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MILESTONE REPORT

Contracted personnel for Theo4Exp VA in place and first codes available for users in the virtual facility

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Abstract: This document outlines the integration of contracted personnel into each installation of Theo4Exp, as well as the opening and the availability of the first codes to users worldwide of the Virtual Access (VA) infrastructure accessible via https://institutional.us.es/theo4exp.

Delivery Slip

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Executive summary

This document outlines the integration of contracted personnel, as well as the selection process of this personnel into each installation of Theo4Exp, a virtual access infrastructure.

It also describes in some detail the infrastructure and the codes that are already available in each of the three installations.

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 started being developed within the first months of the beginning of 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 EURO-LABS has been a key opportunity to set up a framework in which certain relevant computer codes, and calculations obtained therefrom, have been made available to the community on open access platforms for the first time. Therefore, the EU funding of personnel to establish these common platforms can be expected to create a virtuous circle of increased collaboration between theorists and experimentalists. Additionally, new collaborations among theorists and/or other forms of networking can be expected. The key point is that now some codes are accessible to every scientist, and the associated results can be easily compared. This is on par to an easier and more effective access to experimental facilities.

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). Two meetings through Zoom have already been held on 8th September 2022, and 20th September 2023.

2. CONTRACTED PERSONNEL

The project EURO-LABS has provided funding for contracted personnel, one for each installation, in order to develop the three installations and start the operation of the VA infrastructure as a whole. Each beneficiary institution has made its own selection process according to the local rules. The integration of the three contracted computer scientists has taken place at different dates, but all of them before the 18th month, as required by the GA no. 101057511.

2.1 MEANFIELD4EXP

The position of "*Environmental Research Equipment Specialist*" was created at IFJ PAN and assigned to the MeanField4Exp installation. The goal was to program and manage a user-friendly web environment for performing advanced mean-field calculations for nuclear structure. The job announcement appeared on August 1st, 2022 on the IFJ PAN recruitment portals (in Polish and English) and on the EURAXESS website (in English) and on the EURO-LABS website. Applications could be submitted until September 15, 2022. The selection committee assessed the three candidates, who applied, and offered the position to Dr. Abdelghafar Gaamouci, who is employed at IFJ PAN from February 2nd, 2023, to January 31st, 2025.

2.2 REACTION4EXP

The computer scientist who has been contracted for the installation Reaction4Exp is Dr. Carla Tatiana Muñoz Chimbo. The contract has been managed by *Fundación de Investigación Universidad de Sevilla* (FIUS) and started on 11th September 2023, for a period of two years.

The application to the contract was officially open on 12/05/2023 for a period of ten days and was published in the FUIS webpage https://fius.us.es/sites/default/files/Convocatoria_24.pdf. It was also announced through various mailing lists. Before the application opening, the job offer was disseminated internationally, including the EC portal EURAXESS (https://euraxess.ec.europa.eu).

2.3 STRUCTURE4EXP

The person who has been hired to set up this installation is Dr Imane Moumene. She has been contracted by the University of Milano on March 1st, 2023, and her contract ends on February 29th, 2024. The job announcement, dated October 14th, 2022, has been published in the web pages of the University of Milano, both in English and Italian, and it has also been advertised internationally through various mailing lists. In particular, the announcement has been sent to potentially interested candidates via well-known mailing lists like NUSTAR etc. Dr Moumene has been selected by a selection committee, including nuclear physicists and computer scientists.

Dr. Moumene has started from scratch to create the VA infrastructure at the University of Milano, which now includes two mean-field codes (HF-RPA and HFBCS-QRPA), plus a shell-model code (KSHELL), as described later in the text.

