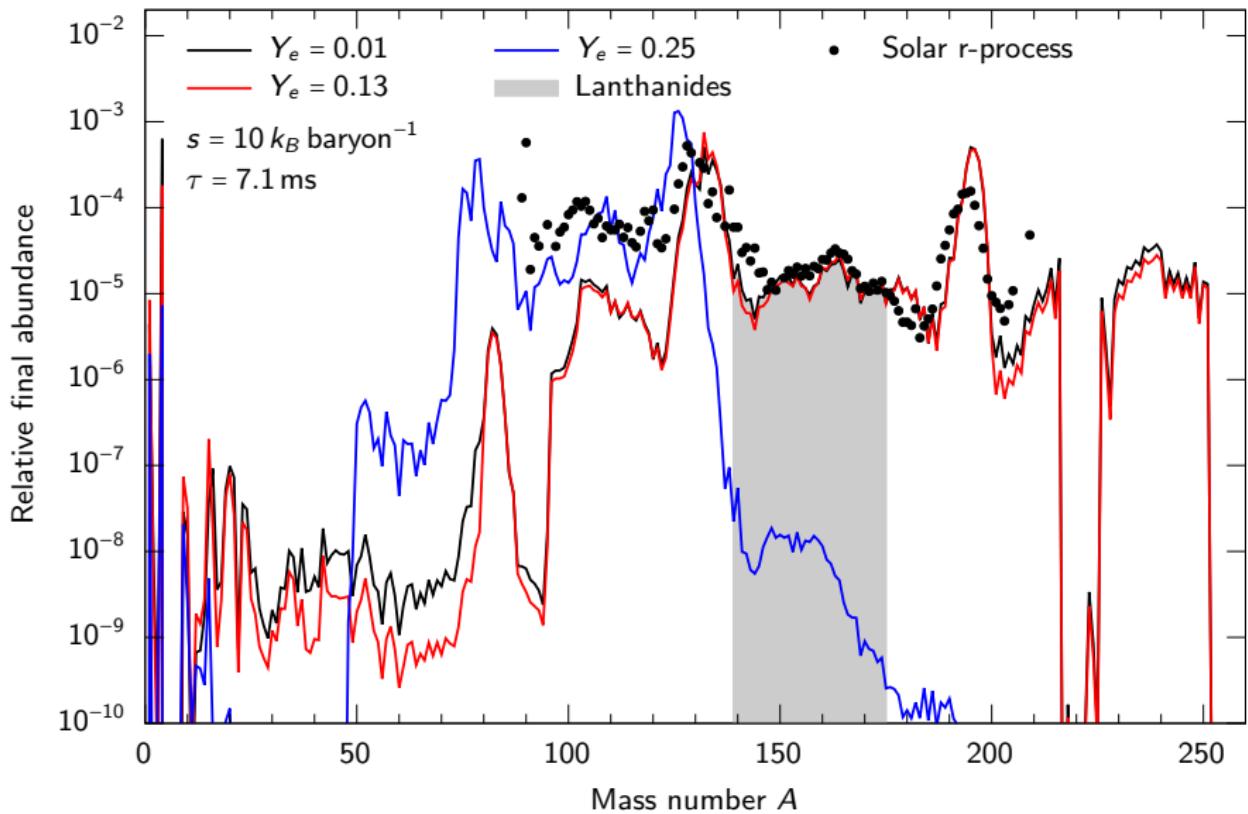
Science

- ▶ Helmholtz equation of state (EOS)
- ▶ Calculate nuclear statistical equilibrium (NSE)
- ▶ Calculate inverse rates from *detailed balance* to be consistent with NSE
- ▶ NSE evolution mode

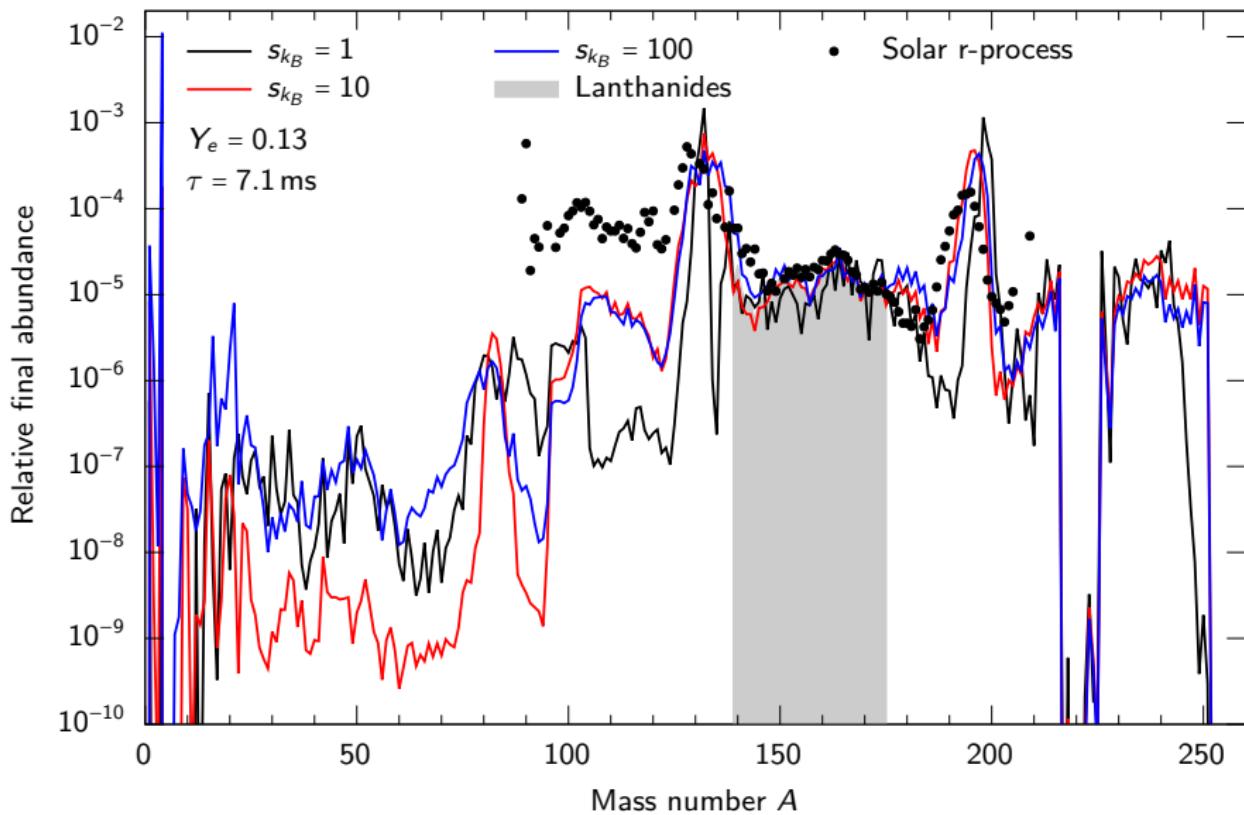
Code

- ▶ Object-oriented C++11
- ▶ Python bindings
- ▶ Uses REACLIB rates, but can easily be extended
- ▶ Convenient HDF5 output
- ▶ Make movie with chart of nuclides

