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Service for the EURO-LABS Community: The THEO4EXP Virtual Access Facility

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Service for the EURO-LABS Community: The THEO4EXP Virtual Access Facility

Nuclear physics is a mature field of research that has reached a high level of sophistication in dealing with the complexity of the nuclear many-body problem and numerous phenomena manifested by nuclei. Still, stronger links between theory and experiment are mandatory to further advance nuclear physics and optimize the realization of the new experimental research programs, like those to be carried out at the radioactive beam facilities or focusing on super-heavy nuclei. In order to discover new physics, one cannot simply rely on previous discoveries but must model them with controlled theoretical uncertainties. To give only one example, if new spectroscopic data have to be unveiled, the mechanism of the reaction that populates the states must be under control; or, conversely, new reaction mechanisms can be discovered only if the states of the involved nuclei are well known. If the goal is a new discovery, all the competing processes that take place in the experimental environment should be simulated at best.

To perform a new search, experimentalists as a rule access complex facilities but this can be seen as a usual, nearly standard proceeding. The access to theoretical predictions is much less standard though. The exchanges between theorists and experimentalists through dedicated meetings, conferences, and workshops, or using any sort of media, ranging from e-mails to chats and video conferences, are valuable and remain the backbone of every scientific advance. Still, when the tools for theoretical predictions and simulations are already public, learning how to use them (or use them extensively) may be time-consuming and difficult in practice. To use these tools effectively, the discussed project provides standard and easy access for nonexperts. This is the underlying motivation for creating a virtual access (VA) facility; namely, a platform within which computer codes that allow predictions of nuclear phenomena in the user-defined context and format can be easily run.

So far, there is a limited choice of theory software that allows experimentalists to have easy access to state-of-the-art predictions for nuclear observables. Although several computer codes have been made avaliable to the community during the last decades, through publication in specialized journals and/or dedicated web pages, not all of them have user-friendly tutorials and input. The creation of a theory platform in which nonexpert users can perform calculations without excessive prior knowledge or training has been a long-awaited step.

We report here on the first virtual access facility for nuclear structure and reactions, created within the framework of the European Union (EU) EURO-LABS project, and open to researchers worldwide. The EU has granted the installation and commissioning of a VA facility called Theo4Exp (https://institucional.us.es/theo4exp/). Here, experimentalists can access software and data in a user-friendly way. Results can be easily downloaded, compared, and communicated. The facility can also foster mutual understanding and new collaborations among theorists. All this is in keeping up with the fact that the nuclear physics community is heading toward open science: publications in open access journals, reproducibility of calculations, and more to come.

The Theo4Exp facility is based on three different installations. The one called MeanField4Exp, installed in Kraków, offers codes for the calculation of nuclear energy surfaces throughout the nuclear mass table, also as a function of angular momentum. The installation Structure4Exp, developed in Milano, offers codes for the calculation of collective excitations in normal and superfluid spherical nuclei throughout the isotope table, and shell model codes for the detailed calculation of the low-energy spectroscopic properties of light- and medium-mass nuclei. The installation Reaction4Exp, developed in Seville, offers a range of tools for the calculation of direct nuclear reactions.

The three installations have been open to users since 1 February 2024. The main portal can be found at https://institucional.us.es/theo4exp. Users are granted access to each installation through the application https://iam-eurolabs.ijclab.in2p3.fr (also developed within the EURO-LABS project). They can access either by providing their institution credentials (if they belong to the EDUcation Global Authentication INfrastructure network, or EDUGAIN) or using Open Researcher and ORCID ID.

The installation MeanField4Exp is based on the numerical applications [1–3] of the realistic phenomenological mean field approach, developed by J. Dudek and collaborators at the University of Strasbourg. The codes have been implemented by Irene Dedes and Abdelghafar Gaamouci at the Institute of Nuclear Physics of the Polish Academy of Sciences in Kraków. The functioning of the MeanField4Exp service benefits from the integration of advanced methods of nuclear structure theory and quantum mechanics with advanced mathematical tools. These include inverse problem theory and Monte Carlo simulations for parameter optimization, group and group representation theories to handle symmetries, and graph theory for studying shape transitions, such as nuclear fission. The service provides access to advanced codes as well as to a comprehensive database containing precalculated results. Users can produce diagrams of nucleonic energy levels or total nuclear energies as functions of various deformation parameters. Potential energy maps allow studying shape coexistence and evolution as functions of proton and neutron numbers, as well as of angular momentum, addressing Jacobi and Poincaré shape transitions. Two examples of the results are shown in Figures 1 and 2.

