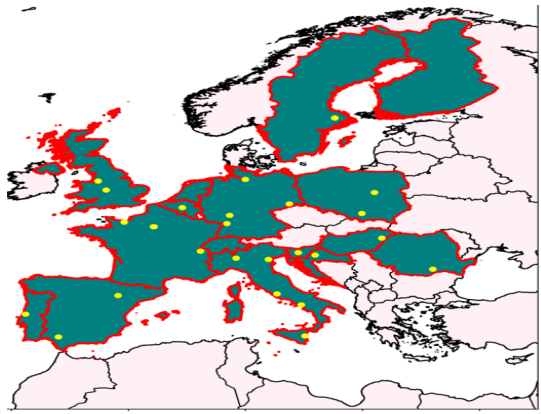


# Virtual Access to theoretical tools (EURO-LABS)

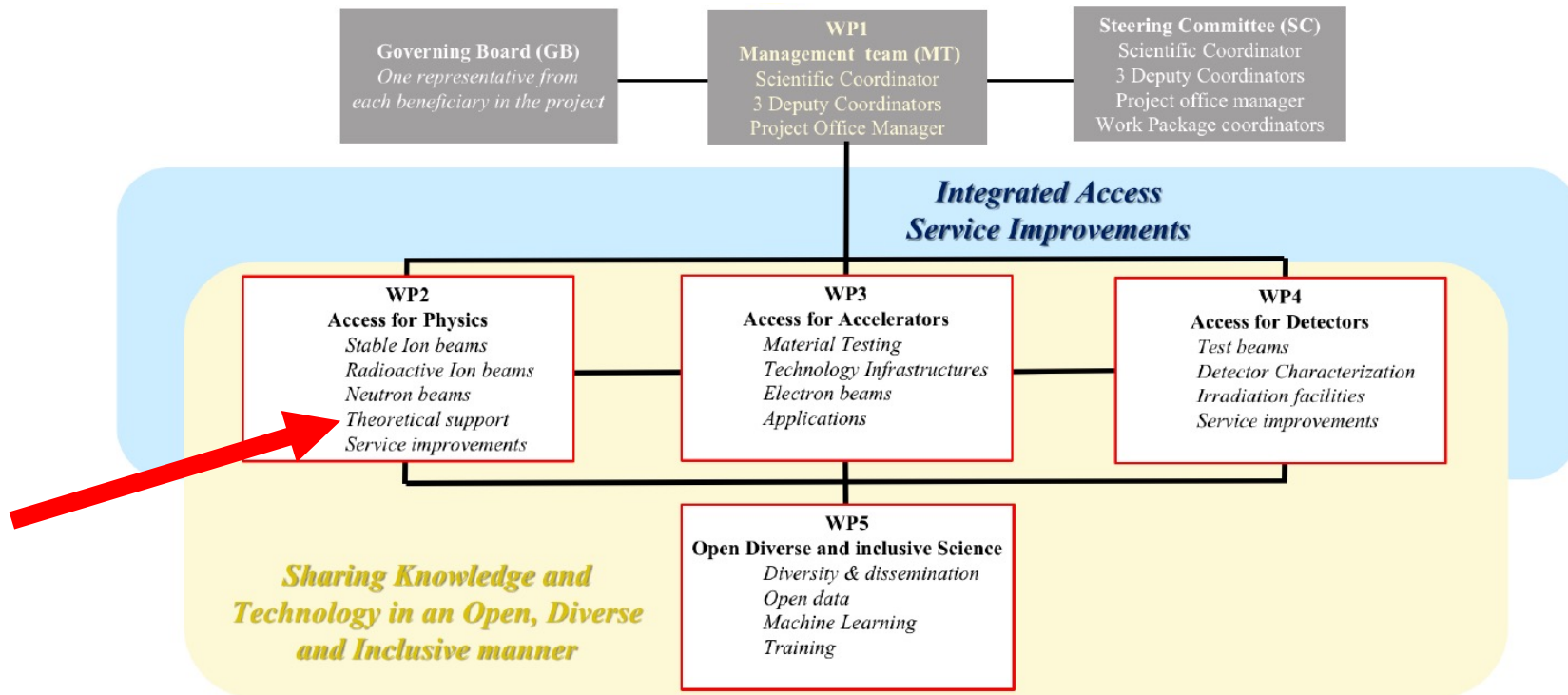
Enrico Viguzzi

**INFN Milano**





EURO-LABS is a consortium of **thirty nine** Research Infrastructures (RIs) from twelve countries in Europe  
*Finland in the north and Italy to south to Romania in the east and Portugal in the west*



a) Task and sub-Task leaders

b) **Each facility will have a well identified Facility Coordinator**

who will follow all aspects related to the TA, and the scientific and technical work related to facilities improvements for EURO-LABS at that facility. He/she will be the contact point to the corresponding Task and WP leaders and the project office.