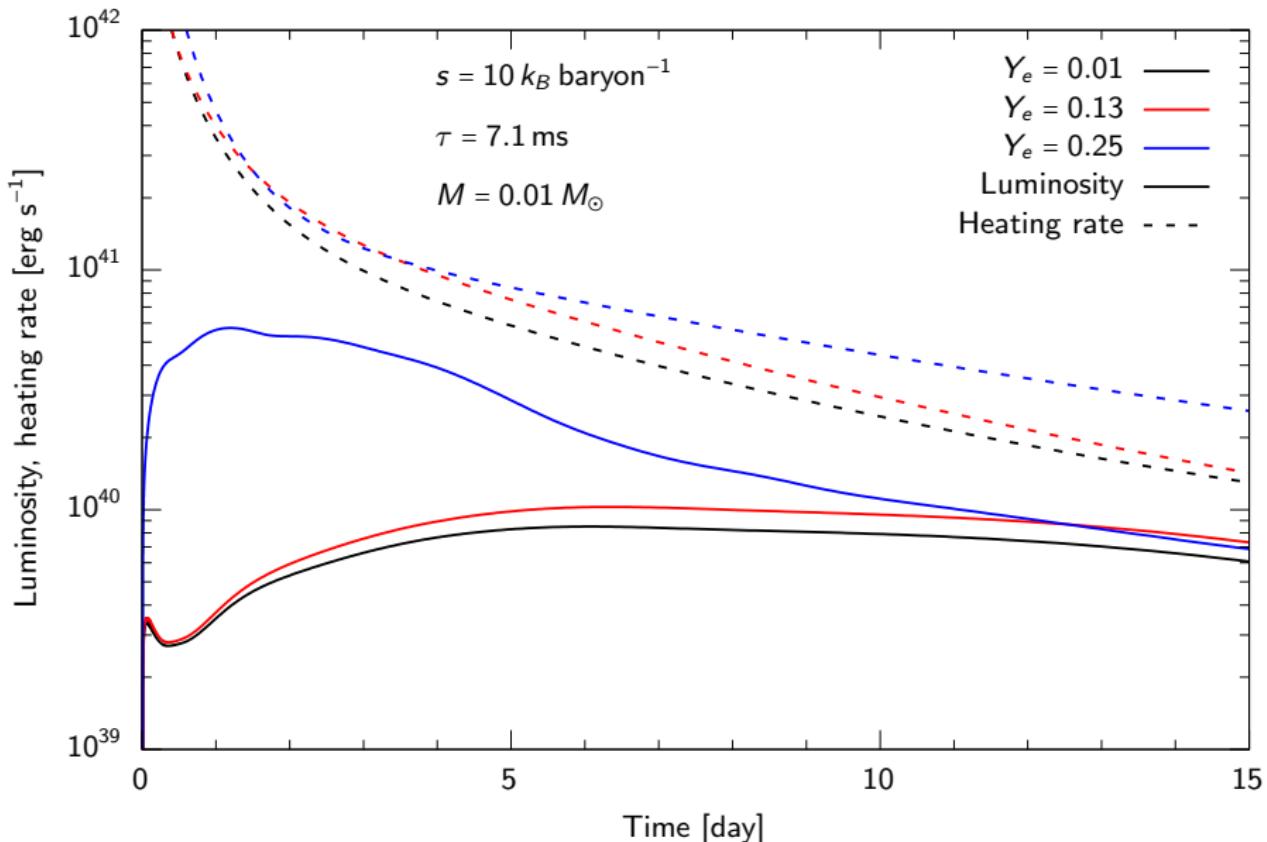
Final abundances vs. electron fraction



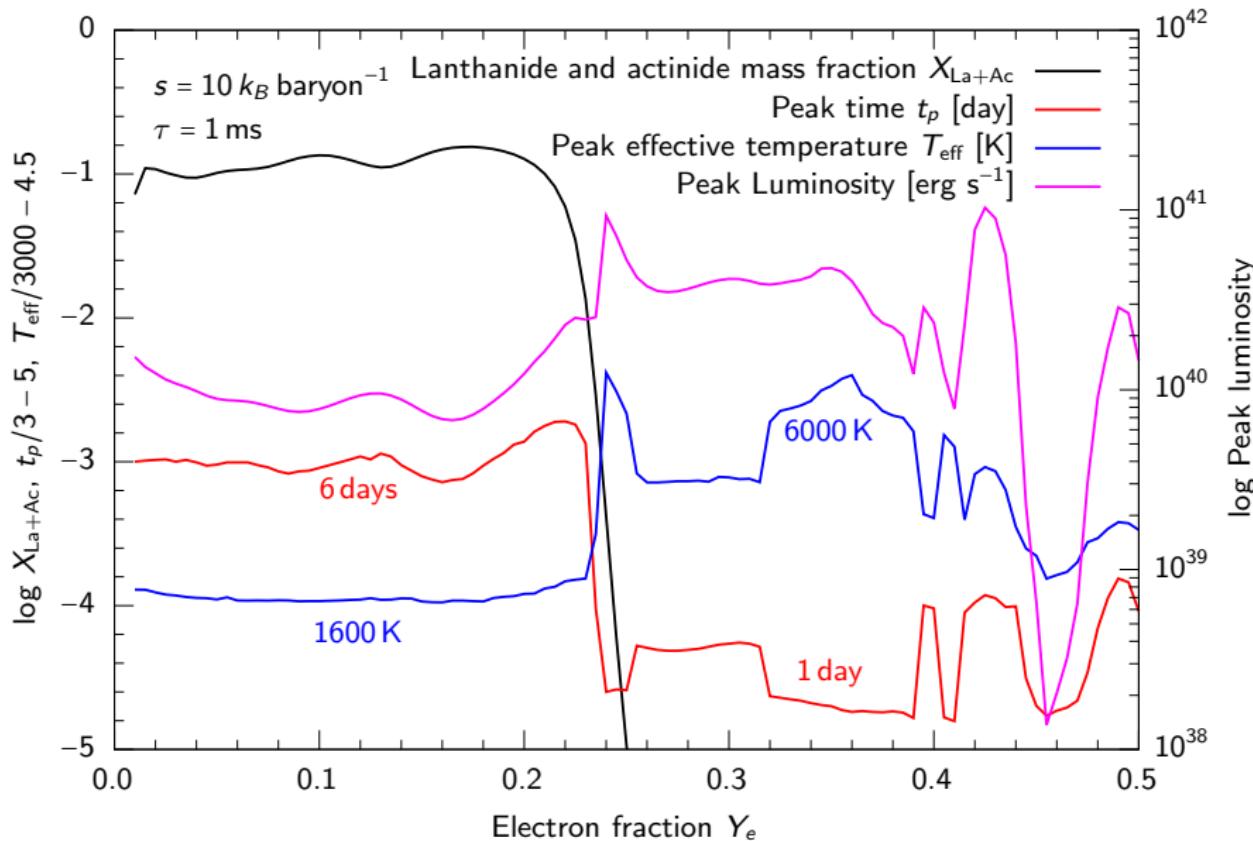
Final abundances vs. entropy

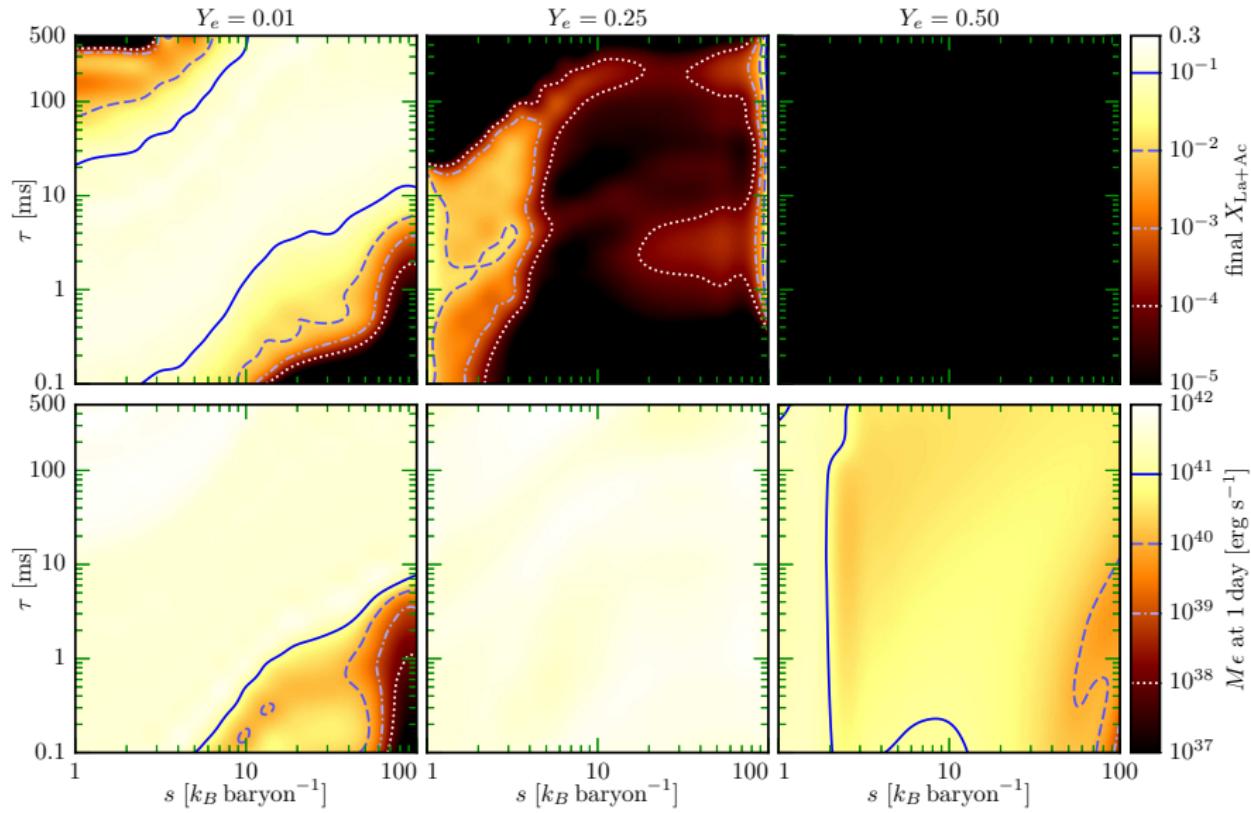


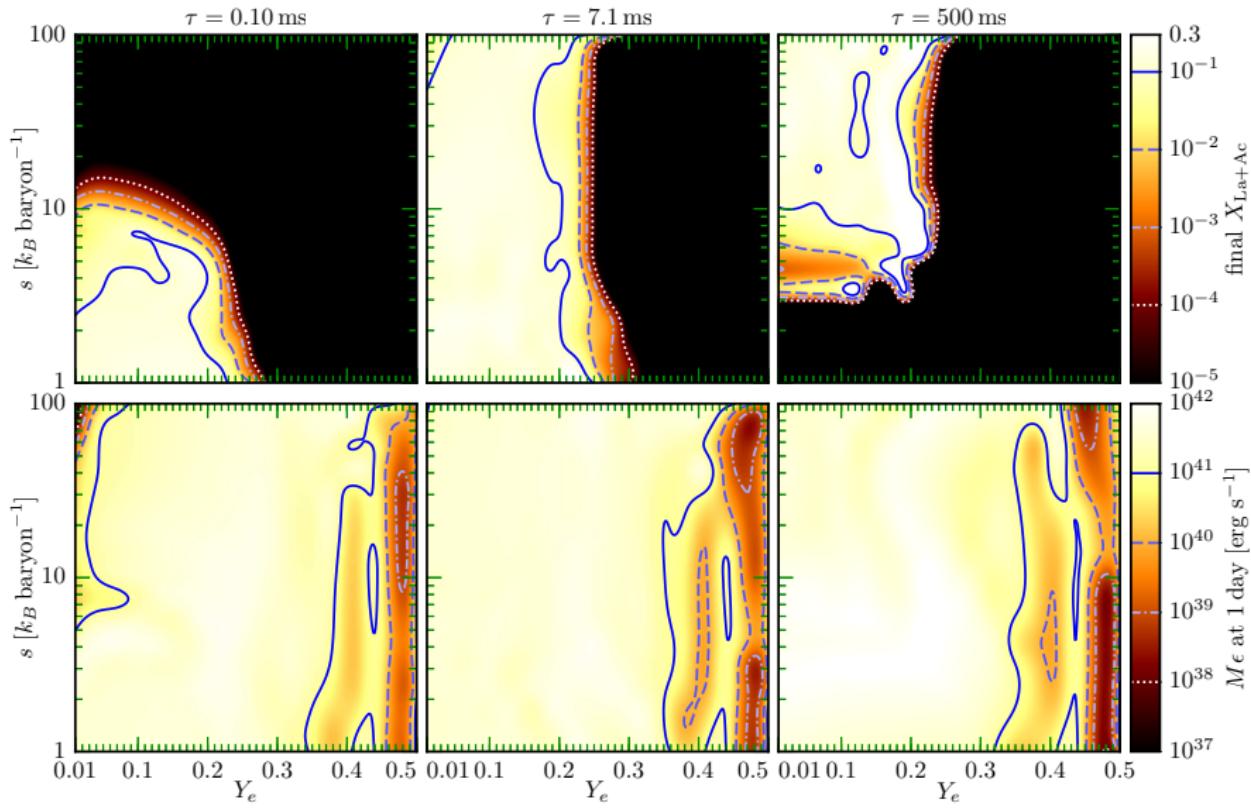
Example light curves



Light curves vs. electron fraction





τ slices

- ▶ Lanthanides and actinides have big impact on kilonova light curve
- ▶ Lanthanide-rich for $Y_e \lesssim 0.22 - 0.30$, except:
 - ▶ High s and small τ : neutron-rich freeze-out
 - ▶ Low s and large τ : restarted r-process at high Y_e
- ▶ Uniform heating rate for $Y_e \lesssim 0.4$

Additional slides

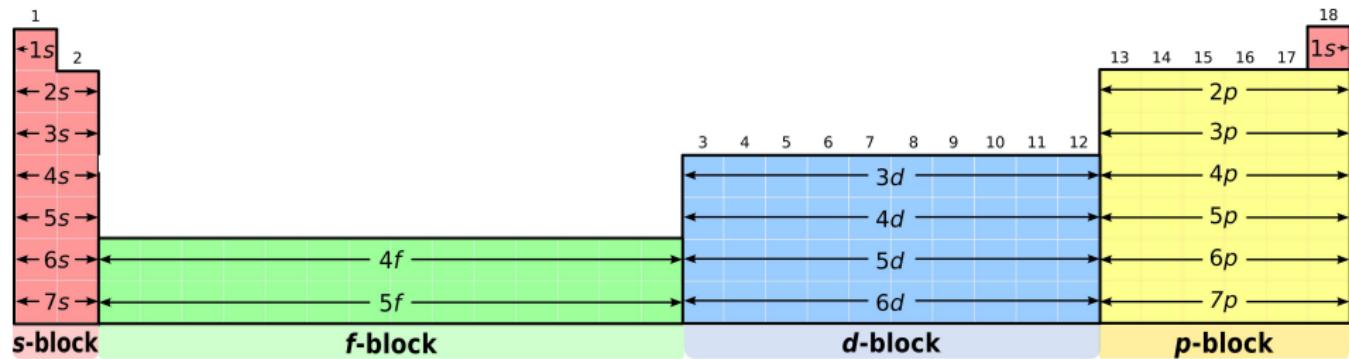
Lanthanides and actinides

1 H																				2 He
3 Li	4 Be																			10 Ne
11 Na	12 Mg																			18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr			
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe			
55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn			
87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo			
119 Uun																				
* Lanthanides		57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu				
** Actinides		89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr				

Credit: <http://www.sciencegeek.net>

Lanthanides and actinides

Credit: <http://www.sciencegeek.net>



Credit: User:DePiep (Wikipedia)

19 Jonas Lippuner

- ▶ Creating nuclides out of nucleons (protons and neutrons)
- ▶ Cost: overcoming Coulomb barrier (but there is a loophole)
- ▶ Reward: ~ 8 MeV per nucleon binding energy
- ▶ Sources
 - ▶ Big Bang
 - ▶ Stellar fusion
 - ▶ Supernovae
 - ▶ Neutron star mergers (NS–NS and NS–BH)

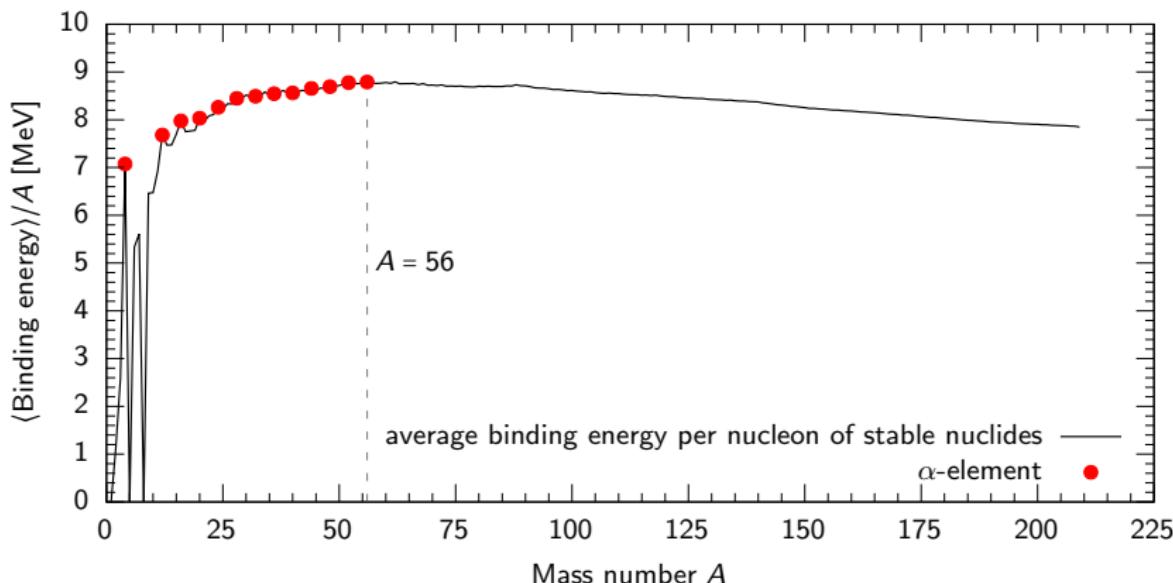
- ~ 100 s after Big Bang, $T \sim 1$ GK

H	^4He	D/H	$^3\text{He}/\text{H}$	$^7\text{Li}/\text{H}$
75.2%	24.8%	3×10^{-5}	1×10^{-5}	1.5×10^{-10}
by mass	by mass			predicted 5×10^{-10} , 4σ discrepancy

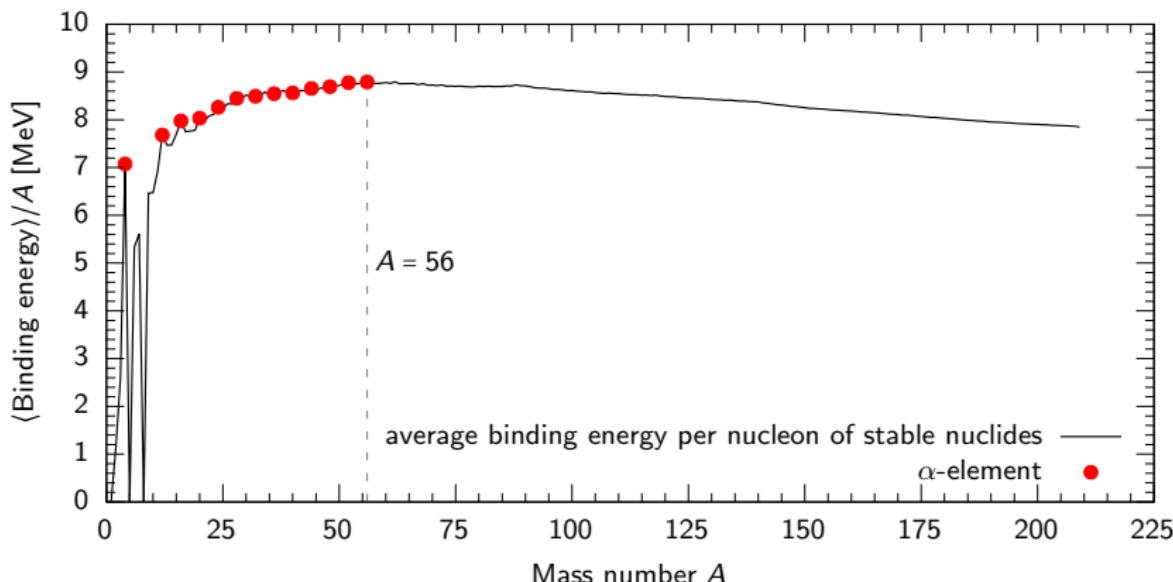


Credit: NASA / CXC / M. Weiss, note that such big nuclides were not produced in BBN

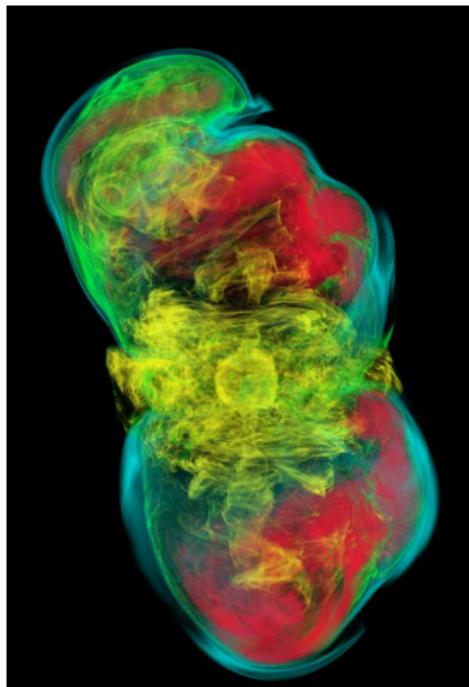
- ▶ p-p Coulomb barrier: $\sim 1 \text{ MeV} \sim 10^{10} \text{ K}$
- ▶ Sun's core temperature: $\sim 1.6 \times 10^7 \text{ K}$
- ▶ Produces mostly α -elements: ${}^4\text{He}$, ${}^{12}\text{C}$, ${}^{16}\text{O}$, ${}^{20}\text{Ne}$, ${}^{24}\text{Mg}$, ${}^{28}\text{Si}$, ${}^{32}\text{S}$, ${}^{36}\text{Ar}$,
 ${}^{40}\text{Ca}$, ${}^{44}\text{Ti}^*$, ${}^{48}\text{Cr}^*$, ${}^{52}\text{Fe}^*$, ${}^{56}\text{Ni}^*$ (* = unstable)



- ▶ p-p Coulomb barrier: $\sim 1 \text{ MeV} \sim 10^{10} \text{ K}$
- ▶ Sun's core temperature: $\sim 1.6 \times 10^7 \text{ K}$ Quantum tunneling!
- ▶ Produces mostly α -elements: ${}^4\text{He}$, ${}^{12}\text{C}$, ${}^{16}\text{O}$, ${}^{20}\text{Ne}$, ${}^{24}\text{Mg}$, ${}^{28}\text{Si}$, ${}^{32}\text{S}$, ${}^{36}\text{Ar}$, ${}^{40}\text{Ca}$, ${}^{44}\text{Ti}^*$, ${}^{48}\text{Cr}^*$, ${}^{52}\text{Fe}^*$, ${}^{56}\text{Ni}^*$ (* = unstable)

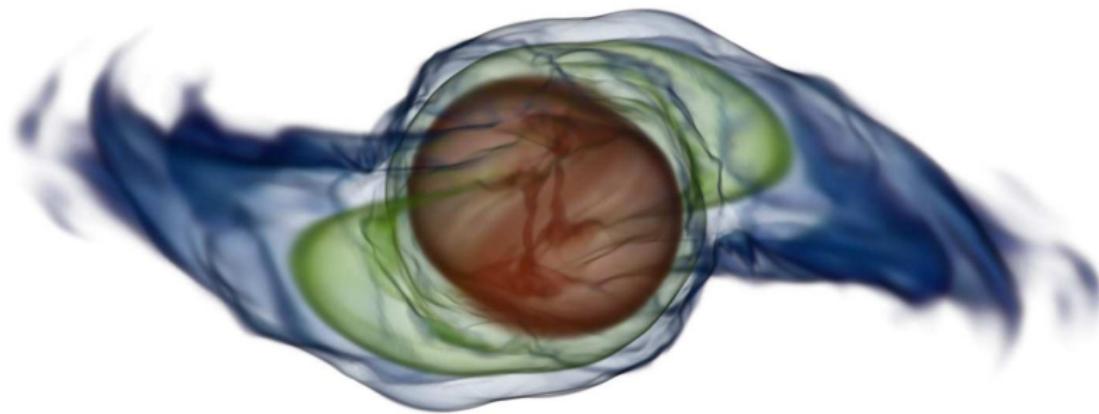


- ▶ Thermonuclear (Type Ia)
 - ▶ Thermonuclear explosion of one or two (?) white dwarf(ves)
 - ▶ Produces mostly iron-peak elements through nuclear statistical equilibrium (NSE): Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn
- ▶ Core-collapse (Type II, Ib/c)
 - ▶ Fluorine (ν knocks out a p from ^{20}Ne)
 - ▶ Produces some iron-peak elements
 - ▶ Ejects s-process elements
 - ▶ Maybe r-process



