

WP4 "Astronuclear HPC"

- Marco Pignatari — Konkoly Observatory/HUN-REN, Hungary; BGI, Bayreuth University, Germany

WP4 main team: U. Battino (INAF*), J. Keegans (UHULL), S. Martinet (ULB), A. Sanz-Lechuga (UPC), R. Hirschi (UKEELE), J. Jose (UPC), S. Goriely (ULB)

JRA2/WP4 Members and Status (2024)

- A) WP members, communication / coordination:
 - WP4 mailing-list = 38 members
- B) Status of staff hiring for the person-months inside this WP.
 - PDRA ~~UHULL~~ **UKEELE** (until December 2024 @ U.Battino)
 - ~~PDRA UKEELE~~ **Teaching Fellow UHULL** (**permanent** @ J. Keegans)
 - PDRA ULB (until September 2024 @ S. Martinet)
 - PhD UPC (4 years; ongoing, up to October 2027 @ A. Sanz-Lechuga)
- C) Associated partners
 - University of York, University of Edinburgh

JRA2/WP4 Members and Status (today)

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 - PDRA ~~UKEELE~~ **Naples/Teramo** (**PDRA** @ U.Battino)
 - Teaching Fellow UHULL (permanent @ J. Keegans)
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TASKS

- **Task 4.1** Stellar Nucleosynthesis Software Tools for Access to HPC (PI: R. Hirschi, UKEELE, participants: CSFK, UHULL)
- **Task 4.2** Nuclear Astrophysics Software Pipeline (PI: M. Pignatari, Konkoly/CSFK, participants: UKEELE, UPC, GUF, ULB, UPC, HZDR, York, Edinburgh)
- **Task 4.3** EXNUC Explosive Nucleosynthesis Codes (PI: J. José, UPC, participants: ULB, UKEELE)

TASK 4.1

User Training and Online Training Course: HPC Nucleosynthesis Calculations

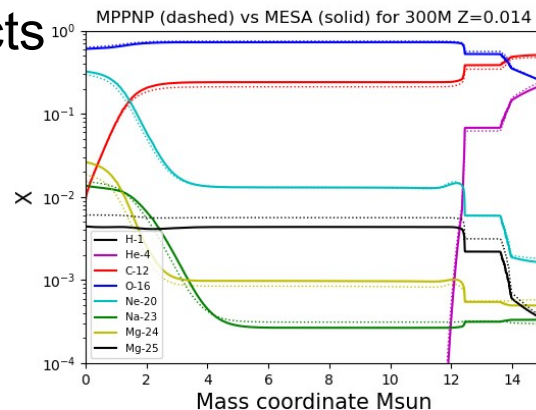
GOAL: provide the stellar nucleosynthesis tools and user-friendly support to access these capabilities within an HPC framework

Activity:

- training for 4 PhDs and 2 Postdoc
- training material on the **ChETEC-INFRA YouTube channel**
- broad spectrum of help and support activities for new and ongoing projects



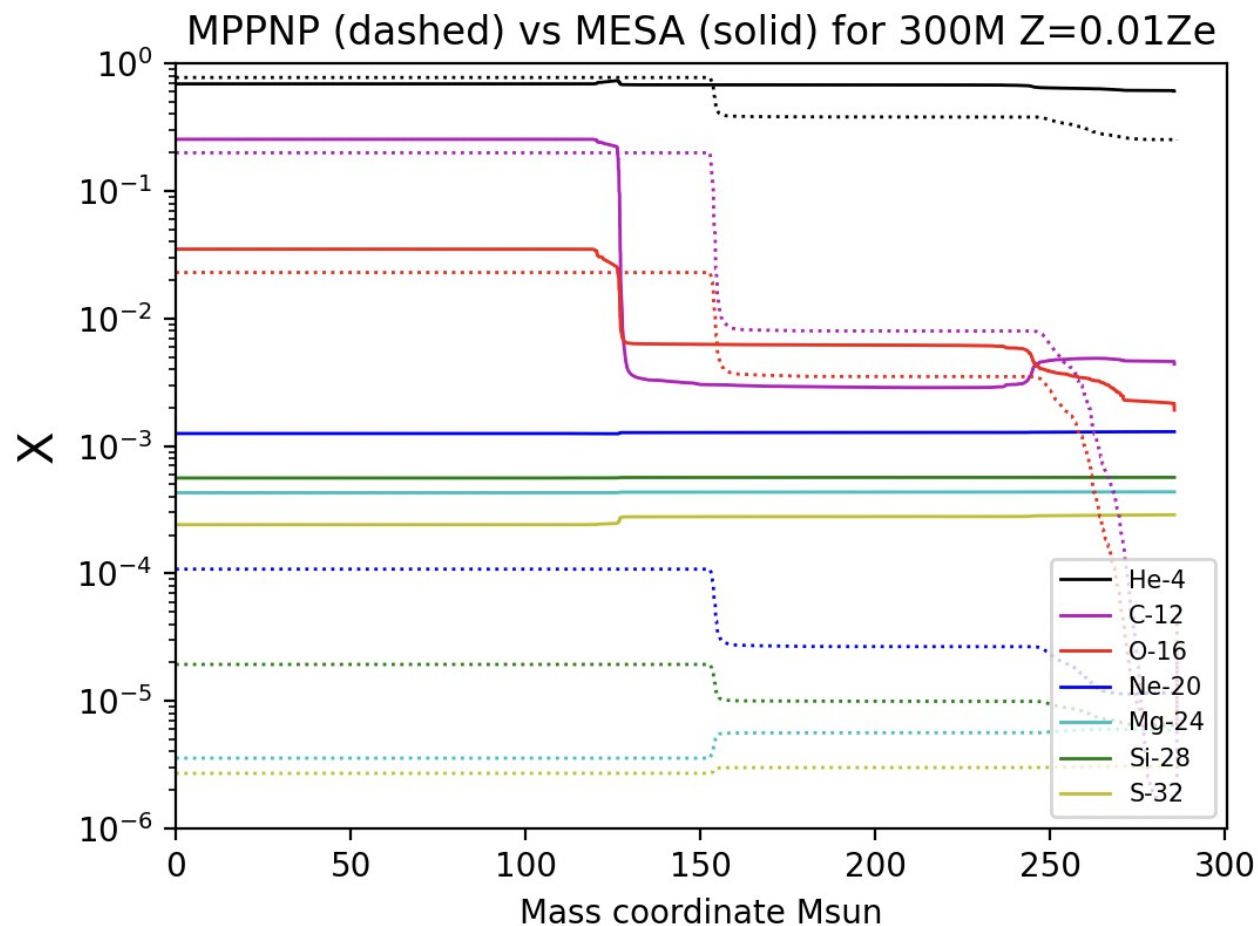
HPC UHull VIPER racks of nodes for computation