Town meeting every year

## THEORY SUPPORT, WP 2.4

2 pillars:

- **ECT\***, European Centre for Theoretical Studies in Nuclear Physics and Related Areas  
Trento, Italy – Gert Aarts
- **Theo4Exp**: Virtual Access to well-established computing codes  
Manuela Rodríguez-Gallardo (Universidad de Sevilla)

**Theo4Exp** virtual access infrastructure: provide theoretical tools for the **EURO-LABS** project and wider experimental nuclear physics community

3 installations:

- **MeanField4Exp** (Krakow): access to mean-field theory service in the domain of nuclear structure physics. Deputies: Jerzy Dudek (IPHC Strasbourg)/Piotr Bednarczyk (Krakow)
- **Reaction4Exp** (Sevilla): codes used for nuclear reaction calculations. Coordinator: Manuela Rodríguez-Gallardo
- **Structure4Exp** (Milano): virtual access to other codes that use advanced tools of nuclear structure theory. Deputy: Gianluca Coló

website: [institucional.us.es/theo4exp/](http://institucional.us.es/theo4exp/)

# THEORY – Theo4Exp

Personnel (milestone for month 18):

- **MeanField4Exp** (IFJ PAN, Krakow): 2-year contract  
computer scientist to implement mean-field theory codes for large-scale calculations of nuclear structure; responsible for programming and management of user-friendly web interface
- **Reaction4Exp** (U. Sevilla): 2-year contract  
computer scientist for programming and management of user-friendly web interface
- **Structure4Exp** (U. Milano): 1-year contract  
computer scientist to improve existing nuclear structure codes; responsible for programming and management of user-friendly web interface

Servers: codes will run on new or existing servers, agreed with university computer centres

## Coordinating Team (CT)

- Coordinator: Manuela Rodríguez-Gallardo
- Deputies: Jerzy Dudek and Gianluca Coló

## International Review Panel (IRP)

- Piotr Bednarczyk (Chairperson) and Krzysztof Rusek
- Antonio M. Moro and Ian J. Thompson
- Enrico Viguzzi and Angela Gargano

IRP will meet annually to produce yearly internal assessment reports.

CT will provide the IRP a comprehensive list of results and achievements, access statistics and user feedback.

First IRP meeting: September 8 2022

## Reaction4Exp, Sevilla

FRESCO, a general code for direct reactions

EPM\_SEV, a code for semiclassical calculations of high-energy collisions

DFPOT, SPP, codes for double folding potentials from density distributions



# Fresco

Coupled Reaction Channels Calculations

[www.fresco.org.uk](http://www.fresco.org.uk)

Documentation

Download

Input examples

Frescox

Reactions book

Related Programs

Special Functions

Contact

Site Information

Computer Program FRESKO

## About Fresco

**Fresco** is a program developed by Ian Thompson over the period 1983 - 2006, to perform coupled-reaction channels calculations in nuclear physics. It uses Fortran 90 or Fortran 95 on Unix, Linux, Vax and Windows machines.

**Sfresco** is an additional version of Fresco, to provide Chi-squared searches of potential and coupling parameters, and to fit additional R-matrix terms in hybrid models.

**Frescox** has the recent developments after 2006.

[Overview talk](#), March 2015.  
Ian Thompson's [home page](#).


### Nuclear Reactions for Astrophysics: Principles, Calculation and Applications of Low-Energy Reactions

#### **New Textbook**

by Ian J. Thompson (Lawrence Livermore National Laboratory, California and University of Surrey)  
and Filomena M. Nunes (Michigan State University)

**Published 2009**. Information at [fresco.org.uk](http://fresco.org.uk), and at [publisher](#)

## About Xfresco

**Xfresco** is a graphics interface for Fresco developed by Antonio Moro. Xfresco helps you to create and modify interactively input files to be later used by fresco. Xfresco is written in C. To provide graphical display, it uses the graphical toolkit **GTK+**, so before installing Xfresco you will need to have GTK+ installed in your system. 

