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Massive Stars: Nucleosynthesis, Nuclear Uncertainties & GCE

Raphael HIRSCHI

in collaboration with: SHYNE team @ Keele: L. Scott, E. Kaiser GVA code: G. Meynet, A. Maeder, C. Georgy, S. Ekström, P. Eggenberger and C. Chiappini (IAP, D) VMS: N. Yusof, H. Kassim (UM, KL, Malaysia), P. Crowther (Sheffield), O. Schnurr (IAP) Nucleo: F.-K. Thielemann, U. Frischknecht, T. Rauscher (Basel, CH/Herts, UK) N. Nishimura NUGRID: F. Herwig (Victoria, Canada), M. Pignatari (Hull), C. Fryer, S. Jones (LANL), Laird (York), C. Ritter (UVic), J. den Hartogh (Konkoly Obs. Hungary), UChicago, UFrankfurt, ... MESA: B. Paxton (KITP), F. X. Timmes, (UArizona, US) SNe: K. Nomoto (IPMU, J), C. Frohlich, M. Gilmer (NCSU), A. Kozyreva (Tel Aviv,II), T. Fischer (W,P) HYDRO: C. Meakin, D. Arnett (UArizona), C. Georgy (GVA), M. Viallet (MPA), F. Roepke (HITS, D), P. Edelmann (Newcastle, UK), A. Cristini (Uoklahoma,US), I. Walkington (ULiverpool)

Recent work

- Massive stars and the (not always) weak s process:
- Large grid of massive star models + weak s proc (Frischknecht+2016, MNRAS):
- Nugrid: set 1 (Pignatari+2016, ApJ), set1extension (Ritter+in prep),
- s process with new convective boundary mixing (CBM): (Battino+ ApJ 2016)
- Nuclear uncertainties: MC-based sensitivity studies for gamma-process (Rauscher+2016, MNRAS), weak s process (Nishimura+2017, MNRAS), main s process (Cescutti+in prep)
- Stellar uncertainties:
- Multi-D tests of convection (Cristini+ 2017, MNRAS) and rotation (Edelmann+2017, A&A)
- Reviews/book chapters: Springer Handbook of Supernovae

"Pre-supernova Evolution and Nucleosynthesis in Massive Stars and Their Stellar Wind Contribution" (doi:10.1007/978-3-319-20794-0_82-1)

- "Very Massive and Supermassive Stars: Evolution and Fate" (doi:10.1007/978-3-319-20794-0_120-1)
- ChETEC COST Action started in April 2017: see www.chetec.eu for details



- Nucleosynthesis in massive (rotating) stars
- Comparison to observations using GCE
- Nuclear uncertainties
- Final remarks/ChETEC

Stars: Importance for Mucleosynthesis



Rotation-Induced Transport

Zahn 1992: strong horizontal turbulence

Transport of angular momentum:

$$\rho \frac{\mathrm{d}}{\mathrm{d}t} \left(r^2 \bar{\Omega} \right)_{M_r} = \underbrace{\frac{1}{5r^2} \frac{\partial}{\partial r} \left(\rho r^4 \bar{\Omega} U(r) \right)}_{\text{advection term}} + \underbrace{\frac{1}{r^2} \frac{\partial}{\partial r} \left(\rho D r^4 \frac{\partial \bar{\Omega}}{\partial r} \right)}_{\text{diffusion term}}$$

Transport of chemical elements:

$$\rho \frac{\mathrm{d}X_i}{\mathrm{d}t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\rho r^2 \left[D + D_{eff} \right] \frac{\partial X_i}{\partial r} \right) + \left(\frac{\mathrm{d}X_i}{\mathrm{d}t} \right)_{\mathrm{nucl}}$$

D: diffusion coeff. due to various transport mechanisms (convection, shear)

D_{eff}: diffusion coeff. due to meridional circulation + horizontal turbulence



Meynet & Maeder 2000



Rotation induced mixing @ Low Z



Raphael Hirschi

Keele University (UK)

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Galactic Chemical Evolution: Primary ¹⁴N

1) Evolution of [N/O] reproduced

← using Z=10⁻⁸ yields

2) Upturn of [C/O]

Observations: Spite et al 2004 (asterisks) Israelian et al 2004 (squares)