3. VIRTUAL ACCESS INFRASTRUCTURE OPEN TO USERS

The VA infrastructure is available since 1st February 2024, at https://institutional.us.es/theo4exp. The information about opening this VA infrastructure to the users was posted on the EURO-LABS web page and in social media, as well as distributed widely via various mailing lists. The link to each installation, MeanField4Exp, Reaction4Exp and Structure4Exp, can be easily found in this webpage (cf. Fig. 1). 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.
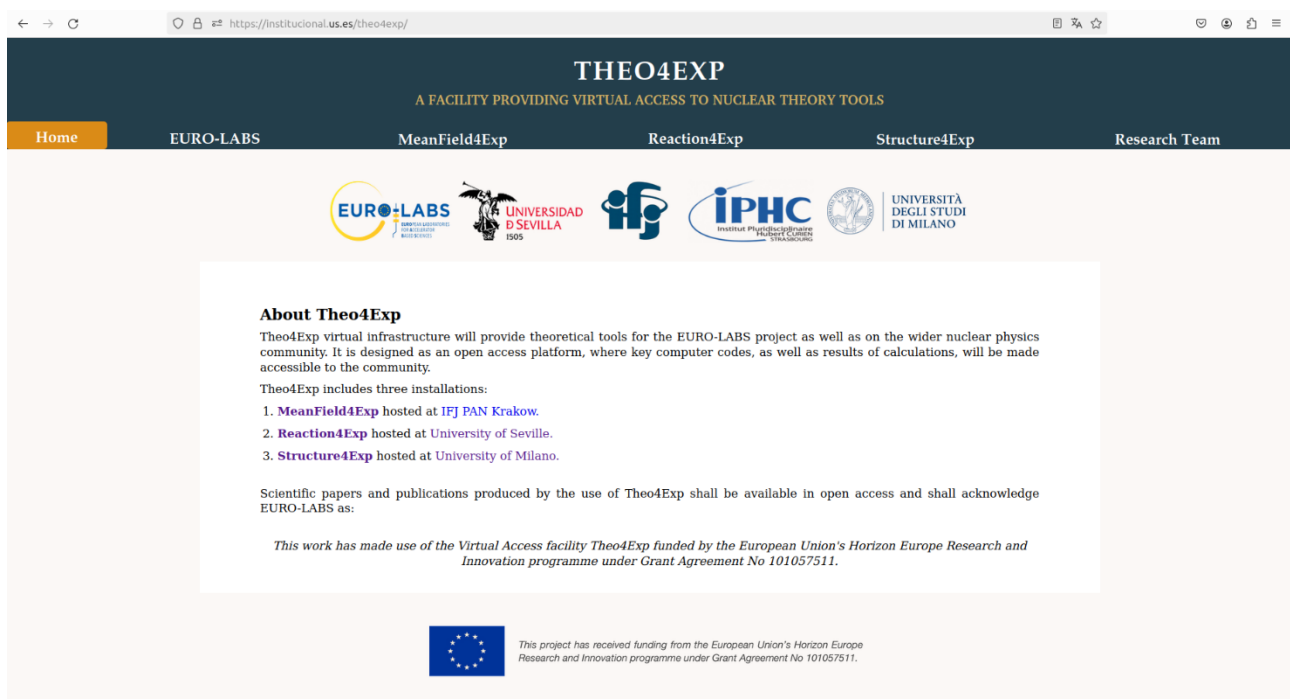
Figure 1. *Home page of the VA infrastructure Theo4Exp.*

3.1 MEANFIELD4EXP

The service referred to as MeanField4Exp (https://meanfield4exp.ifj.edu.pl) belongs to the nuclear theory package Theo4Exp, the latter being a part of even broader project uniting the interests of the EURO-LABS). It is based on the nuclear structure applications of the realistic, phenomenological realisation of the nuclear mean field theory. As its name suggests, the service is dedicated mainly, even though not exclusively, to experimentalists associated in their research with the European accelerator centres. The principal goals behind combining modern accelerator and detector technologies with powerful theory methods are to optimise the way towards innovative experiments, thus opening the perspectives for new discoveries and exploiting to the full the use of European accelerators and associated facilities. The service Theo4Exp facilitates profiting on the every-day basis from the theory interpretation of the experimental results, overviewing selected theory predictions as well as optimising the newly proposed experiments at the level of proposal writing.

The theory modelling methods selected for the service form a part of the standards well known today, very often used and/or cited in numerous publications and frequently addressed in textbooks. The service MeanField4Exp is optimised to facilitate the applications by non-specialists in nuclear structure theory and allows for an easy dialogue with the site. It is equipped with several options for preparing the theory results in the form of the "ready to publish" diagrams and complementary latex format tables.

The functioning of the MeanField4Exp internet site has been possible thanks to the installation of advanced nuclear structure computer programs which provide both modern mean-field approach results, as well as their associated graphical representation. The theory methods and related computer programs were developed by Professor Jerzy Dudek of the University of Strasbourg and implemented by young physicists from the Department of the Structure of Atomic Nucleus IFJ PAN (Dr Irene Dedes and Dr Abdelghafar Gaamouci). The site also provides access to the voluminous database storing results of advanced calculations with multiprocessor computing systems. The database is continually expanded with the help of a multi-processor cluster enlarging the already existing data bank equivalent of many years of CPU time.

The service employs combinations of advanced 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 processes in multi-dimensional deformation spaces, or *Group Theory* and *Group Representation Theory* in treating the nuclear symmetry issues.

Results, which can be obtained with the help of this service, 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].

In what follows we are going to make a brief close-up of a number of options available to the users with the present version of the installation.

3.1.1 Single Nucleon Energies as Functions of Nuclear Shapes

Overviewing nuclear physics articles, one finds that certain authors try to generate the single particle energy diagrams needed for their physical interpretations often by re-editing very ancient diagrams of the Nilsson type thus often not optimal for their actual context. Thanks to the proposed service the user will be able to generate the single-nucleon energy diagrams for any given (Z, N)-nucleus selecting the deformation axis from a choice displayed on the user's screen in the form of the standard multipole deformations: quadrupole, octupole and hexadecapole. The user will need to specify her/his optimal deformation range as well as one of the so-called standard choices of the nuclear mean-field Hamiltonian parameterisation, what offers an extra practical option: Checking to what extent the standard parameterisations of the mean field potential can be considered compatible/equivalent/close.