Antonio Moro's [home page](#).

Reviving the Nuclear Reactions  
Video Project  
<http://nrv.jinr.ru/nrv/>



# Nuclear Reactions Video

## Low Energy Nuclear Knowledge Base

Supported by  
Russian Foundation for Basic Research

Nuclear Properties	Nuclear Models	Nuclear Decays	Nuclear Reactions
<b>Nuclear Map Systematics</b> 	<b>Shell Model</b>	<b>Alpha - decay</b>	<b>Available beams</b> Stable beams: EU Institutions, FLNR (Dubna) U400, FLNR (Dubna) U400M RIBs: GANIL, MSU
	<b>Liquid Drop Model</b>	<b>Beta - decay</b>	<b>Elastic scattering</b> Classical Semiclassical Optical Model (Tutorial in Russian) Phase analysis
	<b>Two-Center Shell Model</b>	<b>Fission</b>	<b>Inelastic Scattering:</b> DWBA model (DWUCK4 code) Adiabatic rotational model (FRESCO code) Coulomb excitation Direct process (DWBA) Channel coupling Deep inelastic collision
		<b>Decay of excited nuclei</b>	<b>Transfer reactions:</b> Direct process (DWBA)   Semiclassical approach (GRAZING code) 3-body classical model Two-nucleon transfer Massive transfer
			<b>Fragmentation</b> EPAX v.3 Break-up (DWBA) Semiclassical model
			<b>Fusion</b> Empirical model Channel Coupling Langevin equations
			<b>Driving potentials</b> Synthesis of SHE (movie)
			<b>Evaporation residues</b> Monte-Carlo
			<b>Radiative capture</b> Potential model
			<b>Pre-equilibrium LP formation</b> 4-body classical model Semiclassical model Moving sources
			<b>Kinematics:</b> 2-body   // 3-body Q-values // Detector loading

Please, quote us as...

 **Warning:** sections marked by this icon or without any icons require installation of **Java** and a Java-compatible browser

All resources of the NRV Knowledge Base are free to use. We, nevertheless, need a support of our project by official establishment for further development of it. New models of nuclear dynamics and much more experimental data on nuclear reactions have to be included. If you get useful results, **please, quote the NRV** in your papers and talks. In a case of elastic scattering, for example, appropriate reference could be V.I. Zagrebaev et al., OM code of NRV, <http://nrv.jinr.ru/nrv/>, and so on.



### NRV: Optical Model



Elastic scattering of  $^4\text{He} + ^{208}\text{Pb}$  at  $E/A = 5.5$  MeV

#### Optical Model parameters

Coulomb $r_0(R)$ , fm	Real part			Imaginary part		
	$V_0$ , MeV	$r_0(R)$ , fm	$a$ , fm	$W_0$ , MeV	$r_0(R)$ , fm	$a$ , fm
1.2 (9.015)	-96.44	1.085 (8.151)	0.625	-32	0.958 (7.197)	0.42
Volume						
Surface						
Spin-Orbit						
Proximity						
Folding						

