Grant Agreement No: 101057511

EURO-LABS

EUROpean Laboratories for Accelerator Based Sciences

HORIZON-INFRA-2021-SERV-01-07 Project EURO-LABS

MILESTONE REPORT

ALL CODES INSTALLED AT THEO4EXP VA AND INTEROPERABILITY AMONG DIFFERENT NODES ESTABLISHED

MILESTONE: MS11

Document identifier:	EURO-LABS-MS11-Theo4Exp
Due date of milestone:	End of Month 42 (February 2026)
Report release date:	28/02/2026
Work package:	WP2: TA1/VA1-RIs for Nuclear Physics; Task 4.B: Description of research infrastructures offering theoretical support for experiments
Lead beneficiary:	USE, IFJ-PAN, UMIL
Document status:	Final

Abstract:

This document outlines the inclusion, into each installation of Theo4Exp, of all envisaged codes in the project application. These codes are being used by researchers worldwide at the Virtual Access (VA) infrastructure accessible via https://institutional.us.es/theo4exp. Although, the final part, interoperability among the different nodes, could not be implemented, the three nodes are accessible from the same webpage and registration access, and are currently in use. Additionally, a workshop has been conducted at ECT* to demonstrate its functionality and provide training.

For more information on EURO-LABS, its partners and contributors please see https://web.infn.it/EURO-LABS/

The EUROpean Laboratories for Accelerator Based Sciences (EURO-LABS) project has received funding from the Horizon Europe programme dedicated to Research Infrastructure (RI) services advancing frontier knowledge under Grant Agreement no. 101057511. EURO-LABS began in September 2022 and will run for 4 years.

Delivery Slip

	Name	Partner	Date
Authored by	M. Rodríguez-Gallardo, J. Dudek and G. Colò	USE, IFJ-PAN, UMIL	27/02/2026
Edited by	M. Rodríguez-Gallardo, J. Dudek and G. Colò	USE, IFJ-PAN, UMIL	27/02/2026
Reviewed by	U. van Kolck [Task coordinator] A. Maj [WP coordinator]	FBK-ECT* IFJ-PAN	27/02/2026
Approved by	A. Navin [Scientific coordinator]	GANIL	28/02/2026

TABLE OF CONTENTS

Executive summary

This milestone reports the successful implementation and deployment of all planned computer codes within the Theo4Exp Virtual Access (VA) infrastructure, developed under Task 4.B of Working Package 2 of the EURO-LABS project. Theo4Exp provides worldwide access to theoretical tools supporting nuclear physics experiments through three installations: MeanField4Exp, Reaction4Exp, and Structure4Exp, hosted at IFJ-PAN, the University of Seville, and the University of Milan, respectively.

The platform has been publicly accessible since February 2024, and all envisaged codes were fully installed and operational by January 2025. Access is provided through a common authentication system based on eduGAIN and ORCID. The infrastructure currently serves more than 400 registered users and has been actively promoted through workshops and dissemination activities.

The platform enables nuclear structure and reaction calculations through user-friendly interfaces, providing graphical and numerical results. The three installations are accessible through a common entry point, and initial interoperability between services has been established. Theo4Exp is fully operational and represents an important achievement of EURO-LABS, improving access to theoretical support and strengthening collaboration between theorists and experimentalists.

1. INTRODUCTION

Task 4 in the Work Package 2 “Research Infrastructures for Nuclear Physics” of EURO-LABS project encompasses two research infrastructures targeted to offer theoretical support for experiments, including Transnational Access (TA) and Virtual Access (VA): ECT* FBK Trento (TA) and Theo4Exp (VA). Theo4Exp is a new virtual infrastructure that has been developed within the EURO-LABS project and includes three installations: MeanField4Exp (hosted at IFJ PAN, Krakow), Reaction4Exp (hosted at University of Seville) and Structure4Exp (hosted at University of Milano).

The infrastructure is open to users worldwide since February 2024, first with some part of the envisaged programs and progressively incorporating the remaining programs until the planned scope is fully completed. The EU funding of personnel to carry out this VA platform is creating a virtual circle of increased collaboration between theorists and experimentalists. The key point is that now some codes are accessible to every scientist, and the associated results can be easily compared. This provides an easier and more effective access to submit proposals at experimental facilities. Additionally, a workshop has been conducted at the ECT* to demonstrate its functionality and provide training, attended by a significant group of participants, mostly experimentalists.

An International Review Panel (IRP) meets every year to review and validate the progress made on the VA infrastructure at its three installations. The IRP is composed of the following members: Piotr Bednarczyk (IFJ-PAN, Chairperson), Antonio Moro-Muñoz (University of Seville), Enrico Vigezzi (INFN-Milano), Krzysztof Rusek (University of Warsaw), Ian J. Thompson (Lawrence Livermore National Laboratory, LLNL) and Angela Gargano (INFN-Napoli). The last review will be held before the end of the project.

2. ALL CODES INSTALLED AT THEO4EXP VA

As already reported on the previous MS10 report, the VA infrastructure is available since 1st February 2024, at https://institutional.us.es/theo4exp. The link to each installation, MeanField4Exp, Reaction4Exp and Structure4Exp, can be easily found in this webpage. The user access to the installations is provided by the application https://iam-eurolabs.ijclab.in2p3.fr/login, that has been developed in task 2 of WP5 of the present EURO-LABS project. This application provides the access either via eduGAIN (https://edugain.org/) or ORCID (https://orcid.org/), ensuring access to any researcher affiliated to a scientific institution.

The infrastructure started operating with some of the codes and was progressively expanded until the incorporation of all the planned codes (more precisely, the different types of calculations) that was completed in January 2025. It has been operating successfully since its public launch, with a high number of registered users (more than 400) and a significant number of calculations performed. The platform has been widely disseminated through several activities, including an invited talk at the Zakopane Conference 2024 in Nuclear Physics [1], a workshop at the ECT* aimed at explaining its operation through practical examples (https://www.ectstar.eu/workshops/theory-service-for-the-low-energy-nuclear-physics-community-a-hands-on-workshop/), and a publication in Nuclear Physics News [2]. Furthermore, two articles on the platform have been published in the EURO-LABS project newsletter, one in July 2024 and another in December 2025 (see https://web.infn.it/EURO-LABS/category/news/newsletter/). In addition to the above, an article has also been published in the Spanish edition of The Conversation [3].

2.1. MEANFIELD4EXP CODES

The service referred to as MeanField4Exp (https://meanfield4exp.ifj.edu.pl) combines a series of applications representing branches of the global approach usually referred to as Nuclear Mean-Field Theory. The present realisation evolved from the so-called Realistic Universal Phenomenological Mean Field approach using deformed Woods-Saxon Hamiltonian with its universal parameterisation employing typically 9 parameters optimised once for all whereas addressing about 3000 nuclei of the Mass Table.

The service employs numerous advanced computer codes based on combinations of selected methods of nuclear structure theory and quantum mechanics, with advanced techniques of Applied Mathematics such as Inverse Problem Theory and Monte Carlo Simulations in optimising Hamiltonian parameters, Graph Theory in analysing the description of nuclear shape transitions in multi-dimensional deformation spaces, or Group Theory and Group Representation Theory in treating the nuclear symmetry issues.

The user ready applications — thanks to installation of the advanced computer codes — address the following low energy nuclear structure physics issues:

- Single Nucleon Energies as Functions of Nuclear Shapes
- Nuclear Energies According to Macroscopic-Microscopic Method (1D Multi-nucleus Representation)
- Nuclear Energies According to Macroscopic-Microscopic Method (2D Potential Energy Maps)
- Shape Evolution with Spin According Macroscopic Models
- Single Nucleon Routhians as Functions of Rotational Frequency

- 3D Representations of Nuclear Surfaces for User Chosen Deformation Parameters
- Effective GDR Strength Functions for Given Spin and Temperature
- 3D Representations of Single Nucleon Probability Density Functions

Results, which can be obtained with the help of the programs underlying the above services, can be seen as follow-up of 'pilot project articles' already published. An interested reader will find an introduction and illustrations to the issues of confidence intervals of our nuclear structure predictions as well as predictive power and improvements of predictive power in Refs. [1-2]. Examples of realistic predictions of nuclear equilibrium deformations, shapes and exotic shape coexistence with the help of the mean-field Hamiltonian without parametric correlations can be found in Ref. [3]. Illustrations focusing on the exotic symmetries and new forms of shell-effects and underlying new concepts of "magic numbers" or shell closures are published in Refs. [4-6].

2.1.1. Single Nucleon Energies as Functions of Nuclear Shapes

The user will be able to generate the single-nucleon energy diagrams of the global structure illustrated on the example below after specifying the proton and neutron numbers of the nucleus needed for the project. One needs to select the nuclear multipole mean field deformation types and ranges, and the nucleon level labelling according to proposed standards used typically in the literature.

The following types of labelling are possible:

• Cartesian labels $[n_x, n_y, n_z]$:
States are labelled by the quantum numbers of the Cartesian Harmonic Oscillator basis-state dominating in the expansion of the solution.

• Nilsson labels $[N, n_z, \Lambda]\ \Omega$:
States are labelled by the quantum numbers of the Cylindrical Harmonic Oscillator basis-state dominating in the expansion of the realistic wave function found, here using axial coordinate system, where N is the principal harmonic oscillator quantum number, n_z is the number of nodes along nuclear symmetry axis (O_z-axis), Λ is the projection of the nucleonic orbital angular momentum on the nuclear symmetry axis, and Ω is the projection of the total nucleonic angular momentum on the same axis.

• Spherical labels $[N, \ell, j]\ j_z$:
States are labelled by the quantum numbers of the Harmonic Oscillator basis-state dominating in the expansion of the realistic wave function found, here using spherical coordinate system, where N is the principal shell quantum number, ℓ is the nucleonic orbital angular momentum quantum number, j is the total nucleonic angular momentum, and j_z is the corresponding z-projection.

The two figures below illustrate typical diagrams in this category, here for a relatively light nucleus.