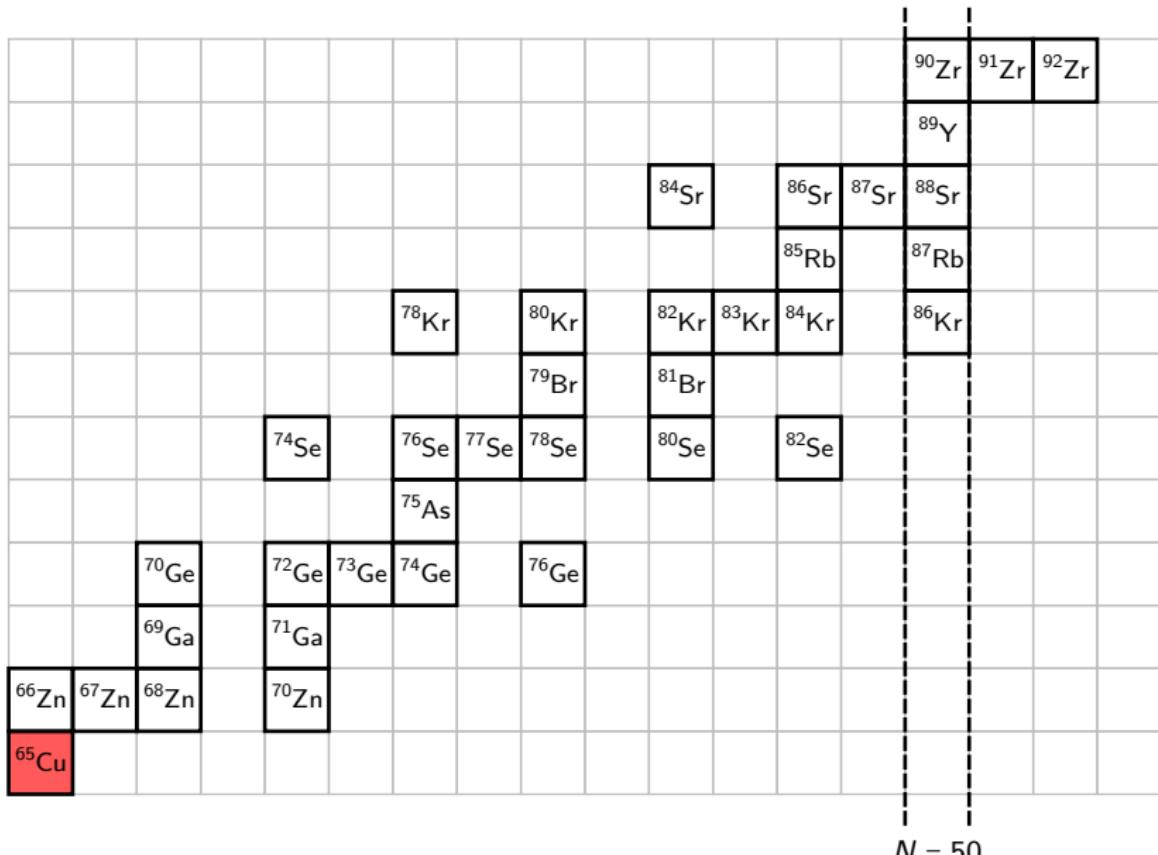
Credit: S. Richers, P. Mösta

- ▶ r-process in neutron-rich ejecta
- ▶ Ejecta: $\sim 10^{-3} - 10^{-2} M_{\odot}$