The users may wish to compare the physical significance of the generated drawings with the analogous ones found in the literature. For that purpose, disposing of an option for choosing the single particle labels among the so-called Cartesian, Nilsson and spherical formats of the level labelling will be a very useful and facilitating factor.

An example of the single proton energies on a non-axial octupole deformation, α_{32}, is shown in Fig. 2 with the user specified deformation range between -0.30 and $+0.30$.
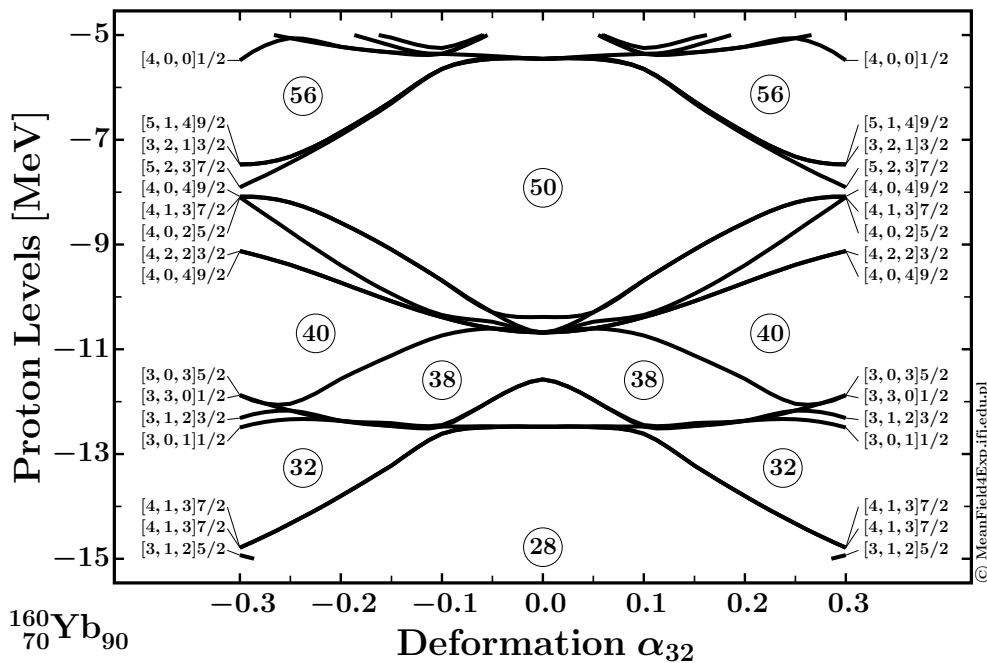
Figure 2: *Proton single particle energies for the ^{160}Yb nucleus ($Z = 70, N = 90$) as functions of the non-axial octupole deformation, α_{32}, usually called tetrahedral symmetry deformation in the literature. As seen from the figure, the reader may appreciate the confirmation of the shell openings (gaps) at the so-called octupole magic numbers $Z = 32, 40, 56...$ known in the literature.*

3.1.2 Nuclear Energies According to Macroscopic-Microscopic Method: Contour Plots of Potential Energy

One of the most sought mean-field information about nuclei addressed in experiments has the form of the so-called potential energy surfaces (or contour plots) representing 2D projections out of usually much richer deformation spaces, typically of 4 or 5 dimensions. The latter are usually specifically selected, depending on the addressed context. The number of possible projections increases with the space dimension. For instance, in the case of a 3D space of deformation variables (d_1, d_2 and d_3) the user would have 3 possibilities, selecting as horizontal vs. vertical axes either (d_1, d_2) or (d_1, d_3) or (d_2, d_3). Obviously, the number of choices increases with the original space dimensions: in the case of 4D the user will have 12 possibilities, in the case of 5D, 20 possibilities etc. The possibility of selecting the projection axes can be seen as a new degree of freedom which can allow a better imagination and can better represent the shape properties, evolution, or competition - as compared to predefined fixed choices found in the literature.