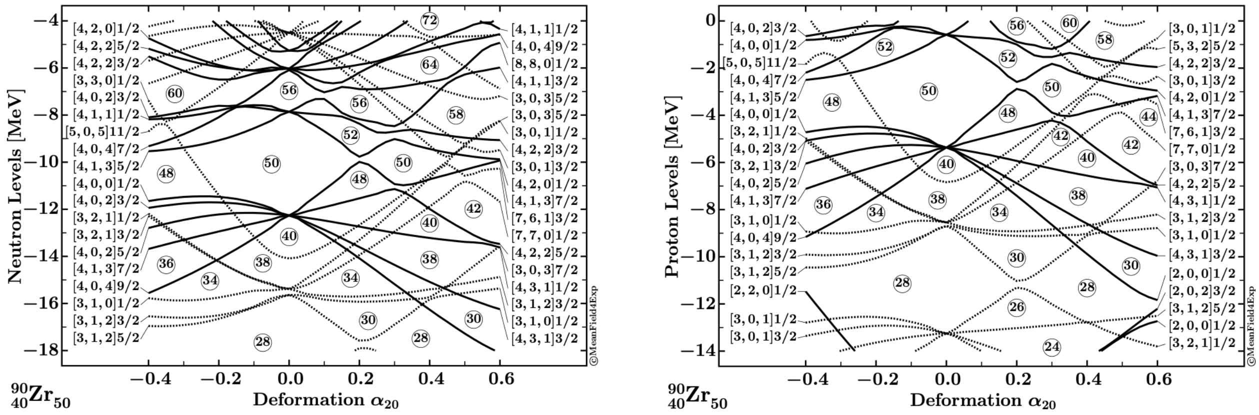


Figure 1: *Single particle levels as function of α_{20} for ^{90}Zr for neutrons (left) and protons (right).*

2.1.2. Nuclear Energies According to Macroscopic-Microscopic Method (1D Multi-nucleus Representation)

This option allows generating comparative 1D nuclear energy diagrams employing the phenomenological Macroscopic-Microscopic Method for a chain of isotopes and/or isotones. Our algorithms employ the Realistic Phenomenological Nuclear Mean-Field Theory Approach with the Universal Woods-Saxon Hamiltonian.

The user needs to select a central nucleus by entering the proton and neutron numbers, and select the range of nuclei by adjusting the intervals *ΔZ* and *ΔN*. Selected nucleon numbers become the labels of the plotted curves (see below). As usual in the present system of programs the user selects a parameter set for the Woods-Saxon Hamiltonian from the dropdown menu.

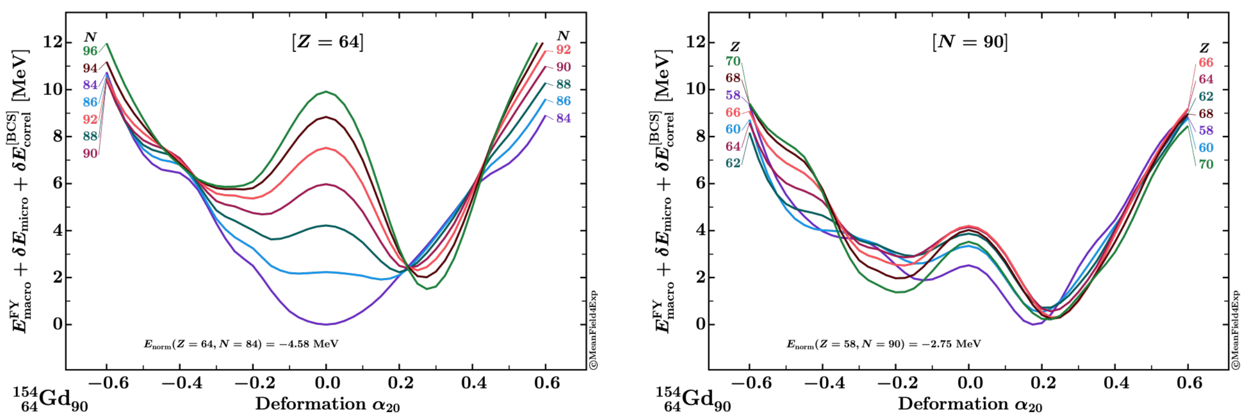


Figure 2: *Isotopes and isotones total nuclear energy as function of quadrupole deformation for ^{154}Gd*

2.1.3. Nuclear Energies According to Macroscopic-Microscopic Method

After selecting *Z* and *N* number of the nucleus of interest the user may specify the design and the appearance of the potential-energy map of interest by employing the provided formatting table. The user has a freedom of choosing the variant of the total Macroscopic-Microscopic energy formula according to which

$$E_{tot} = E_{macro} + E_{micro} + E_{pairing} \quad (1)$$

The macroscopic energy, E_{macro}, appears in two variants, the so-called Yukawa-folded [E(FYU)] and the Lublin-Strasbourg Drop [E(LSD)] liquid drop models. The standard Strutinsky shellcorrection energy is denoted E_{micro}, whereas the pairing term, $E_{pairing}$, can be chosen in the form of the so-called pairing correlation energy with a simple (BCS) approximation or a more advanced Particle Number Projection (PNP) approximation. Illustrations below are arbitrarily chosen - whereas the user will be able to adapt the final choice to her/his needs.

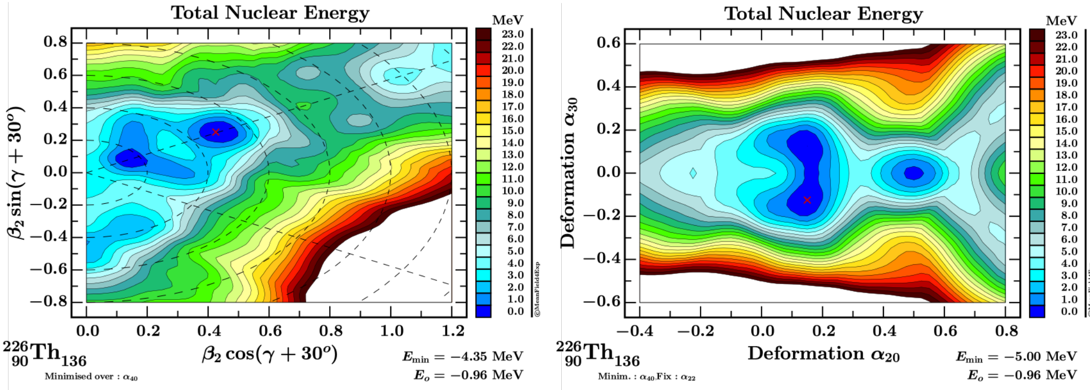


Figure 3: *Examples of the total energy maps for the axial and non-axial quadrupole deformation choice – left, as opposed to axial-octupole (pear-shape) vs axial quadrupole (elongation) – right.*

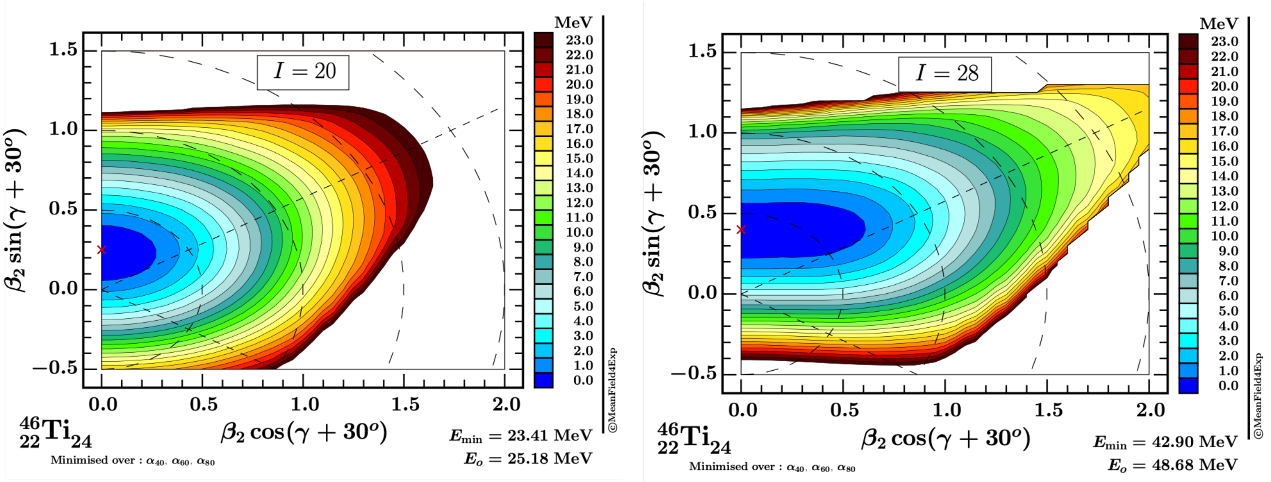
2.1.4. Shape Evolution with Spin According Macroscopic Models

The user of this option is invited to select the proton and neutron numbers of the nucleus needed from the pre-calculated data base containing the results for even-even nuclei only. Potential energy surfaces were pre-calculated using multiprocessor computer systems within an ensemble of 5-dimensional original deformation spaces. The graphical representation corresponds to choosing two deformation variables as x-, and y-coordinates. The total energies are minimised over the remaining variables at the disposal. Next, one needs to choose the variant of the total energy formula according to which

$$E_{tot} = E_{macro} + E_{rotation} \tag{2}$$

The macroscopic energy, E_{macro}, appears in two variants, the so-called Lublin-Strasbourg Drop [E(LSD)] and "traditional" Myers-Swiatecki [E(M-S)]. The rotational energy part is defined as in the classical rotor case. Those interested can find the original references [6-9].

Map appearance and the format specifications are also at the user disposal. The size of the colour stripes [in MeV] for the energy contour plotting can be chosen as well as the aesthetic aspects such as the smoothness of the contour lines - via the corresponding input fields.



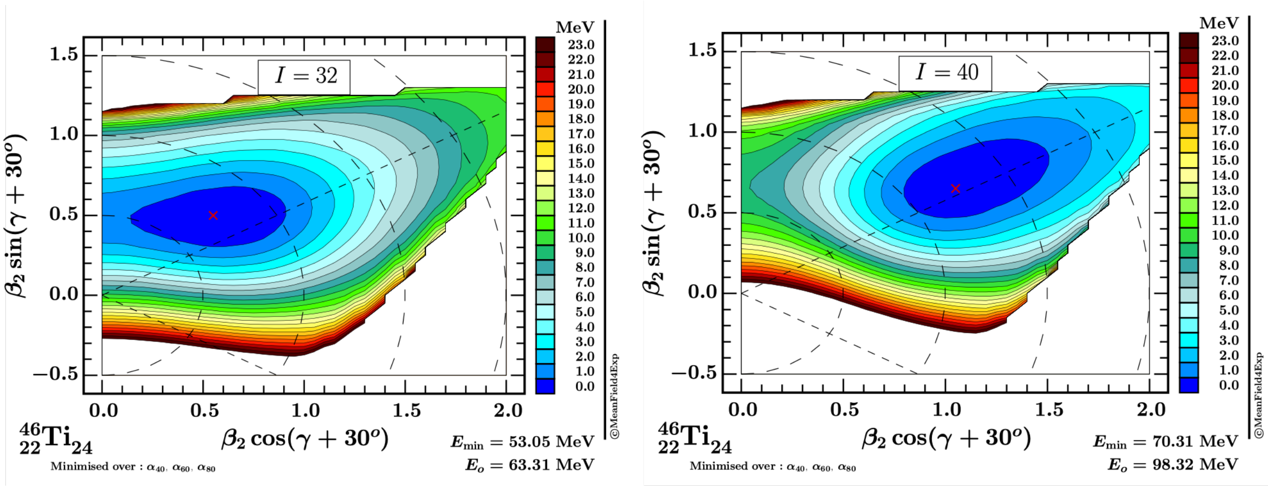


Figure 4*: Shape evolution with spin for ^{46}Ti.*

2.1.5. Single-Nucleon Routhians as Functions of Rotational Frequency

This option allows generating the single particle Routhians (single-nucleon energies in the rotating coordinate frame) calculated using the so-called 3D-Cranking approach. Mean-field Hamiltonian describing the motion of a single particle under collective rotation in the Cranking approach is defined as follows:

$$\hat{H}_\omega = \hat{H}_0 - \vec{\omega} \cdot \vec{\hat{j}} \tag{3}$$

where $\hat{H}_0$ is the deformed mean-field Hamiltonian, whereas the so-called cranking term

$$\vec{\omega} \cdot \vec{\hat{j}} = \omega_x \hat{j}_x + \omega_y \hat{j}_y + \omega_z \hat{j}_z \tag{4}$$

represents the scalar product of the total single nucleon angular-momentum $\vec{\hat{j}}$ and the rotational frequency $\vec{\omega}$.