Fabbian et al 2008 DLAs Pettini et al 2008



Raphael Hirschi

Galactic Chemical Evolution: ¹²C/¹³C ratio

3) Evolution of $[^{12}C/^{13}C]$ (Chiappini et al 08, A&A) 105 better reproduced 104 \leftarrow using Z=10⁻⁸ yields Hirschi 07: - - - - -1000 JE1/J21 Large differences 100 expected at [Fe/H]~-5 10 4) Primary evolution -5 -2 of Be & B [Fe/H] **Observations:** Spite et al 2004 Prantzos (2012)

Rotation-Induced Mixing \rightarrow Primary ¹⁴N & ²²Ne

Frischknecht, Hirschi et al, MNRAS, 2016, 456, 1803



Mixing between He and H-burning layers

S Process in Massive Stars

Kaeppeler, et al, 2011, RvMP, 83, 157, ... Weak s process: (slow neutron capture process) during core He- and shell C-burning



At solar Z: rotating models may produce up to 3x more s process (See also Chieffi, Limongi, 2012ApJS..199...38L)

How much s process do massive rotating stars produce at low Z?

S-Process Models of Massive Rotating Stars





Frischknecht et al, A&A letter 2011, 2016

• STELLAR EVOLUTION CALCULATIONS WITH 600/700-ISOTOPE NETWORK!

22 Ne production almost primary but still varies with Z & especially V_{ini} . M_{ini}

- Secondary seeds (Fe) limit production (²²Ne cannot act as seed)
- Strong variations in [Sr,Y/Ba] up to 2 dex dep. on Z,V $_{ini}$, and $^{17}O(a,g)$
- Possibility of explosive n-capture process in He-shell
- FULL GRID NOW PUBLISHED! Frischknecht, Hirschi et al, MNRAS, 2016

S-Process Models of Massive Rotating Stars

• FULL GRID NOW PUBLISHED!

Frischknecht, Hirschi et al, MNRAS, 2016, 456, 1803



STELLAR EVOLUTION CALCULATIONS WITH 600/700-ISOTOPE NETWORK!

New S-Process Models Compared to EMP * & Bulge GC



- Strong variations in [Y/Ba] >~ 2 dex matches well observed range! (EMP *: Frebel et al 2010)
- New models also explain abundances in one of the oldest clusters in galactic bulge

Other processes cannot explain all the observed stars in bulge GC NGC6522

New S-Process Models Compared to EMP * & Bulge GC

* 5 signatures of rotation at low Z Cescutti,..., Hirschi et al, 2013, A&A, 553, A51 rise of N/O and C/O, low 12C/13C, and a primary-like evolution of Be and B, s process
* Models explain abundances in one of the oldest clusters in galactic bulge Chiappini et al, Nature Letter, 2011 Inhomogeneous GCE models by Cescutti et al 2013 A&A,553,51, 2015 A&A, 577, 139

 Strong variations in [Sr/Ba] > 1 dex matches well observed range for EMP stars (black circles)!

(no main s process included so cannot explain CEMP-s stars in blue)



	(EMP	*.	Frebel	et al	201	0
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Model name	panels in Fig. 5	s-process	r-process
ſ-	Upper	No s-process from massive stars	standard + extended r-process site (8 - 30 M_{\odot})
as-	middle	average rotators $(v_{ini} / v_{critic} = 0.4)$	standard r-process site (8 - 10 M_{\odot})
fs-	lower	fast rotators ($v_{ini}/v_{critic} = 0.5$) and 1/10 for ¹⁷ $O(\alpha, \gamma)$ reaction rate	standard r-process site (8 - 10 M_{\odot})



- Nucleosynthesis in massive (rotating) stars
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- Final remarks/ChETEC

S Process in Massive Stars: Nuclear Physics Uncertainty



Hirschi et al 2008, NICX Pignatari et al 08, ApJ letter, 687,95 ¹⁶O(n, γ)¹⁷O: - ¹⁶O poison if ¹⁷O(α , γ)²¹Ne dom. - ¹⁶O absorber if ¹⁷O(α ,n)²⁰Ne dom.

Measurement of ¹⁷O(a,g)²¹Ne at TRIUMF Taggart et al NICXI: ¹⁷O(a,g) lower than CF88! Best et al 2011 (@ Notre Dame): But much higher than Descouvemont 1993!