This service proposes, to start, the most standard deformation choices as found in the textbooks such as *Nuclear Structure* by A. Bohr and B. Mottelson, i.e. the quadrupole shapes (α_{20}, α_{22}) minimised over the hexadecapole deformation α_{40}, but the more exotic choices are being prepared; they include all 4 components of the octupole (mass asymmetry) variables, α_{30} (pear-shape), α_{31} (C$_{2v}$, water molecule symmetry), α_{32} (tetrahedral symmetry) and α_{33} (D$_{3h}$ molecular symmetry). These corresponding shapes are more and more addressed in the contemporary literature.
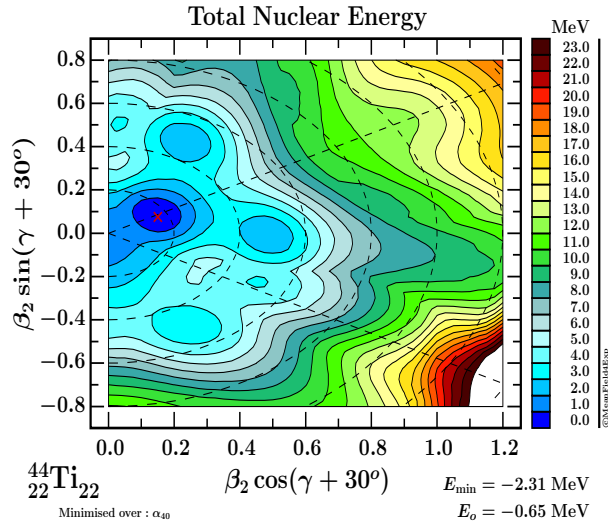
Strasbourg-Krakow Collaboration

Nucleus $^{44}_{22}$Ti$_{22}$

- **Total Energy:** E(FYU) + Shell[e] + Correlation[BCS]
- **Minimum Energy:** $E_{min} = -2.31$ MeV
- **Spherical-point Energy:** $E_o = -0.65$ MeV

Energy [MeV]	$\beta_2 \cos(\gamma + 30^o)$	$\beta_2 \sin(\gamma + 30^o)$	α_{40}	β	$\gamma(^o)$
0.0000	0.150	0.075	0.225	0.168	-3
1.6567	0.000	0.000	0.000	0.000	0.000
2.1789	0.225	0.425	0.100	0.481	32
2.1912	0.475	0.000	0.100	0.475	-30
3.2532	0.250	-0.425	-0.025	0.493	-90
3.9001	0.450	-0.225	-0.275	0.503	-57
3.9044	0.025	0.500	-0.275	0.501	57

Table 1: Map Energy minima for Z = 22, N = 22; Com-OxCaCANiZrSnGdPb. Dark-red rows mean minimum at the edge of the rectangle

$^{44}_{22}$Ti$_{22}$

Minimised over : α_{40}

$E_{min} = -2.31$ MeV

$E_o = -0.65$ MeV

Figure 3: *Example of the quadrupole shape properties of the nucleus ^{44}Ti with the often employed (β, γ) shape representation equivalent to (α_{20}, α_{22}) [with $\alpha_{20} = \beta \cos \gamma$, $\alpha_{22} = \frac{1}{\sqrt{2}} \beta \sin \gamma$], here minimised over α_{40}. On the right, the table of various local minima and the corresponding energy values.*

3.1.3 Nuclear Energies According to Macroscopic-Microscopic Method: Comparing Results for Isotopes or Isotones

Quite often the nuclear reactions used in experiments populate several neighbouring nuclei providing valuable information for several of the reaction products. It follows that the related publications address comparisons of the nuclear properties for varying neutron or proton numbers, what brings us to the interest in providing the similar type of information from theory viewpoints.

The service provides options, which allow comparing the energy dependence on various deformation degrees of freedom for neighbouring isotopes or isotones. The user may define the shape degrees of freedom to be addressed, the ranges of the corresponding deformations as well as the ranges of the proton and neutron numbers. The following drawing illustrates the comparison for a number of Thorium isotopes.
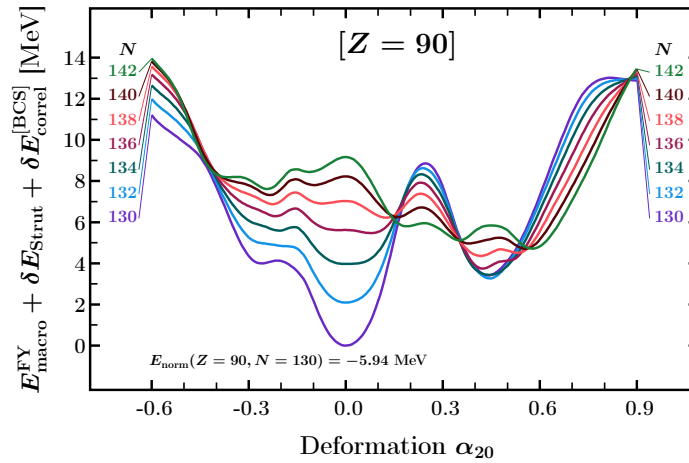
Figure 4: *Illustration of a competition among various quadrupole, axial symmetry minima, together with their evolution with neutron number. One notices the dominating spherical shape at $N = 140$ (and its quick vanishing with varying N) and relatively elongated shape at $\alpha_{20} \sim 0.45$.*

3.1.4 Shape Evolution with Angular Momentum: Towards Jacobi and/or Poincare Shape Transitions

In this part of this service, we help exploring the shape evolution with angular momentum employing macroscopic nuclear models. The user may choose between the Lublin Strasbourg Drop (LSD) Approach and a more traditional realisation of the model due to Myers and Swiatecki. The user selects the deformation space (the number of actually available possibilities is being enlarged; and new options are being introduced) indicating the nucleus (Z, N) as well as the angular momentum of interest.