The user specifies her/his choice among three universal parameterisations (three parameter sets employing among 9 to 12 parameters, optimised once for all for 3000 nuclei of the Mass Table (wherefrom the term “universal”), the actual nucleus and its deformation in terms of $\alpha_{\lambda\mu}$.

The presented option can be seen as one of the most powerful on the market since the user may control the 3D aspect of nuclear rotation by specifying the orientation of the cranking vector with respect to the nucleus with the help of three cranking frequency components at her/his disposal. The diagram below represents arbitrarily chosen type of rotation and nuclear shape.

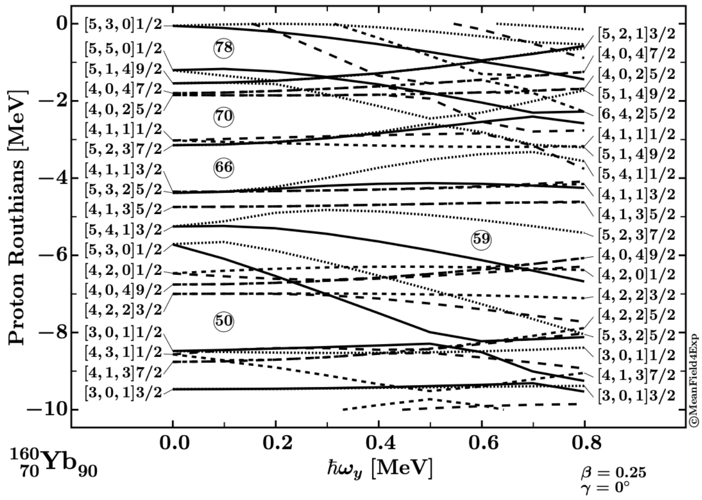


Figure 5: *Proton single particle Routhians for ^{160}Yb nucleus, at fixed deformation* $\beta = 0.25$.

2.1.6. Nuclear Shapes and 3D Nuclear Surfaces

This option can be seen as providing pedagogical representations of the nuclear shapes and in particular shape symmetries. The user can model nuclear surfaces based on specified deformation parameters, $\alpha_{\lambda\mu}$, employing an expansion in terms of spherical harmonics

$$\Sigma: R(\vartheta,\varphi) = R_0 C(\alpha)\left[1 + \sum \alpha_{\lambda\mu} Y_{\lambda\mu}(\vartheta,\varphi)\right]. \tag{5}$$

This expression represents the distance from the centre of the reference frame to the points at the surface. Above, $\alpha_{\lambda\mu}$ represents the nuclear deformation parameters, according to standard notation: $(\lambda = 2)$ quadrupole, $(\lambda = 3)$ octupole, and $(\lambda = 4)$ hexadecapole. The user can combine up to 6 independent multipole deformations parameters. Some typical illustrations are shown below.

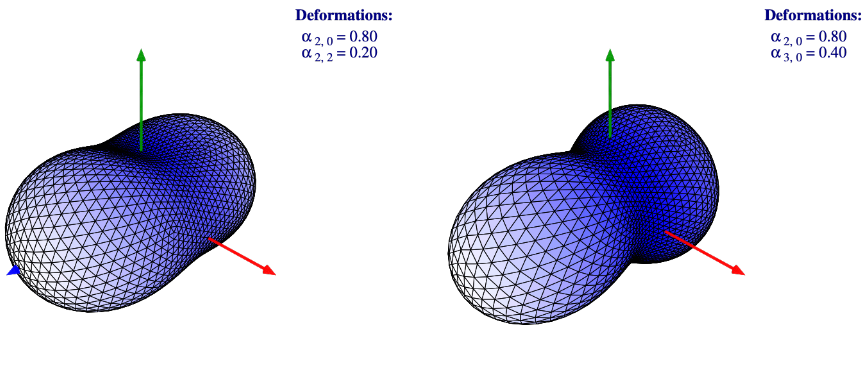


Figure 6: *3D shape representations at the deformations indicated; Here super-deformed elongation was selected.*

2.1.7. Generating effective GDR strength function for given angular momentum and temperature

This option allows the user to model the Giant Dipole Resonance (GDR) strength function in terms of the evolution with nuclear angular momentum and temperature according to macroscopic nuclear models. The user may choose the nucleus and the model parameters after consulting the provided elementary references. Graphical aspects are controlled with self-explanatory input data.

The user has a parameter choice limited by a pre-calculated data base containing results for even-even nuclei only. The Macroscopic Energy maps represent the sum of the Lublin-Strasbourg-Drop

macroscopic and rigid body rotation energies for selected spins minimised over α_{30}, $\alpha_{40}$and α_{50} deformation parameters.
The following diagrams show arbitrarily chosen cases focussed on illustrations of the GDR strength.

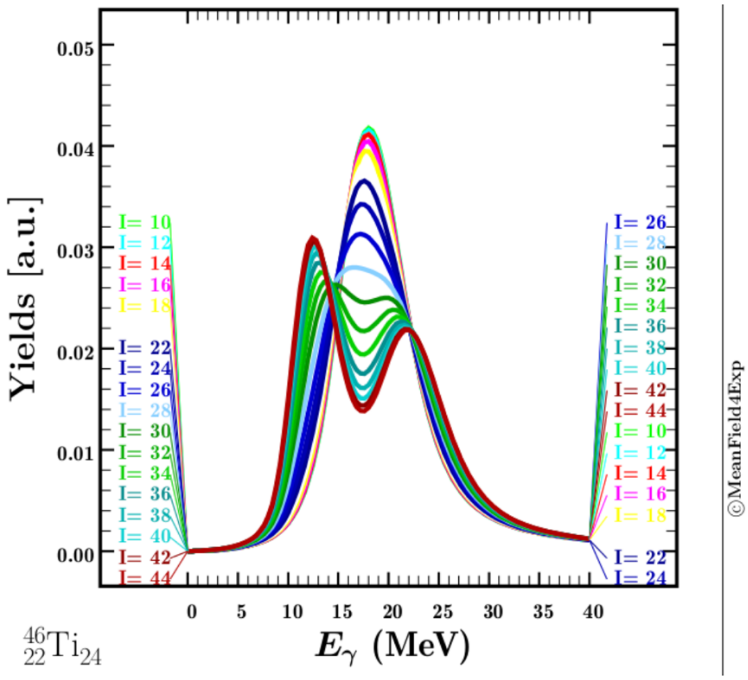


Figure 7: *Effective GDR strength functions in ^{46}Ti for varying spins (from 10 to 44).*

2.1.8 Single Nucleon Probability Density Functions

This option provides illustrations of the spatial behaviour of the nucleonic wave functions employing the densities $\rho_n(r) = |\Phi_n(r)|^2$, for either protons or neutrons. This is done by constructing simplified projection type illustrations of the nucleonic orbital densities in space, to enable the user to construct images of various projections of the wave functions but at the same time mutual relative placements of density distributions of various orbitals.

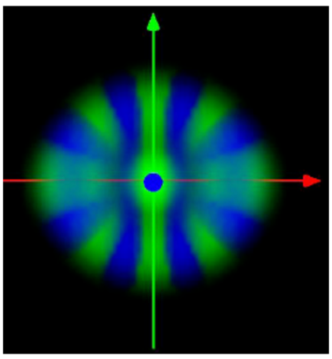


Figure 8: *Example of single nucleon probability density functions for two neighbouring orbitals.*