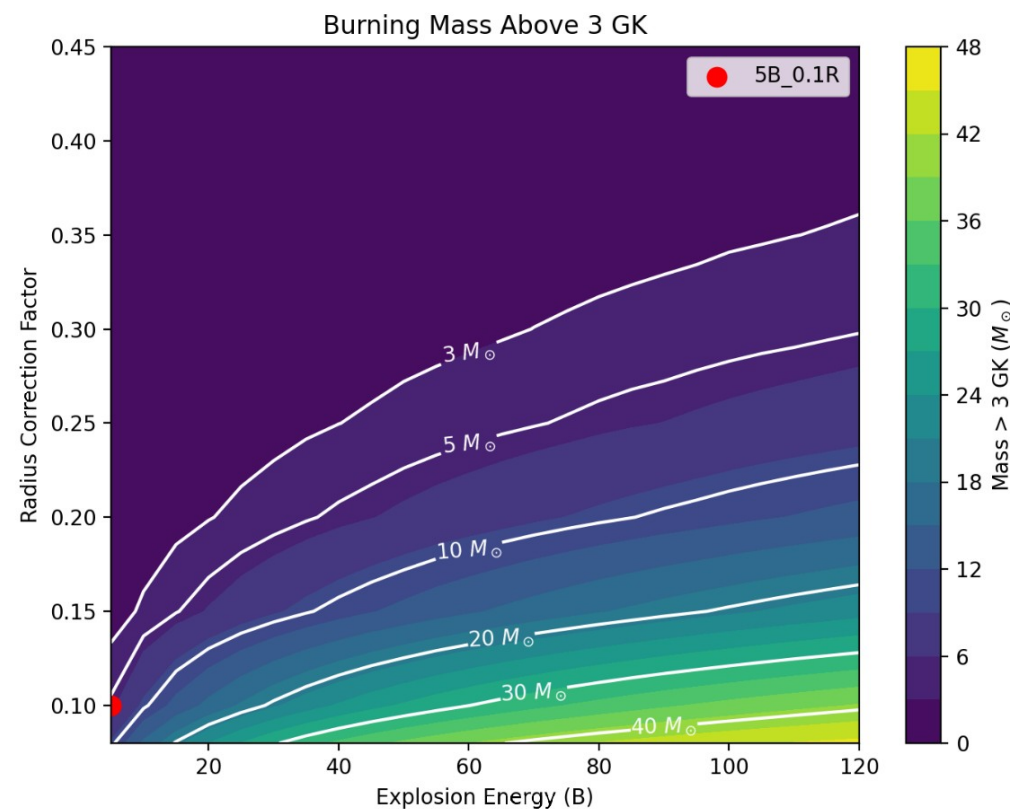
M=300Msun star, Z=0.014
Stellar model vs nucleosynthesis model

@ PhD P. Fong - HPC simulations

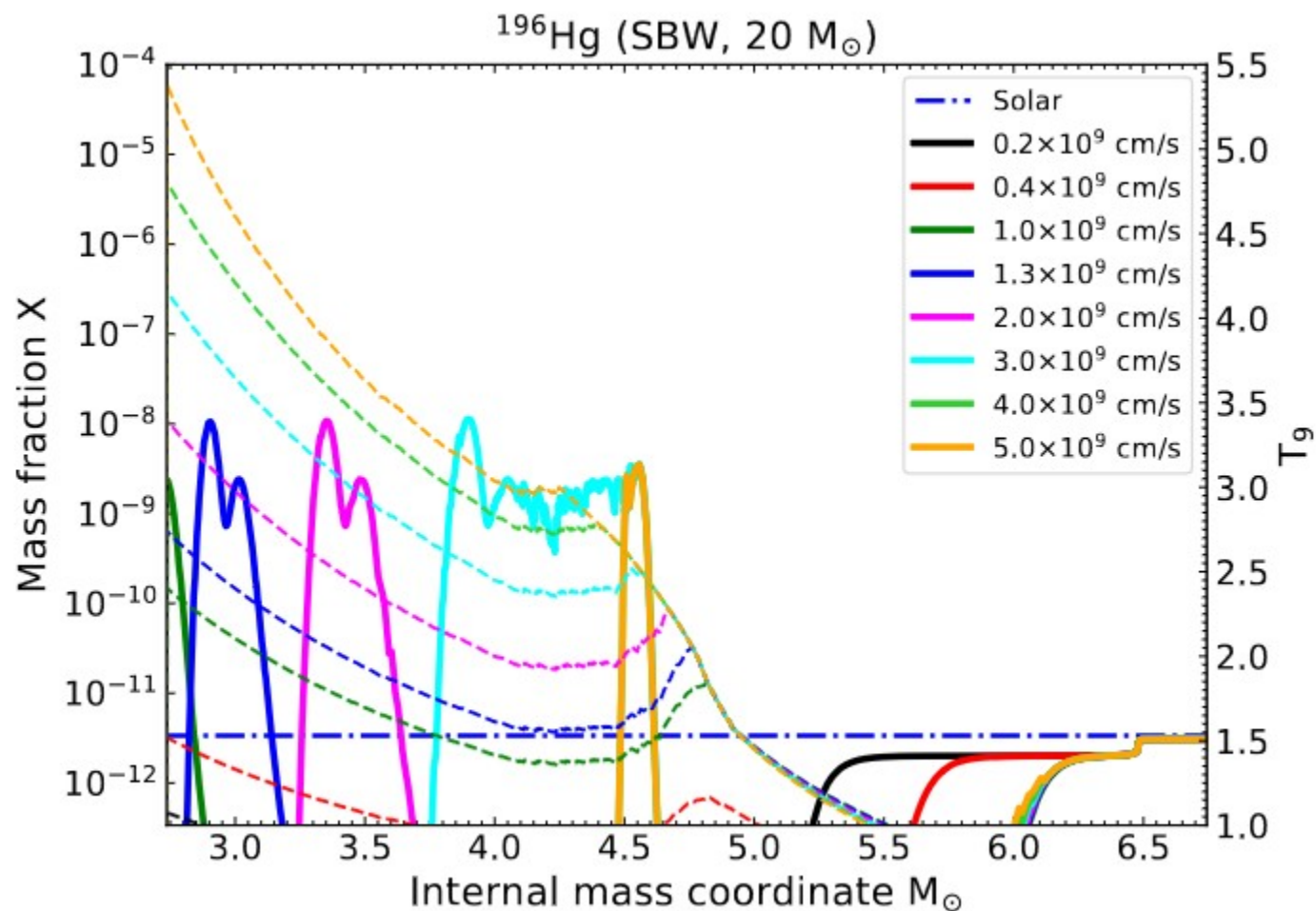
TASK 4.1



$M=300M_{\text{sun}}$ star, $Z=0.00014$
Stellar model vs nucleosynthesis model &
parametric PISN explosions
@ PhD P. Fong - HPC simulations



TASK 4.1



$M=20 M_{\text{sun}}$ star, $Z=0.02$

γ -process production for different explosion energies (Roberti+ 2024 A&A L)

@ PDRA L. Roberti - HPC simulations

^{197}Pb 8.10 m β^+	^{198}Pb 2.40 h β^+	^{199}Pb 1.50 h β^+	^{200}Pb 21.50 h β^+	^{201}Pb 9.33 h β^+
^{196}Tl 1.84 h β^+	^{197}Tl 2.84 h β^+	^{198}Tl 5.30 h β^+	^{199}Tl 7.42 h β^+	^{200}Tl 1.09 d β^+
^{195}Hg 10.13 h β^+	^{196}Hg 0.15 204 mb	^{197}Hg 2.67 d β^+	^{198}Hg 9.97 173 mb	^{199}Hg 16.87 374 mb
^{194}Au 1.58 d β^+	^{195}Au 186.11 d β^+	^{196}Au 6.17 d β^+	^{197}Au 100 582 mb	^{198}Au 2.70 d 840 mb, β^-
^{193}Pt 50.01 a 1123 mb, β^+	^{194}Pt 32.967 365 mb	^{195}Pt 33.832 860 mb	^{196}Pt 25.242 183 mb	^{197}Pt 19.89 h β^-