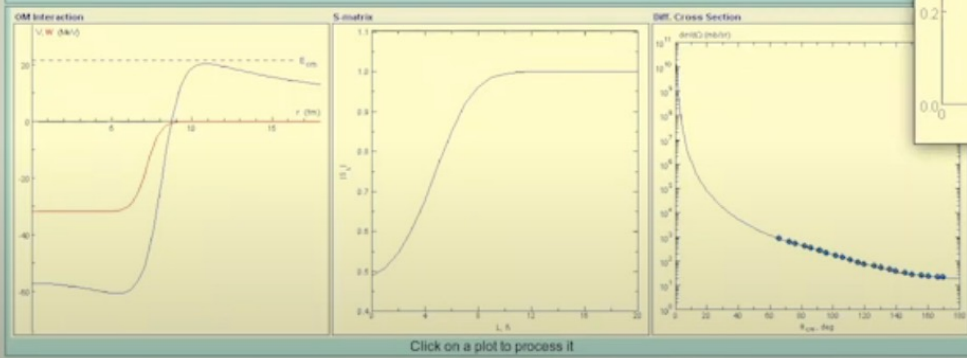
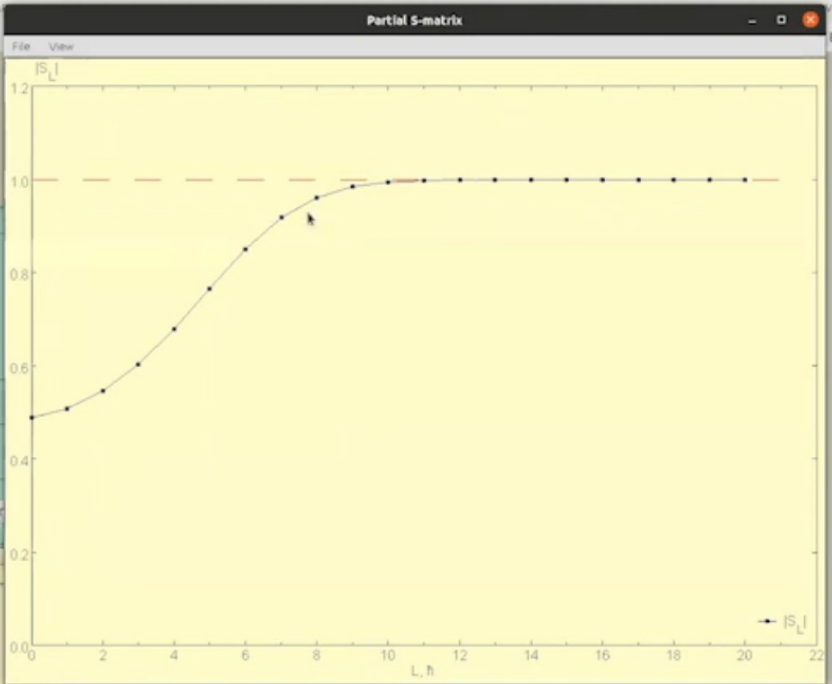
#### Other quantities

$E_{lab} = 22$  MeV  
 $E_{cm} = 21.585$  MeV  
 $k = 2.013 \text{ fm}^{-1}$   
 $\eta = 11.011$   
 $R_{max} = 25$  fm  
 $dr = 0.15$  fm

#### Fitting process

$N_{steps} = \text{no fit}$   
 $\Delta\chi^2/\chi^2 = \text{no fit}$   
 Use obtained OMP in  
 DWBA: Inelastic scattering (exit channel)

	Before fitting	After fitting
$\sigma_R$ , mb	220.84	-
$\sigma_{tot}$ , mb	285.09	-
$\chi^2/N_{points}$		-



Click on a plot to process it  
Java blocked?

## MeanField4Exp, Krakow

Large sets of pre-calculated potential energy surfaces, electric and mass moments as a function of spin and temperature

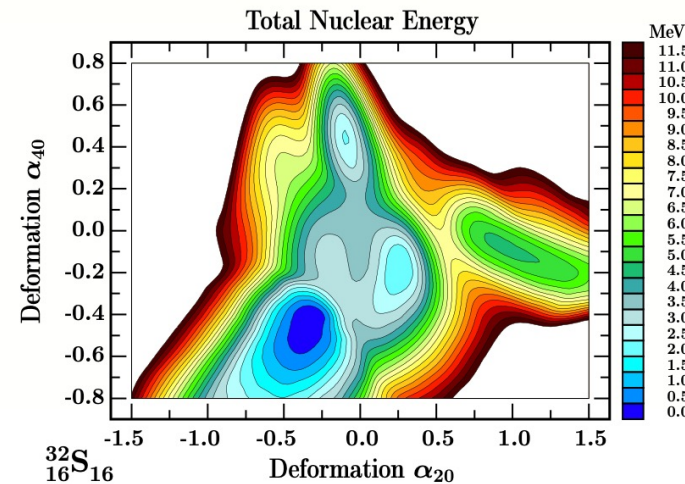
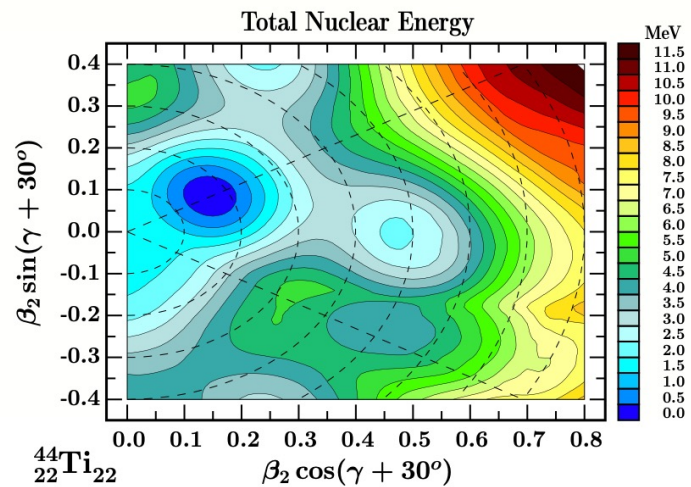
HFB cranking calculations of rotational band structures