The installation Reaction4Exp, hosted at Universidad de Sevilla (Spain) and implemented by Carla Muñoz-Chimbo, provides codes for the calculation of observables measured in various kinds of direct reactions, including Coulomb breakup, as well as elastic and inelastic scattering and transfer reactions. All the results are presented in text format as well as graphically and can be downloaded. The production of double-folding potentials from nuclear density distributions, is envisioned. Coulomb breakup is calculated in a semiclassical formalism, the equivalent photon model (EPM) [7], and makes use of the code developed by José A. Lay-Valera at the University of Seville [8]. This program provides differential Coulomb breakup cross-sections from external transition probabilities, as functions of angle and energy. Elastic scattering

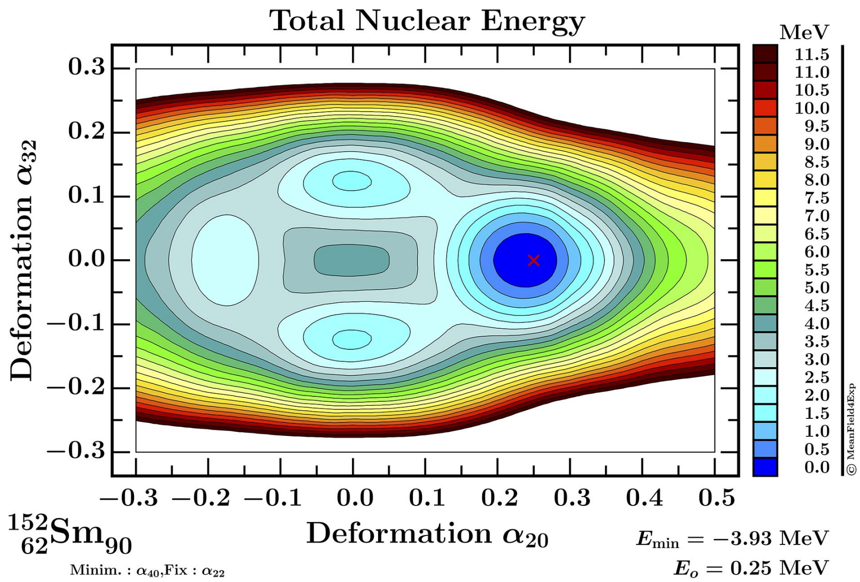

Figure 1. *Potential energy surface for ^{152}Sm nucleus according to the macroscopic–microscopic method as a function of axial quadrupole deformation α_{20} and octupole (tetrahedral symmetry) deformation α_{32} showing in addition to two coexisting axal prolate and oblate minima at $\alpha_{20} \approx +0.28$ and -0.18, respectively, also the tetrahedral symmetry minima at $\alpha_{32} \approx \pm 0.12$, the latter affirmed experimentally as the world's first identification in Ref. [4].*