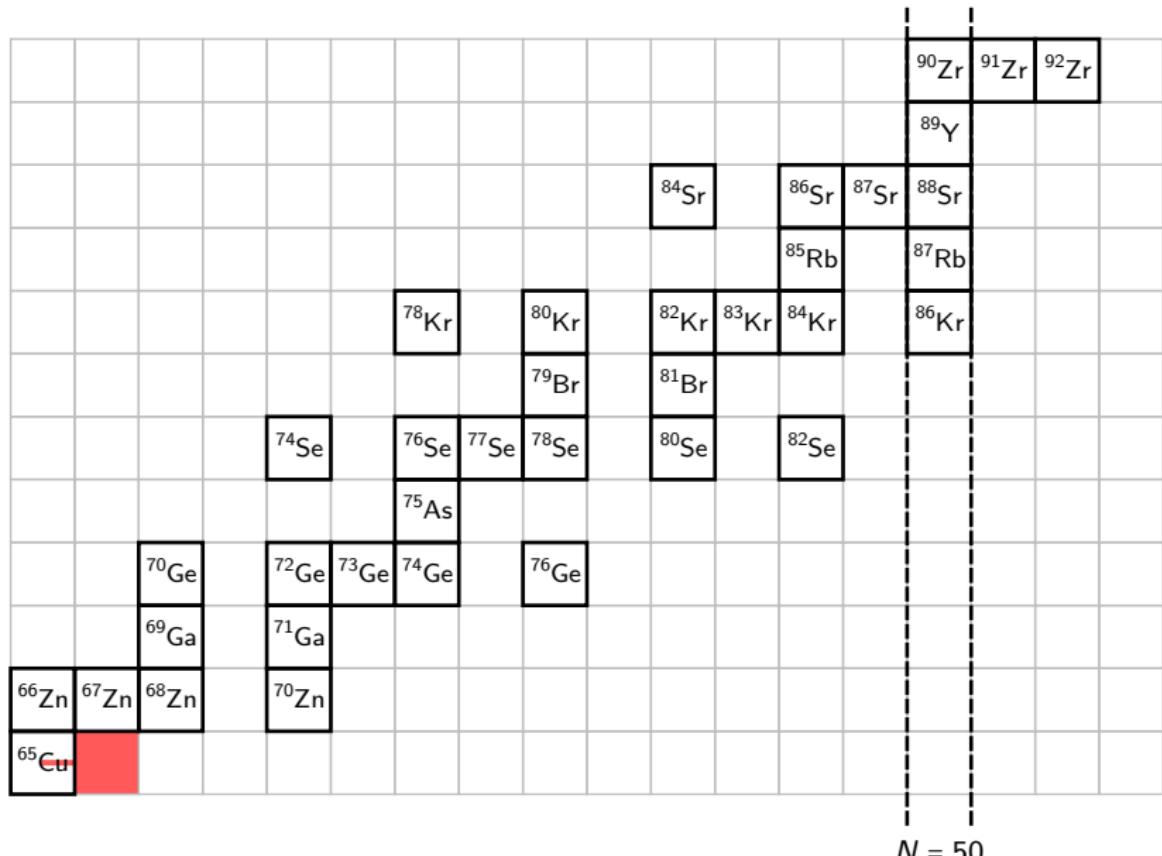


Credit: R. Haas

s-process Path

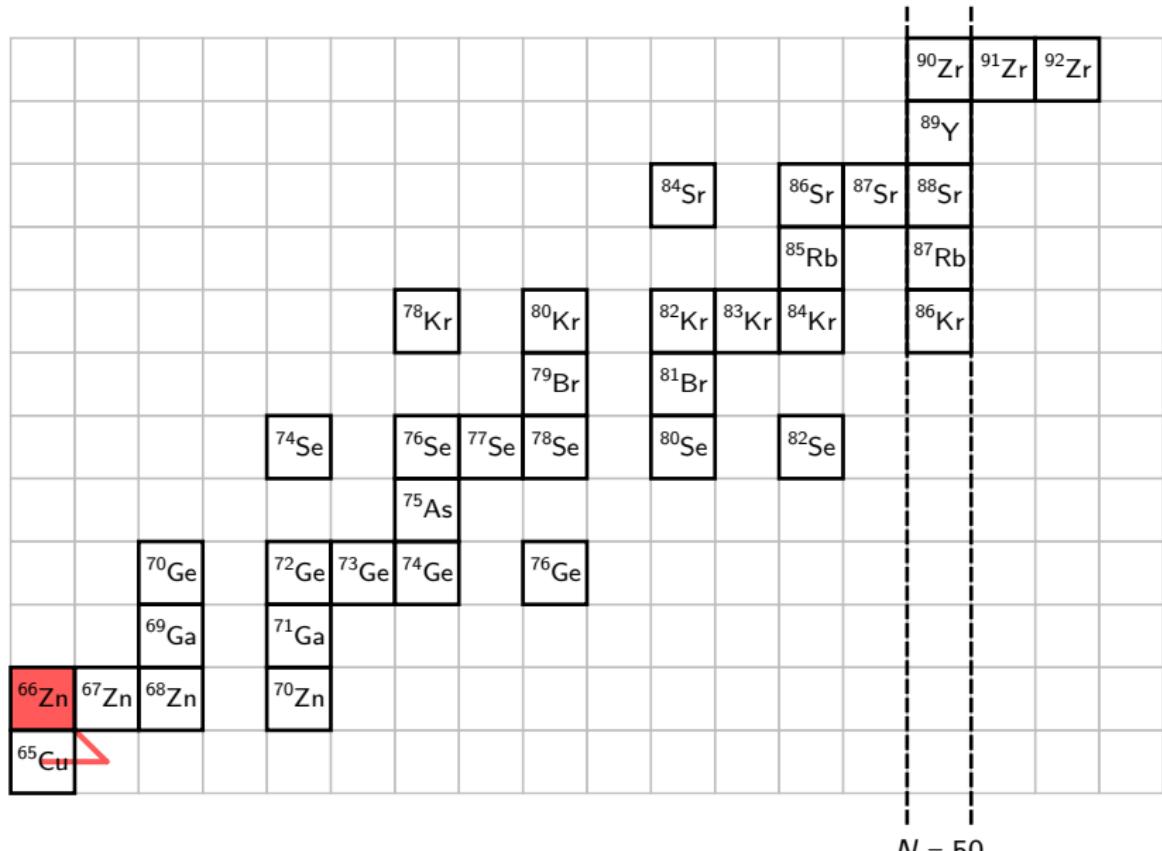


s-process Path



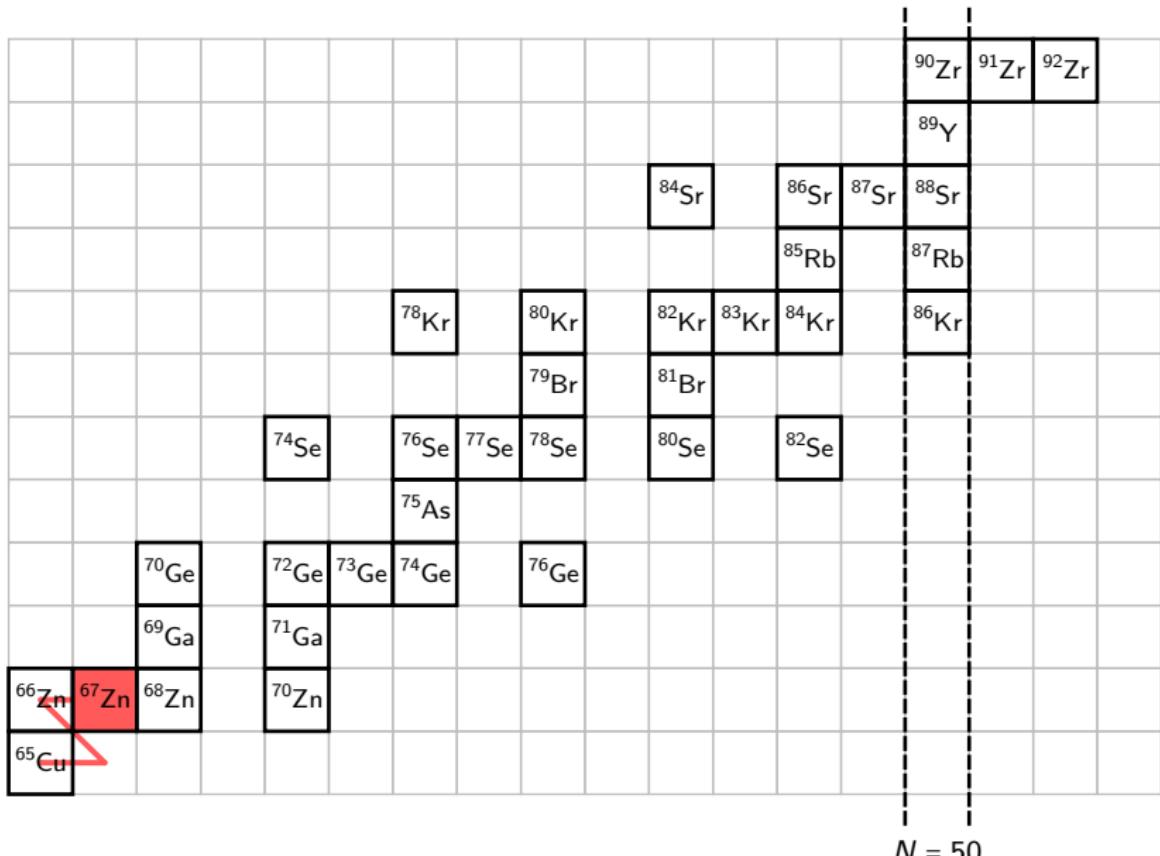
$N = 50$

s-process Path

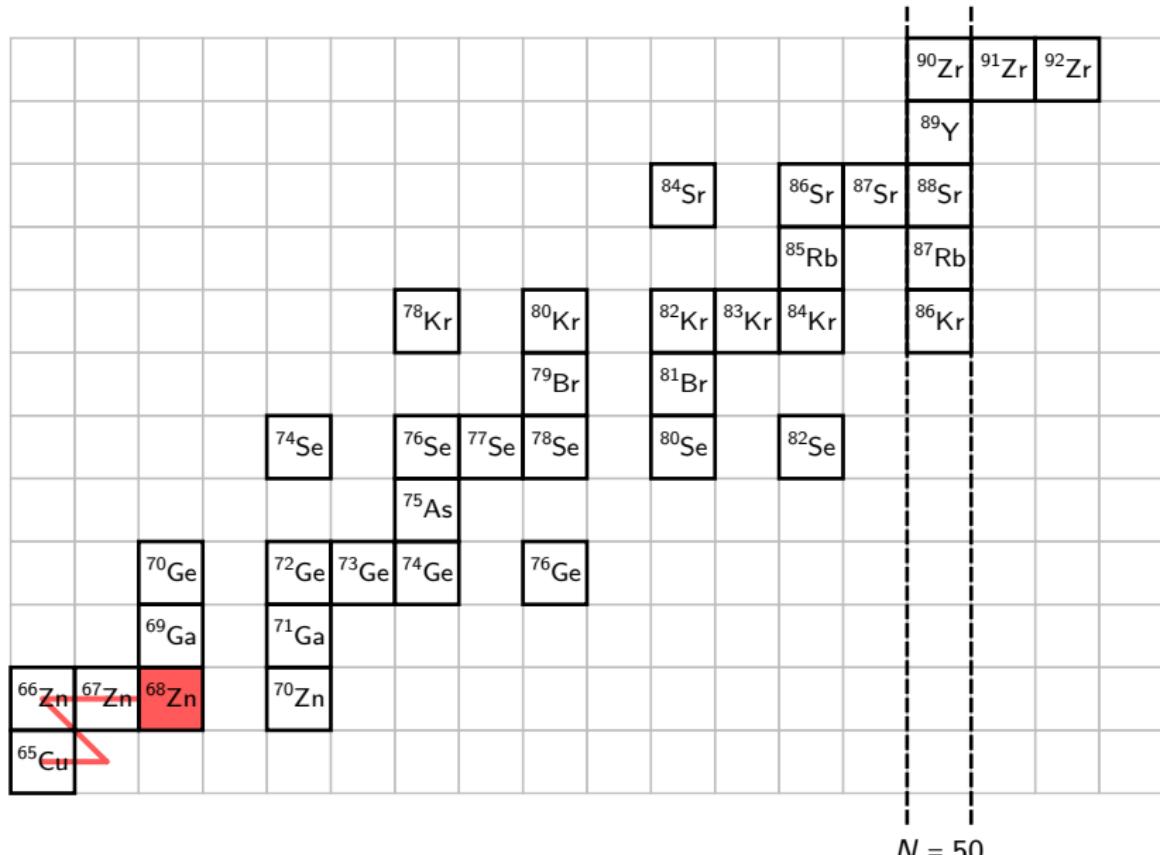


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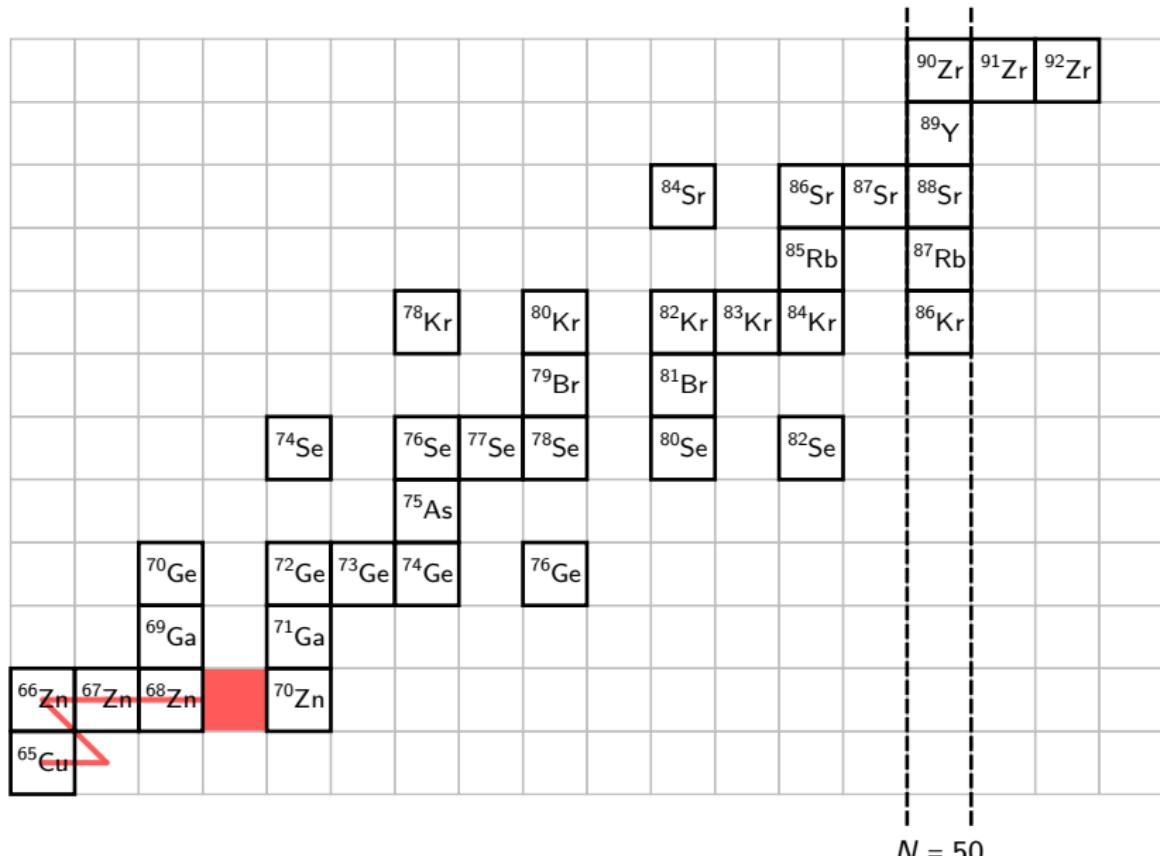
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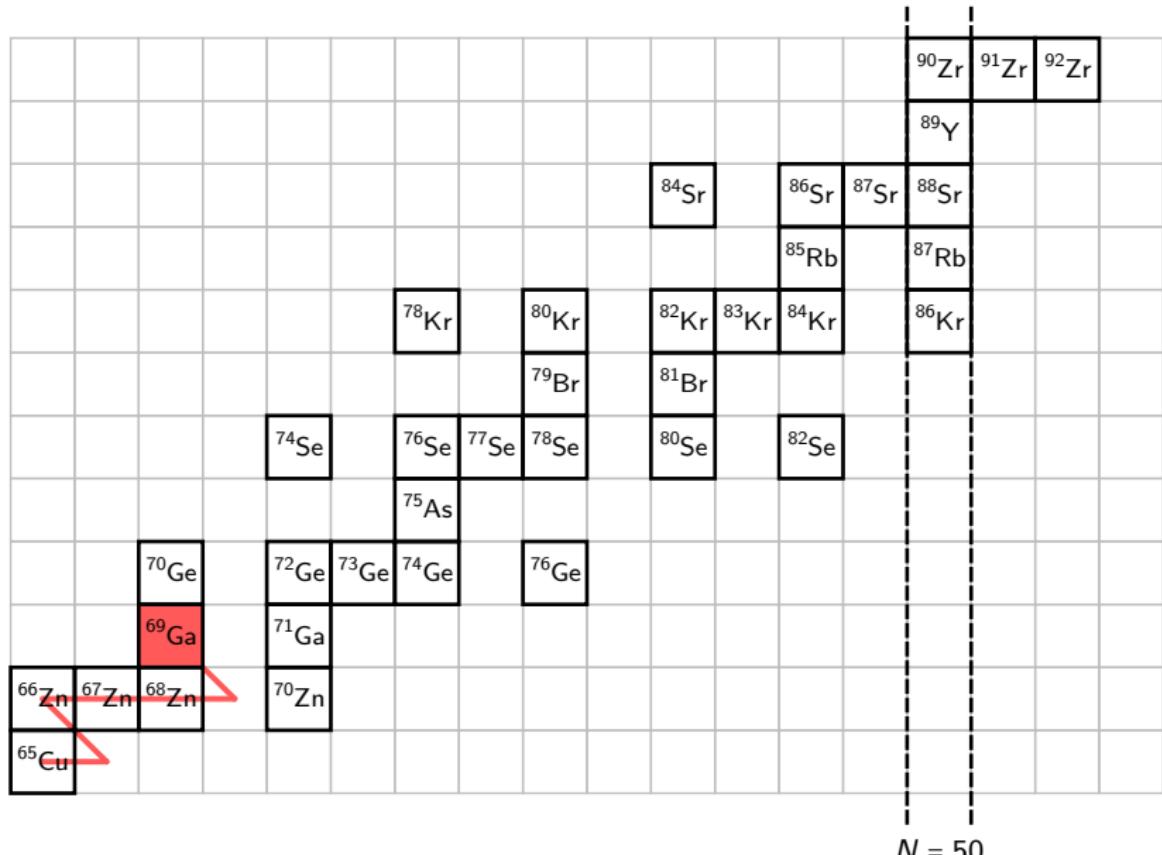
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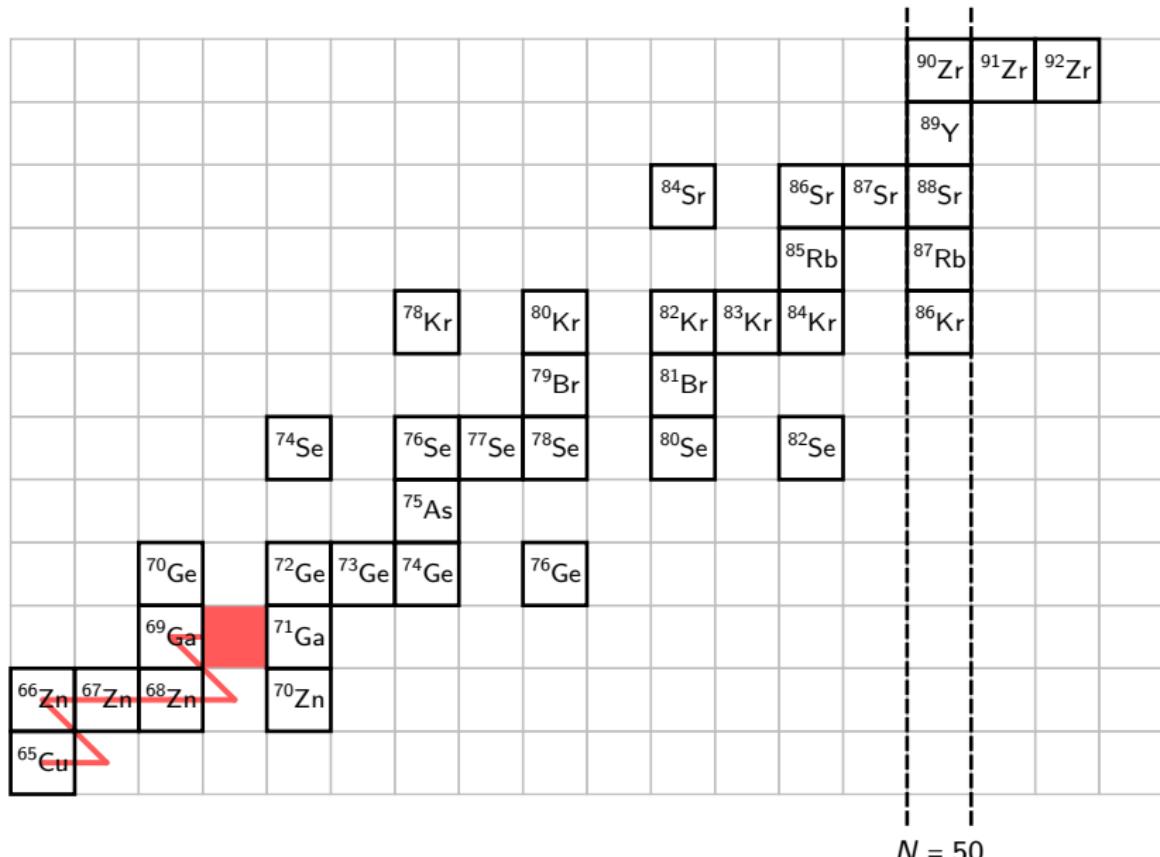
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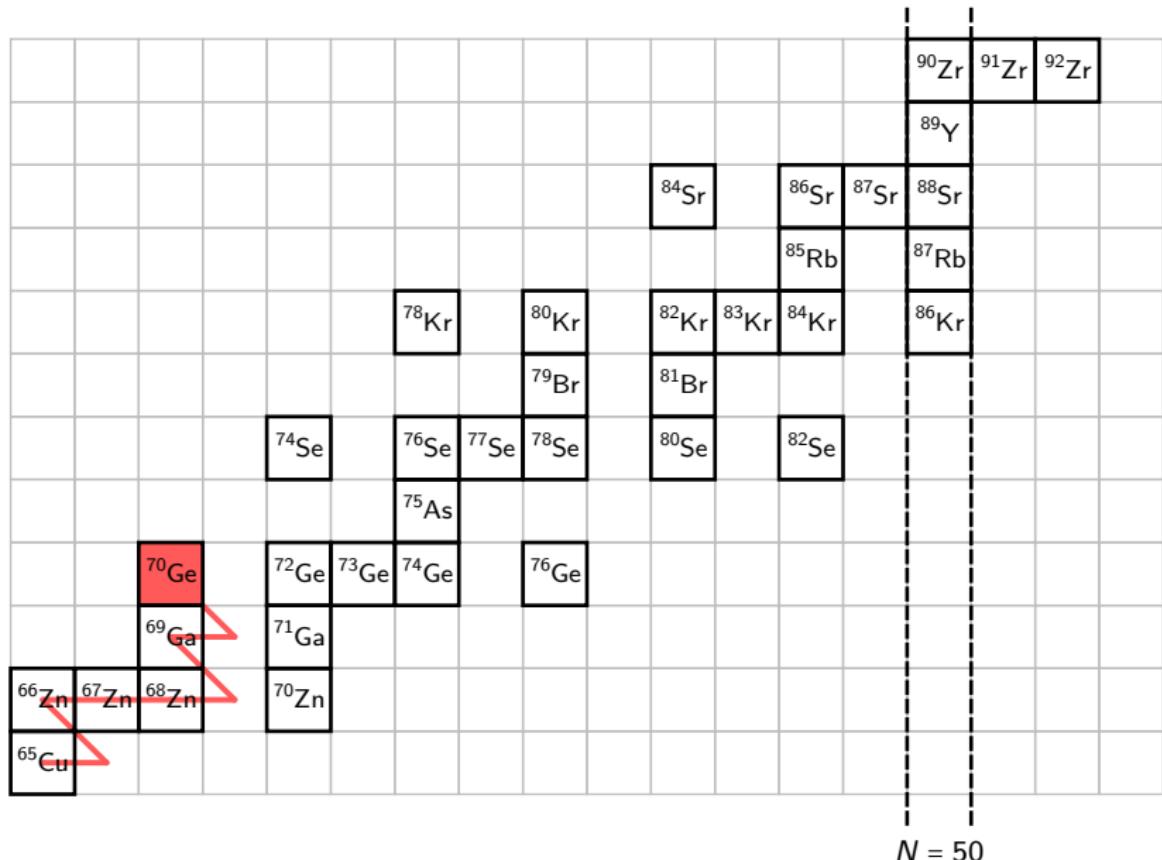
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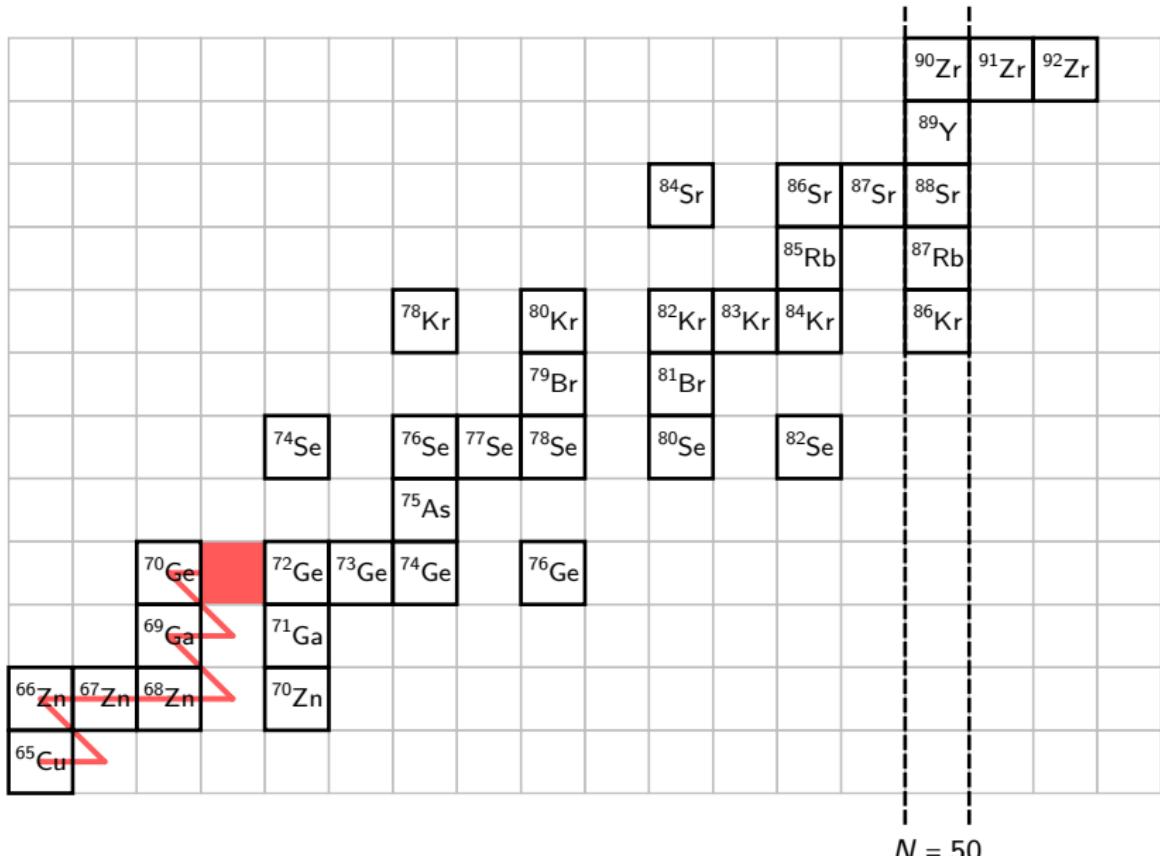
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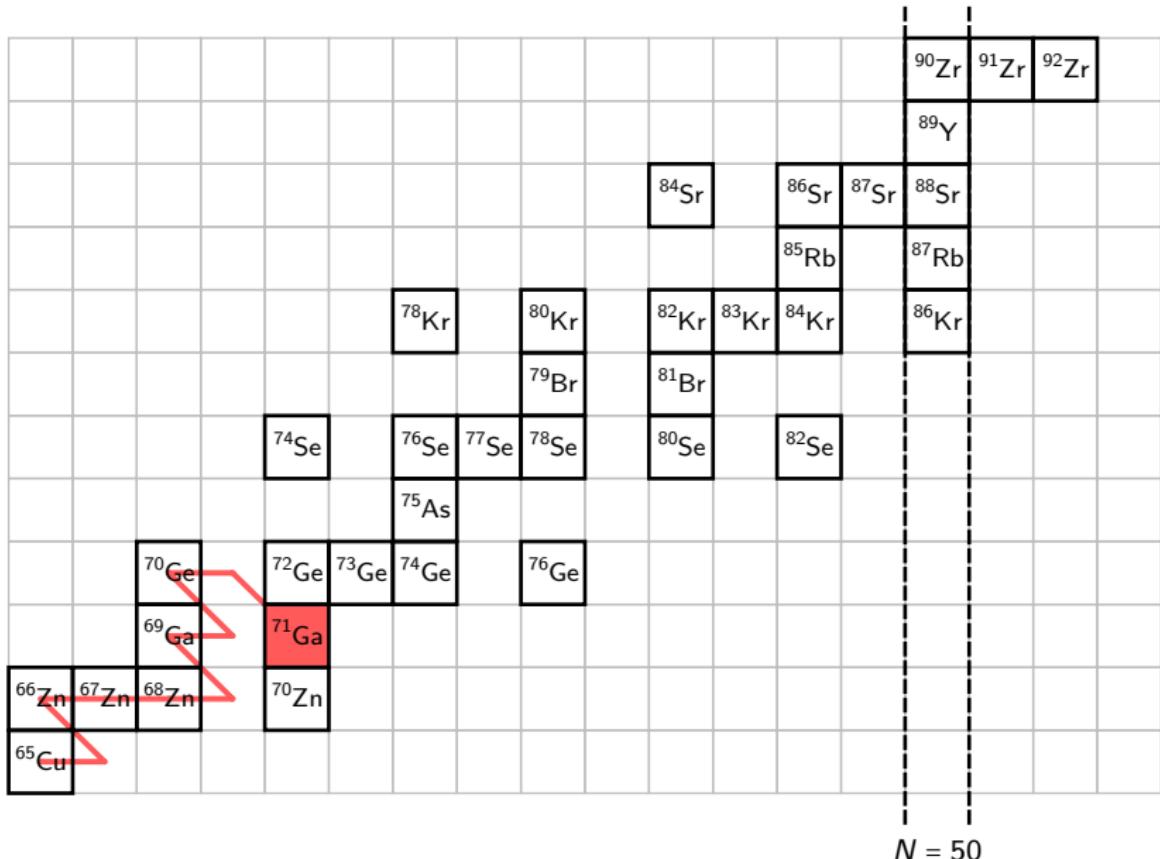
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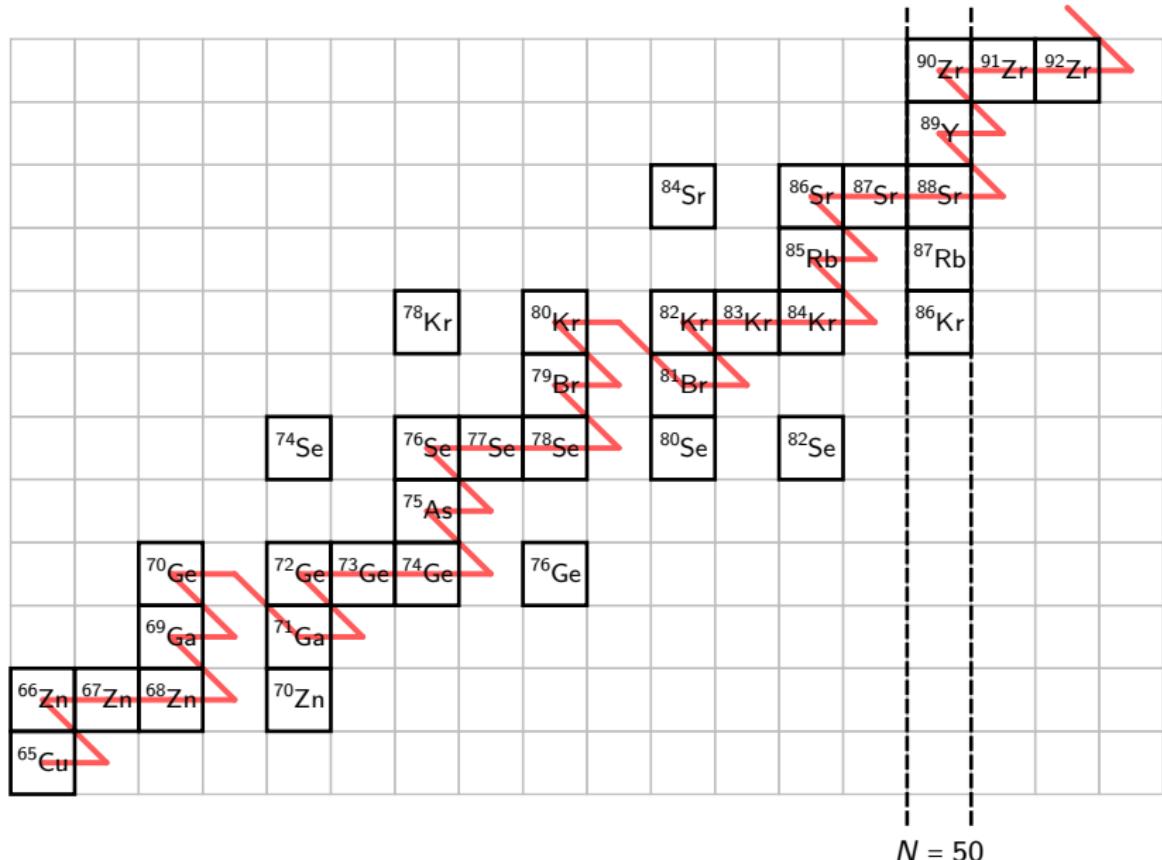
s-process Path