Structure of isomers

Giant dipole resonances as a function of temperature and spin

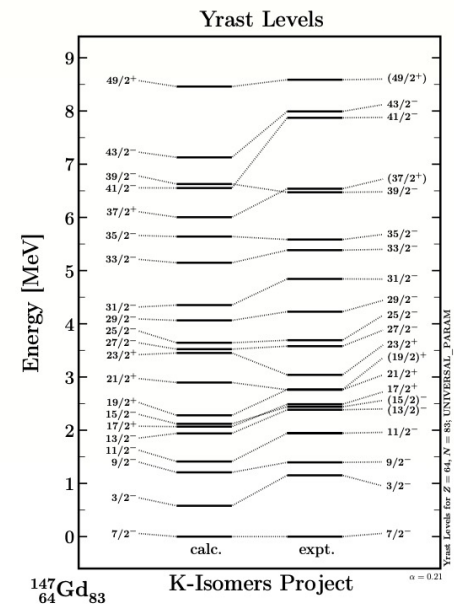
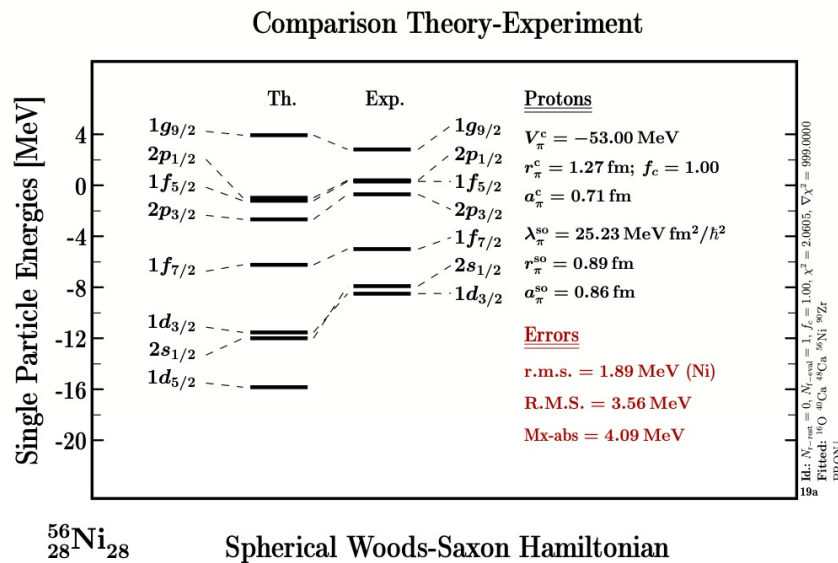
Nuclear densities of deformed nuclei

- **GOAL 1:** Construct a user-friendly, web-based interface allowing to access OUR theory data-bases with results of the large-scale calculations to RI experimentalists;
- **Nota bene:** “OUR theory-data-base” contains the results of large scale calculations with  $\sim 10^5$  processors, months of the c.p.u. time, to be extended if project accepted
- **This means selecting plots you want among  $\sim 10^5$  plots\*) in the base, for instance:**



\*) Prepared in collaboration with Ms Jie YANG, PhD student, Prof. Dudek Group

- **GOAL 1:** Construct a user-friendly, web-based interface allowing to access OUR theory data-bases with results of the large-scale calculations to RI experimentalists;
- **GOAL 2:** Provide possibilities of performing on line modelling for nuclei of interest for an experimentalist-user with the help of the standard theory tools (details below);
- **DudWare+** will be a web-based software, running on MacOSX/Linux/Windows, with a intuitive Graphic User Interface, having 'clicable' buttons and dialog windows



## Structure4Exp, Milano

SKYRME\_RPA, HFBCS\_QRPA, codes for calculations of energies and transition probabilities of collective states

Charge-changing transitions

Beta-decay half lives

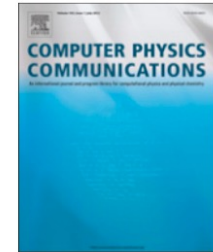
KSHELL, a general shell model code (A. Gargano, G. De Gregorio, Napoli)