Jacobi Transitions. The shape evolution diagrams, which can be generated by this service, allow describing an increase in nuclear triaxiality imposed by increasing rotation. This mechanism is usually referred to as Jacobi shape transition. According to this scenario, the transition begins at slightly oblate nuclear equilibrium corresponding to the lowest spins, followed, above certain critical spin, by a sequence of tri-axial shapes with gradually increasing elongation, terminating at axially symmetric strongly elongated forms leading eventually to fission.

Poincare Transitions. The user can also study a competition between the just described shape transitions and other ones, according to which the system may develop gradually the left-right asymmetry. For certain proton/neutron number combinations, this type of transitions may be privileged leading at the end to the mass-asymmetric fission.

A typical illustration of the Poincare type shape transition is shown below in Fig. 5.
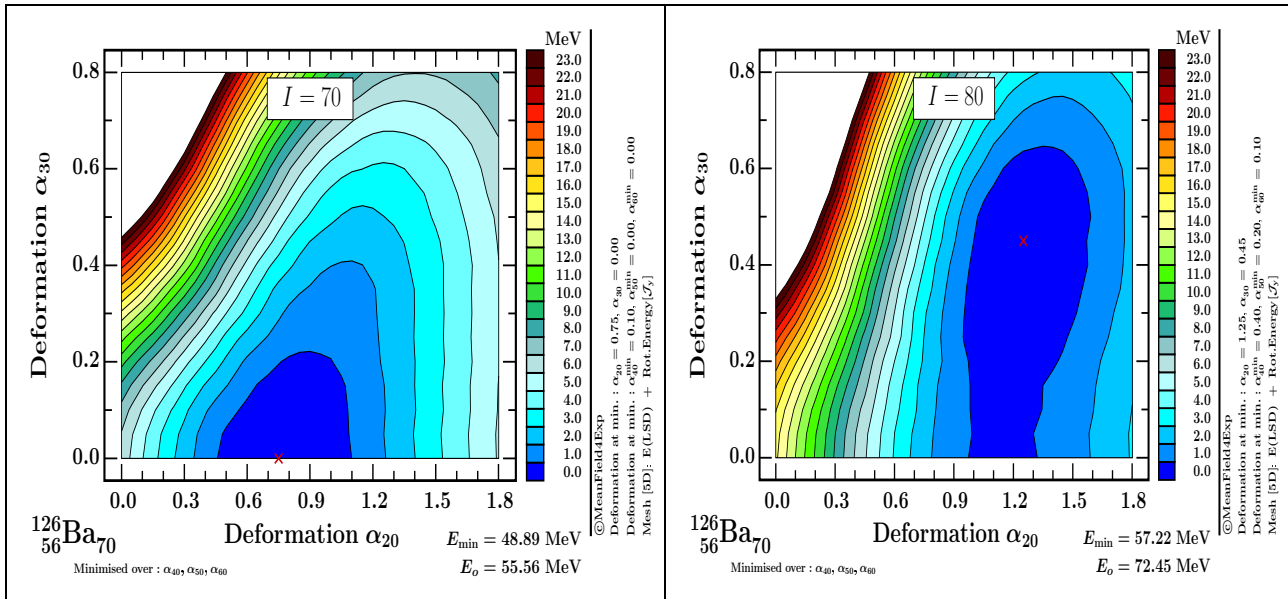
Figure 5. *Left: Nuclear macroscopic energy diagram for ^{126}Ba at angular momentum $I = 70\hbar$, showing an onset of the octupole shape instability manifested by a flatness of the landscape with increasing octupole pear-shape deformation α_{30}. Right: A follow up of the shape transition which began at lower spins as suggested by the previous diagram, here for angular momentum $I = 80\hbar$.*

3.2 REACTION4EXP

In the main page of Reaction4Exp (https://reaction4exp.us.es) we have included an option for each type of calculation that it is available at present: Equivalent Photon Model (EPM) [7,8] calculation (in a semiclassical formalism), and Optical Model (OM) calculation with the FRESCO [9] code. In the following, a short explanation is given about the services available in the present version of the installation.

3.2.1 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 a function 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 probability distribution (the inelastic/breakup distribution divided by the Rutherford cross section).