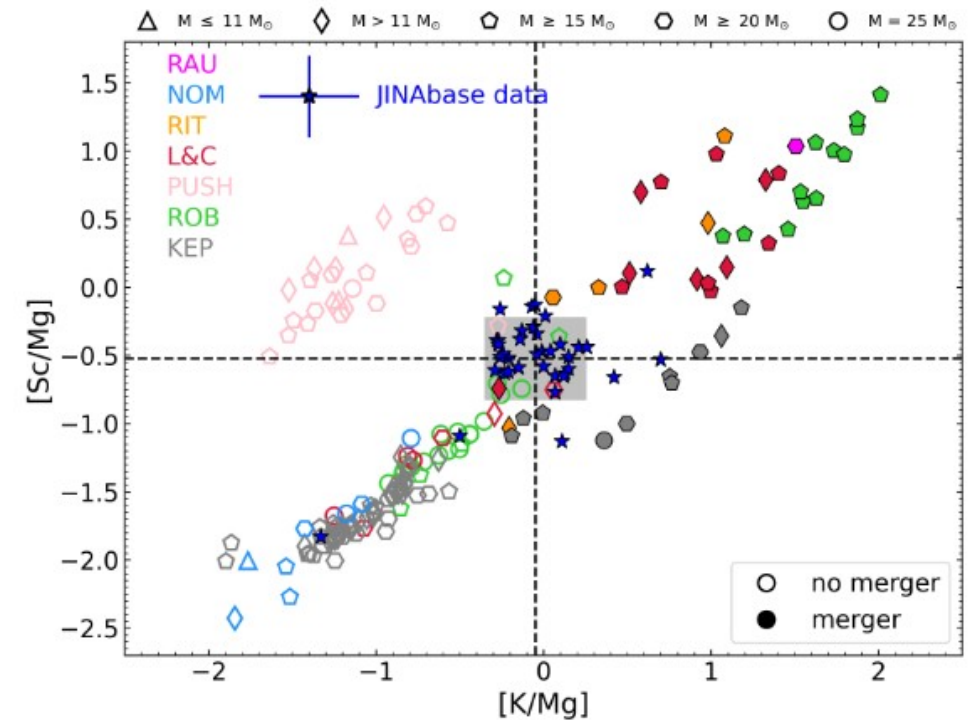
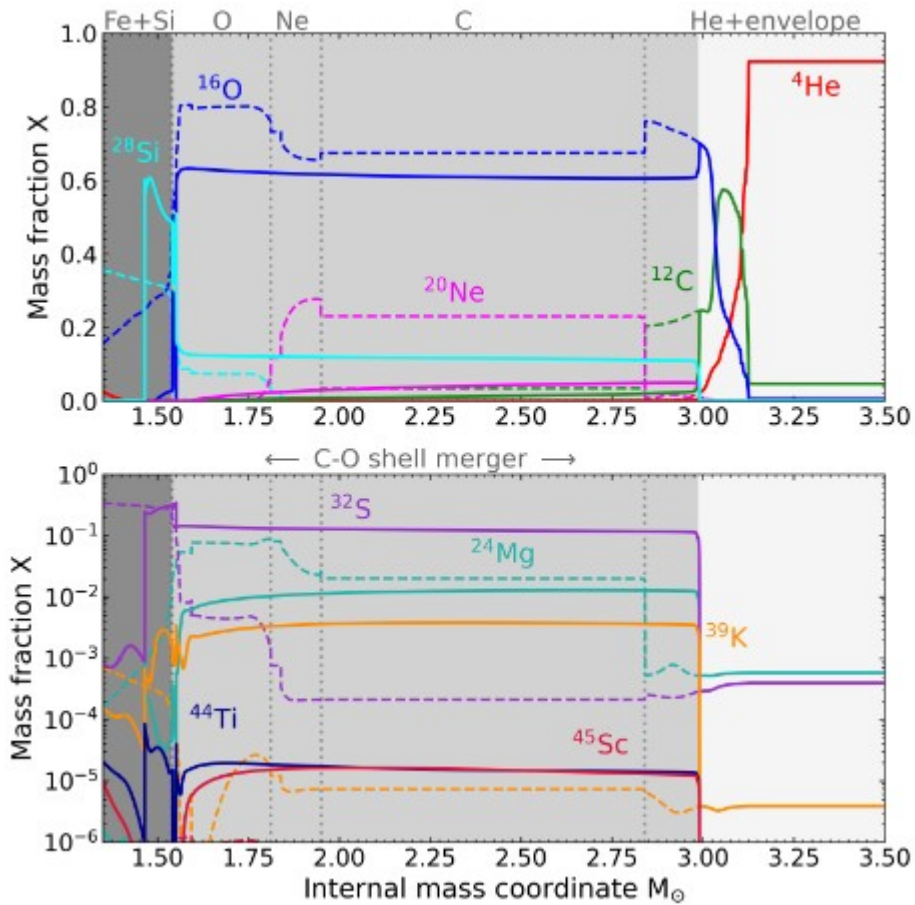
TA Projects: 22102724-ST and 23103142-ST

TASK 4.1

M=15 Msun star, Z=0.02

CO shell merger study (Roberti+ 2025 A&A)