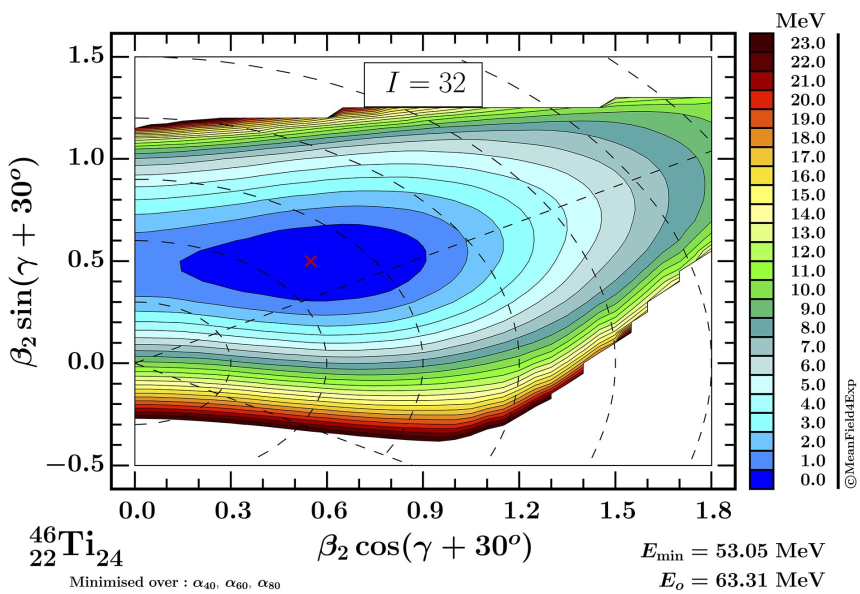

Figure 2. *Illustration of the Jacobi shape transition occurring at high nuclear temperatures following an increase of angular momentum (here at I = 32) with the nuclear energy modeled with the help of the macroscopic Lublin-Strasbourg-Drop approach, Ref. [5]. This shape transition was for the first time discovered experimentally in Ref. [6].*

calculations are performed according to the Optical Model (OM) formalism, by introducing an optical potential to describe the interaction between the projectile and the target. The code provides the elastic angular distributions, at a given energy in the laboratory frame. It is also possible to obtain the classical trajectories and deflection functions as a function of the impact parameter [9], using a code developed by Mario Gómez-Ramos at the University of Seville. The inelastic scattering code provides cross-sections for the population of the excited states of the projectile or the target, making use of transition probabilities obtained from a collective model. It is based on the coupled-channels (CC) formalism and the cross-sections can also be computed in first-order approximation, known as the distorted-wave Born approximation (DWBA). The transfer reaction calculations are performed in DBWA formalism and provide cross-sections for channels in which one particle from the projectile is transferred to the target or vice-versa. The OM, CC and DWBA calculations are performed with the code Fresco (www.fresco.org.uk) [10], which was developed by Ian J. Thompson, formerly at the University of Surrey and Lawrence Livermore National Laboratory. An example of inelastic cross-section calculation, as displayed in the facility, is shown in Figure 3.

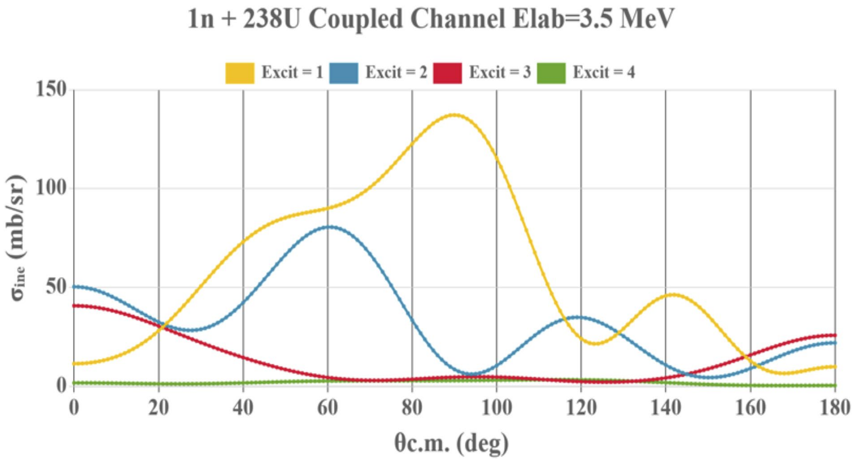

Figure 3. *Example of differential cross-sections for the inelastic excitation to the first excited states of the target in the reaction n+^{238}U at 3.5 MeV.*

