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Do you know how to use the Structure4Exp platform

ECT* workshop
Trento-Italy
9 July 2025

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In collaboration with: G. Colò, E. Vigezzi, A. Gargano, G. Degregorio

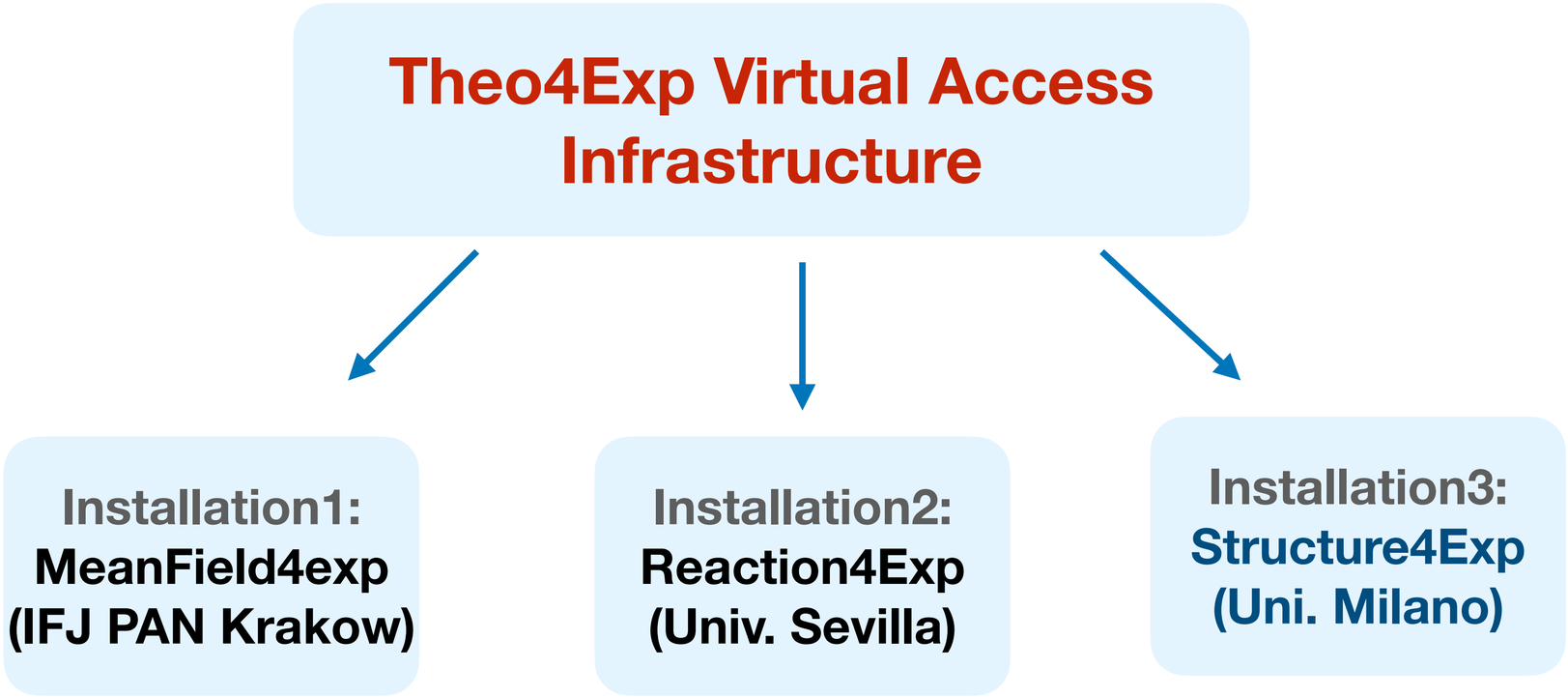
Outline

- Introduction
- Hartree Fock (HF) plus Random Phase Approximation (RPA)
- HF_Bardeen_Cooper_Schrieffer-Quasiparticle RPA (HFBCS-QRPA)
- KSHELL code
- Conclusion