@ PDRA L. Roberti - HPC simulations

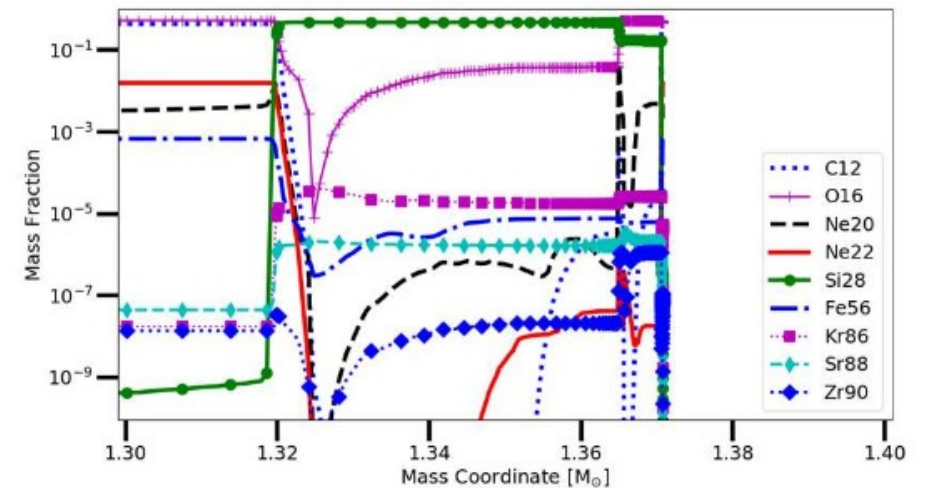
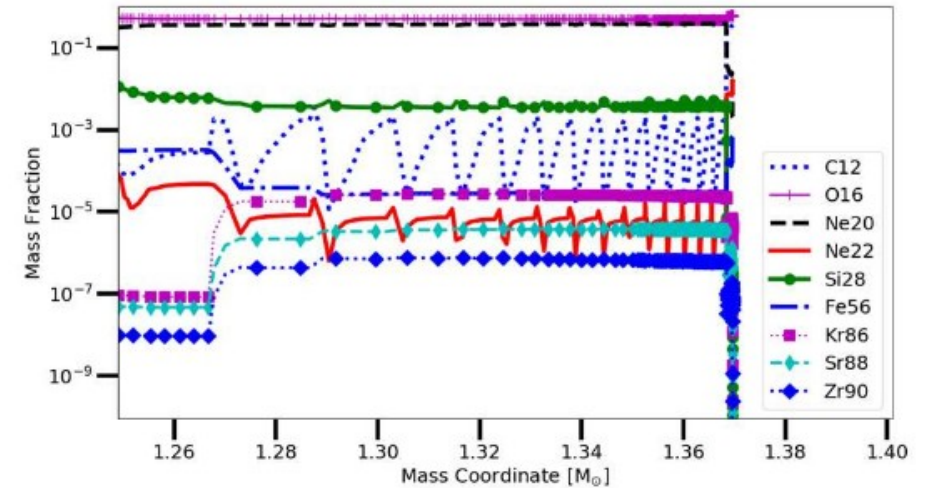
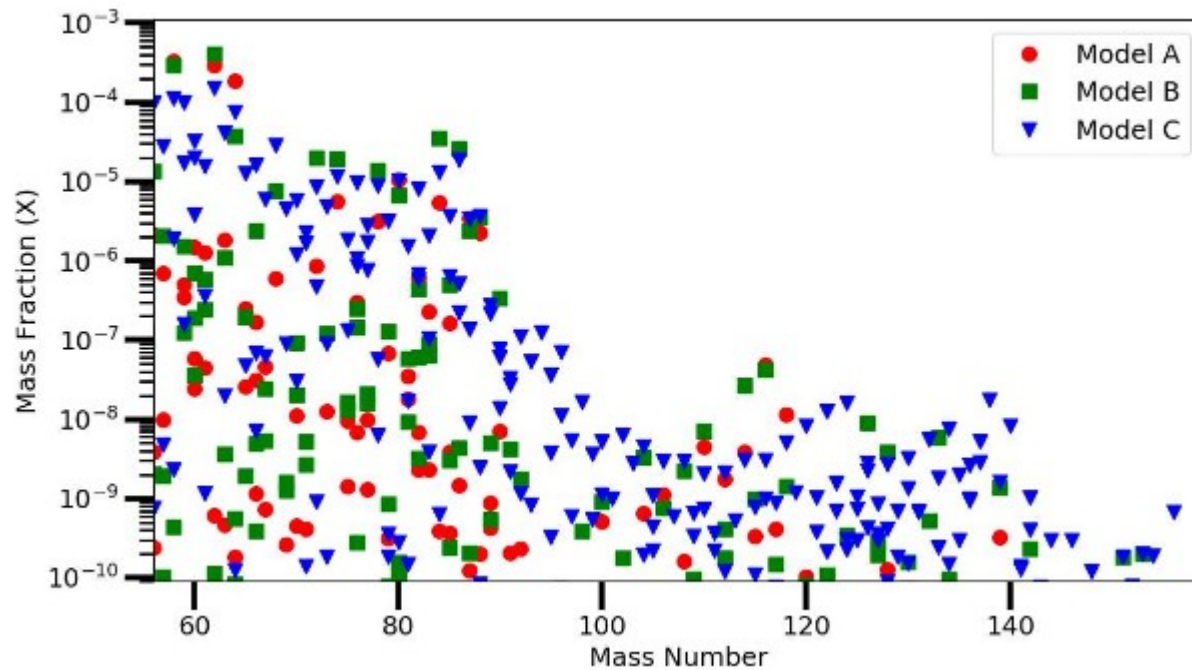


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TASK 4.1

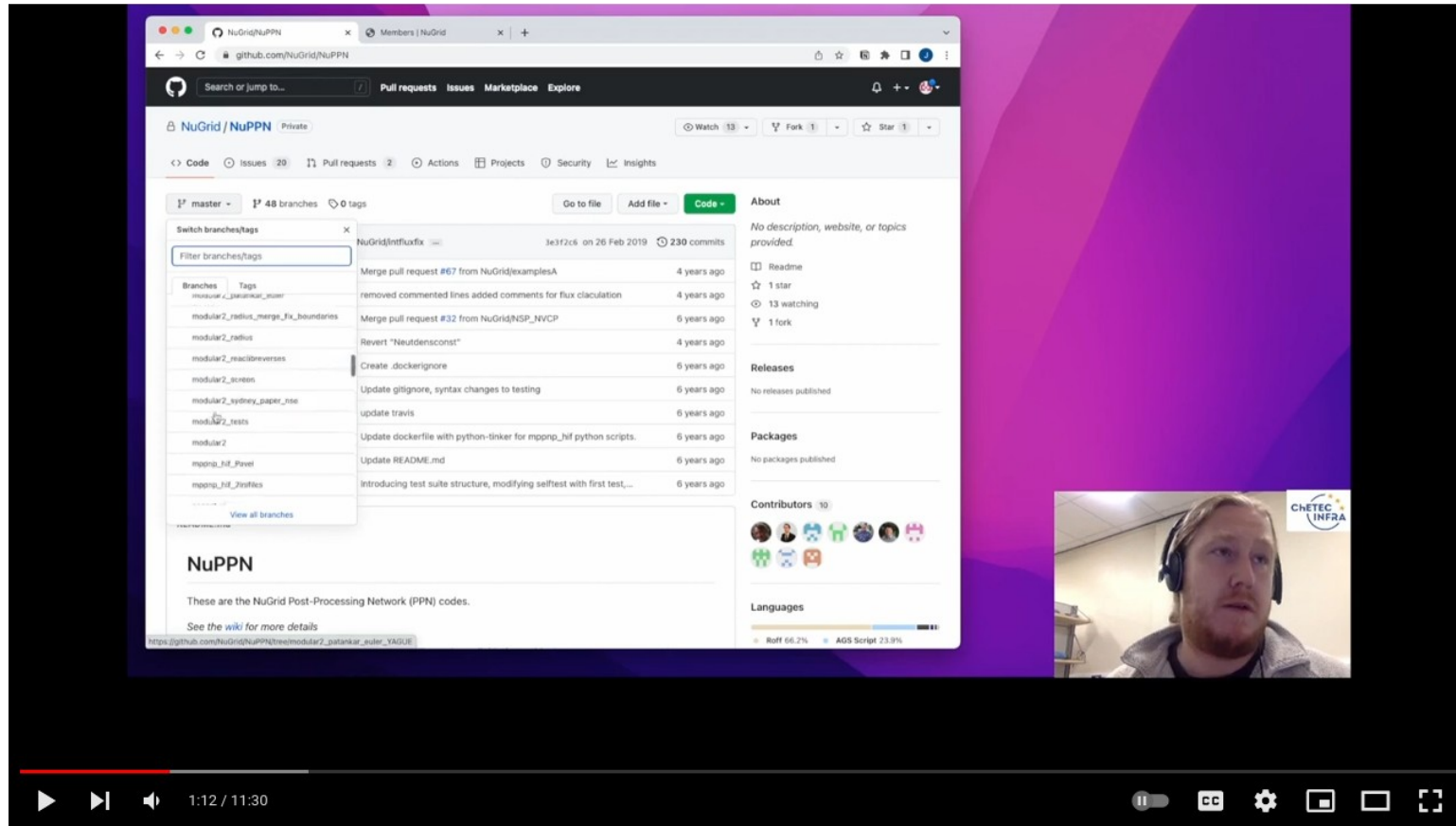
Trans-Fe elements from Type Ia Supernovae

Battino+ 2025 A&A accepted; arXiv



TASK 4.1

Tutorials!