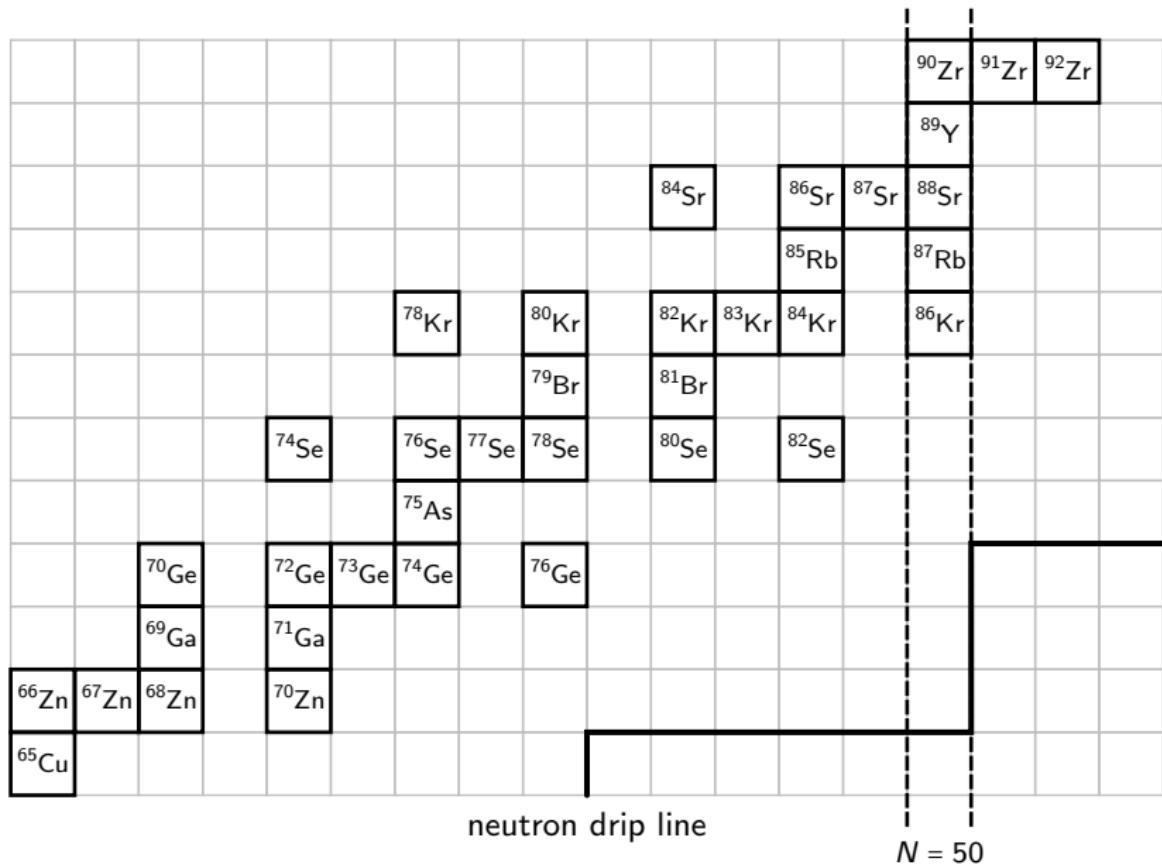
s-process Path



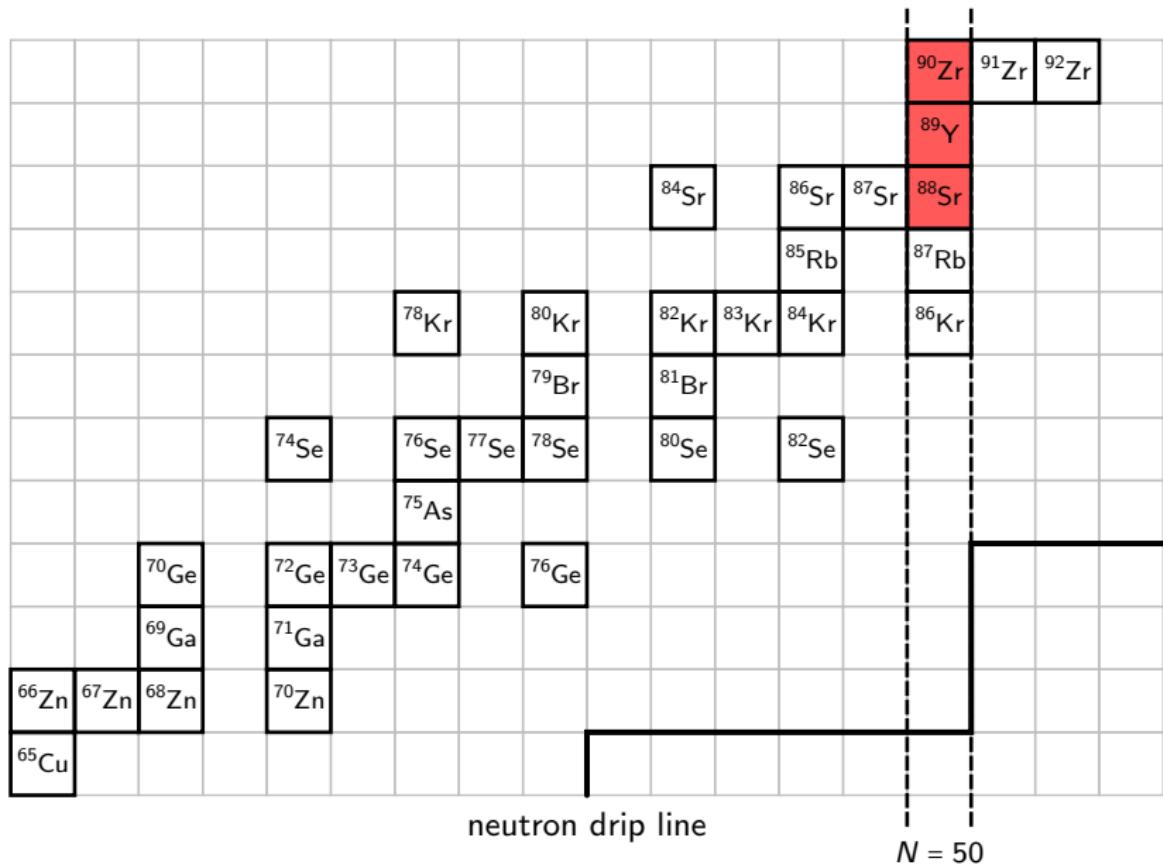
s-process Path



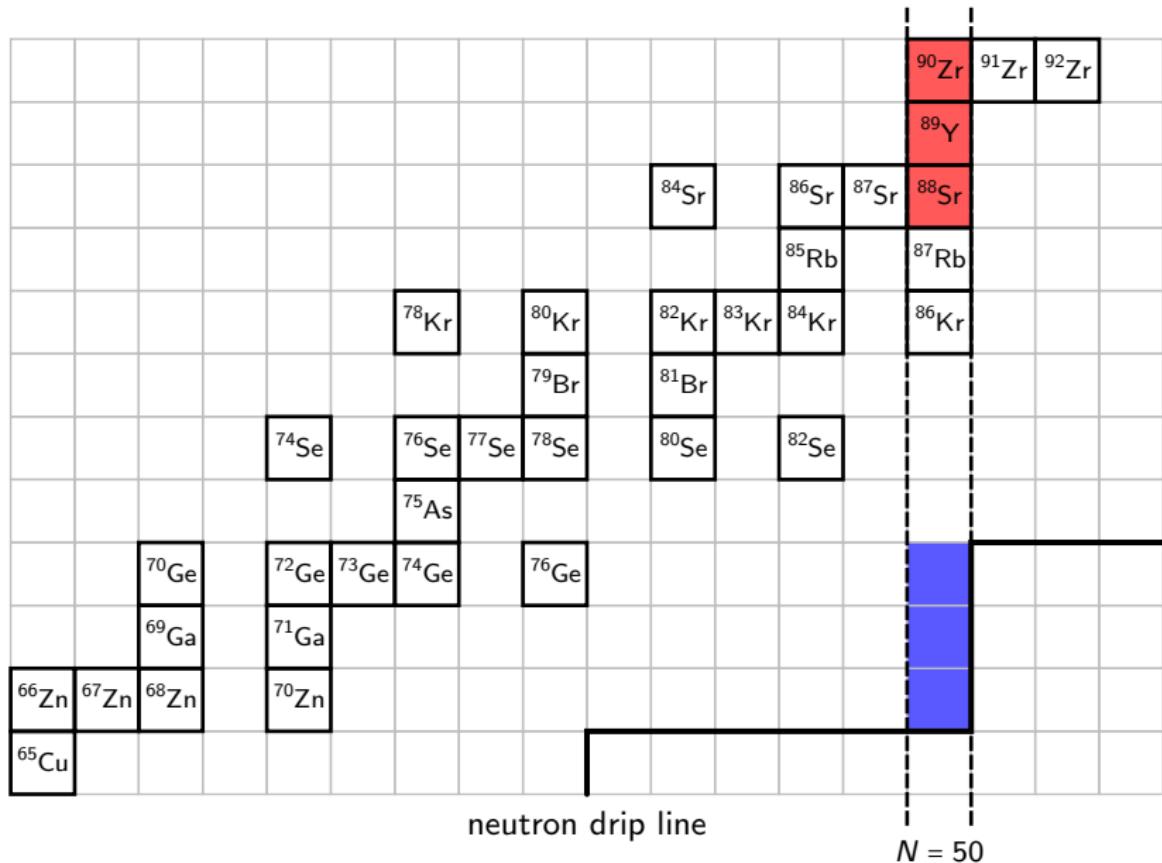
Double Peaks due to Closed Neutron Shells