Introduction

- Computational tools are essential for advancing research in nuclear physics.
- THEO4EXP serves as a gateway to advanced computational resources for nuclear physicists.
- Focuses on user-friendliness, easy navigation, and accessibility to bridge the gap between theory and experiment.
- The infrastructure consists of three key installations:

Introduction



Introduction

Structure4Exp Overview:

- Hosted at the University of Milano.
- The platform is available online at: https://ns4exp.mi.infn.it
- Integrates three specialised codes adapted to various nuclear structure models:
  - Skyrme HF-RPA — Talk by G.Còlo
  - HFBCS-QRPA — Talk by E.Vigezzi
  - KSHELL (Shell Model) — Talk by A. Gargano

Introduction

Structure4Exp Overview:

- Codes are designed to address key aspects of nuclear structure:
  - From closed-shell to open-shell nuclei
  - From mean-field to shell-model approaches
- Provide access to nuclear observables such as: energy spectra, excited states, transition probabilities.
- Offer a unified framework for nuclear structure studies.

1* Hartree Fock (HF) plus Random Phase Approximation (RPA)

HF-RPA

- Based on Hartree-Fock + Random Phase Approximation (RPA).
- Applicable to even-even, spherical nuclei, typically closed shells or sub-shells.
- Uses **Skyrme effective interaction** for fully self-consistent calculations.
- Provides:
  - Ground state properties.
  - Excitation spectra for **natural parity states**.
  - Transition strengths for isoscalar, isovector, and electromagnetic modes.

1* Hartree Fock (HF) plus Random Phase Approximation (RPA)

Input Interface

Input Parameters for *HF plus RPA calculation*

To perform the *HF plus RPA calculation* , please enter the parameter values for the system under study