Installing mppnp



Subscribe



<https://www.youtube.com/channel/UCB2SFPWEpNFfeWZURED8PXZw/videos>

TASK 4.2

Platform for the Exchange of Nuclear Astrophysics Data - ChANUREPS

GOAL: share and distribute new published nuclear reaction rates as open source and with the same simple format.

Tool: Wordpress software; hosted by Frankfurt Uni.

Activity:

- Nuclear rates available: 54 rates for 38 reactions
- Link to major nuclear reaction libraries
- Portal: <http://chanureps.chetec-infra.eu/>
- **New project to support stellar simulations (MESA or else) and alignment stellar simulations with post-processing nucleosynthesis**



How to use ChANUREPS?

Create your reaction rate file

Click below to download your template and fill it up with your data. Add as many rows as you want (temperature in GK, lower and upper limit rate at the level of 1 sigma, and median rate in $\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$), just keep the same, standard, format. Please, if your reaction rate is of one of the nuclear reactions listed [here](#), consider uploading your rate also in the MESA format.

Download "template"
rate_template-3.txt – Downloaded 58
times – 294.00 B

Upload your reaction rate

Use the contact form in the "Contact" section to contact the webmaster and request permission to have your rate uploaded. Please, do include the link to your published paper and any additional relevant information.

Download a reaction rate

Use the search engine below to find the rate you want, or click on the relevant category to browse by reaction type (e.g., click on 'p_g' to get a list of published (p,gamma) reactions).

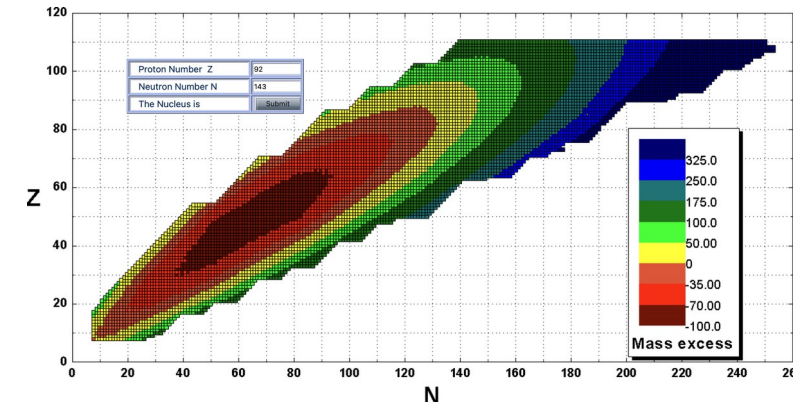
TASK 4.2

The Brussels BRUSLIB nuclear library and the nuclear network generator NETGEN (ULB)

GOAL: Provide to the community an extended library of computed data of astrophysics relevance and a user-friendly nuclear network generator including experimental and theoretical rates

Activity:

- Update the sets of experimental nuclear reaction rates
- Update the theoretical library on the basis of state-of-the-art microscopic models
- Improve the website design
- Portal: <http://www.astro.ulb.ac.be/pmwiki/IAA/NuclearData>



TASK 4.2

Newly available!

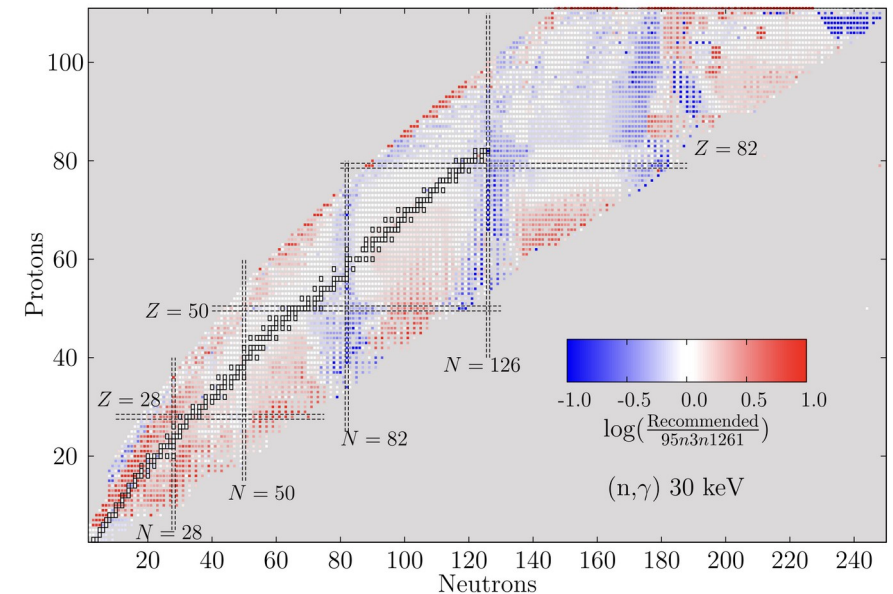
TENDL-astro 2023

Cross sections, reaction rates and MACS for astrophysics

D. Rochman, A. Koning, S. Goriely, S. Hilaire, Nuclear Physics A 1053 (2025) 122951

<http://www.astro.ulb.ac.be/bruslib/nucdata/TENDL-astro/>

Based on the TALYS-evaluated Nuclear Data Library (TENDL), 8892 reaction cross sections, MACS and rates of astrophysical interests have been calculated including model uncertainties.



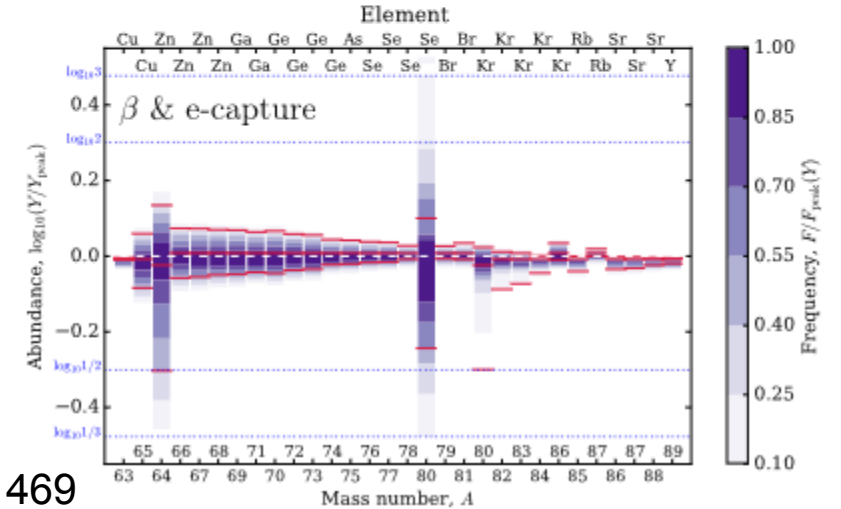
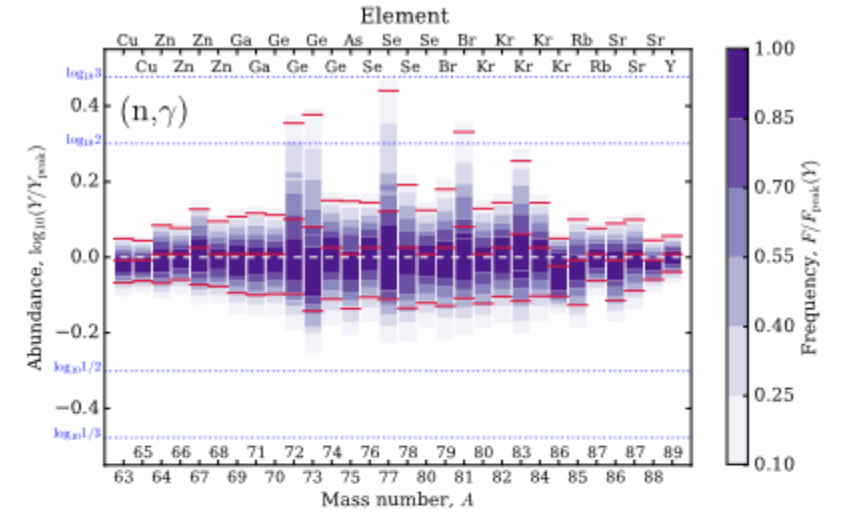
TASK 4.2