Keele University (UK)

S Process in Massive Stars: Nuclear Uncertainty: ²²Ne+a

²²Ne+α are well known important reactions for s process, that are still uncertain. see R. Longland, C. Iliadis, and A. I. Karakas, PRC, 065809, (2012) and references therein



FIGURE 4. Abundance ratios of different reaction rates for α -captures by ²²Ne. All of the results are based on a one-zone trajectory mimicking the conditions in a 20 M_{\odot} star of $Z = 10^{-6}$ (described in [10]) without rotation (upper) and with "effective rotation" via ¹⁴N-enhancement (lower). Both panels show results using different reaction rate sets.

Nishimura et al 2013, OMEG12 proceedings Reactions also strongly affect weak s process at low Z Stellar HYdrodynamics Nucleosynthesis & Evolution (SHYNE) Project

ERC Starting grant: 5 year; 2 Postdocs; 2 PhDs; 1000+ CPU cluster $TOOL SUITE \rightarrow DATASETS \rightarrow IMPACT$ Nuclear



Efficient pipeline: nuclear/hydro/astro

The s-process in massive stars: uncertainties



- <u>Stellar thermal evolution</u>
 - ZAMS mass and metallicity
 - convection, rotation and magnetic fields
- <u>core He-burning</u>
 - main fusion reactions: triple- α , ¹²C(a,g)¹⁶O, ...
 - n-source and n-poison reactions: ²²Ne(a,n)²⁵Mg, ... (see e.g., Nishimura et al., AIPC 1594 p 146, 2014)

Network calculation Monte-Carlo simulation

- <u>Nucleosynthesis</u>
 - (n,g) reactions
 - beta-decays



uncertainty in the final abundances

feedback (find key uncertain reactions/decays)



Monte-Carlo network code

- Monte-Carlo framework
 - PizBuin MC-driver (T. Rauscher)
 - a simple "Brute-force" approach
 - parallelized by OpenMP for shared memory architectures (easier implementation)



Piz Buin mountain

- Nuclear Reaction network
 - Network solver:
 - WinNet: latest Basel network, Winteler et al., 2012
 - Reaction rates:
 - Reaclib: (Rauscher & Thielemann 2000)
 - T-dependent beta-decay (Takahashi & Yokoi 1987, Goriely 1999)
 - T-dependent uncertainty:
 - Provided by Reaclib format, based on Rauscher 2012

<u>Stellar Environment</u>: \leftarrow trajectories: T & ρ vs time

T-dependent uncertainty: (n,g) (T. Rauscher, ApJL, 775, 2011)

- <u>Theoretical</u>
 - basic rates: Reaclib (Rauscher & Thielemann 2000)
 - a constant factor 2
- <u>Experimental</u>
 - base rates: KADoNiS v0.3 (Dillemann el al., 2009)
 - the formula: Rauscher, ApJ, 775, 2011

$$U(T) = U_{g.s.}X + U_{e.s.}(1 - X)$$

- ground state (experimental based): $u_{g.s.} \sim 1.0 - 1.3$
- excited states (theory based): $u_{\text{e.s.}} = 5$ (given constant)
- X(T): the fraction of particles in the ground state



X for 83 Kr(n,g) 84 Kr

T-dependent uncertainty: beta-decay based on T. Rauscher (2011, 2012, 2013)

beta-decay: only the ground state 1.3 (30%)
beta-decay: T-dependent

(Takahashi & Yokoi 1987, Goriely 1999)





s-process flow: which reaction produces each isotope?



<u>Rules of the game</u>:
(1) nucleosynthesis flow goes from lower A to higher A
(2) (n,γ): right (→)
(3)beta-decay: diagonal (∧ or ∧)



Key Reaction Levels 1-3:

N. Nishimura+ 2017

- Level 1 key rates dominate the uncertainty for a given isotope

- Once level 1 rates are fixed, *then* Level 2 rates become dominant

• • •

We adopt the Pearson product-moment correlation coefficient Pearson (1895) to quantify the correlation between rate variation and the final abundances (also used in Rauscher et al. 2016), defined by

$$r_{\rm cor} = \frac{\sum_{i}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i}^{n} (x_i - \bar{x})^2} \sqrt{\sum_{i}^{n} (y_i - \bar{y})^2}}$$
(4)

where x_i and y_i are variables with \bar{x} and \bar{y} being their arithmetic mean value, respectively. The summation is applied to all data for the MC runs $i = 1, 2, 3, \dots, n$. Here, x and y in Equation 4 correspond to variation factors f and final abundances Y.