Contents lists available at [SciVerse ScienceDirect](#)

## Computer Physics Communications

journal homepage: [www.elsevier.com/locate/cpc](http://www.elsevier.com/locate/cpc)



# Self-consistent RPA calculations with Skyrme-type interactions: The `skyrme_rpa` program<sup>☆</sup>


Gianluca Colò<sup>a,\*</sup>, Ligang Cao<sup>b,c,a</sup>, Nguyen Van Giai<sup>d</sup>, Luigi Capelli<sup>a,1</sup>

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<sup>b</sup> *Institute of Modern Physics, Chinese Academy of Science, Lanzhou 730000, PR China*

<sup>c</sup> *Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator of Lanzhou, Lanzhou 730000, PR China*

<sup>d</sup> *Institut de Physique Nucléaire, Univ. Paris-Sud and IN2P3-CNRS, F-91406 Orsay Cedex, France*

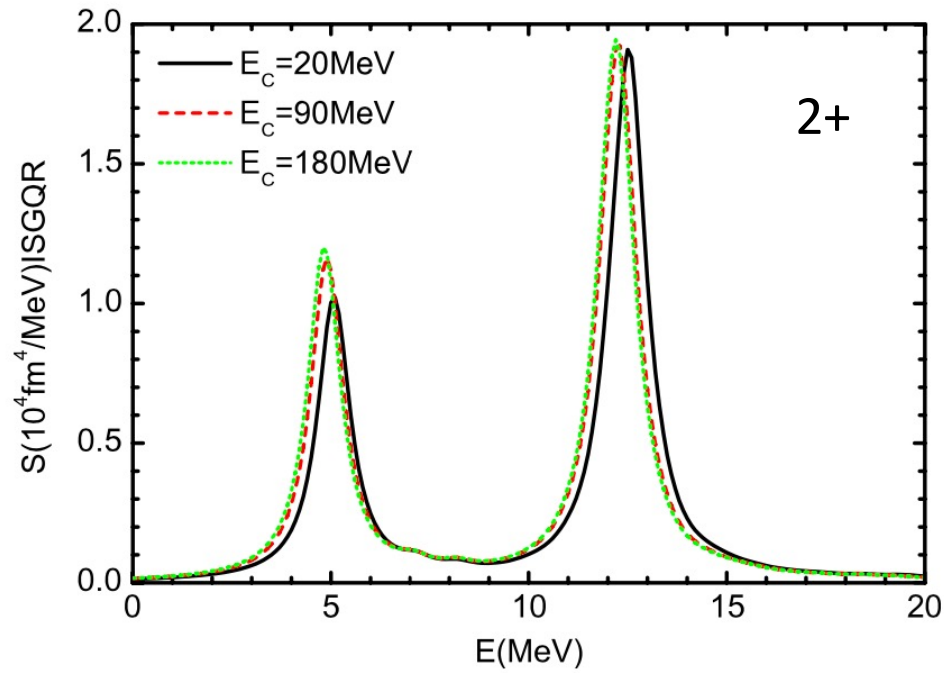
 > nucl-th > arXiv:2102.06562

## User guide for the `hfbcq-rpa(v1)` code

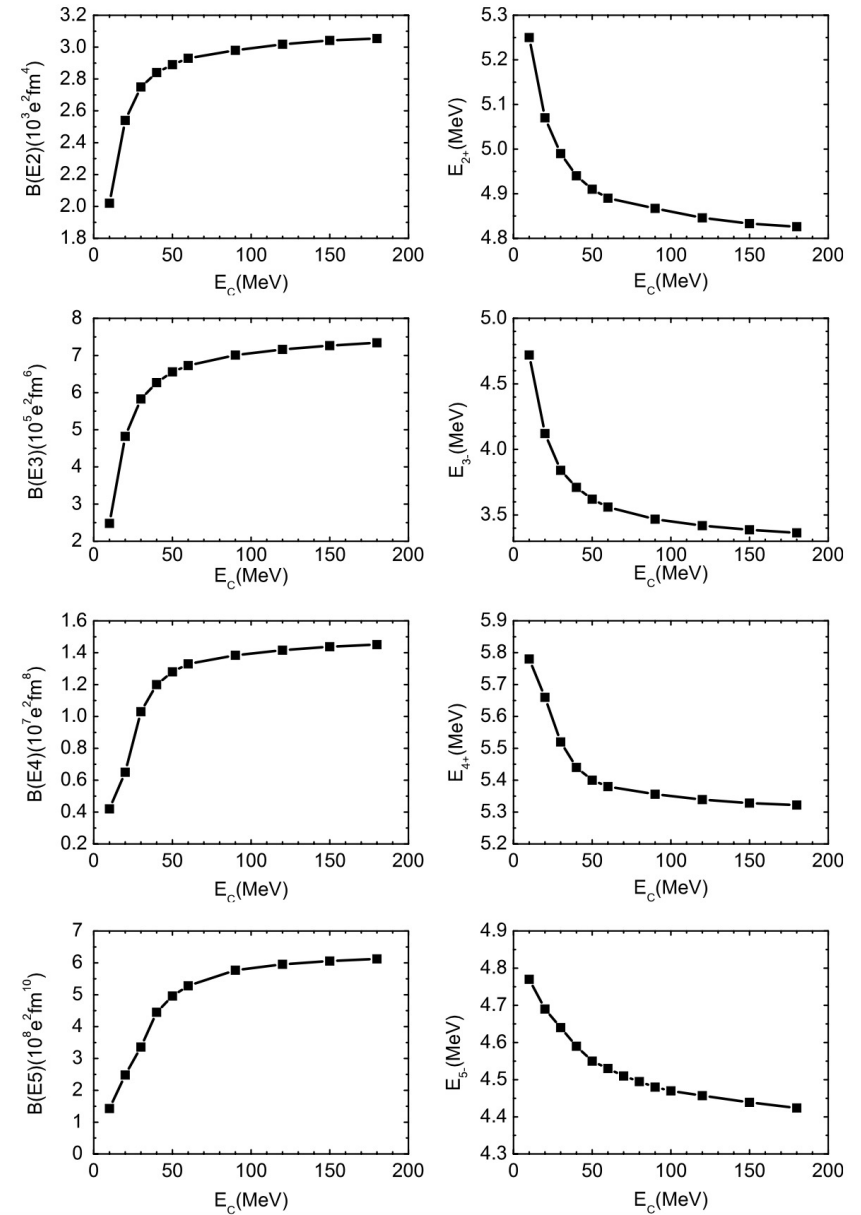
Gianluca Colò, Xavier Roca-Maza



$^{208}\text{Pb}$



G. Colò et al., Comp. Phys. Comp. 184 (2013) 142





"KHELL"  
code for  
nuclear shell-  
model  
calculations

Cover page for "KHELL"  
code

Download

Links

# Nuclear shell-model calculations "KHELL" code

This page is for "KHELL", nuclear shell-model calculation code.

Noritaka Shimizu, Center for Computational Sciences, University of Tsukuba

"KHELL" code is a shell-model code that was recently developed by N. Shimizu and collaborators.

It works in a similar manner to traditional shell-model codes, such as "OXBASH", "NuShell", "ANTOINE", "MSHELL64", and so on.

"KHELL" code enables us to perform nuclear shell-model calculations with M-scheme basis representation with the thick-restart block Lanczos method. This code is easily used on a Linux PC with a many-core CPU and OpenMP library. It is also used on a state-of-the-art massive parallel computer with hybrid MPI+OpenMP parallel programming. This manual explains how to use this code.

This code is equipped with a user-friendly dialogue interface to generate a shell script to run a job. By modifying this script, the code runs on various computers including supercomputers. Intel Fortran compiler with a Linux OS is most recommended. It can compute energy levels, spin, isospin, magnetic and quadrupole moments, E2/M1 transition probabilities, and one-particle spectroscopic factors. Up to hundreds of billions M-scheme dimensions is capable if enough memory is available on the computers.

The ground-state energy of  $^{56}\text{Ni}$  with a pf-shell and KB3 interaction (one billion M-scheme dimensions) was computed in 53 seconds using 144 nodes (8064 CPU cores) with the Oakbridge-CX supercomputer, at the University of Tokyo.