Example:
$^{132}Sn(1^-)$

Mass Number: 132

Atomic Number: 50

Skyrme Interaction: SLy4

Spin: 1

Parity : -1

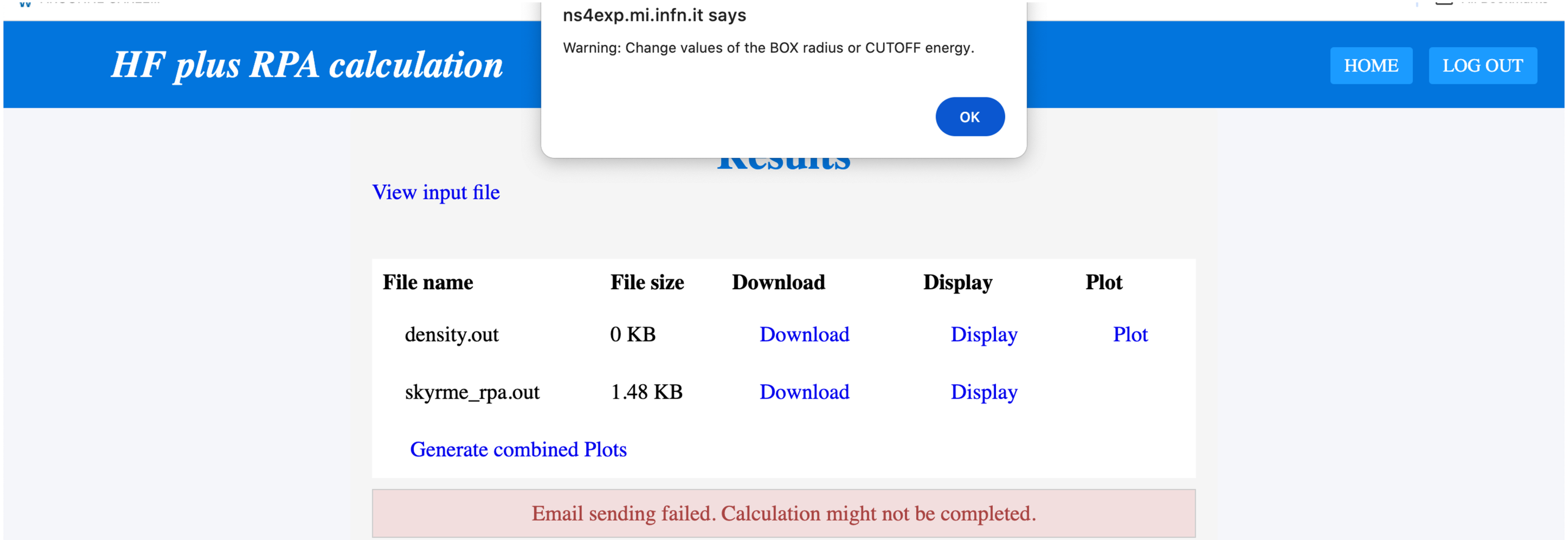
Default Parameters

Can be modified if needed for specific cases

Back | Reset | Submit

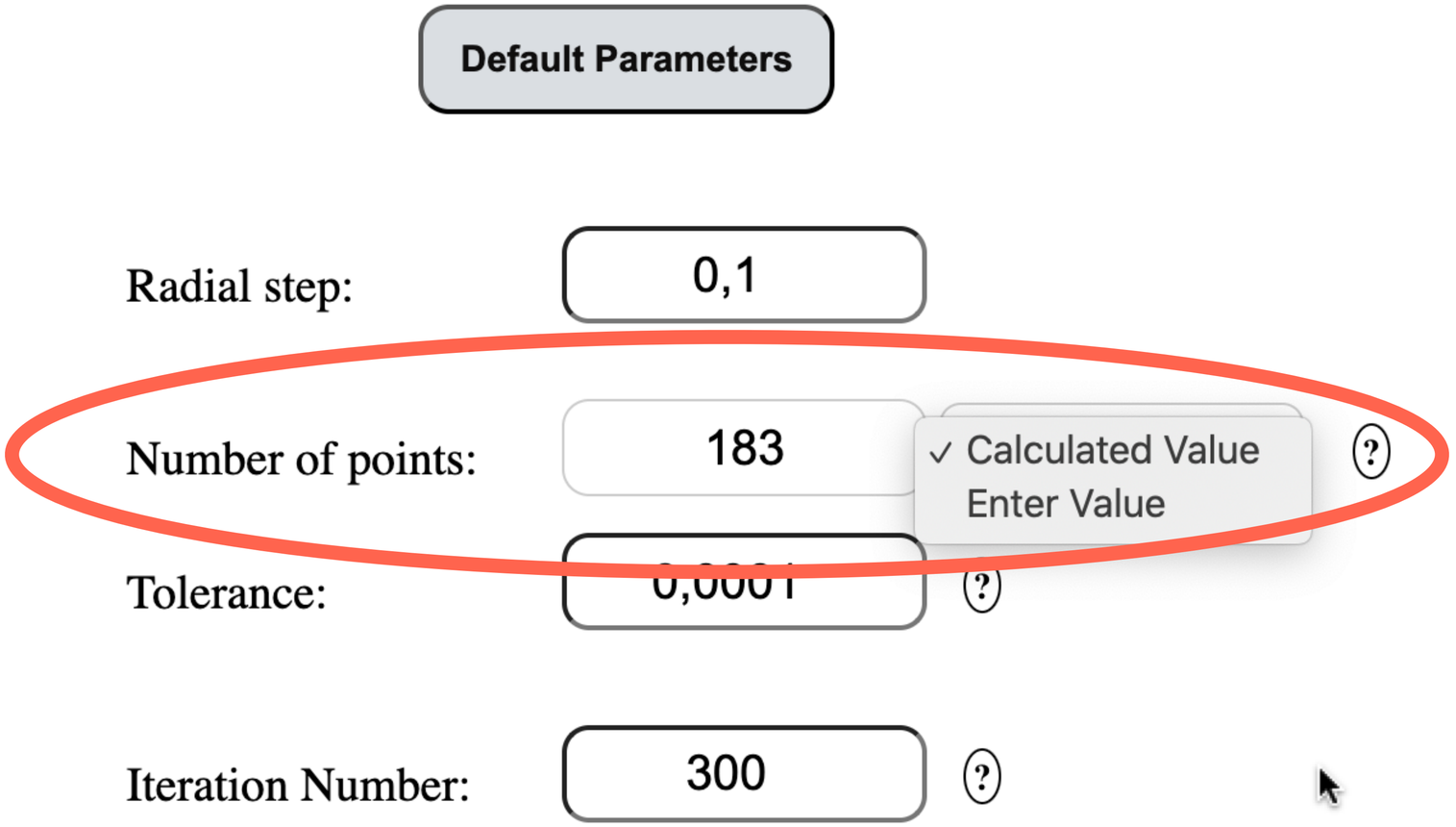
1* Hartree Fock (HF) plus Random Phase Approximation (RPA)