2.2. REACTION4EXP CODES

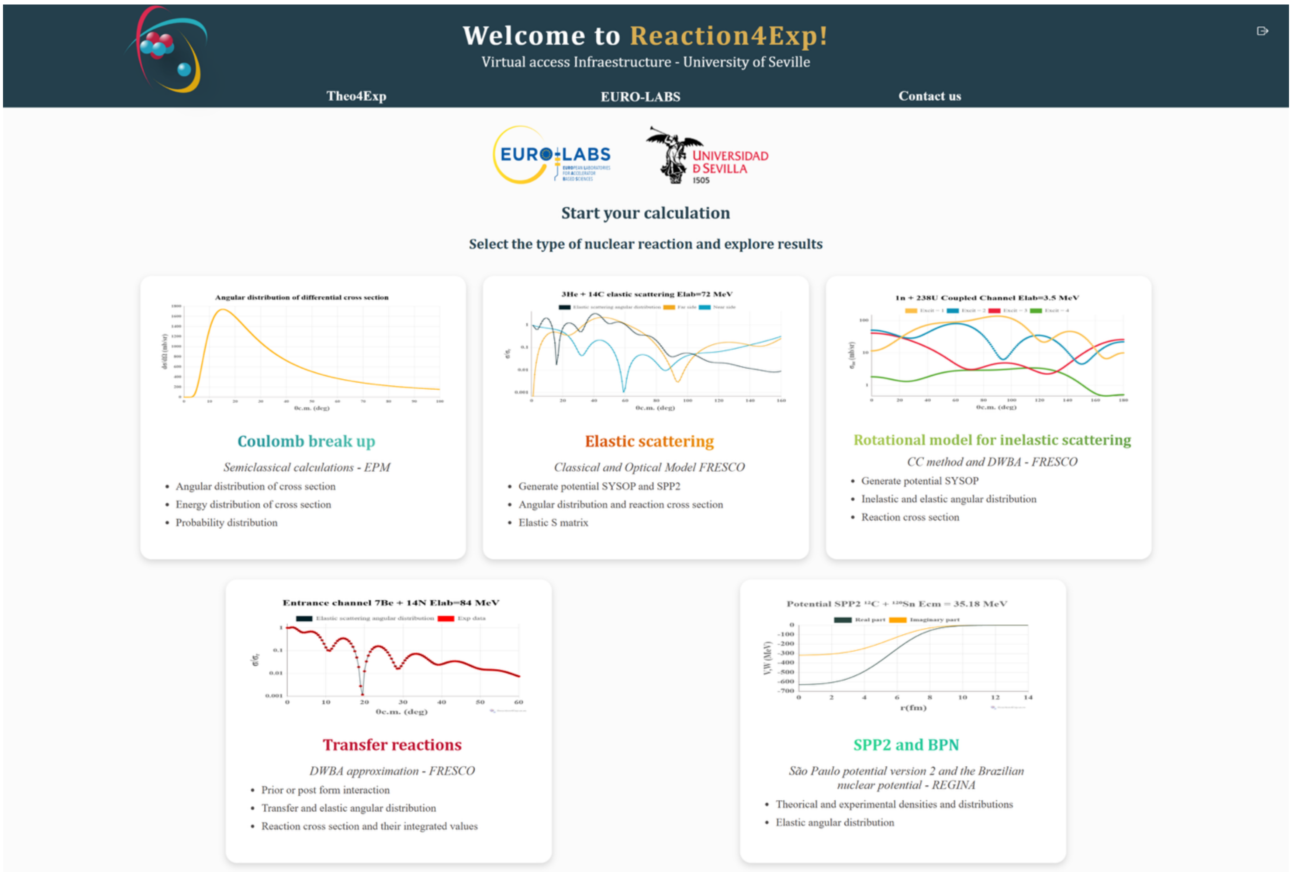


Figure 9: *Homepage for Reaction4Exp showing the five types of calculations*

In the main page of Reaction4Exp (https://reaction4exp.us.es) we have included an option for each type of calculation that it is available (see Fig.): (1) Coulomb Breakup, (2) Elastic Scattering, (3) Inelastic Scattering, (4) Transfer Reactions and (5) folding potentials with SPP2 and BNP. To perform these calculations the codes used are an Equivalent Photon Model (EPM) [10,11] code developed at Universidad de Sevilla, FRESCO [12] code, REGINA [13] code and a classical scattering program [14], also developed at Universidad de Sevilla to be included in the installation. In the following, a short explanation is given about the services available in the installation.

2.2.1 Coulomb Breakup (Equivalent Photon Model)

The EPM code (developed by J. A. Lay Valera at University of Seville) calculates differential Coulomb breakup cross sections from external transition probabilities, as functions of both angle and energy. Multipolarities included are dipole and quadrupole for electric transitions and only dipole for magnetic transitions. The results are presented in text format and graphically displayed. As output, the code provides: the angular distribution of inelastic/breakup cross section, the energy distribution of inelastic/breakup cross section, and the inelastic/breakup probability distribution.

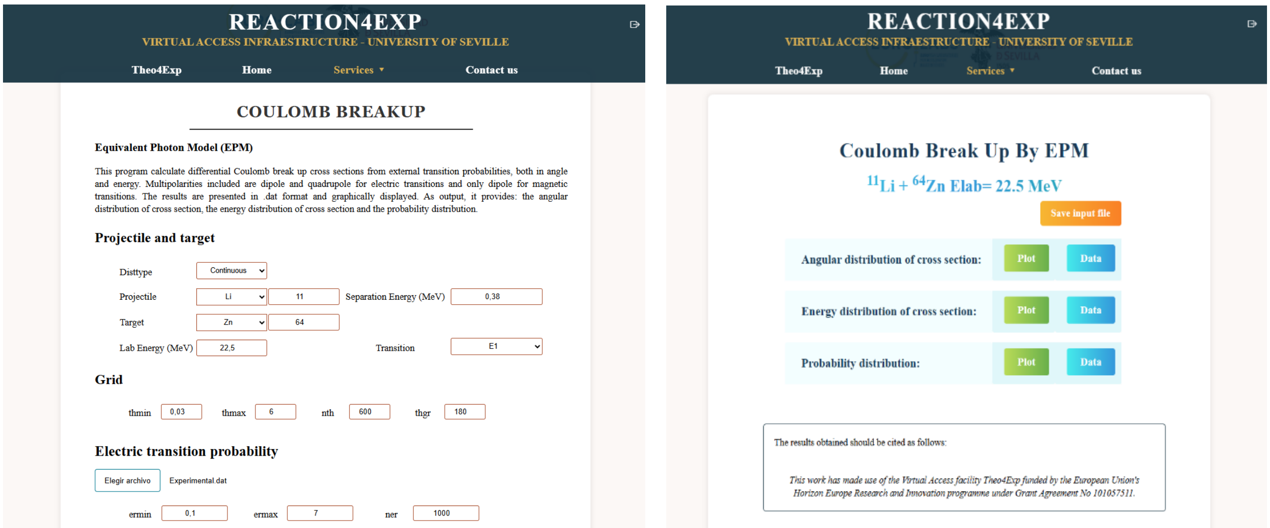


Figure 10: *Examples of the input data page and the results page*

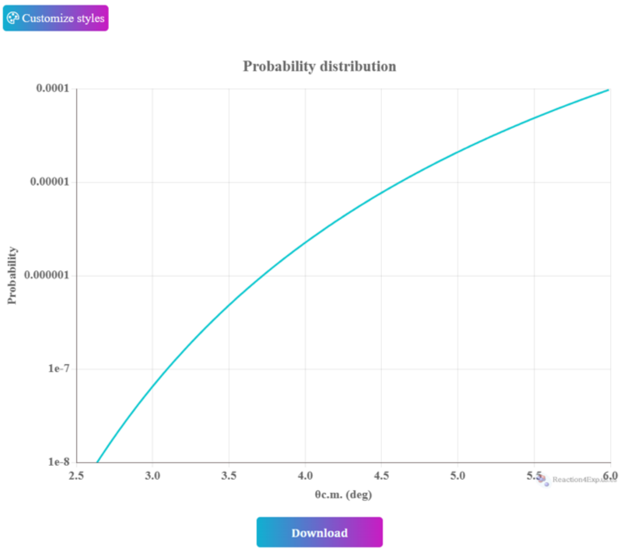


Figure 11: *Breakup probability distribution for ^{11}Li+^{64}Zn at 22.5 MeV.*

2.2.2 Elastic Scattering (Optical Model and Classical)

The Elastic Scattering calculation allows us to choose between the Optical Model (OM) or a classical model. The OM provides the elastic cross section of the reaction considered, at a given energy in the laboratory frame, when an optical potential is provided in order to describe the interaction between projectile and target. The code used for this is FRESCO [9], developed by I.J. Thompson (LLNL, USA), and close collaborator of the group at the University of Seville. The results are presented in text format and graphically displayed. As an output, it provides: the angular distribution for the elastic cross section, the absorption and total reaction cross section as a function of the total angular momentum, and the modulus of the elastic S-matrix as a function of the total angular momentum. On the other hand, the classical model [14] program in Reaction4Exp was developed by Mario Gomez-Ramos from University of Seville, and it provides results that include deflection functions, trajectories and turning points.

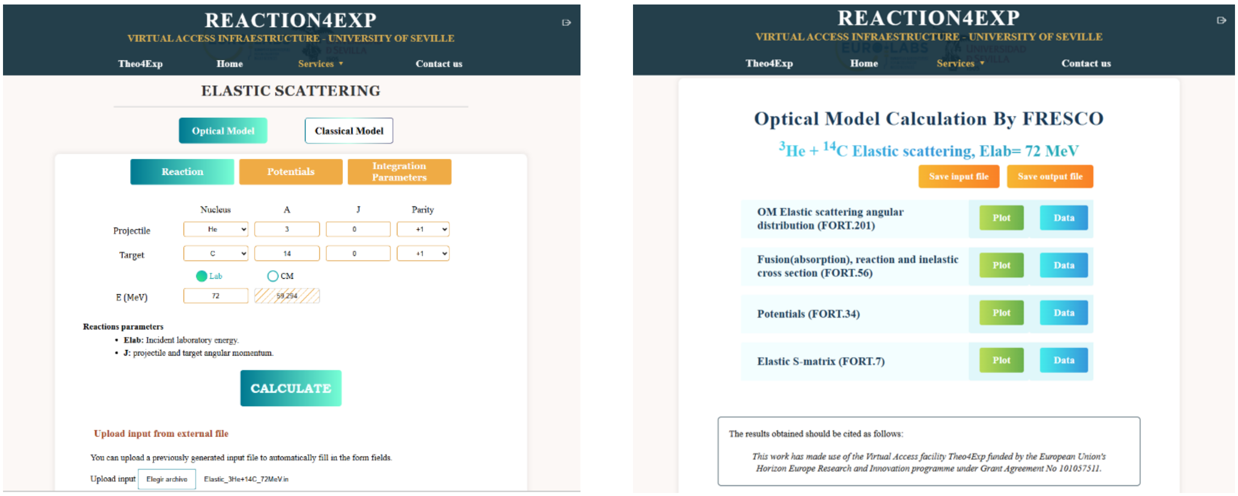


Figure 12: *Examples of the input data page and the results page for the optical calculation*

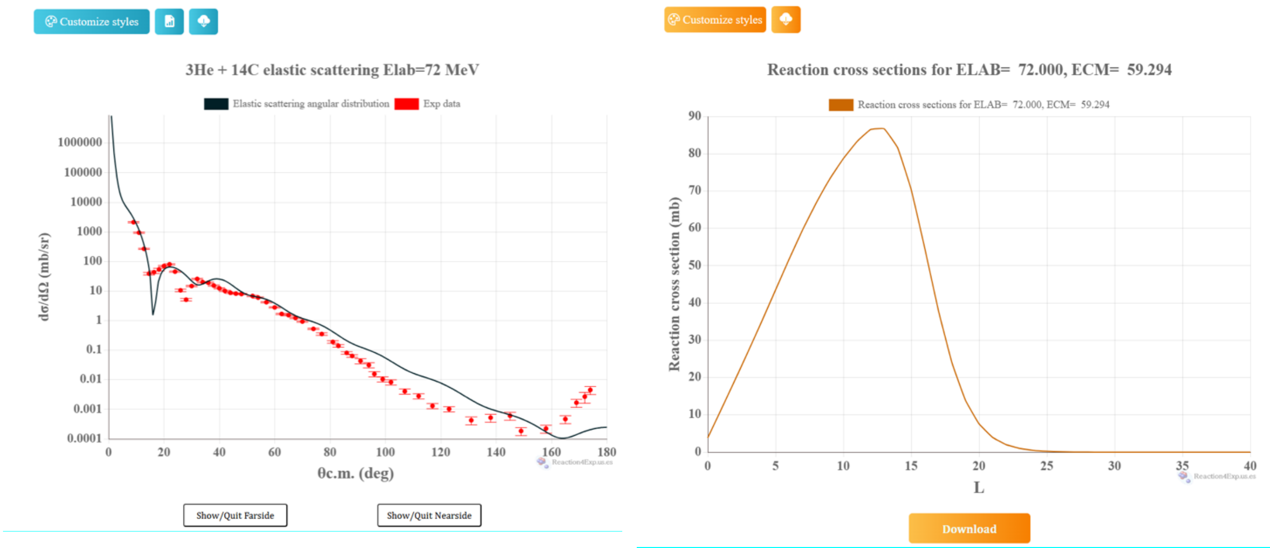


Figure 13. *Angular distribution for the elastic cross section of reaction $^{3}He+^{14}C$ at 72 MeV compared with experimental data (left). The reaction cross section as a function of the angular momentum for the same reaction (right).*

As novelty with respect to the past report is that this calculation includes an optical potential generator with two options (see Fig. 14):

- Systematic Optical Model Potentials (SYSOP): a generator for nuclear optical model potentials. It supports several well-known models, including Becchetti-Greenless, Koning-Delaroche, CH89, Watson and others. SYSOP allows users to compute potentials for various projectile-target combinations over a wide energy range. Developed by Danyang Pang, it incorporates the frontend code of TWOFNR, maintained by Jeffrey A. Tostevin.
- The REGINA [13] code calculates the São Paulo potential version 2 (SPP2) and the Brazilian nuclear potential (BNP), using nuclear densities and distributions for a large variety of nuclei. With theorical and experimental densities for the calculations.