Key Reaction Lists for Weak s Process

N. Nishimura+ 2017: http://adsabs.harvard.edu/abs/2017MNRAS.469.1752N

Nuclide	r _{cor,0}	$r_{\rm cor,1}$	$r_{\rm cor,2}$	Key Rate Level 1	Key Rate Level 2	Key Rate Level 3	X_0 (8, 30 keV)	Weak Rate (8, 30 keV)
[€] Zn	0.76			${}^{64}\mathrm{Cu}(\beta^{-}){}^{64}\mathrm{Zn}$				1.30, 1.36
	-0.46	-0.73			${}^{64}{ m Cu}(e^-, \nu_e){}^{64}{ m Ni}$			e ⁻ capture
⁶⁷ Zn	-0.67			${}^{67}\mathrm{Zn}(\mathrm{n},\gamma){}^{68}\mathrm{Zn}$			1.00, 1.00	
72 Ge	-0.85			$^{72}\text{Ge}(n,\gamma)^{73}\text{Ge}$			1.00, 1.00	
73 Ge	-0.84			$^{73}\text{Ge}(n,\gamma)^{74}\text{Ge}$			0.88, 0.81	
74 Ge	-0.44	-0.54	-0.67			$^{74}\mathrm{Ge}(\mathrm{n},\gamma)^{75}\mathrm{Ge}$	1.00, 1.00	
^{75}As	-0.50	-0.59	-0.70			$^{75}\mathrm{As}(\mathrm{n},\gamma)^{76}\mathrm{As}$	1.00, 1.00	
77 Se	-0.86			$^{77}\mathrm{Se}(\mathrm{n},\gamma)^{78}\mathrm{Se}$			1.00, 1.00	
78 Se	-0.71			$^{78}\mathrm{Se}(\mathrm{n},\gamma)^{79}\mathrm{Se}$			1.00, 1.00	
	0.38	0.68			${ m ^{68}Zn}({ m n},\gamma){ m ^{69}Zn}$		1.00, 1.00	
80 Se	-0.76			${}^{80}{ m Br}(\beta^{-}){}^{80}{ m Kr}$				1.31, 4.70
	0.27	0.73			${}^{80}{ m Br}(\beta^+){}^{80}{ m Se}$			1.31, 4.70
	0.16	0.44	0.88			${}^{80}{ m Br}(e^-,\nu_e){}^{80}{ m Se}$		e ⁻ capture
$^{79}\mathrm{Br}$	-0.64	-0.73			$^{79}\mathrm{Br}(\mathrm{n},\gamma)^{80}\mathrm{Br}$		1.00, 1.00	
$^{81}\mathrm{Br}$	-0.80			${}^{81}\mathrm{Kr}(\mathrm{n},\gamma){}^{82}\mathrm{Kr}$			1.00, 0.98	
⁸³ Kr	-0.76			${}^{83}\mathrm{Kr}(\mathrm{n},\gamma){}^{84}\mathrm{Kr}$			0.81, 0.74	
⁸⁴ Kr	-0.49	-0.65	-0.76			${}^{84}\mathrm{Kr}(\mathrm{n},\gamma){}^{85}\mathrm{Kr}$	1.00, 1.00	
⁸⁶ Kr	0.84			${}^{85}\mathrm{Kr}(\mathrm{n},\gamma){}^{86}\mathrm{Kr}$			1.00, 1.00	
	-0.30	-0.70			${}^{86}\mathrm{Kr}(\mathrm{n},\gamma){}^{87}\mathrm{Kr}$		1.00, 1.00	
	-0.34	-0.62	-0.90			${}^{85}\mathrm{Kr}(\beta^{-}){}^{85}\mathrm{Rb}$		1.30, 1.30
87 Rb	-0.56	-0.65	-0.95			${}^{87}\mathrm{Rb}(\mathrm{n},\gamma){}^{88}\mathrm{Rb}$	1.00, 1.00	

Other Key Reaction Lists

Priority lists established for: - Enhanced (weak) s proc. in low-Z fast rotating stars: N. Nishimura+ 2017



- Gamma (aka p) process in CCSNe: T. Rauscher+ 2016 http://adsabs.harvard.edu/abs/2016MNRAS.463.4153R

- Gamma (aka p) process in Sne Ia: Nishimura et al (2018): http://adsabs.harvard.edu/abs/2018MNRAS.474.3133N

- Main s process (C13-pocket) Cescutti + subm.