- **Adjusting the Box Radius**



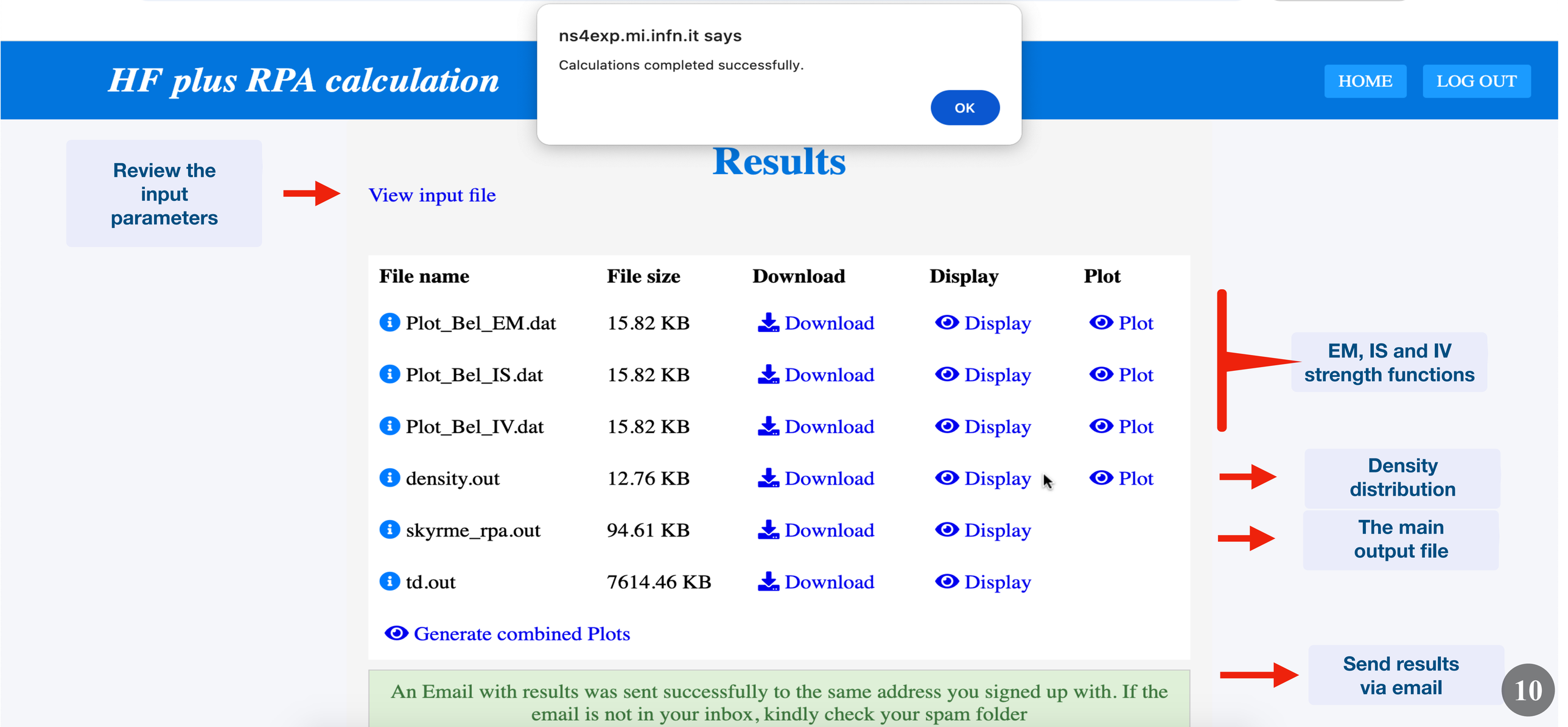
1* Hartree Fock (HF) plus Random Phase Approximation (RPA)