Stellar Trajectories - ORChESTRA

GOAL: publish fully documented library of verified trajectories for nuclear astrophysics simulations, covering a wide range of stellar conditions.

Activity:

- Portal: <https://zenodo.org/communities/chetec-infra-wp4>
- Preliminary version with 4 published trajectories
- The nucleosynthesis for the s-process and Novae is covered
- More trajectories on preparation – coming * soon *



Nishimura+2017 MNRAS 469

TASK 4.2

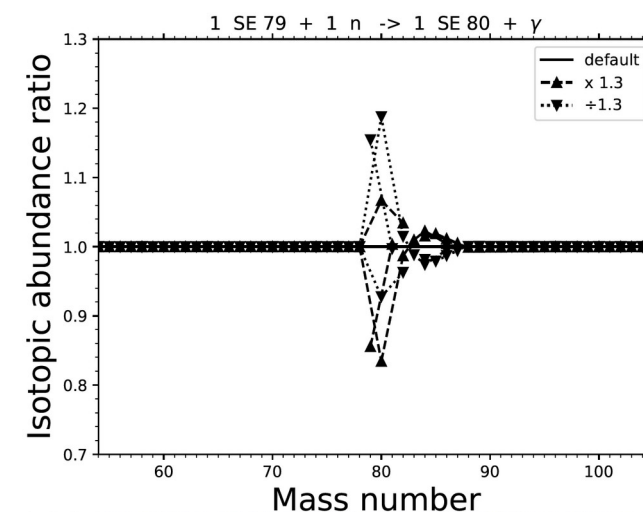
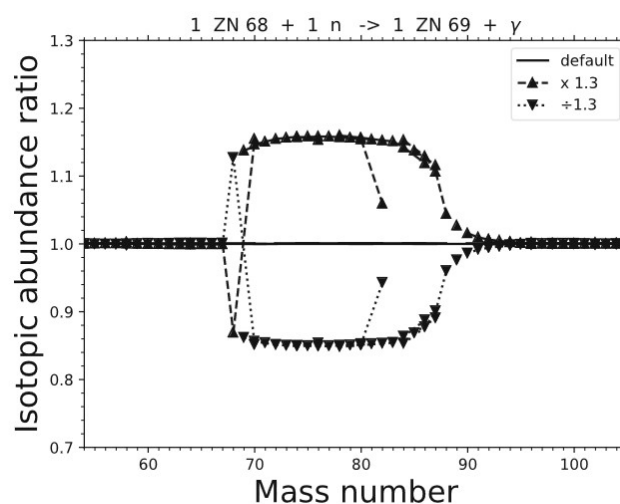
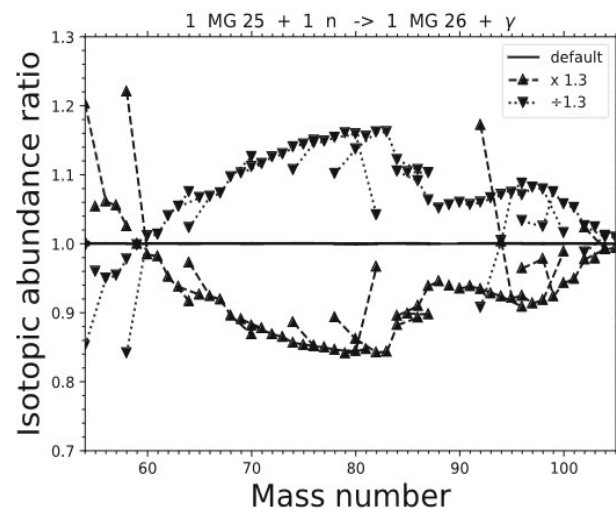
Example of an application:



EPJA volume
in honour of
Franz
Käppeler

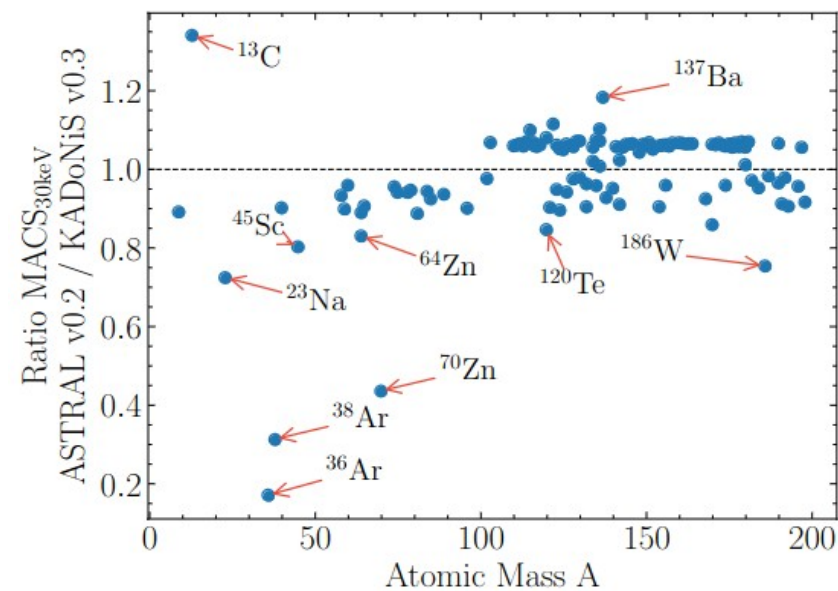
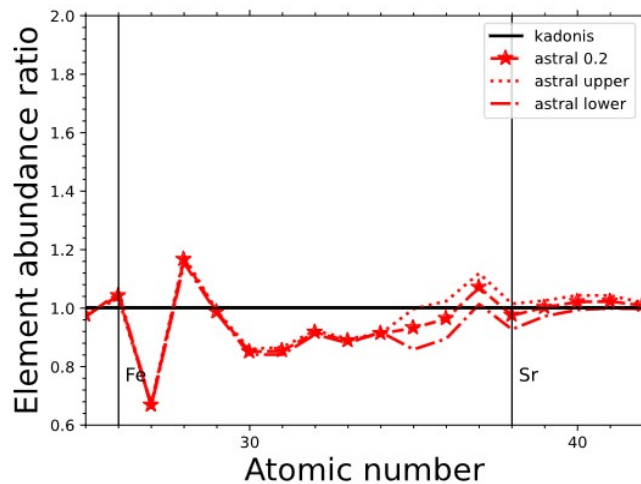
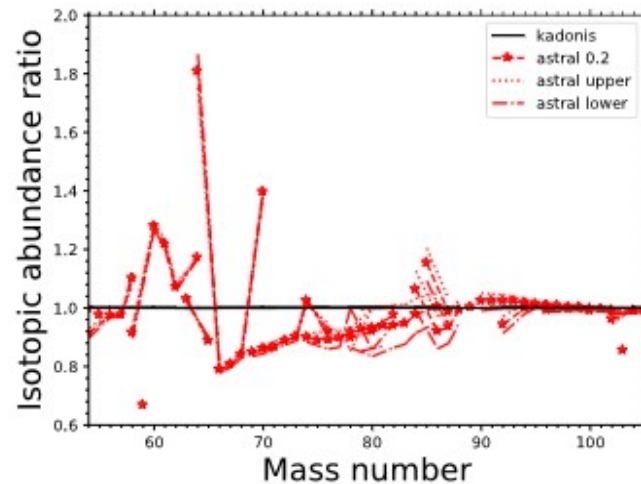