Figure 6. *The EPM calculation page in* https://reaction4exp.us.es/ *with input data for the reaction $^{11}Be+^{197}Au$ at 27.9 MeV and the excitation of ^{11}Be from the ground state to the first excited state via E1 transition.*
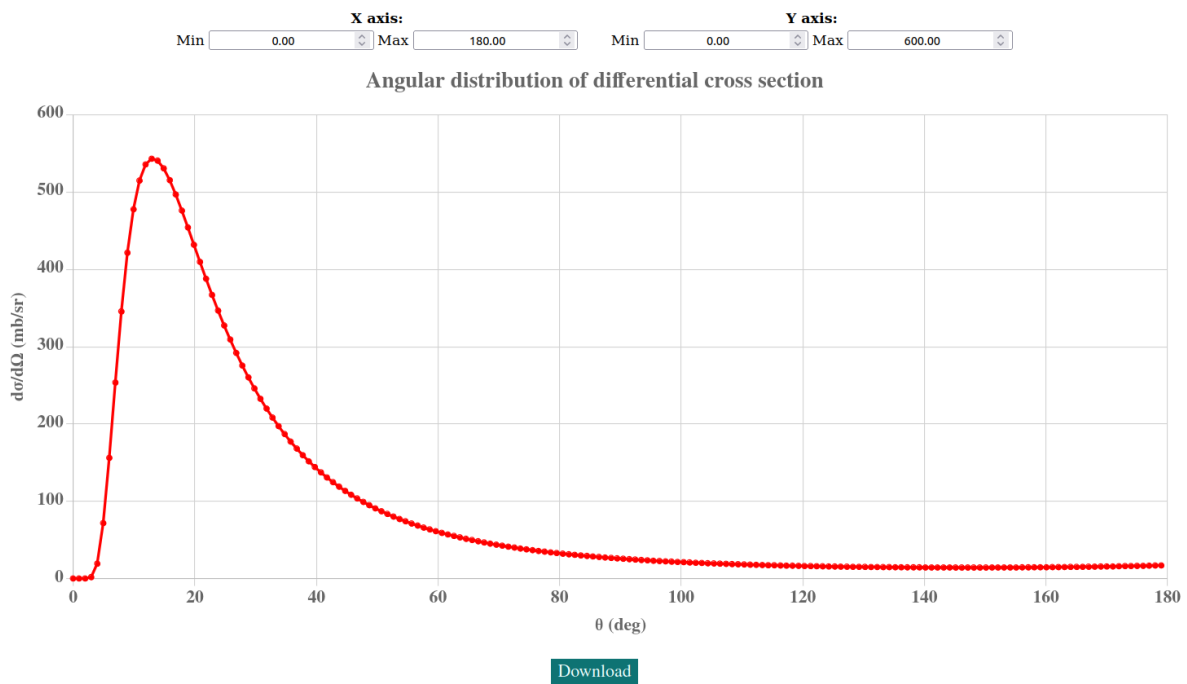
Figure 7: *Example of the angular distribution obtained with the EPM formalism. It is the inelastic cross section of ^{11}Be to the first excited state (bound state).*

3.2.2 Optical Model

The OM calculation provides the angular distribution for the elastic scattering 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 aim is FRESCO [9], developed by I.J. Thompson (LLNL, USA), and close collaborator of the group at the University of Seville. This code will be used also for Coupled-Channels (CC) calculations briefly. 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.

Figure 8. *The OM calculation page in https://reaction4exp.us.es/, with input data for the reaction $^4He+^{58}Ni$ at 25 MeV incident energy.*