The second option corresponds precisely to the fifth type of calculation that was planned and represents an important step towards interoperability within the installation.

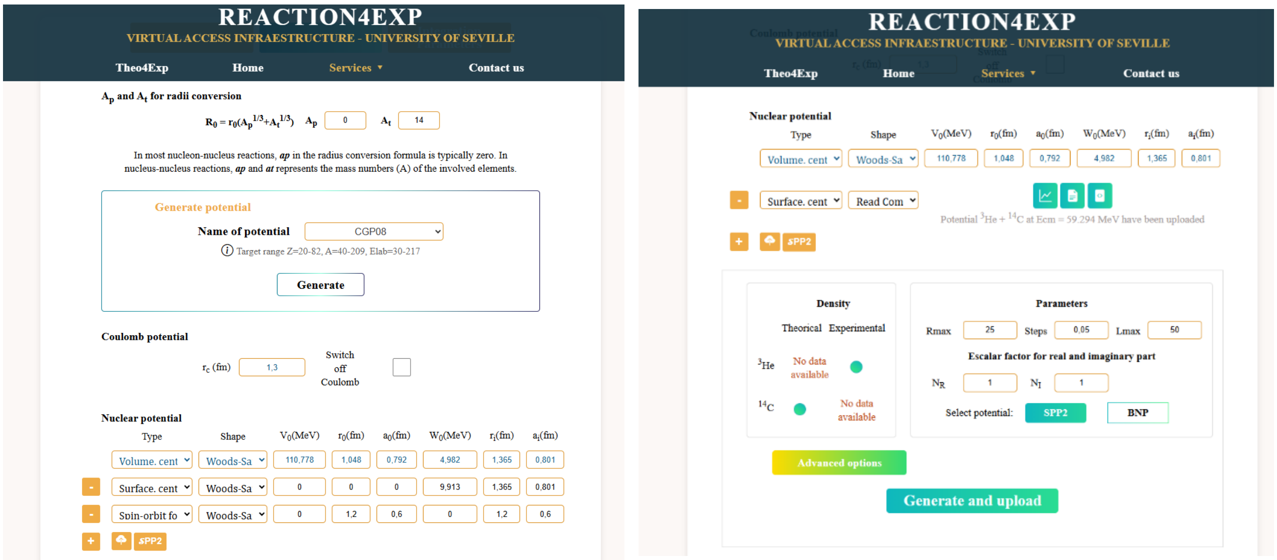


Figure 14. *The potential generator with SYSOP (left) and with the inclusion of a SPP2 potential (right).*

2.2.3 Inelastic Scattering (CC and DWBA)

The Inelastic Scattering calculation, using a rotational model, provides the inelastic scattering to excited states. The model used is a Coupled-Channels (CC) formalism using a rotational model for the excited states of the projectile or the target. Also, it is possible to perform the calculation in first order, what is called the Distorted Wave Born Approximation (DWBA). As an output, it provides: reaction cross sections, the elastic angular distribution and inelastic angular distributions to the different excited states. Additionally, it includes the integrated cross section for all states. The code used for this is again FRESCO [9]. Also, the potential generator is included in this type of calculation.

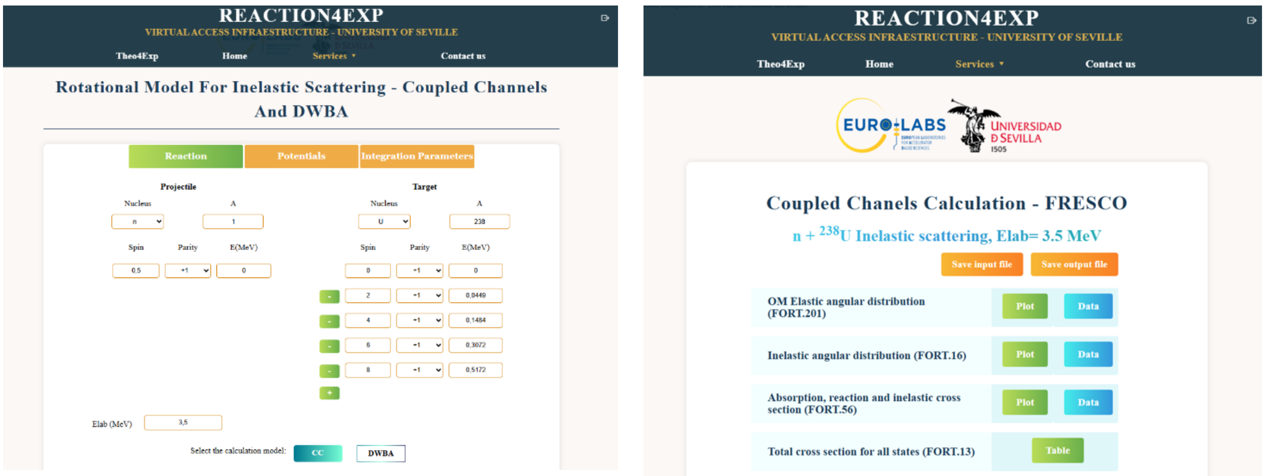
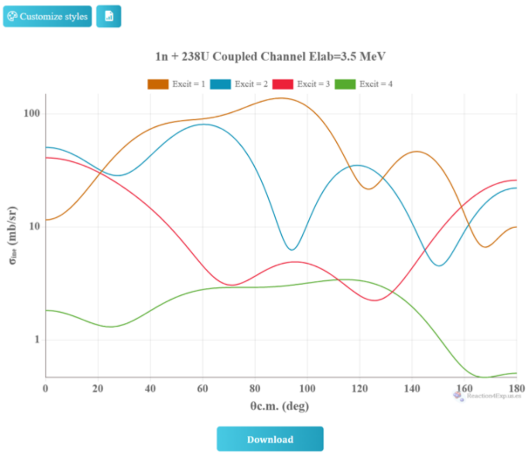


Figure 15. *Examples of the input data page and the results page.*



Integrated cross section 1n + 238U Coupled Channels, Elab= 3.5 MeV

Reaction cross section (mb)	2756.1
Absorbtion cross section (mb)	1269.33156

Projectile			Target			Integrated cross section (mb)
J	Parity	E (MeV)	J	Parity	E (MeV)	
0.5	1	0	2	1	0.0449	931.42
0.5	1	0	4	1	0.1484	425.84
0.5	1	0	6	1	0.3072	97.699
0.5	1	0	8	1	0.5172	31.833

Figure 16. *Angular distributions of the inelastic scattering cross section to different excited states for the reaction n+^{238}U at 3.5 MeV (left) and the integrated cross sections to each state (right).*

2.2.3 Transfer reactions

The transfer calculation provides the cross-section distributions for reactions in which one particle from projectile is transferred to the target (or vice versa) using the DWBA formalism, both in prior or post form. The program used to perform the calculations is FRESCO [9]. The installation provides now the options for the initial partition, projectile and target, and the final one, ejectile and residual nucleus. It is necessary to include a couple of binding potentials together with several optical potentials. All these ingredients are clearly specified for the users. As an output, it provides: the angular distribution for the elastic and transfer cross sections, the reaction cross section, and also a table with the integrated transfer cross section to the states considered in the final partition.

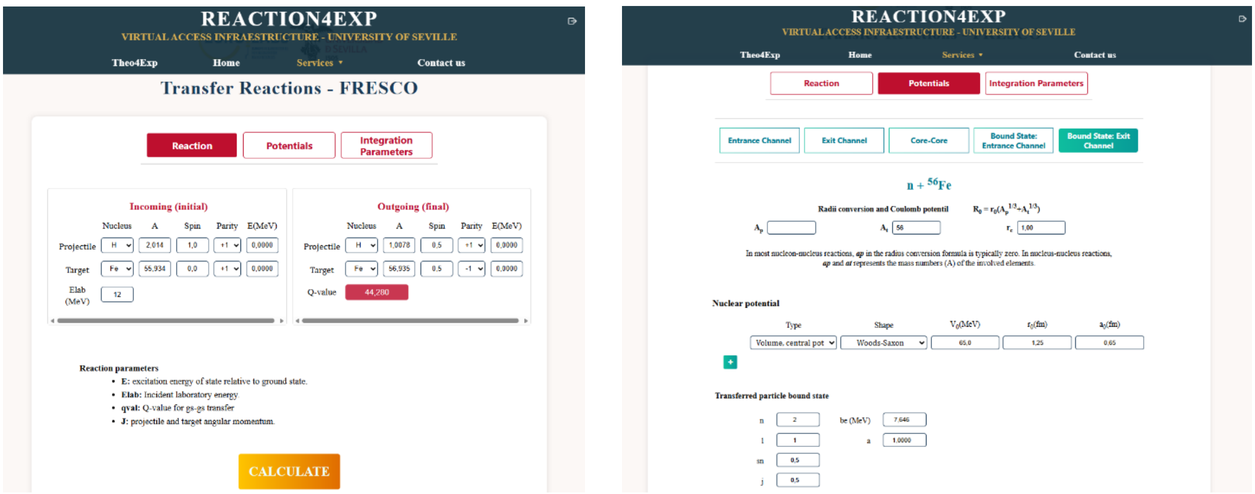
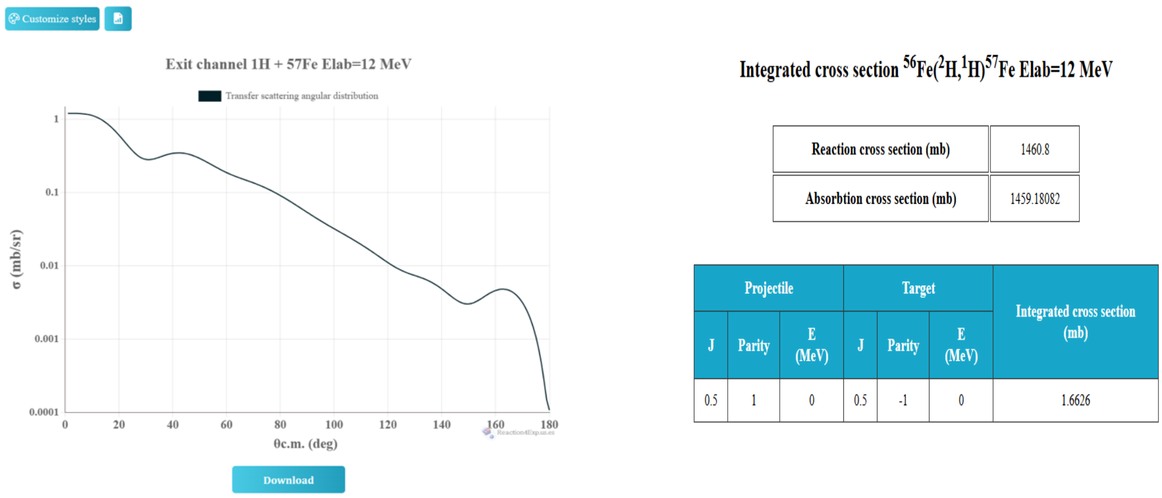