Constraints from stellar evolution: ${}^{12}C-{}^{12}C$ rate, 30x

• Full stellar models + post-processing using MPPNP (Nugrid)



See Suda et al 2011 for a study constraining 3α reaction

Stellar HYdrodynamics Nucleosynthesis & Evolution (SHYNE) Project



Efficient pipeline: nuclear/hydro/astro

Tool Suite: Parallel Programming Platform

TOOL SUITE: Current Platform \rightarrow Future Platform



(shared memory: OpenMP / Distributed mem.: MPI)

SHYNE Computer Cluster

 The cluster comprises a total of 1056 AMD-based CPU-cores
 with 2GB RAM per core.
 The main specifications are the following:

288 cores Numascale

- 8 x 3 socket servers (each socket has 12-core CPUs, AMD opteron 6172, 2.1 MHz)
- Single memory image 576GB
- Single operating system image
- Numascale inter-connect

768 cores QDR Infiniband

- 12 x 4 socket servers (each socket has 16-core CPUs, AMD opteron 6272, 2.1MHz)
- 1 O/S per server
- Distributed memory image 128 GB per server
- Unified cluster management for both architectures
 - IBM Platform HPC
 - 2 LSF queues Numa and IB
 - Numa nodes visible as single machine with 288 cores and 576 GB RAM
- Dedicated water cooled environment up to 30kW in 1 rack



Link with Industry

numascale

Norwegian HPC company





 FROM: distributed memory clusters
 TO: scalable shared memory clusters

 For the same cost!

- Super-desktop: single OS, 288 cores, RAM 576 GB
- Large scale: better balance between shared/distributed memory

The Memory Hierarchy & Scaling

OpenMP easier to implement than MPI but might be harder to scale

Memory access time:



OPM Subsamples/hour Scaling 80 16 32 48 64 96 112 128 Number of Threads

Excellent scaling possible on Numascale system!

Scaling:

Monte Carlo Sensitivity Studies

- PizBuin Monte Carlo wrapper (T. Rauscher)
- + WinNet (Winteler+ 12) < Reaclib
- = McWinNet



- beta-decay & (n,g) uncertainties are T-dependent
- Largest simulations: 1000 trajectories x 1hr run x 10,000 iterations

The Memory Hierarchy & Scaling

Speed up

10

5

0

٥

5

10

Number of core

15

Memory access time:





p = 1

20

p = 0.99

p = 0.999 Loop = 2000

25

ChETEC COST Action (2017-2021) www.chetec.eu



30 countries have joined ChETEC to coordinate research efforts in Nuclear

Astrophysics: Austria, Belgium, Bulgaria, Croatia, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Ireland, Israel, Italy, Lithuania, Malta, The Netherlands, Norway, Poland, Portugal, Romania, Serbia, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and United Kingdom

ChETEC Objectives

www.chetec.eu

What is ChETEC about? (pronounced [ketek])

Main challenge: tackle key open questions and link European facilities.



Working Groups (WG) & Management Structure (MC)

- WG1: nuclear data for astrophysics: needs, coordination and dissemination
- WG2: modelling pipelines connecting nuclear processes to astronomical observables
- WG3: astronomical data coordination, analysis and interpretation
- WG4: tools, techniques, knowledge exchange and innovation

Management Committee (MC): 2 members per country (+2-3 substitutes)

CORE group/Steering Committee (each CORE group member represents a team, see "Key Info" for more details) Action Chair: R. Hirschi

Vice Chair: M. Lugaro

WG leaders:Alessandra Guglielmetti (WG1),
Andreas Korn (WG3),Georges Meynet (WG2),
Daniel Bemmerer (WG4)

- Gender coordinator: Maria Lugaro
- Pan-European coordinator: Sevdalina Dimitrova
- Inter-sectoral (bi-direction Knowledge Transfer) coordinator: Daniel Bemmerer
- **STSM manager: Neven Soic**
- **Dissemination coordinator: Jordi Jose**