CONTRACTED PERSONNEL FOR THEO4EXP VA IN PLACE AND FIRST CODES AVAILABLE FOR USERS IN THE VIRTUAL FACILITY

Milestone: MS10

Date: 28/02/2024
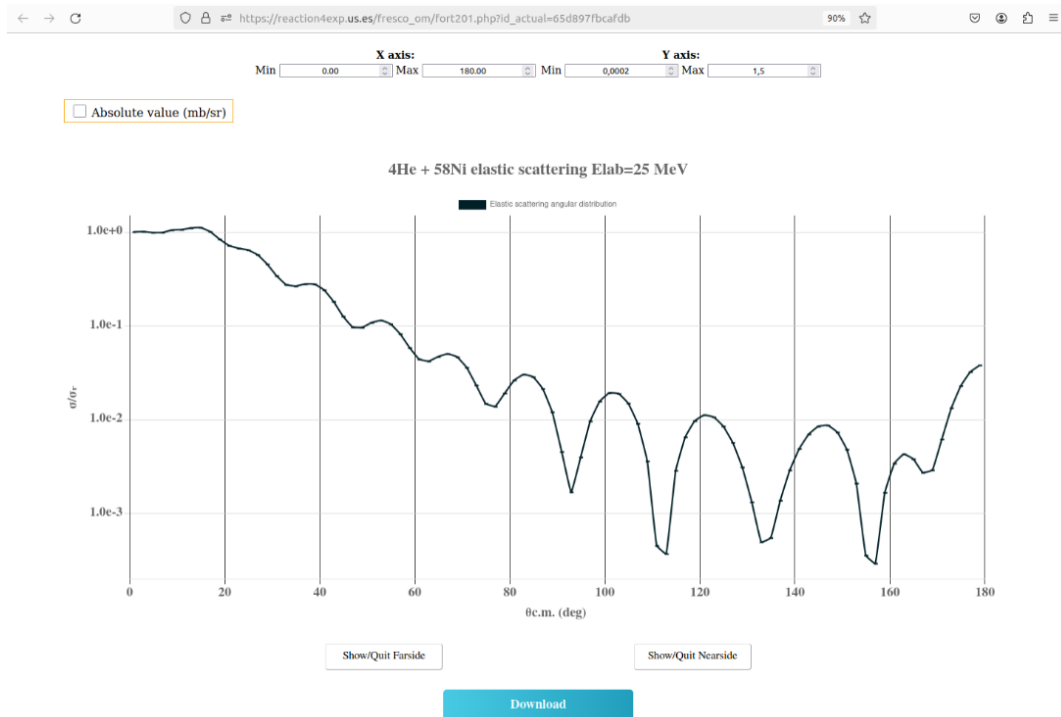
Figure 9. *Example of the angular distribution for the elastic cross with OM (FRESCO) formalism. The result is for the reaction $^4He+^{58}Ni$ at 25 MeV.*
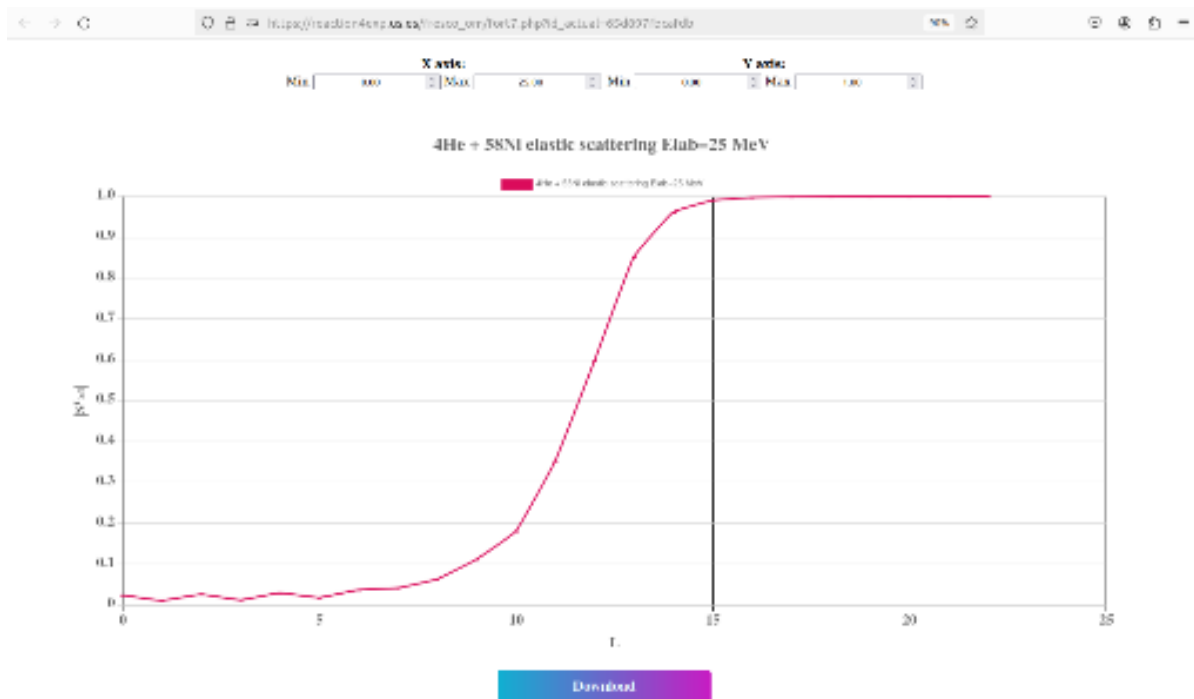
Figure 10. *Example of the elastic scattering S-matrix (modulus) as a function of the total angular momentum, obtained with OM (FRESCO) formalism. The result is for the reaction $^4He+^{58}Ni$ at 25 MeV.*

3.3 STRUCTURE4EXP

A brief general explanation, about the overall purpose of the installation and the different computer codes that are available, is currently 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 are available so far. Two codes can carry out self-consistent computations of the ground and excited states of spherical nuclei, using Skyrme effective interactions. The HF-RPA [10] code works within the framework of the Hartree-Fock + Random Phase Approximation, and can be applied to closed-shell nuclei, while the HFBCS-QRPA [11] can take also pairing correlations into account, and can be used for open-shell nuclei. In addition, the KSHELL code [12] can perform shell model calculations, selecting an appropriate core and an appropriate interaction among valence nucleons. The choice of possible interactions is limited for the moment, but an extension is planned in the near future. 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 presently available in the installation, and show some typical result.