Figure 17. *Examples of input data pages. (Left panel) The incoming and outgoing partitions. (Right) The different potentials to be included.*



Reaction cross section (mb)	1460.8
Absorbtion cross section (mb)	1459.18082

Projectile			Target			Integrated cross section (mb)
J	Parity	E (MeV)	J	Parity	E (MeV)	
0.5	1	0	0.5	-1	0	1.6626

Figure 18. *Angular distribution of the transfer cross section for the reaction $^{56}Fe(^{2}H,^{1}H)^{57}Fe$ at 12 MeV (left) and a table with the integrated cross sections (right).*

2.2.3 Folding potentials (SPP and BNP)

The REGINA [13] code calculates the São Paulo potential version 2 (SPP2) and the Brazilian nuclear potential (BNP), using nuclear densities and distributions for a large variety of nuclei, including theorical and experimental densities for the calculations. These folding potentials can later be used in the elastic, inelastic and transfer calculations within this installation or in other programs outside the platform. The output provides the folding potential and the elastic cross section angular distribution obtained with that potential (taking the imaginary as a parameter times the real part).

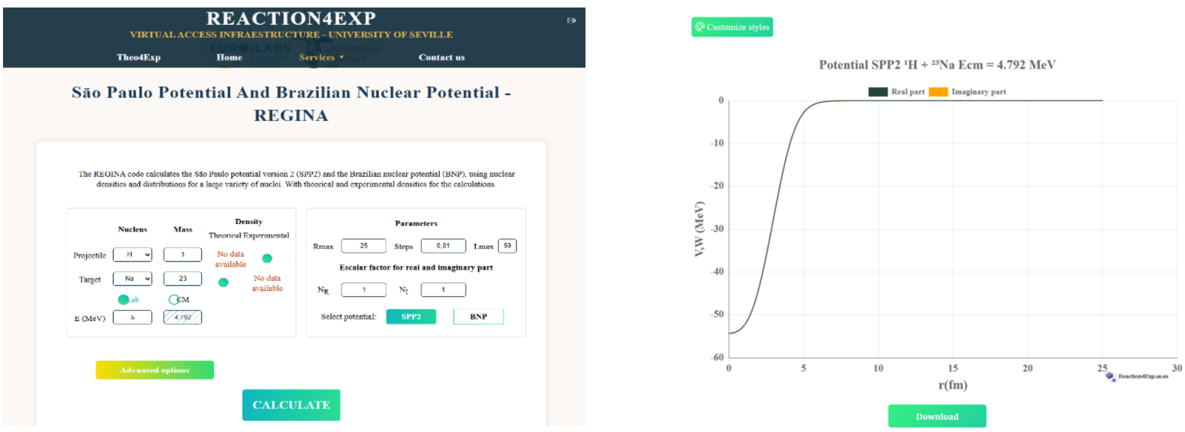


Figure 19. *Example of input data page (left). The SPP2 folding potential for the reaction of p+^{23}Na at 5 MeV (right).*

2.3. STRUCTURE4EXP

A brief general explanation, about the overall purpose of the installation and the different computer codes that are available, is presented in the main page of the Structure4Exp installation (https://ns4exp.mi.infn.it). The user can specify which code he/she is interested in, and then access specific pages with more detailed explanations. In particular, the user is guided to prepare correct inputs through a user-friendly interface.

Three computer codes have been made available. Two codes can carry out self-consistent computations of the ground and excited states of spherical nuclei, using Skyrme effective interactions. The HF-RPA [15] code works within the framework of the Hartree-Fock + Random Phase Approximation, and can be applied to closed-shell nuclei, while the HFBCS-QRPA [16] can take also pairing correlations into account, and can be used for open-shell nuclei. In addition, the KSHELL code [17] can perform shell model calculations, selecting an appropriate core and an appropriate interaction among valence nucleons. The choice of possible interactions has been extended as compared to the last report. The limits of the three codes are clearly spelled out. Shell model calculations can place significant demands on CPU and RAM resources. Therefore, a preliminary estimation is conducted to assess the computing resources necessary to complete the calculation specified in the user input, aiming to prevent the submission of overly demanding computations.
The web pages have been extensively tested, and comprehensive accounting information is available, concerning the number of users and their CPU usage.

In the following, we provide some details about the use of each of the three programs that are available in the installation, and show some typical result.

2.3.1 HF-RPA

This is a software tool designed to perform self-consistent calculations of the ground-state properties of spherical atomic nuclei, as well as of their excitation spectra (spectra of vibrational excitations in this context), including multipole strength functions and other related properties. The strength functions are associated with the typical isoscalar, isovector, or electromagnetic operators that are widely employed in the literature. The program is based on the Hartree-Fock (HF) + Random Phase Approximation (RPA) theoretical framework, and makes use of Skyrme-type interactions or energy functionals. The code is limited to even-even, spherical nuclei, neglecting pairing correlations and operating within closed shells or sub-shells. Certain widely used Skyrme sets are built in the code and can be chosen from a simple menu, but the user has the possibility to input the parameters of a different interaction.

By solving, first, the HF equations, the program determines the mean fields and densities associated with the nucleus specified in the input. The HF equations are solved in coordinate space, on a predefined radial mesh with box boundary conditions. If the user has selected the HF option, the calculation stops here. The HF calculations are carried out, as a rule, with a set of default parameters that should be suitable for most situations. However, the user can modify these parameters in order to check the stability of the results and the accuracy of the convergence. In particular, the user can modify the radial mesh, the number of points and the maximum number of iterations used to solve the HF equations, as well as the tolerance used to determine the convergence of the solution.

The RPA code, which relies on the HF results, carries out fully self-consistent calculations of the RPA equations. The RPA equations are solved on a basis of particle-hole (p-h) configurations, in the usual matrix form. As a result, one obtains the excitation spectrum for a selected value of the total angular momentum J and parity π. For each excited state, the code provides the transition strengths associated with isoscalar, isovector, and electromagnetic operators. In addition, the discrete RPA peaks are smeared out with a Lorentzian function. In this way, a continuous strength function is obtained, in the isoscalar, isovector, and electromagnetic cases.

After the run is completed, the user has access to a set of files, containing information about the run and the strength functions in digital form. In addition, plots of the strength functions are also provided.

The same files are also sent to the user's e-mail address. In case of some error, pop-up windows alert the user.

In Figs. 20, 21 and 22, we provide, as an example, the images of the web pages associated to a calculation of the isoscalar quadrupole response of ^{208}Pb. At the end of the run, the list of files that is presented to the user can be seen in Fig. 11. The calculated density profile of the ground-state of ^{208}Pb is shown in Fig. 12. It has to be noted that detailed information about the moments of the density distributions can be found in the output file: the user interested in e.g., the charge radius or the neutron skin, can find easily these values. The quadrupole isoscalar strength is shown in Fig. 13. It displays a low-lying peak at excitation energy E* ≈ 5 MeV, which is the low-lying 2^+_1 excitation, as well as a high-lying peak at E* ≈ 12.5 MeV, which represents the well-known Giant Quadrupole Resonance (GQR). The user can also check whether the energy-weighted sum rule (EWSR) is well satisfied by the calculation.

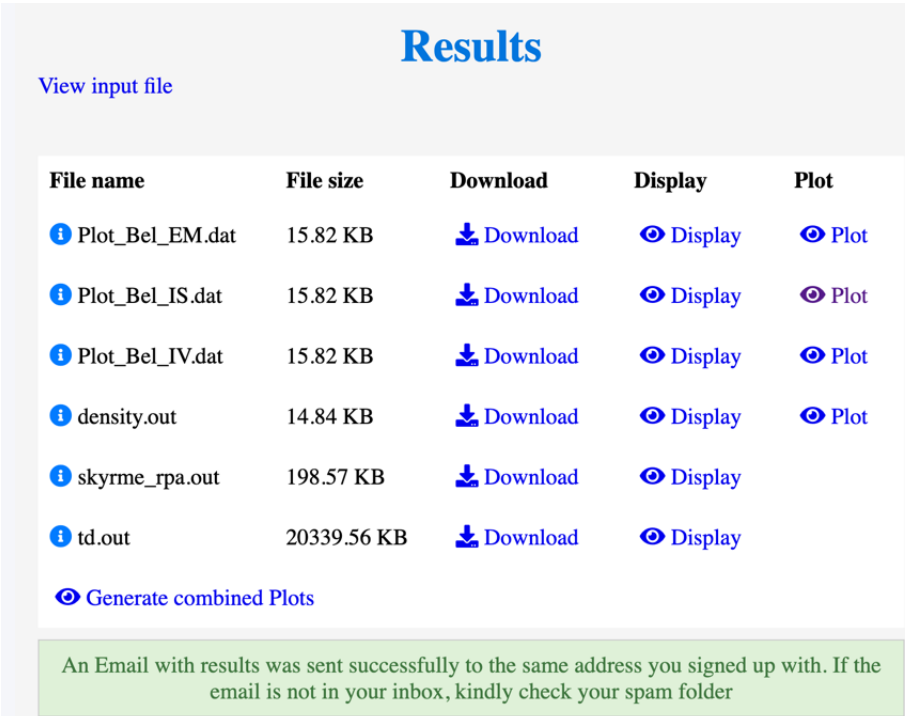


Figure 20. *List of files produced by the HF-RPA code after the calculation of the quadrupole excitations in ^{208}Pb. The specific calculation has been carried out using the SLy4 Skyrme interaction. Information about the convergence of the calculation, the basic properties of the ground-state (binding energy, radii, densities), the transition densities as well as the plots of the isoscalar, isovector and electromagnetic strengths are provided. They can be displayed online or downloaded, and are also automatically sent to the user's e-mail.*