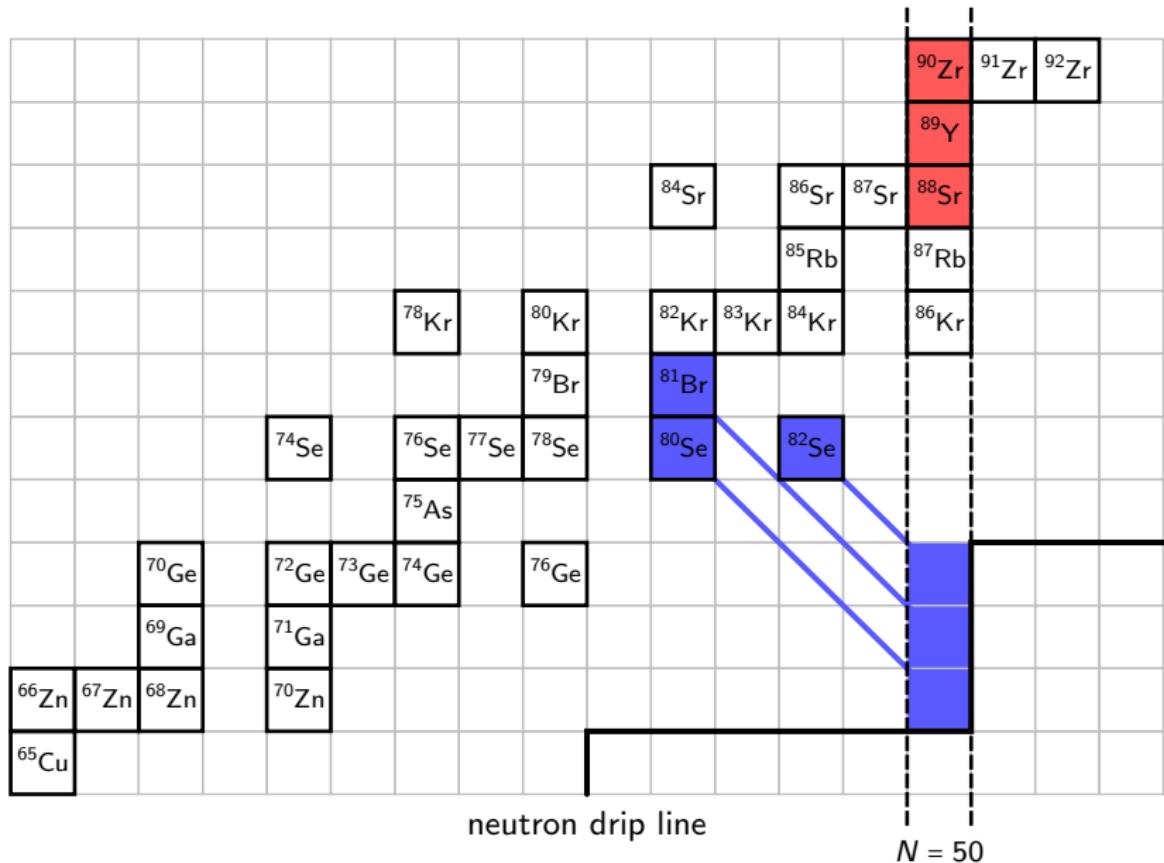
Double Peaks due to Closed Neutron Shells