3.3.1 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 pre-defined 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. At the moment, this is restricted to natural parity states, namely to electric excitations. An extension to magnetic excitations can be envisioned. 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. 11, 12 and 13, 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 11. *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.
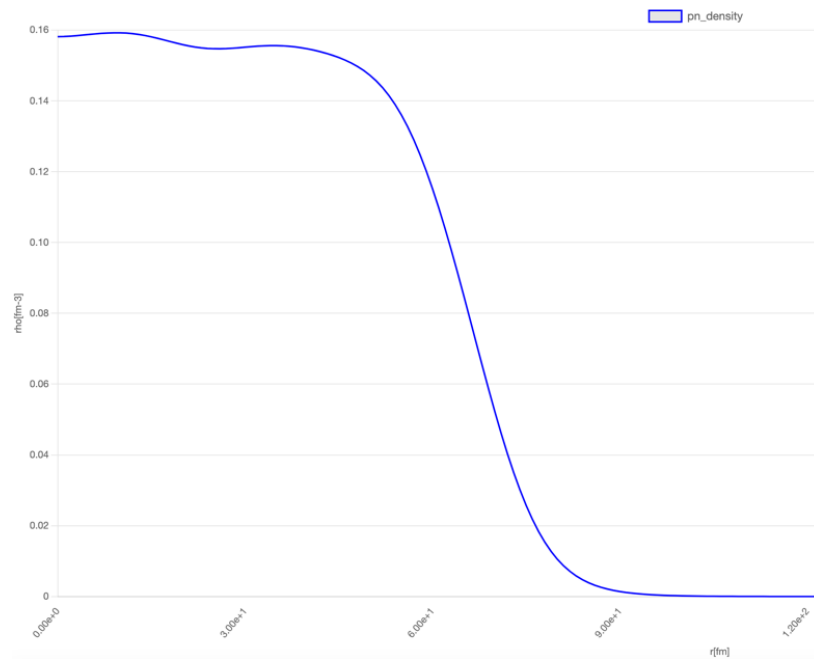

Figure 12. *Density of ^{208}Pb calculated by the HF code. Here only the total density is shown but proton, neutron and charge densities can be displayed as well.*
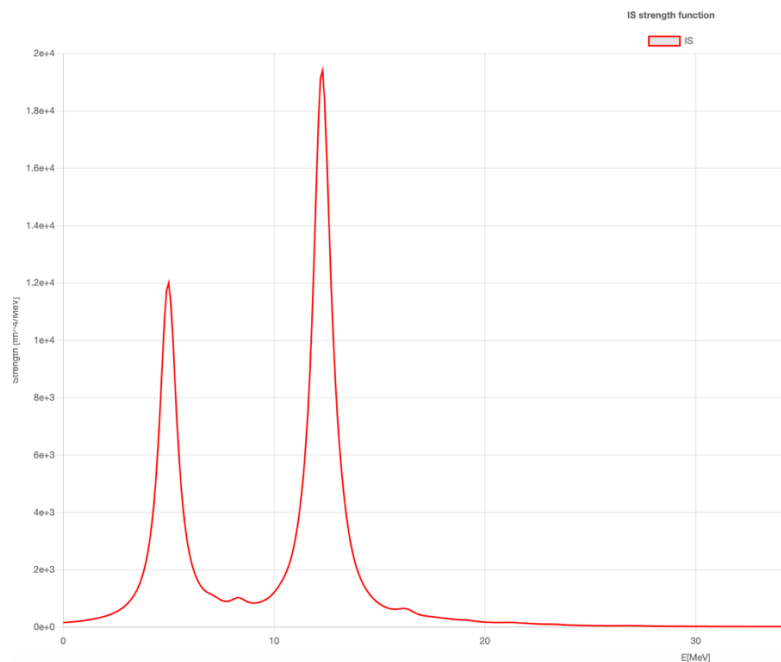

Figure 13. *Isoscalar quadrupole strength function of ^{208}Pb, highlighting the low-lying peak and the Giant Quadrupole Resonance (GQR). The isovector and electromagnetic strengths can be displayed as well.*

3.3.2 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.

3.3.3 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.

At the moment, only one effective Hamiltonian is available for each valence space, but we plan to overcome this restriction in the next future. 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 14. *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 15. *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.*

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

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Figure 16. *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.

4.   SUMMARY

Although the Theo4Exp Virtual Access facility, consisting of 3 installations: MeanField4Exp, Reaction4Exp and Structure4Exp, has been running for less than a month and is still in incomplete form, there is already a lot of interest from external users. This makes it certain that the number of users of the offered services will be high when The4Exp is expanded with new functionalities. New services are planned to be offered and we also envision ways to interact with the users' community.

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