How to Get Involved? www.chetec.eu

COST Actions are open and inclusive

- Everyone can participate ... but budget is limited given scale of network
- (Most countries already have management committee members)
- 1) Join a WG by contacting the WG leader and the Action chair
- 2) Sign up to ChETEC mailing list (to be set up soon)
- 3) Contribute to the "knowledge hubs": including at least one directory of datasets per WG
- 4) "Young" scientists are encouraged to attend the training schools
- 5) Propose, organise, host COST events

http://www.cost.eu/participate/join_action

Activities Planned in 2017-2018 (Year 1) www.chetec.eu

1) Short-term Scientific Missions (STSMs): throughout the year with evaluation deadlines every 3-4 months

2) Proposed Training schools (confirmed by next week):

- Gamma-ray measurements and target preparation (main contact: Livius Trache): April 2018 @ IFIN-HH (ELI-NP), Bucharest, Romania
- R-matrix calculations for nuclear astrophysics (main contact: Fairouz Hammache)
 13-15 September 2017 @ IPN, Orsay, France

3) Main Action workshop involving all WGs: October 9-11, Keele University, UK (main contact R. Hirschi)

COST Acknowledgements

The ChETEC Action (CA16117) is supported by COST (www.cost.eu). COST (European Cooperation in Science and Technology) is a funding agency for research and innovation networks. Our Actions help connect research initiatives across Europe and enable scientists to grow their ideas by sharing them with their peers. This boosts their research, career and innovation.





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Stars are super-rich in Physics! Stellar evolution theory is challenging and fun!

Thanks for your participation!

3D C-shell Simulations: |v| movie

Cristini+ 2017, MNRAS

Gas Velocity $\|\mathbf{v}\|$



http://www.astro.keele.ac.uk/shyne/321D/convection-and-convective-boundary-mixing/visualisation

Methods: performance/resources

for shared memory systems

- Fortran + OpenMP
- parallelized well
- optimized code/matrix library for large scared memory computers (multi threads)

•<u>Computer resources</u> **numascale**



Shyne cluster @Keele (ERC)

performance tests of matrix solvers on shared memory system



Cosmos2 @Cambridge (UK DiRAC facility, STFC)



Some nuclei show higher uncertainty (uncertainty range factor 2 or more)



⁶⁴Zn, ^{72, 73}Ge, ^{77, 80}Se, ⁸¹Br, ^{80, 83}Kr



s-process flow: which reaction produces each isotope?



Key 15 reactions (candidates):

 $\begin{array}{cccc} {}^{60}{\rm Ni}\,({\rm n},\gamma)\,{}^{61}{\rm Ni} & {}^{61}{\rm Ni} & {}^{61}{\rm Ni} \\ {}^{72}{\rm Ge}\,({\rm n},\gamma)\,{}^{73}{\rm Ge} & {}^{73}{\rm Ge} \\ {}^{79}{\rm Se}\,(\beta^-)\,{}^{79}{\rm Br} & {}^{80}{\rm E} \\ {}^{82}{\rm Kr}\,({\rm n},\gamma)\,{}^{83}{\rm Kr} & {}^{83}{\rm Kr} \end{array}$

 ${}^{61}{
m Ni}({
m n},\gamma)\,{}^{62}{
m Ni}$ ${}^{73}{
m Ge}({
m n},\gamma)\,{}^{74}{
m Ge}$ ${}^{80}{
m Br}\,(\beta^+)\,{}^{80}{
m Se}$ ${}^{83}{
m Kr}\,({
m n},\gamma)\,{}^{84}{
m Kr}$

 64 Cu (β^{-}) 64 Zn 76 Se (n,γ) 77 Se 80 Br (β^{+}) 80 Kr 85 Kr (β^{-}) 85 Rb

Candidates key reactions vs All rates

only 15 reactions sampled



all (n,g) & decay varied

Summary: uncertainty in the weak s-process

- •<u>MC nuclear reaction network code</u>
 - applicable to general nucleosynthesis
 - parallelized by OpenMP for shared memory systems
- (weak) s-process in massive stars
 - We evaluated T-dependent uncertainty including the effect of exited states
 - key reactions (n,g) and $\beta^\pm\text{-decay}$ are identified
 - a list of minimum key rates (15 reactions/decay)
 - different uncertainty: higher T and different hydro models
- Further investigation
 - non-standard weak s-process in metal-poor stars
 - other nucleosynthesis, i.e., rp, vp, and r processes