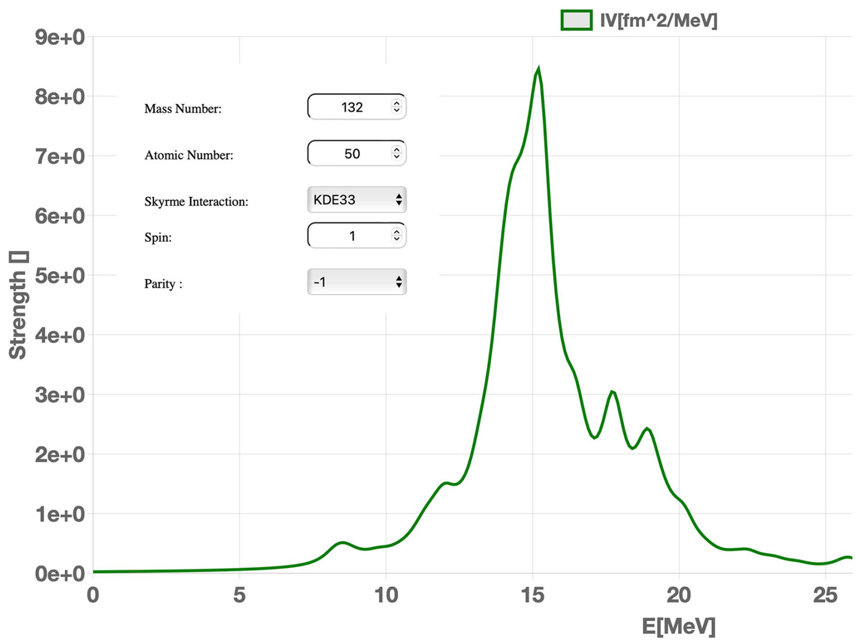

Figure 4. *Example of a result, in the case of the isovector dipole strength calculated in RPA using the Skyrme force KDE033 in ^{132}Sn. The inset shows the input mask that the user has to fill.*

The installation Structure4Exp, hosted at the University of Milan, and set up by Imane Moumene, offers two types of codes. The first category includes two codes that are designed for the calculation of basic spectroscopic properties of spherical nuclei throughout the mass table. Ground state properties like masses and radii, as well as vibrational excited states, are provided. For each excited state, the codes give the transition strengths associated with usual isoscalar, isovector, and electromagnetic operators. One can visualize how this strength is distributed among giant resonances and low-lying vibrational states. One of these two codes is based on self-consistent Hartree-Fock (HF) plus random phase approximation (RPA), developed by Gianluca Colò and coworkers [11]. This is suitable for double-magic nuclei, or for nuclei with closed sub-shells both for neutrons and protons. The other code is based on HF+Bardeen-Cooper-Schrieffer plus Quasiparticle RPA (QRPA), and has been developed by Gianluca Colò and Xavier Roca-Maza. Both codes employ a Skyrme-type effective force [12]. An example of results obtained by using the facility is displayed in Figure 4. The installation also offers the possibility to run the shell-model code KSHELL [13]. This has been developed by N. Shimizu and collaborators at the Centre for Computational Sciences of the University of Tsukuba. The code has been implemented with the help of Giovanni Di Gregorio (Caserta University and Istituto Nazionale di Fisica Nucleare [INFN] Napoli) and Angela Gargano (INFN Napoli). Calculations can be performed in different valence spaces, with a selection of appropriate interactions. Users can specify the energy levels to be determined, and the program provides energy, occupation numbers, main contributing configurations, and, if requested, E2 and M1 electromagnetic transition values.

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LaVA: An Introduction

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The Lattice Virtual Academy (LaVA) is a virtual platform for advanced e-learning in lattice field theory, a computational method developed for nuclear and particle physics. LaVA will provide open-access, inclusive training to beginner and advanced students. It will also serve as a reference hub for scientists working in other fields who wish to become acquainted with some of the aspects of this rich subject.

LaVA was formed in 2022, after the pandemic lockdown abruptly forced many academics to learn how to teach online. Researchers involved in LaVA recognized their newly and unexpectedly gained experience in making video lectures and online teaching material enabled them to make advanced material in support of new lattice research community members.

Lattice field theory is a computational framework for making first-principles predictions about strongly interacting matter, such as the quarks and gluons bound inside the nucleon. As the subject has matured, it is now embedded and widely used in theoretical efforts to make predictions from quantum field theories related to hadron structure and spectroscopy, precision physics of the standard model, and studying matter in the extremes of