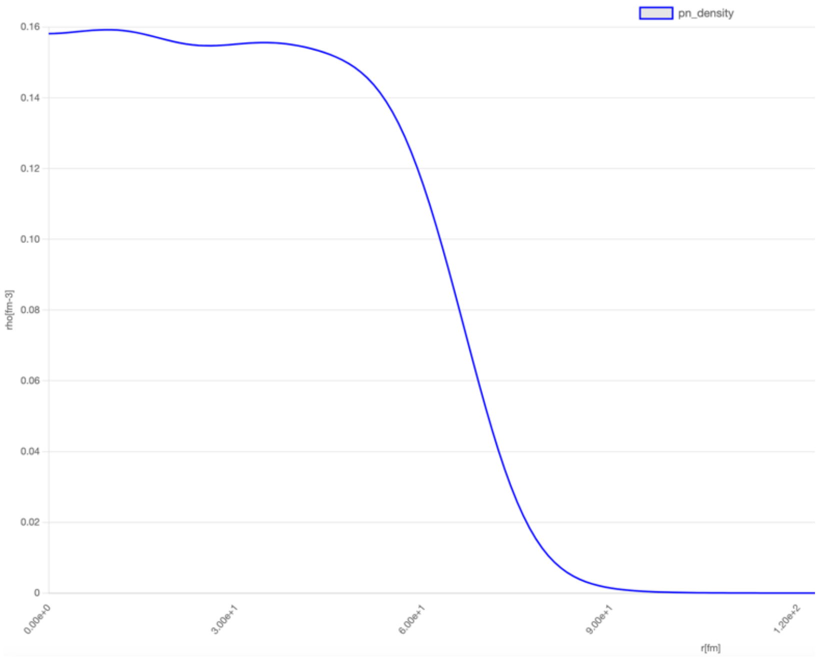


Figure 21. *Density of ^{208}Pb calculated by the HF code. Here only the total density is shown but proton, neutron and charge densities can be displayed as well.*

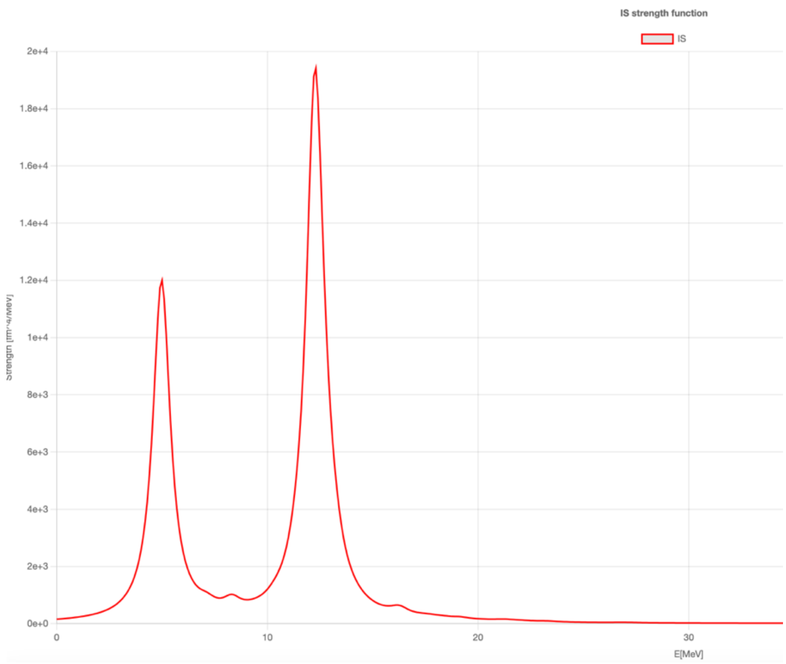


Figure 22. *Isoscalar quadrupole strength function of ^{208}Pb, highlighting the low-lying peak and the Giant Quadrupole Resonance (GQR). The isovector and electromagnetic strengths can be displayed as well.*

2.3.2 HFBCS-QRPA

This software tool has a structure similar to HF-RPA, and will not be described here in detail. It includes the possibility to take into account pairing correlations in the ground-state and in the excited states, calculated in the BCS and in the QRPA, respectively. In this way, the properties of collective states of open-shell nuclei can be assessed. As compared with the previous HF-RPA case, the input also requires to specify the strength of a zero-range pairing interaction, together with an associated energy cut-off.

Both HF-RPA and HFBCS-QRPA are useful tools for experimentalists who aim at studying giant resonances in spherical nuclei, but also low-lying multipole excitations like pygmy states. Charge radii, neutron skins, dipole polarizabilities, and other observables of interest for an experimental proposal or for other purposes can be accessed.

2.3.3 KSHELL

KSHELL is a shell-model code developed by N. Shimizu and collaborators at the Center for Computational Sciences of the University of Tsukuba. The code is complemented by a series of scripts, and the whole package has been made available also thanks to the contribution by Giovanni Di Gregorio (Caserta University and INFN Napoli) and Angela Gargano (INFN Napoli). The KSHELL code enables users to perform realistic nuclear shell-model calculations, using two-body interactions, within the so-called M-scheme basis representation. The diagonalization procedure of the Hamiltonian matrix is based on a variant of the Lanczos method, called the thick-restart block Lanczos method.

Depending on the model space, shell model calculations may require much more computing resources, in terms of CPU and RAM, than the (Q)RPA computations described above. The KSHELL code is capable to handle massive parallel calculations on supercomputers, but the limited capabilities of our server put rather severe constraints to the calculations which can be carried out using our service. Accordingly, for a given input proposed by the user, a preliminary estimate is made of the aforementioned resource, and if the calculation requires the diagonalization of matrices that are larger than 10^6, then the user is warned that the desired calculation is not feasible.

A number of effective Hamiltonians are available for each valence space, and previous restrictions of the code has been overcome. Calculations are performed by considering as reference core the doubly closed-shell nucleus closest to the selected system (e.g., for ^{136}Te, with Z=52, N=84 the closed shell nucleus ^{132}Sn with Z=50, N=82 is taken as core). As valence space for protons and/or neutrons, one major shell is taken (e.g., for ^{136}Te the neutron valence space is spanned by the $0h_{9/2}$, $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$, $2p_{1/2}$, and $0i_{13/2}$ orbitals, whereas the proton valence space by the $0g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, and $0h_{11/2}$ orbitals). To run the code, the user must specify the number of protons and neutrons of the nucleus to be studied, and the number of required states (for one or more values of angular momentum and parity). Default values of the effective charges and gyromagnetic factors are provided, but they can be modified by the user.

The output provides energy levels, their spin and isospin values, their magnetic and quadrupole moments, as well as the E2/M1 transition probabilities. In Figs. 14, 15 and 16, we show the steps needed for the calculation of the lowest states in ^{44}Ca (Z=20, N=44).

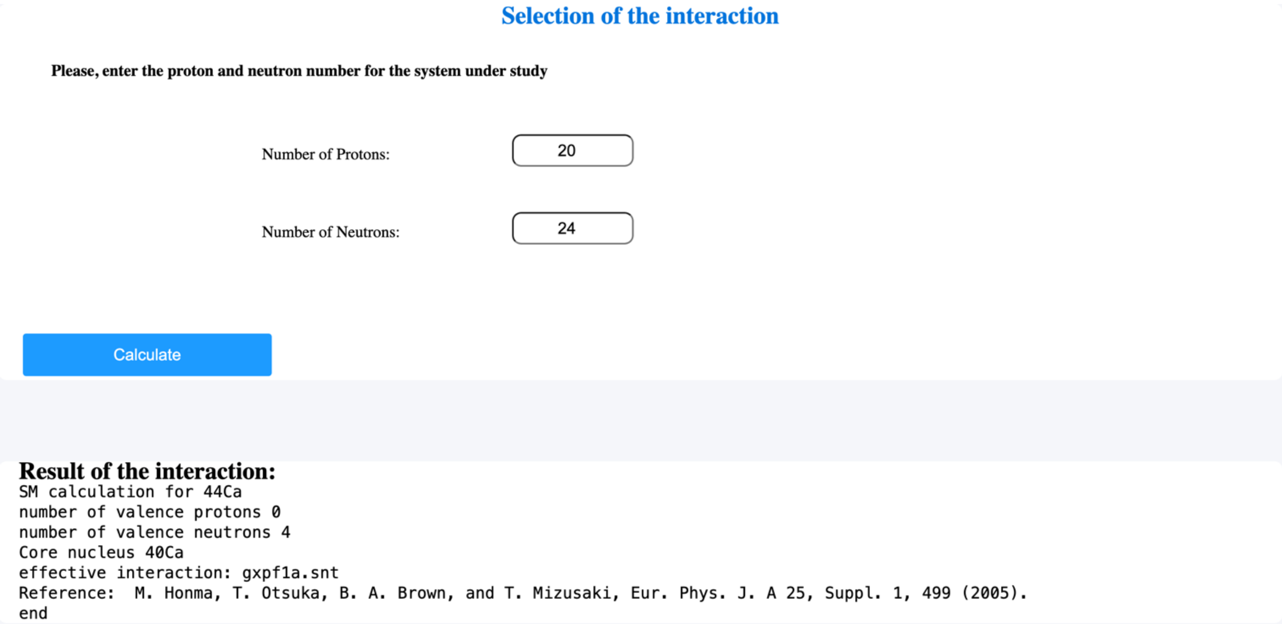


Figure 23. *First step of a KSHELL calculation as described in the text: the user inputs the number of protons and neutrons. The system selects the gxpf1a interaction, based on the ^{40}Ca core.*