Double Peaks due to Closed Neutron Shells

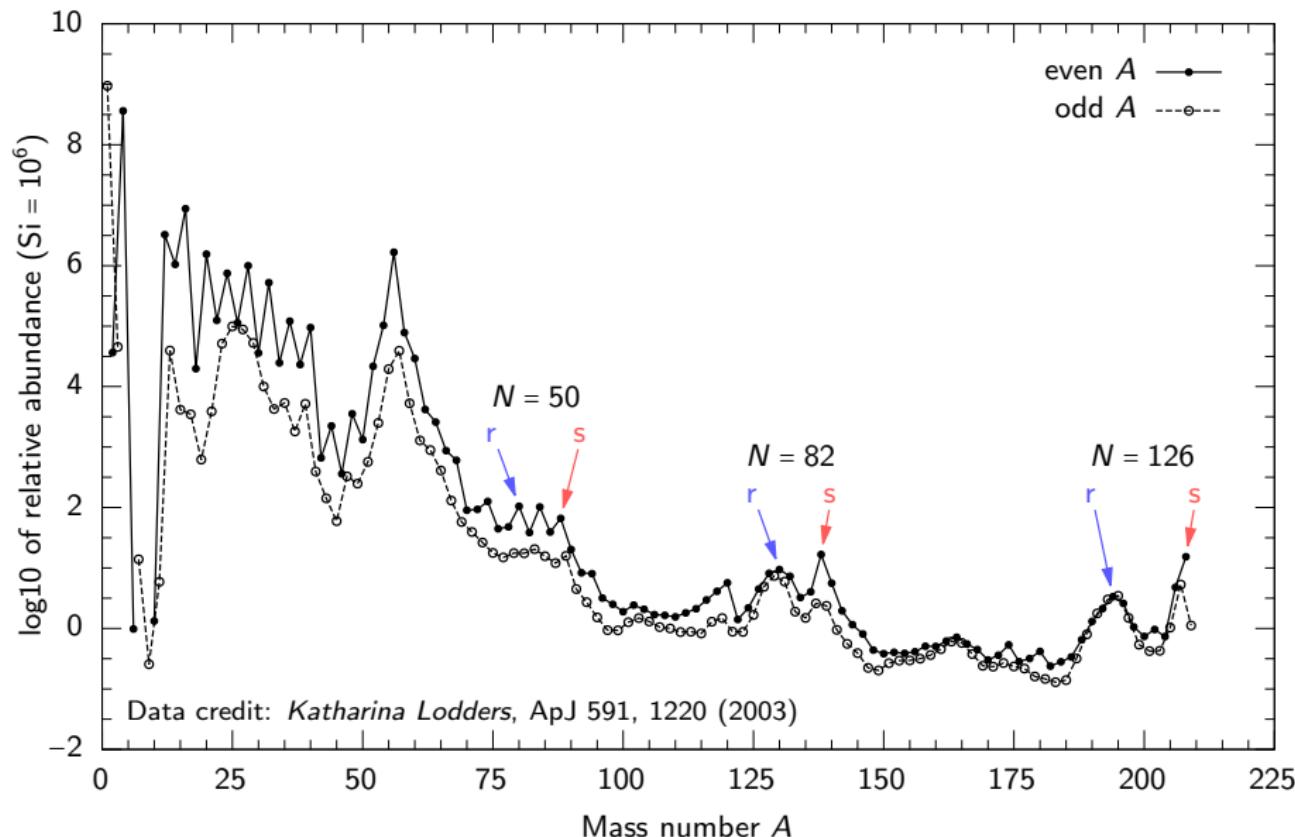


Double Peaks due to Closed Neutron Shells



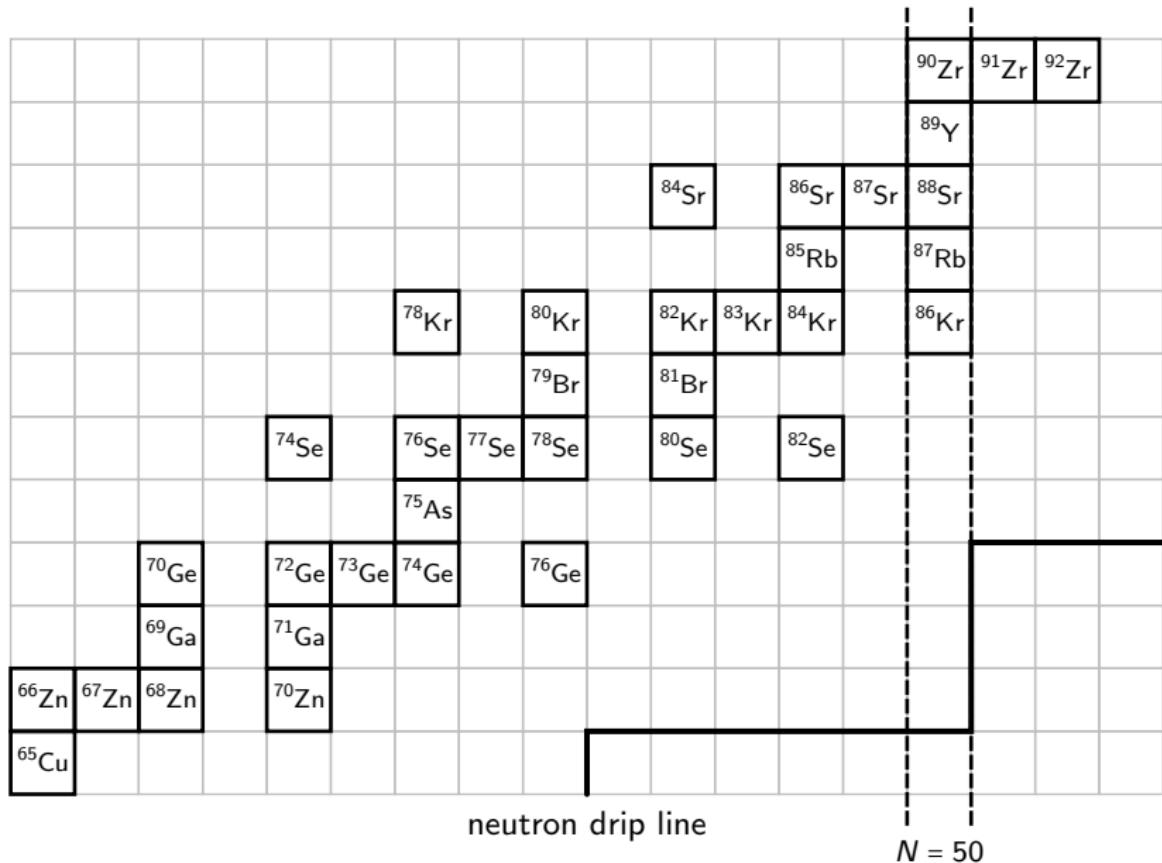
Solar System Abundances

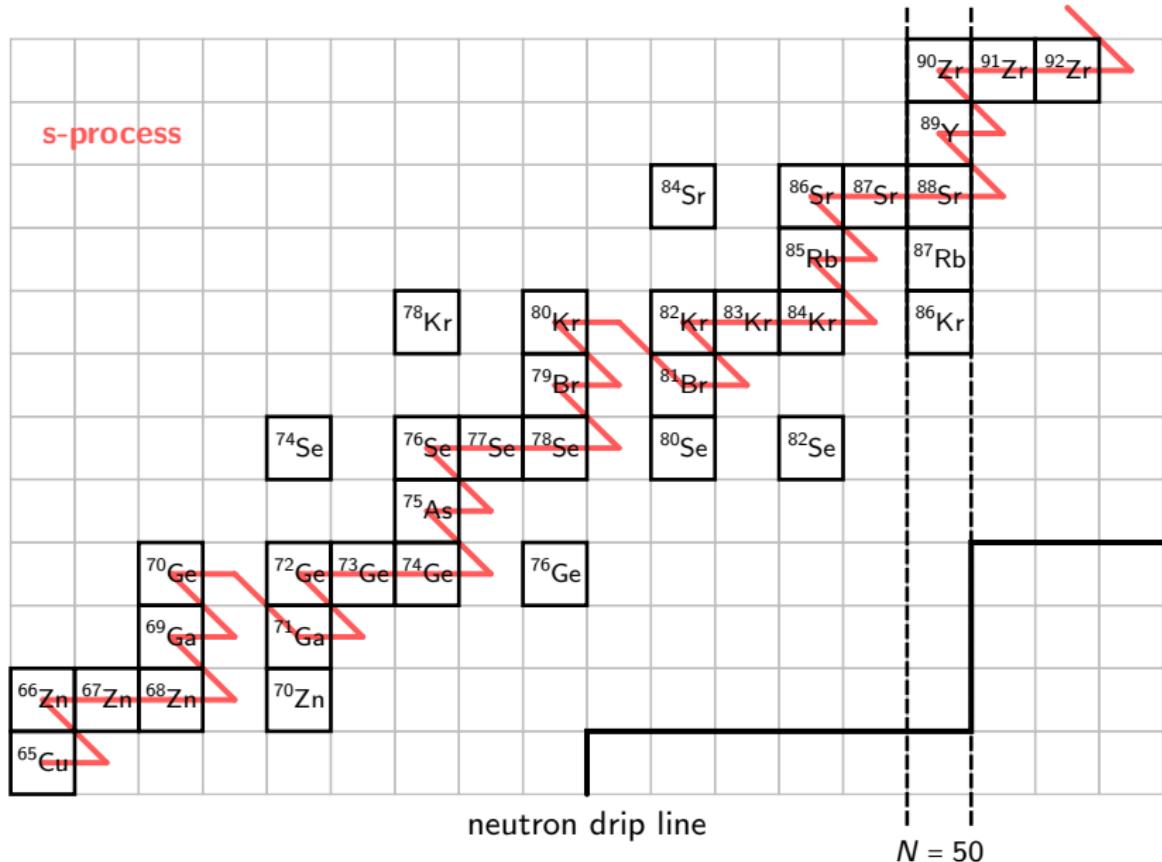
Caltech

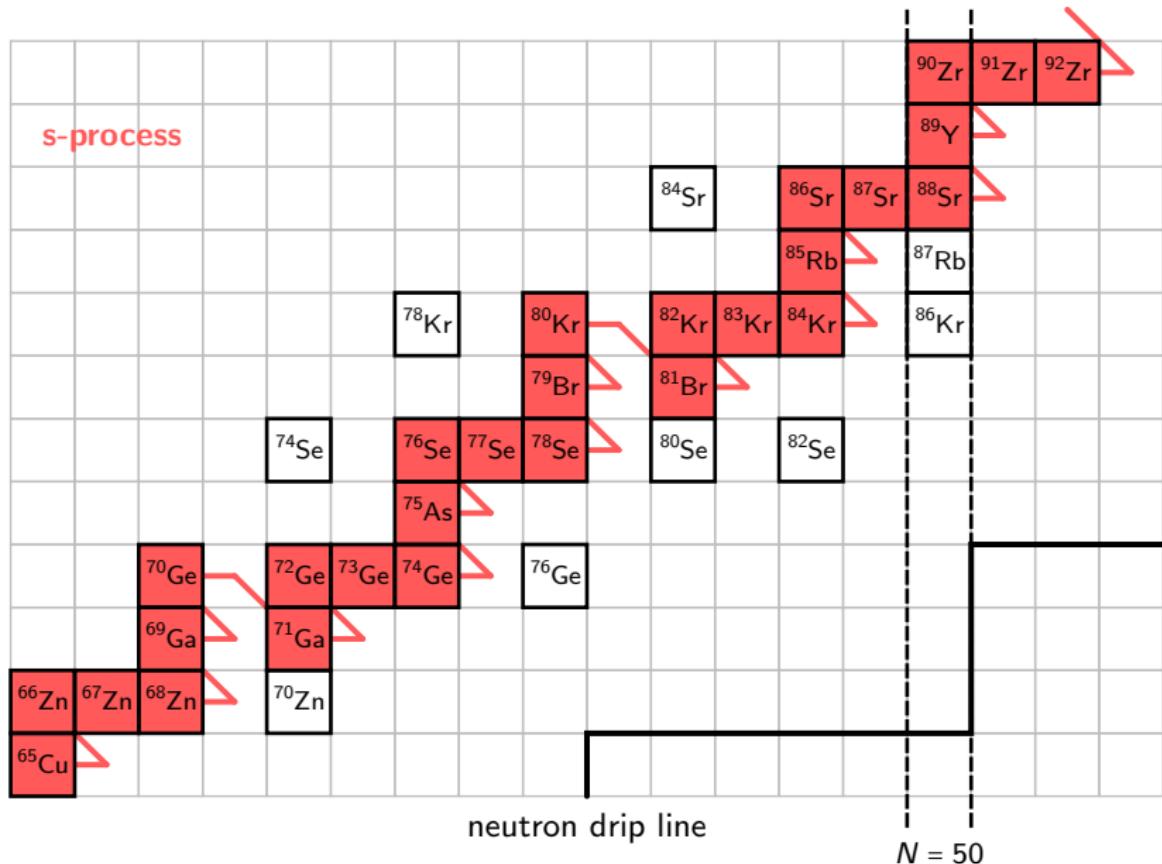


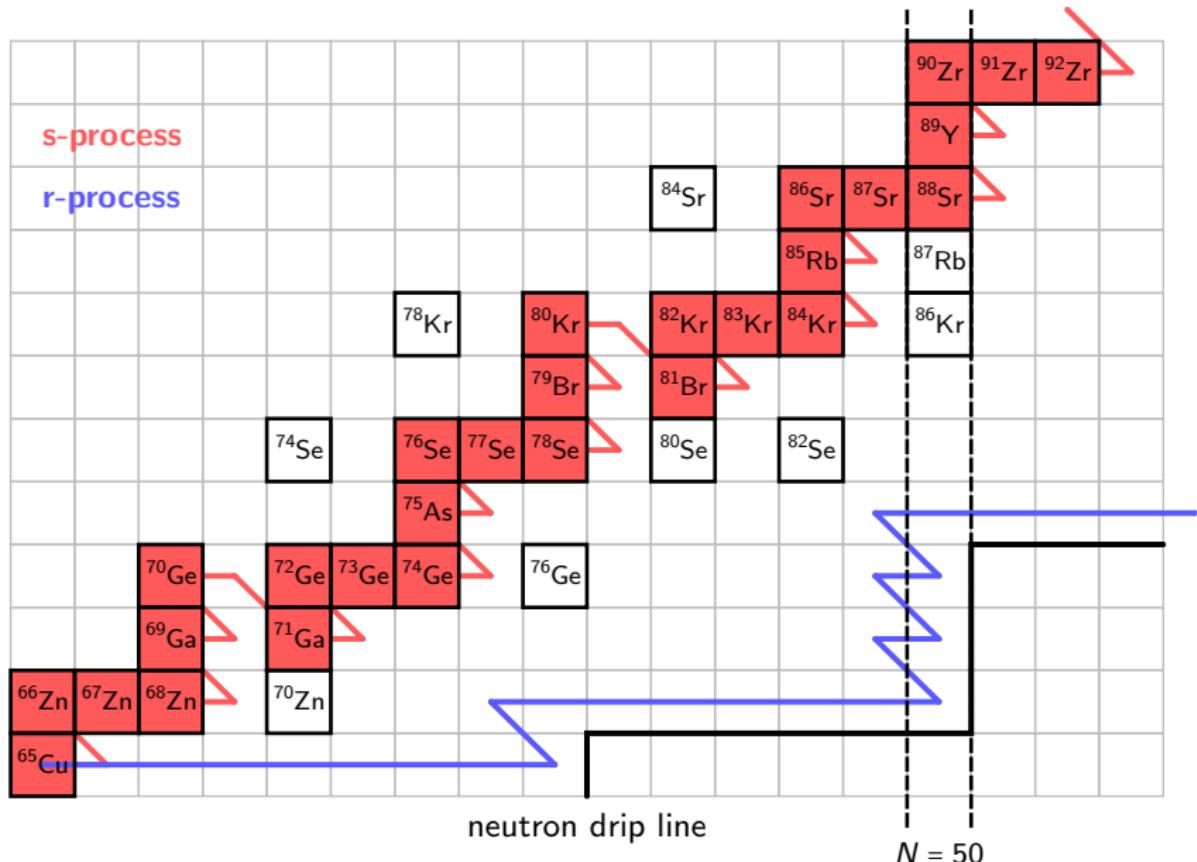
	s-process	r-process
mechanism	neutron capture, β^- decay	No Coulomb barrier!
τ_n	$10^2 - 10^5$ yr	$\ll \tau_{\beta^-}$
τ_{β^-}	$\ll \tau_n$	$0.01 - 10$ s
site	inside massive stars	supernovae? NS-NS/BH mergers?
neutron source	$^{13}\text{C} + ^4\text{He} \rightarrow ^{16}\text{O} + \text{n}$ $^{22}\text{Ne} + ^4\text{He} \rightarrow ^{25}\text{Mg} + \text{n}$	neutrino driven wind tidal ejecta of NS material
path	valley of stability	neutron drip line
peaks*	$A = 88, 138, 208$ strontium, barium, lead	$A = 80, 130, 194$ selenium, xenon, platinum

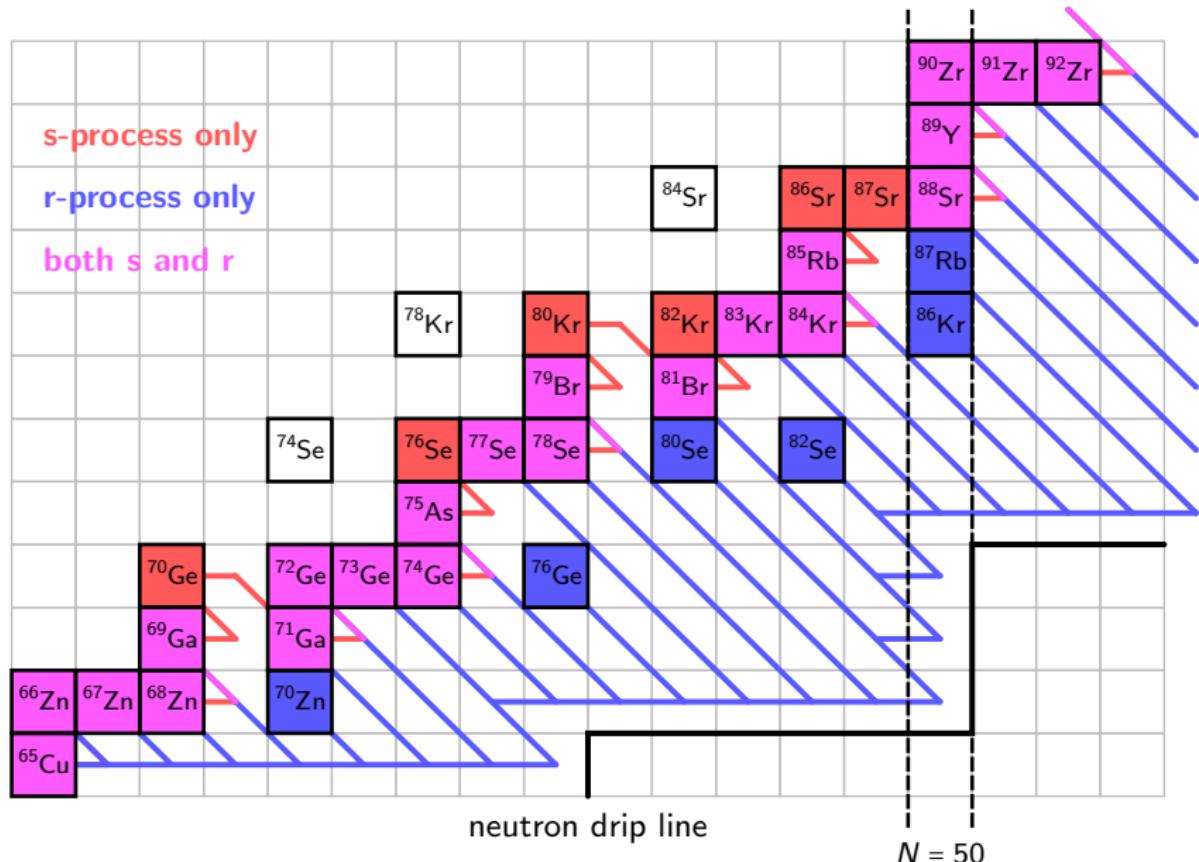
* due to closed neutron shells at $N = 50, 82, 126$











- ▶ General purpose nuclear reaction network
- ▶ Inputs:
 - ▶ List of nuclides (~ 8000)
 - ▶ List of nuclear reactions and rates (~ 100,000)
 - ▶ Initial composition, initial entropy / temperature
 - ▶ Density vs. time
- ▶ Outputs:
 - ▶ Composition vs. time
 - ▶ Temperature, entropy, heating rate vs. time

Science

- ▶ Helmholtz equation of state (EOS)
- ▶ Calculate nuclear statistical equilibrium (NSE)
- ▶ Calculate inverse rates from *detailed balance* to be consistent with NSE
- ▶ NSE evolution mode

Code

- ▶ Object-oriented C++11 (with CMake build system)
- ▶ Python bindings (with SWIG)
- ▶ Support for different matrix solver packages
 - ▶ Sparse: Intel MKL, Trilinos (KLU, UMFPACK, SuperLU), Pardiso
 - ▶ Dense: LAPACK, Trilinos (LAPACK), Armadillo
- ▶ Convenient HDF5 output
- ▶ Make movie with chart of nuclides
- ▶ Open source (soon)

Consider reaction



$$\begin{aligned} \text{cross section} = \sigma &= \frac{\# \text{ of reactions per target } [j] \text{ per second}}{\text{flux of projectiles } [k]} \\ &= \frac{R/(Vn_j)}{n_k v} = \frac{r}{n_j n_k v}, \end{aligned} \quad (2)$$

and so

$$r = \frac{R}{V} = \sigma v n_j n_k = \# \text{ of reactions per second per volume}, \quad (3)$$

where

R = # of reactions per second,

V = volume,

$n_{j,k}$ = number density of species $[j]$, $[k]$,

v = relative speed between $[j]$ and $[k]$.

In general

$$r_{j,k} = \int \sigma(\|\mathbf{v}_j - \mathbf{v}_k\|) \|\mathbf{v}_j - \mathbf{v}_k\| d^3 n_j d^3 n_k, \quad (4)$$

using Boltzmann distribution

$$r_{j,k} = n_j n_k \langle \sigma v \rangle_{j,k} = n_j n_k \left(\frac{8}{\mu \pi} \right)^{1/2} (k_B T)^{-3/2} \int_0^\infty E \sigma(E) e^{-E/(k_B T)} dE, \quad (5)$$

where

$$\mu = \text{reduced mass} = \frac{m_j m_k}{m_j + m_k},$$

T = temperature,

k_B = Boltzmann constant.

Note that $\langle \sigma v \rangle_{j,k} = \langle \sigma v \rangle_{j,k}(T)$.

Define *abundance*

$$Y_i = \frac{n_i}{n_B} = \frac{\# \text{ of species [i]}}{\# \text{ of baryons}}, \quad (6)$$

where n_B is baryon number density, then for $[j] + [k] \rightarrow [m]$

$$\dot{Y}_m = \frac{r_{j,k} V}{\# \text{ of baryons}} = \frac{r_{j,k}}{n_B} = \frac{Y_j n_B Y_k n_B \langle \sigma v \rangle_{j,k}}{n_B} = Y_j Y_k \lambda_{j,k}, \quad (7)$$

where

$$\lambda_{j,k} = n_B \langle \sigma v \rangle_{j,k} = N_A \rho \langle \sigma v \rangle_{j,k}(T) = \lambda_{j,k}(T, \rho), \quad (8)$$

where N_A is Avogadro's number, and ρ is the mass density.

And, of course

$$\dot{Y}_j = \dot{Y}_k = -\dot{Y}_m. \quad (9)$$

In general

$$\dot{Y}_i = \sum_{\alpha} N_i^{\alpha} \lambda_{\alpha}(T, \rho) \prod_{m \in \mathcal{R}_{\alpha}} Y_m^{|N_m^{\alpha}|}, \quad (10)$$

where

α = index running over all reactions,

N_i^{α} = # of species [i] destroyed/created in α ,

\mathcal{R}_{α} = set of reactants of α .

Example:

$$\dot{Y}_{^4\text{He}} = \underbrace{\dots}_{\text{decay}} + \underbrace{\dots}_{\text{producing reaction}} + \underbrace{\dots}_{\text{destroying reaction}} + \dots \quad (11)$$

$^4\text{He} \rightarrow 2\text{d}$ $\text{p} + ^7\text{Li} \rightarrow 2\text{ }^4\text{He}$ $\text{n} + \text{p} + 2\text{ }^4\text{He} \rightarrow ^7\text{Li} + ^3\text{He}$

In general

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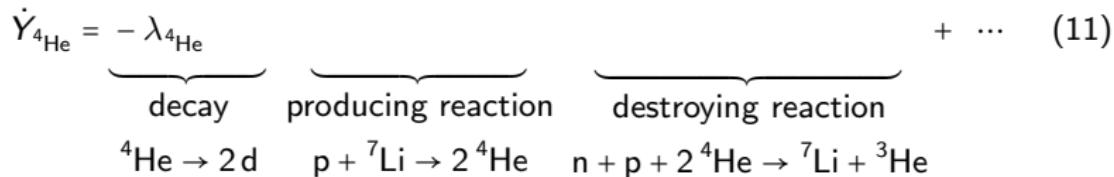
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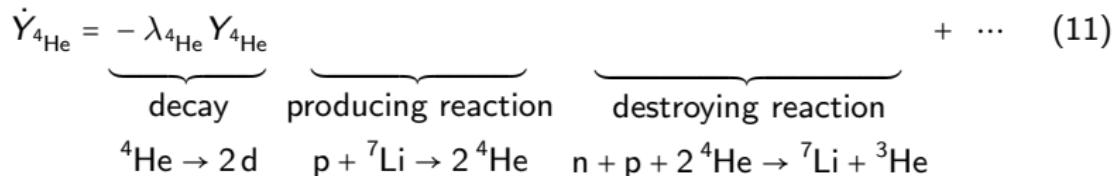
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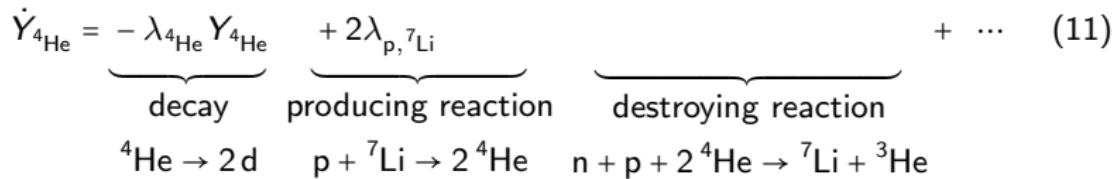
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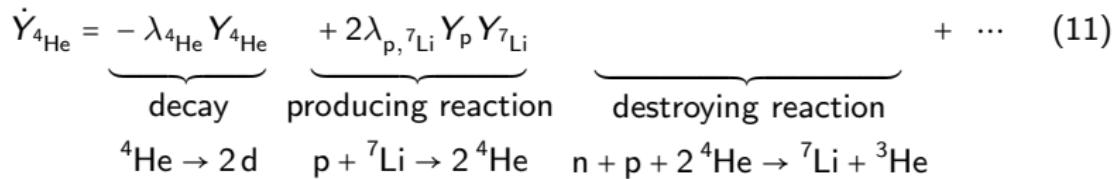
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In general

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Example:

$$\dot{Y}_{^4\text{He}} = \underbrace{-\lambda_{^4\text{He}} Y_{^4\text{He}}}_{\text{decay}} + \underbrace{2\lambda_{p, ^7\text{Li}} Y_p Y_{^7\text{Li}}}_{\text{producing reaction}} - \underbrace{2\lambda_{n,p,2} Y_n Y_p}_{\text{destroying reaction}} + \dots \quad (11)$$

$^4\text{He} \rightarrow 2\text{d}$ $p + ^7\text{Li} \rightarrow 2\text{ }^4\text{He}$ $n + p + 2\text{ }^4\text{He} \rightarrow ^7\text{Li} + ^3\text{He}$

In general

$$\dot{Y}_i = \sum_{\alpha} N_i^{\alpha} \lambda_{\alpha}(T, \rho) \prod_{m \in \mathcal{R}_{\alpha}} Y_m^{|N_m^{\alpha}|}, \quad (10)$$

where

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N_i^{α} = # of species [i] destroyed/created in α ,

\mathcal{R}_{α} = set of reactants of α .