## 1. Introductory part

Textbooks, reviews, notes on shell model, with special focus on technical aspects

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## 2. Shell model codes

### 2.1 KSHELL

2.1.1. User's Guide & materials on the use and the limits of the code

2.1.2 How download and compile the code

2.1.3 Simple scheme of its functions (interactive workflow?)

2.1.4 List of options, for each option add few explicative lines, specify the input, the output

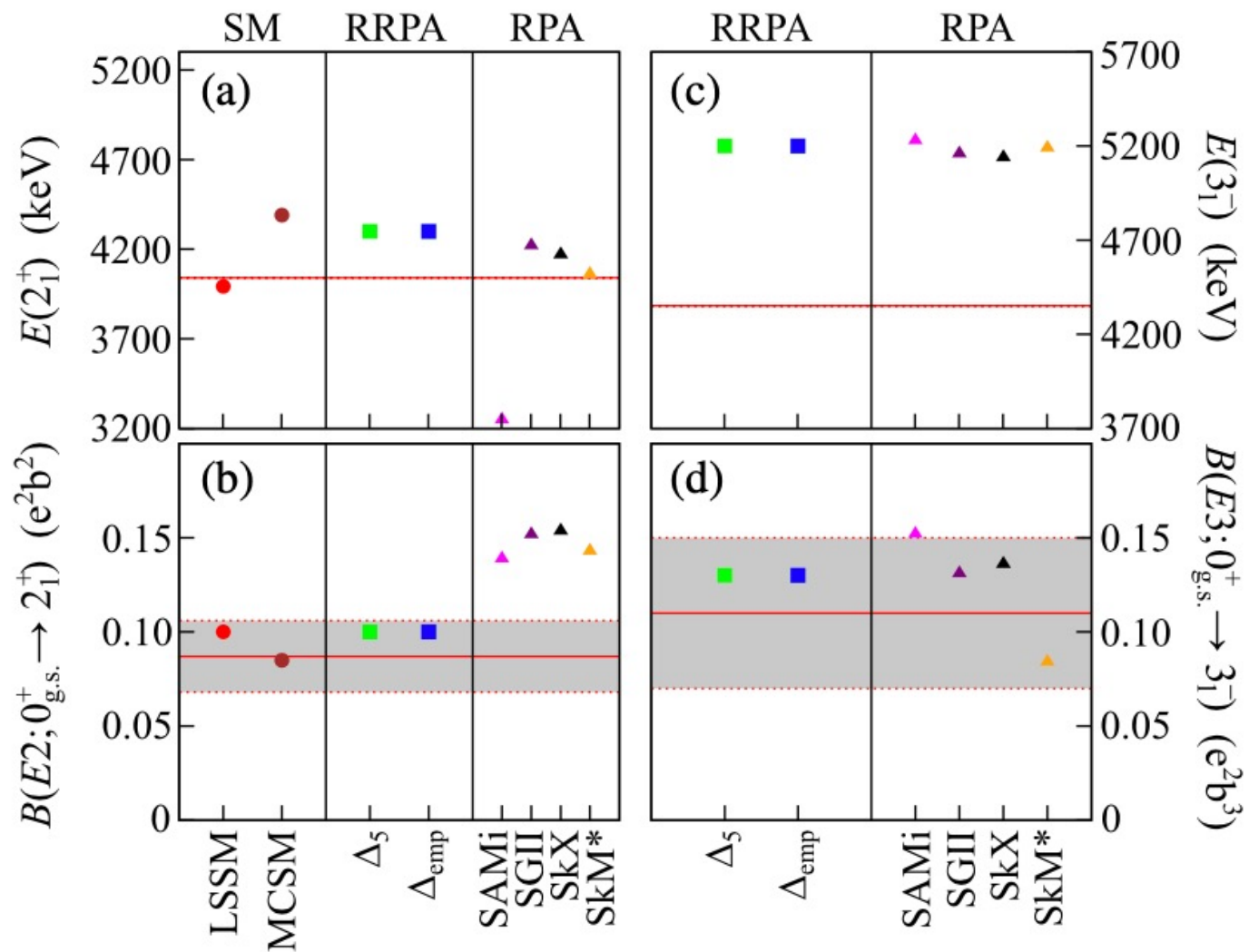
2.1.5. Interaction database with references; converter codes for different interaction format

2.1.6. use of KSHELL user interface (in python) to construct input  
input e output examples for the options of list 2.1.4

2.1.7. Python files to organize the output

## 3. Bibliography with physics cases

$^{132}\text{Sn}$



D. Rosiak et al, PRL 121 (2018) 252501

Some issues:

Management of access, authorization platform

Connection between the three sites

Connection with FAIR Data

Maintenance after the end of EURO-LABS project

Proposal of codes from other groups are welcome  
( possibly to be implemented at a later stage)

Advice from experimentalists about the best ways to serve their needs is welcome