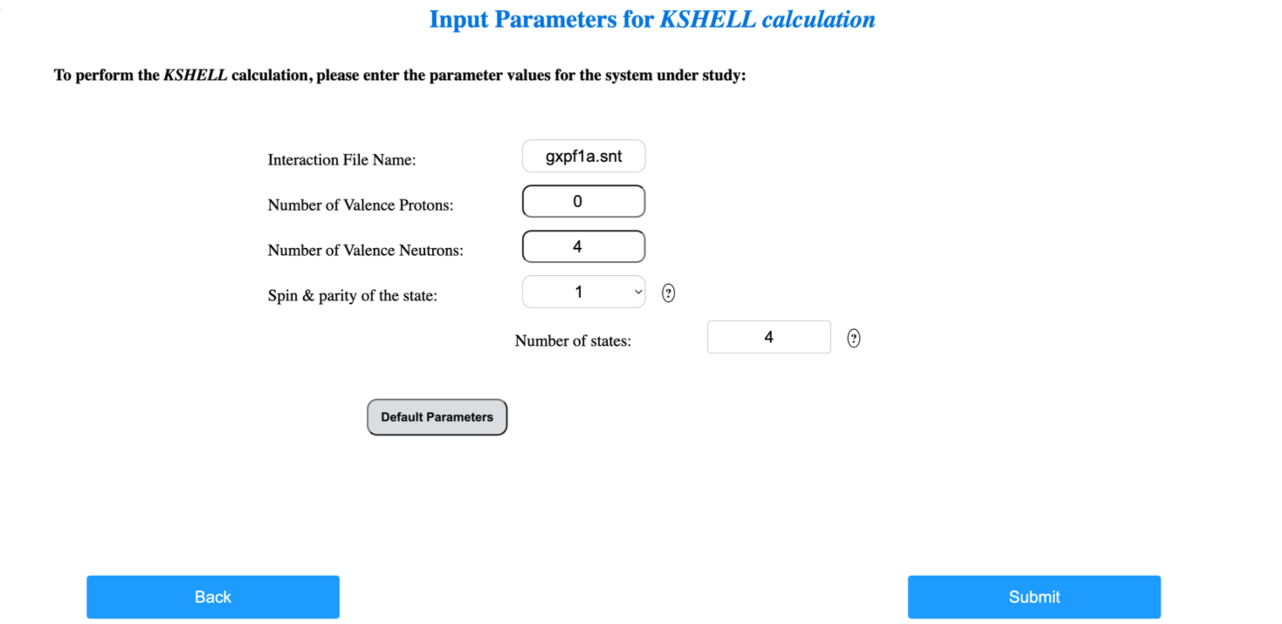
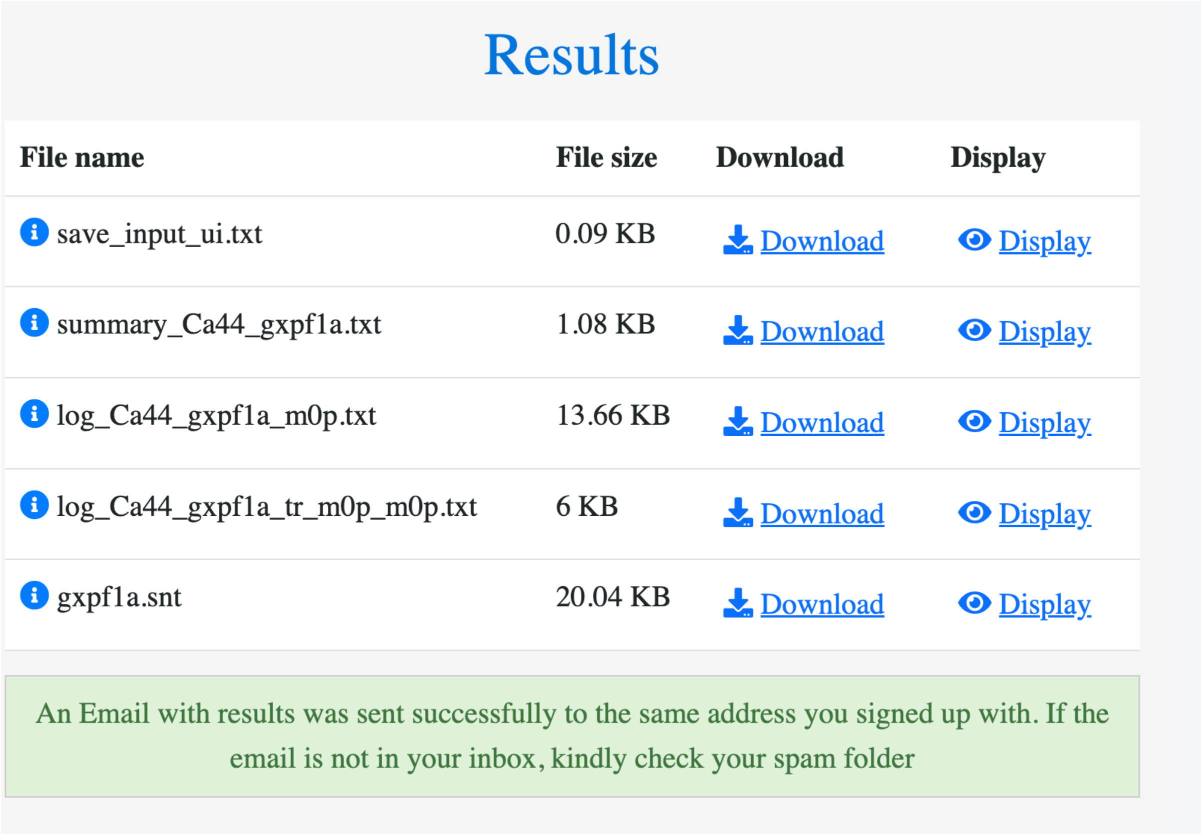


Figure 24. *Second step of a KSHELL calculation as described in the text: the user inputs the number of valence protons (0) and neutrons (4), as well as the number of required states (4). The code will be run, then, with standard values of effective charges and gyromagnetic ratios.*



Results

File name	File size	Download	Display
save_input_ui.txt	0.09 KB	Download	Display
summary_Ca44_gxpf1a.txt	1.08 KB	Download	Display
log_Ca44_gxpf1a_m0p.txt	13.66 KB	Download	Display
log_Ca44_gxpf1a_tr_m0p_m0p.txt	6 KB	Download	Display
gxpf1a.snt	20.04 KB	Download	Display

An Email with results was sent successfully to the same address you signed up with. If the email is not in your inbox, kindly check your spam folder

Figure 25. *Third step of a KSHELL calculation as described in the text: the results obtained for ^{44}Ca are presented, organized in several files. Energies, occupation numbers, and transition probabilities are contained in the summary and log files, while the matrix elements of the gxpf1a interaction are contained in the .snt file.*

Also, in the case of KSHELL, we expect that the service will enable experimentalists to check by themselves the theory predictions for observables of general interest in nuclear physics. Our goal, in making the three codes available at the same time in the first release of the service, is also that of allowing comparison between different theories. Low-lying states of several spherical nuclei can be calculated both using (Q)RPA and shell-model, as is well known.

3. INTEROPERABILITY AMONG DIFFERENT NODES ESTABLISHED

The three facilities in Theo4Exp have achieved very important degree of coordination. The access of the users is done through a common platform, that verifies the identity using the application https://iam-eurolabs.ijclab.in2p3.fr/login, that has been developed in task 2 of WP5 of the present EURO-LABS project. This application provides the access either via eduGAIN (https://edugain.org/) or ORCID (https://orcid.org/), ensuring access to any researcher affiliated to a scientific institution.

The access units are monitored following a common procedure as established in the application project. The scientific committee has identified the key aspects relevant for the interoperability of the systems. These include the evaluation of transition densities in structure models.

As an example of interoperability is the option to use SPP2 and BNP folding potentials as input for the Elastic Scattering and also Inelastic scattering calculations.

The computing infrastructures Theo4Exp, which were developed through the project, have permanent locations in the University of Seville, the University of Milan and IFJ-PAN, and they are fully operational.

The basis has been set up for an expansion of Theo4Exp, increasing the number of relevant codes and developing the interoperability of the codes. This expansion of Theo4Exp will require additional funds, from European on National sources, that will be requested in future calls.

4. REFERENCES

[1] Rodríguez-Gallardo, M, Colò, G and Dudek, J. (2025) Service for the EURO-LABS Community: The THEO4EXP Virtual Access Facility, Nuclear Physics News, 35(1), 33-36.

[2] Rodríguez-Gallardo, M, Colò, G, Dudek, J., Dedes, I. Gaamoucci, Muñoz-Chimbo, C. and Moumene, I. (2025) THEO4EXP: a theory service for euro-labs community. In: Acta Physica Polonica B, Proceedings Supplement, 18 article 2-A10, Zakopane Conference on Nuclear Physics *Extremes of the Nuclear Landscape 25th August-1st September 2024, Zakopane, Poland.*

[3] Rodríguez-Gallardo, M. and Muñoz-Chimbo, C., (2025) Cómo hacer cálculos de Física Nuclear sin ser experto, *The Conversation, 9th September 2025,* https://doi.org/10.64628/AAO.qyu5rauwg.

[4] Dedes, I., Dudek, J. (2018) Predictive power of theoretical modelling of the nuclear mean field: examples of improving predictive capacities, Physica Scripta, Vol. 93, No. 4.

[5] Dedes, I., Dudek, J. (2019) Propagation of the nuclear mean-field uncertainties with increasing distance from the parameter adjustment zone: Applications to superheavy nuclei, Phys. Rev. C, 99, 054310;

[6] Gaamouci, A., Dedes, I., Dudek, J., Baran, A., Benhamouda, N., Curien, D., Wang, H.L. and Yang, J. (2021) Exotic toroidal and super-deformed configurations in light atomic nuclei: Predictions using a mean-field Hamiltonian without parametric correlations, Phys. Rev. C, 103, 054311;

[7] Yang, J., Dudek, J., Dedes, I., Baran, A., Curien, D., Gaamouci, A., Góźdź, A., Pędrak, A., Rouvel, D., Wang, H.L., Burkat, J., (2022) Exotic shape symmetries around the fourfold octupole magic number N = 136: Formulation of experimental identification criteria, Phys. Rev. C, 105, 034348;

[8] Yang, J., Dudek, J., Dedes, I., Baran, A., Curien, D., Gaamouci, A., Góźdź, A., Pędrak, A., Rouvel, D., Wang, H.L., (2022) Exotic symmetries as stabilising factors for superheavy nuclei: Symmetry-oriented generalised concept of nuclear magic numbers, Phys. Rev. C, 106, 054314;

[9] Yang, J., Dudek, J., Dedes, I., Baran, A., Curien, D., Gaamouci, A., Góźdź, A., Pędrak, A., Rouvel, D., Wang, H.L., (2023) Islands of oblate hyper-deformed and super-deformed super-heavy nuclei with D3h point group symmetry in competition with normal-deformed D3h states: Archipelago of D3h-symmetry islands, Phys. Rev. C, 107, 054304;

[10] Bertulani, C.A., Baur, G. (1988) Electromagnetic processes in relativistic heavy ion collisions, Phys. Rep., 163 (5-6), 299-408;

[11] Fernández-García, J.P., Cubero, M., Rodríguez-Gallardo, M. et al. (2013) 11Li Breakup on 208Pb at Energies Around the Coulomb Barrier, Phys. Rev. Lett., 110, 142701;

[12] Thompson, I.J. (1988) Coupled Channels Methods for Nuclear Physics, Comput. Phys. Rep., 7 (4), 167-212;

[13] Chamon, L.C., Carlson, B.V., Gasques, L.R. (2021) *São Paulo potential version 2 (SPP2) and Brazilian nuclear potential (BNP),* Comp. Phys. Comm. 267 108061;

[14] R. Newton, Scattering Theory of Waves and Particles (1966), Ch. 5 & 8, McGraw-Hill.

[15] Colò G., Cao L.G., Giai N.V., Capelli L. (2013) Self-consistent RPA calculations with Skyrme-type interactions: The skyrme_rpa program, Comp. Phys. Comm. 184, 142;

[16] Colò G. and Roca-Maza X. (2021) User guide for the hfbcs-qrpa code, arXiv:2102.06562;

[17] Shimizu N., Mizusaki T., Utsuno T., Tsunoda Y. (2019) Thick-restart block Lanczos method in nuclear shell-model calculations, Comp. Phys. Comm. 244, 372.