Sensitivity study: 86 neutron-capture rates in the mass regions C-Si & Fe - Zr



TASK 4.2

Example of
an application:



Vescovi+2023 ASTRAL (WP8)

<https://www.chetec-infra.eu/resources/#ASTRAL>

TASK 4.3

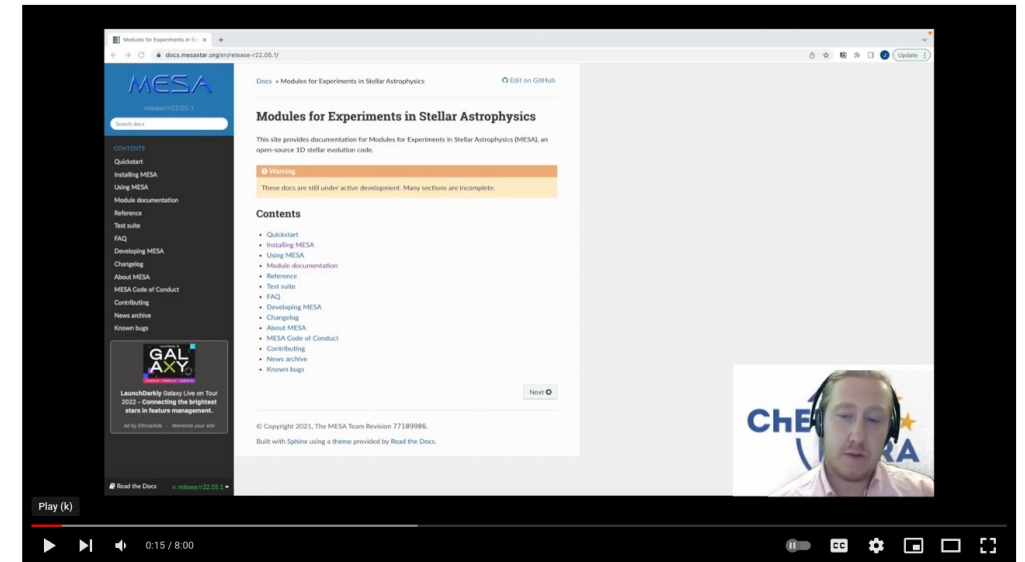
Online Training Course: star and stellar explosion codes

GOAL: provide series of courses/video tutorials for stellar evolution simulations and hydrodynamics simulations for stellar explosions

Activity:

Tutorials published for the stellar code **MESA**;

- * How to run MESA
- * How to write output suitable for post-processing
- * How to install a parallel nucleosynthesis code
- training on the **ChETEC-INFRA YouTube channel**



