ChETEC-INFRA

Chemical Elements as Tracers for the Evolution of the Cosmos - INFRASTRUCTURES for Nuclear Astrophysics



(PI: M. Pignatari, UHULL, participants: KEELE, UPC, GUF, ULB, CSFK)

Task 4.3 EXNUC explosive nucleosynthesis codes (PI: J. Jose, UPC, participants: ULB, KEELE):



Task 4.1 Stellar nucleosynthesis tools for access to HPC (PI: R. Hirschi, Keele; participants: UHULL)

We will provide the stellar nucleosynthesis tools and user-friendly support to use these tools within an HPC framework (**Objective 1**). For this purpose, we will:

- i) help users to generate the "SE" files for their stellar models. Python scripts will be provided to the users for this purpose;
- set up the HPC nucleosynthesis simulations for the SE files. Nucleosynthesis tools for the simulations are version-controlled and made available on github repositories (https://github.com/NuGrid);
- iii) provide dedicated online and in-person training courses for the software tools, and for the data analysis software.
- iv) verify that codes are fully operational at the UHULL HPC facility included in ChETEC-INFRA and, on request, also on additional facilities that are accessible to individual users and may in the future become accessible to all users.
- v) Share common data analysis packages via github repositories.



Task 4.2: objective

- <u>Objective 3</u>: Generate verified nuclear sensitivity studies, extensive or upon specific user requests, to support proposals for experiments at nuclear physics infrastructures. Transparency and reproducibility of the results.
- <u>Objective 4</u>: Provide access to impact studies on stellar nucleosynthesis of new nuclear experiment results, or new theoretical rates from computational simulations.

Task 4.2: Actions

- (i) Create and maintain a **platform on the ChETEC-INFRA web page where nuclear astrophysics data can be exchanged**, connecting theoretical predictions with nuclear experimental data and stellar yields.
- (ii) Create, update and publish regularly a fully documented library of certified trajectories, covering a wide range of stellar conditions for nuclear astrophysics simulations (NuGrid One-Zone Numerical Experiments – OZONE library*). Trajectories will be fully available in github repositories.
- (iii) Upgrade and extend capabilities of the NuGrid Sensitivity study tool (NuSensi), and make available extensive sensitivity studies to the community based on the OZoNE library, to probe the need of new nuclear experiments or of theoretical studies.
- (iv) Provide dedicated online and in-person training courses for the software tools NuSensi, for users
 interested in specific impact studies associated to their research projects. Young researchers at
 postgraduate level mainly represent the user pool in our community.
- (v) Develop a pipeline of full representative stellar models (NuGrid Impact study Pipeline NuGIPi), giving the capability to deliver impact studies of new experimental nuclear reactions measured in nuclear physics infrastructures, and theoretical nuclear reactions calculated with computational simulations.

* Alignment with investments from **CaNPAN** (Canadian Nuclear Physics for Astrophysics Network, project funded **NPDOE** - Nuclear Physics of the Dynamic Origin of the Elements), **IReNA** and **JINA-CEE**.

Task 4.2: Science

Method 2





Task 4.3 EXNUC Explosive Nucleosynthesis Codes (PI: J. José, UPC, participants: ULB, KEELE)

Facilitate and streamline access to existing computer codes, sharing our know-how to shorten down to one month the training period required (**Objective 2**).

- i) Help users to access the codes MESA, FLASH and GADGET-2, reproducing the relevant examples provided online.
- ii) Set up the simulations and data-analysis tools.
- iii) Provide dedicated online and in-person training courses for the software tools, and for the data analysis software.
- iv) Verify that codes are operational, and provide support for simulation setup at selected HPC facilities included in ChETEC-INFRA.

EXAMPLES



3D **FLASH** simulations of mixing at the core-envelope interface in classical nova outbursts

[Ref: Casanova, José, García-Berro et al., *Nature* 2011]



3D **GADGET-2** SPH simulations of the interaction between ejecta, disk, and the stellar secondary in classical nova outbursts [Ref: Figueira, José, García-Berro et al., *A*&A 2018]

Deliverables

- D4.1: First online training course on the use of stellar evolution and explosion codes and software tools for data analysis active on ChETEC-INFRA web page (12 months, UKEELE)
- D4.2: Platform where nuclear astrophysics data can be exchanged online on the ChETEC-INFRA web page (12 months, UHULL).
- D4.3: Publication online of the first version of the OZoNE library as github repository, and make available the list of nuclear reactions identified with high priority for the community (12 months, UHULL).
- 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).
- D4.5: User forum active for support and Q&A (24 months, UHULL).
- D4.6: Review stellar simulations, and report on project web page the list of simulations made and resulting publications (36 months, UKEELE).
- D4.7: Report on sustainability of web platforms beyond the end of the project (42 months, UKEELE)
- 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).

Participants (2020)

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

ChETEC-INFRA WP4 mailing-list (April 2021)



Marco Pignatari Privileged owner, Subscriber

List Options

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Schmidt, Marco Pignatari, Raphael

Hirschi 📝

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First round-table discussion: in the WP4 parallel session.