Example:

$$\begin{aligned} \dot{Y}_{^4\text{He}} = & \underbrace{-\lambda_{^4\text{He}} Y_{^4\text{He}}}_{\text{decay}} + \underbrace{2\lambda_{p, ^7\text{Li}} Y_p Y_{^7\text{Li}}}_{\text{producing reaction}} - \underbrace{2\lambda_{n,p,2} {}^4\text{He} Y_n Y_p Y_{^4\text{He}}^2}_{\text{destroying reaction}} + \dots \quad (11) \\ & {}^4\text{He} \rightarrow 2\text{d} \quad p + {}^7\text{Li} \rightarrow 2 {}^4\text{He} \quad n + p + 2 {}^4\text{He} \rightarrow {}^7\text{Li} + {}^3\text{He} \end{aligned}$$

Given \mathbf{Y} , T , and ρ , we have a (big) system of coupled ODEs:

$$\dot{\mathbf{Y}} = \dot{\mathbf{Y}}(\mathbf{Y}, T, \rho). \quad (12)$$

Use implicit method due to stiffness

$$\dot{\mathbf{Y}}(t + \Delta t) = \frac{\mathbf{Y}(t + \Delta t) - \mathbf{Y}(t)}{\Delta t}. \quad (13)$$

Use Newton–Raphson to find unknown $\mathbf{x} = \mathbf{Y}(t + \Delta t)$ by finding root of

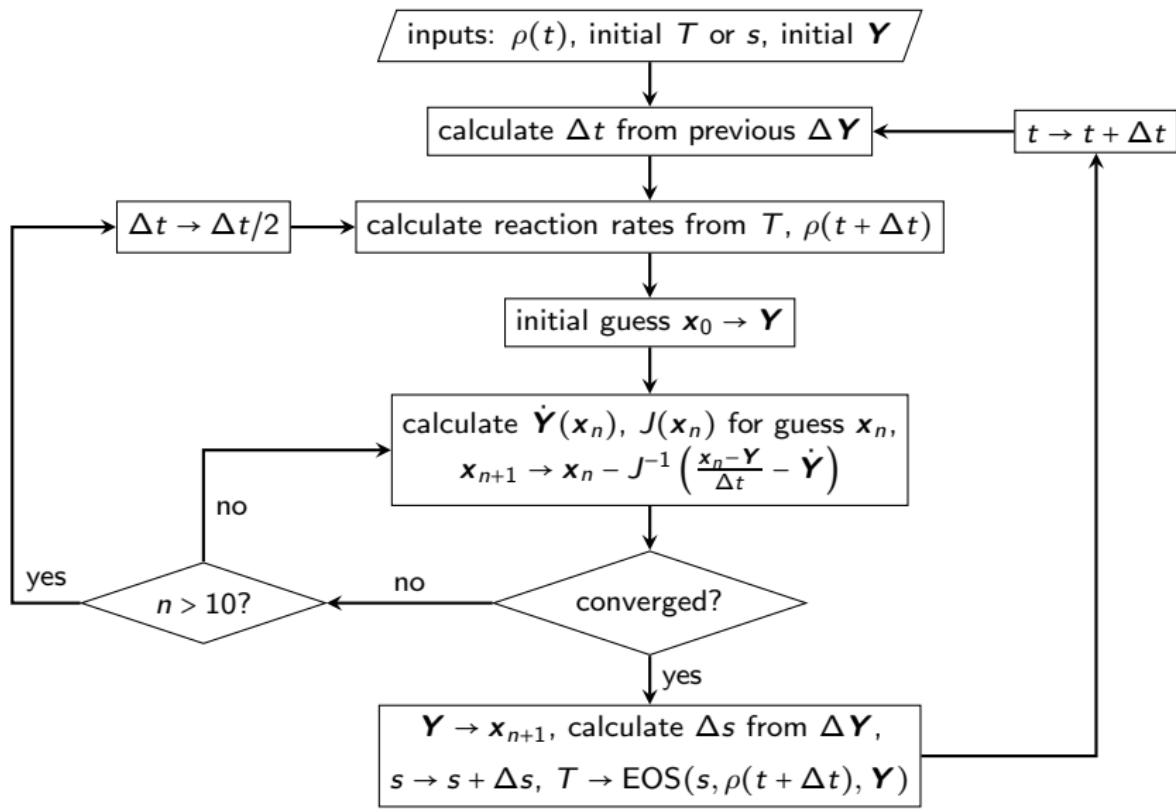
$$\mathbf{F}(\mathbf{x}) = \frac{\mathbf{x} - \mathbf{c}}{\Delta t} - \dot{\mathbf{Y}}(\mathbf{x}, T, \rho) = \mathbf{0}, \quad (14)$$

where $\mathbf{c} = \mathbf{Y}(t)$ is a known constant. Update guess with

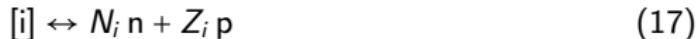
$$\mathbf{x}_{n+1} = \mathbf{x}_n - [J_{\mathbf{F}}(\mathbf{x}_n)]^{-1} \mathbf{F}(\mathbf{x}_n), \quad (15)$$

where the (sparse) Jacobian is

$$(J_{\mathbf{F}})_{ij} = \frac{\partial F_i}{\partial Y_j} = \frac{\delta_{ij}}{\Delta t} - \frac{\partial \dot{Y}_i}{\partial Y_j}. \quad (16)$$



Let species $[i]$ have N_i neutrons and Z_i protons. NSE means the reactions



are in equilibrium so

$$\mu_i = N_i \mu_{\text{n}} + Z_i \mu_{\text{p}}, \quad (18)$$

where μ_x are chemical potentials. Abundance is

$$Y_i = e^{\mu_i/(k_B T)} \frac{G_i(T)}{n_B} \left(\frac{m_i k_B T}{2\pi \hbar^2} \right)^{3/2}, \quad (19)$$

where $G_i(T)$ is internal partition function. Now find μ_{n} and μ_{p} such that

$$1 = \sum_i A_i Y_i \quad \text{and} \quad Y_e = \sum_i Z_i Y_i, \quad (20)$$

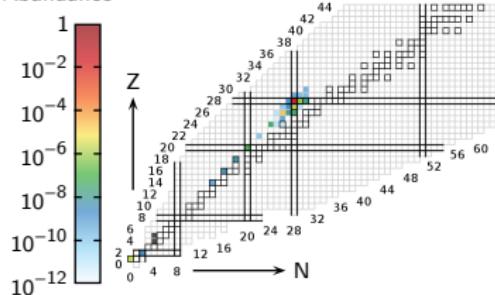
where $A_i = N_i + Z_i$.

Nuclear Statistical Equilibrium (NSE)

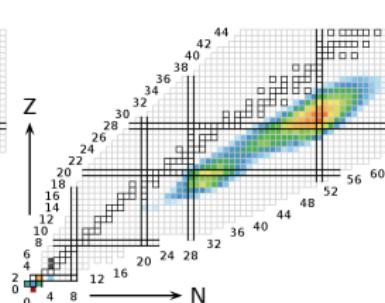
Caltech

$$T = 2.5 \text{ GK}$$
$$\rho = 1.0 \times 10^7 \text{ g cm}^{-3}$$
$$Y_e = 0.50$$

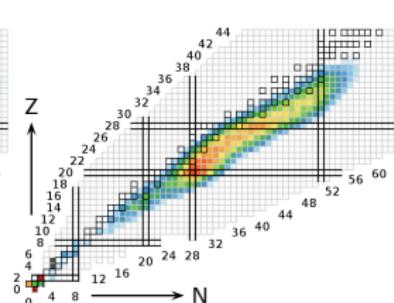
Abundance



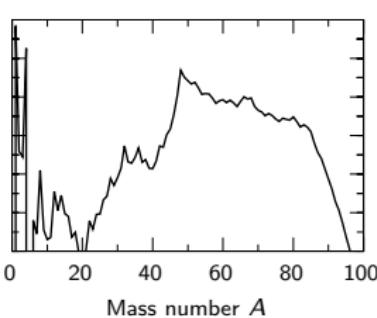
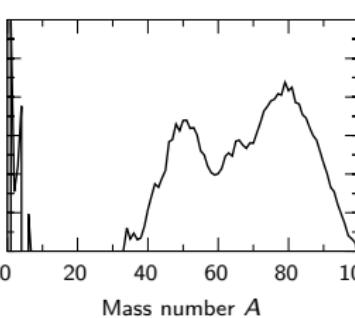
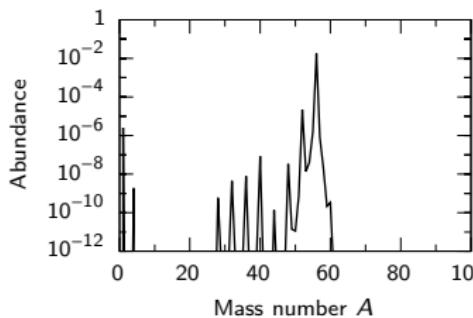
$$T = 7.0 \text{ GK}$$
$$\rho = 2.2 \times 10^8 \text{ g cm}^{-3}$$
$$Y_e = 0.051$$



$$T = 6.9 \text{ GK}$$
$$\rho = 7.8 \times 10^6 \text{ g cm}^{-3}$$
$$Y_e = 0.22$$



Abundance



1. Full GR neutron star–black hole merger simulation (right), up to 10's of ms

Francois Foucart (LBL), *Foucart et al.*,
Phys. Rev. D 90, 024026 (2014)

2. Follow ejecta ($\text{few} \times 10^{-2} M_{\odot}$) in SPH simulation, up to 10 s, get many $\rho(t)$ histories,

Matt Duez (WSU)

3. Nucleosynthesis with SkyNet,
extend $\rho \propto t^{-3}$, 7841 isotopes,
95,467 reactions

JL with Luke Roberts (Caltech)

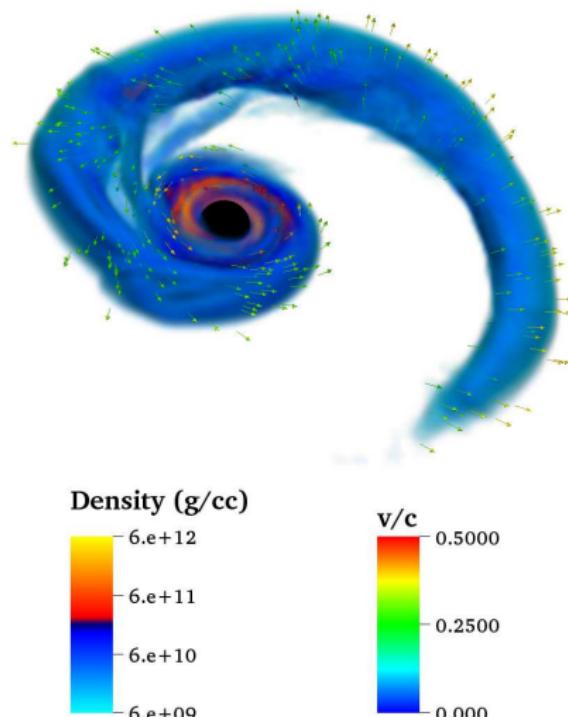
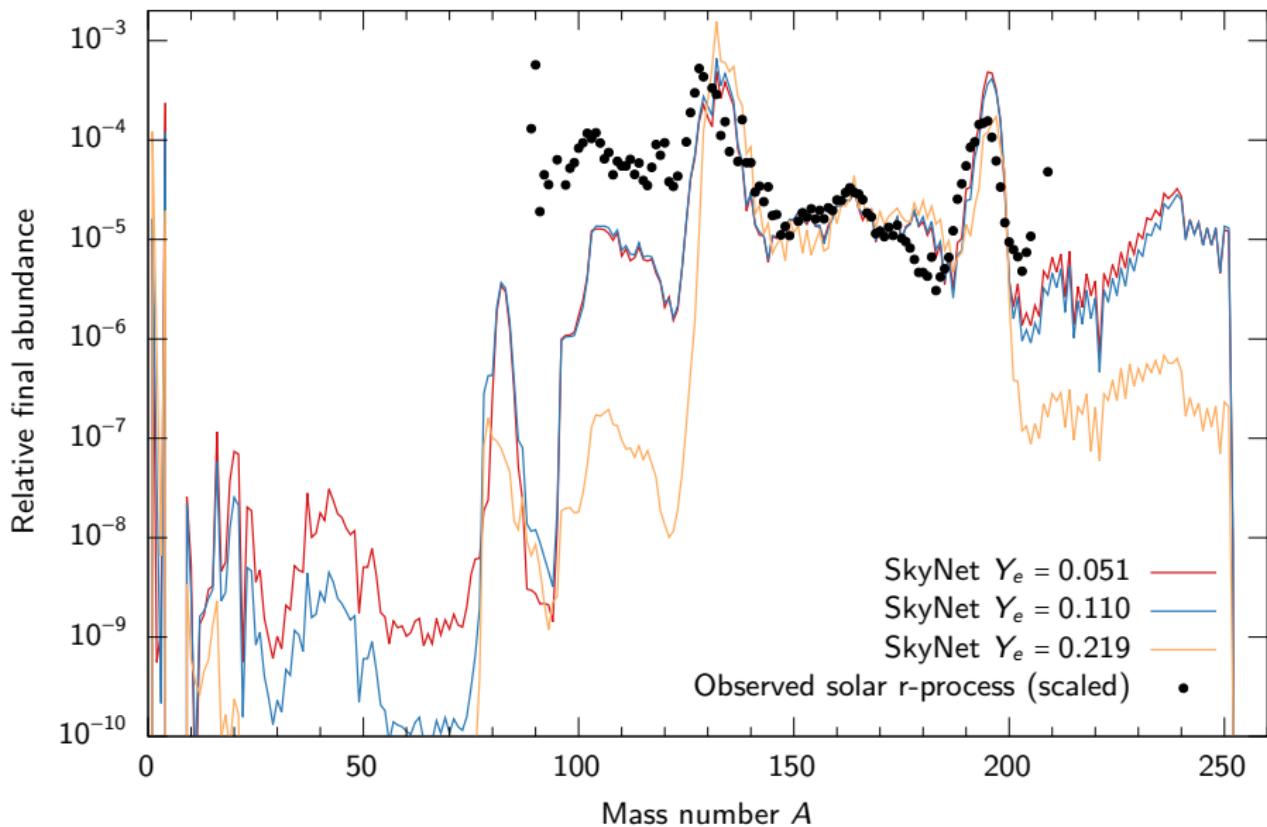


Figure credit: F. Foucart

Neutron Star–Black Hole Merger: Results

Caltech



Parameter Study: Running SkyNet with Python

```
1  #!/usr/bin/env python
2  from SkyNet import *
3  import numpy as np
4
5  init_T9 = 6.0; Ye = 0.01; s = 10.0; tau_ms = 7.1
6  opts = NetworkOptions()
7  opts.ConvergenceCriterion = NetworkConvergenceCriterion.Mass
8  opts.MassDeviationThreshold = 1.0E-10
9  opts.IsSelfHeating = True
10
11 nuclib = NuclideLibrary.CreateFromWebnucleoXML(SkyNetRoot + "/data/webnucleo_nuc_v2.0.xml")
12 helm = HelmholtzEOS(SkyNetRoot + "/data/helm_table.dat")
13 weakReacs = REACLIBReactionLibrary(SkyNetRoot + "/data/reaclib",
14     ReactionType.Weak, False, "Weak reactions", nuclib, opts)
15 strongReacs = REACLIBReactionLibrary(SkyNetRoot + "/data/reaclib",
16     ReactionType.Strong, True, "Strong reactions", nuclib, opts)
17 neutFissReacs = REACLIBReactionLibrary(SkyNetRoot + "/data/netsu_panov_symmetric_Oneut",
18     ReactionType.Strong, False, "Symmetric neutron induced fission reactis", nuclib, opts)
19 spontFissReacs = REACLIBReactionLibrary(SkyNetRoot + "/data/netsu_sfis_Roberts2010rates",
20     ReactionType.Strong, False, "Spontaneous fission reactions", nuclib, opts)
21
22 net = ReactionNetwork(nuclib, [weakReacs, strongReacs, neutFissReacs, spontFissReacs], helm, opts)
23 nse = NSE.CalcFromTemperatureAndEntropy(init_T9, s, Ye, net.GetNuclideLibrary(), helm)
24 density_profile = ExpTMinus3(nse.Rho(), tau_ms / 1000.0)
25 output = net.EvolveSelfHeatingWithInitialTemperature(nse.Y(), 0.0, 1.0E9, init_T9, density_profile,
26     "Ye_%4.2f_s_%07.3f_tau_%07.3f" % (Ye, s, tau_ms)); final_y = output.FinalYVsA()
27 np.savetxt("Y_vs_A", np.column_stack((np.arange(len(final_y)), final_y)), "%6i %30.20E")
```