SE Outputs from MESA for Postprocessing

ChETEC-INFRA
69 subscribers

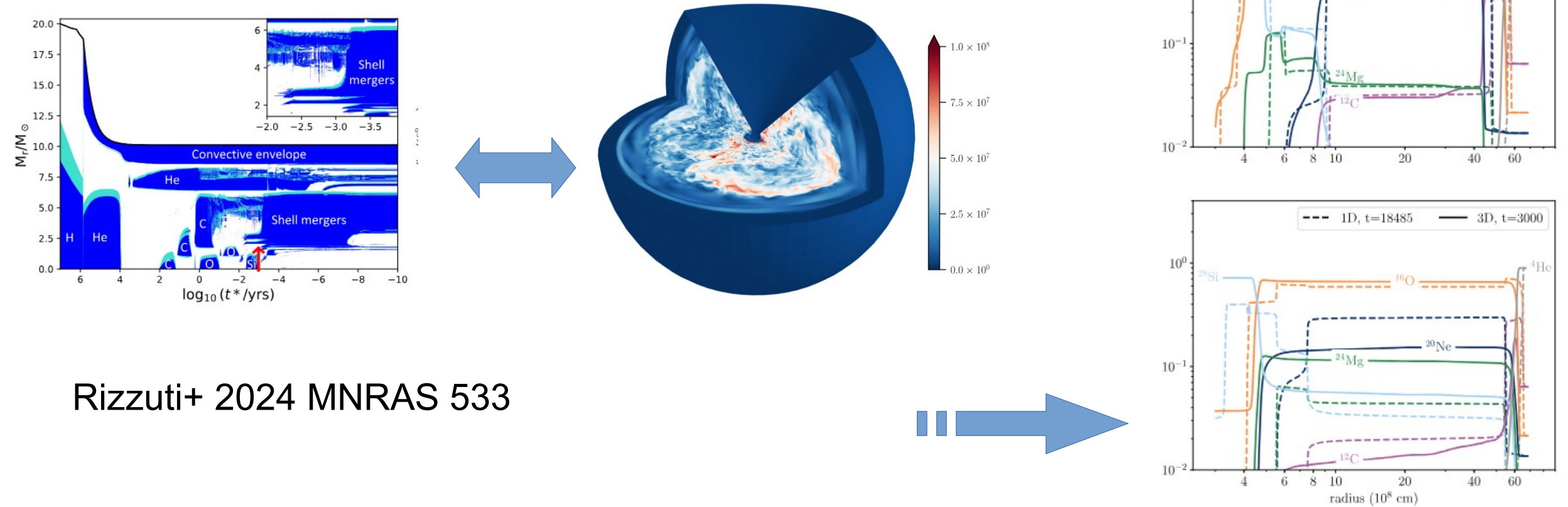
Subscribe

Like Comment Share Clip Save

<https://www.youtube.com/channel/UCB2SFPWEpNFeWZURED8PXZw/videos>

TASK 4.3

1D vs 3D massive star models



Rizzuti+ 2024 MNRAS 533

Deliverable status

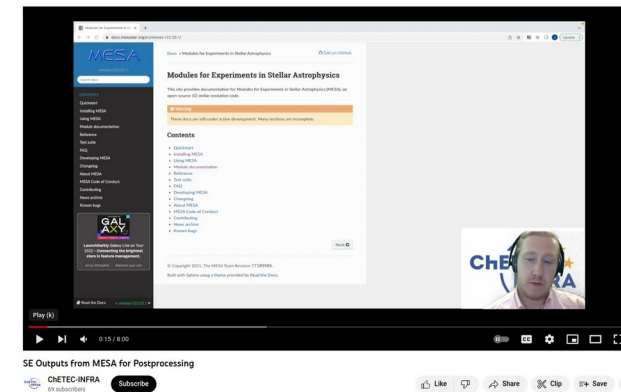
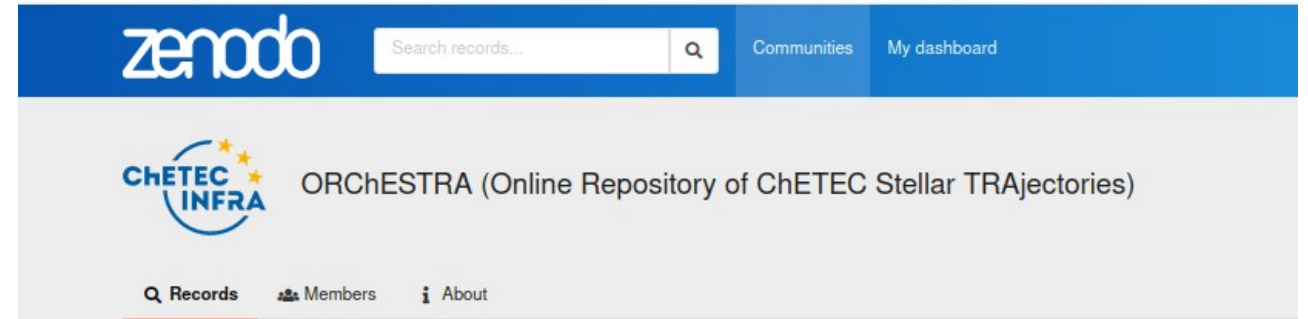
- **D4.1: First online training course on the use of stellar evolution and explosion codes and software tools for data anaAlysis active on ChETEC-INFRA web page (12 months, UKEELE). [Deliverable ready & submitted on time]**
- **D4.2: Platform where nuclear astrophysics data can be exchanged online on the ChETEC-INFRA web page (12 months, UHULL). [Deliverable ready & submitted on time]**
- **D4.3: Publication online of the first version of the library of stellar trajectories as github repository, and make available the list of nuclear reactions identified with high priority for the community (12 months, UHULL/UPC). [Deliverable ready & submitted on time]**
- **D4.4: Review simulations done in the first two years, and report on project web page the list of simulations made and resulting publications (24 months, UKEELE) [Deliverable ready & submitted a week late]**
- **D4.5: User forum active for support and Q&A (24 months, UHULL) [Deliverable ready & submitted on time].**
- **D4.6: Review stellar simulations, and report on project web page the list of simulations made and resulting publications (36 months, UKEELE) [Deliverable ready & submitted on time]**
- **D4.7: Report on sustainability of web platforms beyond the end of the project (42 months, UKEELE) [Deliverable ready & submitted on time] – Confidential, only for consortium members**
- **D4.8: Review simulations done in years 3-4, and report on project web page the list of simulations made and resulting publications (48 months, UKEELE) [Deliverable ready & submitted on time]**

Outlook

About 70 refereed publications related to WP4 activities carry the ChETEC-INFRA acknowledgement;

- Person-power:
 - ~ Mostly covered by ChETEC-INFRA until the middle of year 4, ChANUREPS still working based on other funding (see next slide);
 - ~ A PhD running for the all duration of the project;
 - ~ J. Keegans moved to a permanent position.
- All deliverables submitted on time.
- Deliverable D4.7: no source of funding identified so far in the long-term to support the open-source tools developed/supported within WP4.

D4.7



Updates & News (and some hope...):

- July 2025 Interest to find ways to support it (GIANTS2025)
- July 2025 – Interest to use ChANUREPS as standard platform where to share new LUNA rates (LUNA General meeting)



News and pieces of context for the next chetec-infra

ANNOUNCING: GEOASTRONOMY

erc A **NEW** ERC Synergy project, starting in 2025 and running for 6 years!

cPI. Steve Mojzsis
(Bayreuth, Germany/CSFK, Hungary)

PI. Fabrice Gaillard
(CNRS, France)

PI. Kevin Heng
(LMU, Germany)

TRANSLATE COMPOSITION OF STARS TO PLANETS
Planetary geochemistry and nuclear astrophysics of exoplanets.

PERFORM LAB EXPERIMENTS OF EXOPLANET MAGMAS
Laboratory experiments of outgassing from planetary interiors

INTERPRET SPECTRA OF EXOPLANET ATMOSPHERES
Theory of exoplanet atmospheres

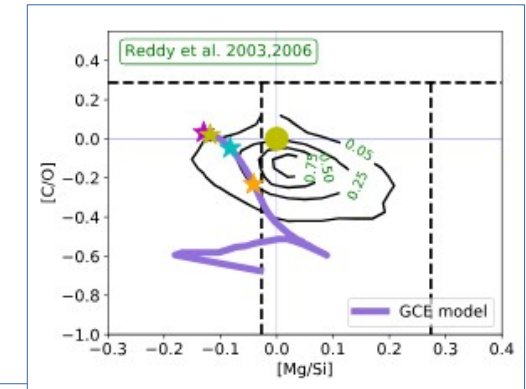
Exoplanetary systems can be markedly different from our own
A non-Earth-centric view is REQUIRED to make progress
We are recruiting Junior and Senior Staff Research Associates and Ph.D. students

“nuclear astrophysics of exoplanets”
(WP1.1, WP1.3)

GCE

Radioactives for planets

First sparkles of ideas and needs...



Experimental Astronomy (2022) 53:225–278
<https://doi.org/10.1007/s10686-021-09754-4>

ORIGINAL ARTICLE



Exploring the link between star and planet formation with Ariel

Diego Turrini^{1,2} · Claudio Codella³ · Camilla Danielski⁴ · Davide Fedele^{2,3} · Sergio Fonte¹ · Antonio Garufi³ · Mario Giuseppe Guarcello⁵ · Ravit Helled⁶ · Masahiro Ikoma⁷ · Mihkel Kama^{8,9} · Tadahiro Kimura⁷ · J. M. Diederik Kruijssen¹⁰ · Jesus Maldonado⁵ · Yamila Miguel^{11,12} · Sergio Molinari¹ · Athanasia Nikolaou^{13,14} · Fabrizio Oliva¹ · Olja Panić¹⁵ · Marco Pignatari^{16,17,18} · Linda Podio³ · Hans Rickman¹⁹ · Eugenio Schisano¹ · Sho Shibata⁷ · Allona Vazan²⁰ · Paulina Wolkenberg¹

Received: 30 June 2020 / Accepted: 13 April 2021 / Published online: 15 October 2021
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News and pieces of context for the next chetec-infra



<https://www.erc-nuclear.uk/>

About the Project

The NUCLEAR project is based at the **University of Edinburgh** and led by **Prof. Marialuisa Aliotta (PI)**. We seek to tackle three long-standing questions in nuclear astrophysics through a synergic approach of nuclear experiments, nuclear theory, and astrophysical computations.

The project involves collaboration with leading experts **Dr Guillaume Hupin**, from the Irène-Joliot-Curie Laboratory (France), **Dr Richard James deBoer** from the University of Notre Dame (US), and **Dr Marco Pignatari** from the Konkoly Observatory (Hungary).

Grant: ERC Advanced, €2.49 million

Period: 01.12.2024 - 30.11.2029

PI: Prof. Marialuisa Aliotta