- **Adjusting the Box Radius**



1* Hartree Fock (HF) plus Random Phase Approximation (RPA)

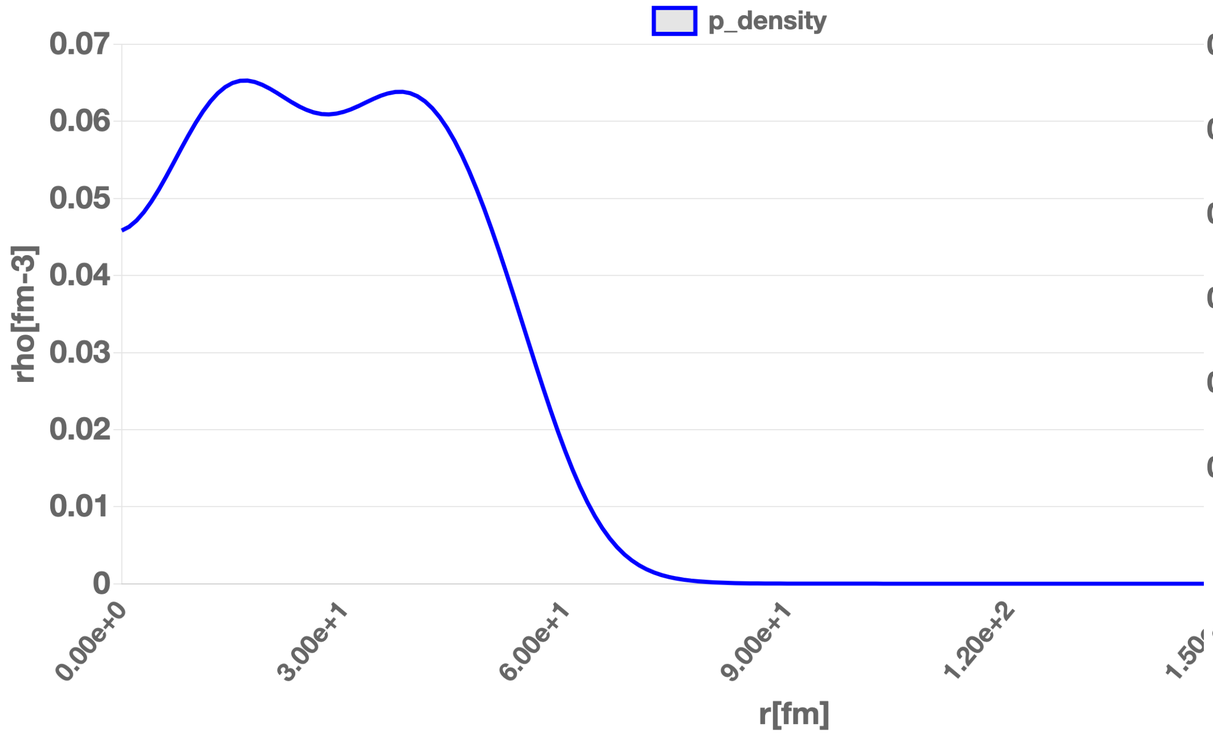
Results page



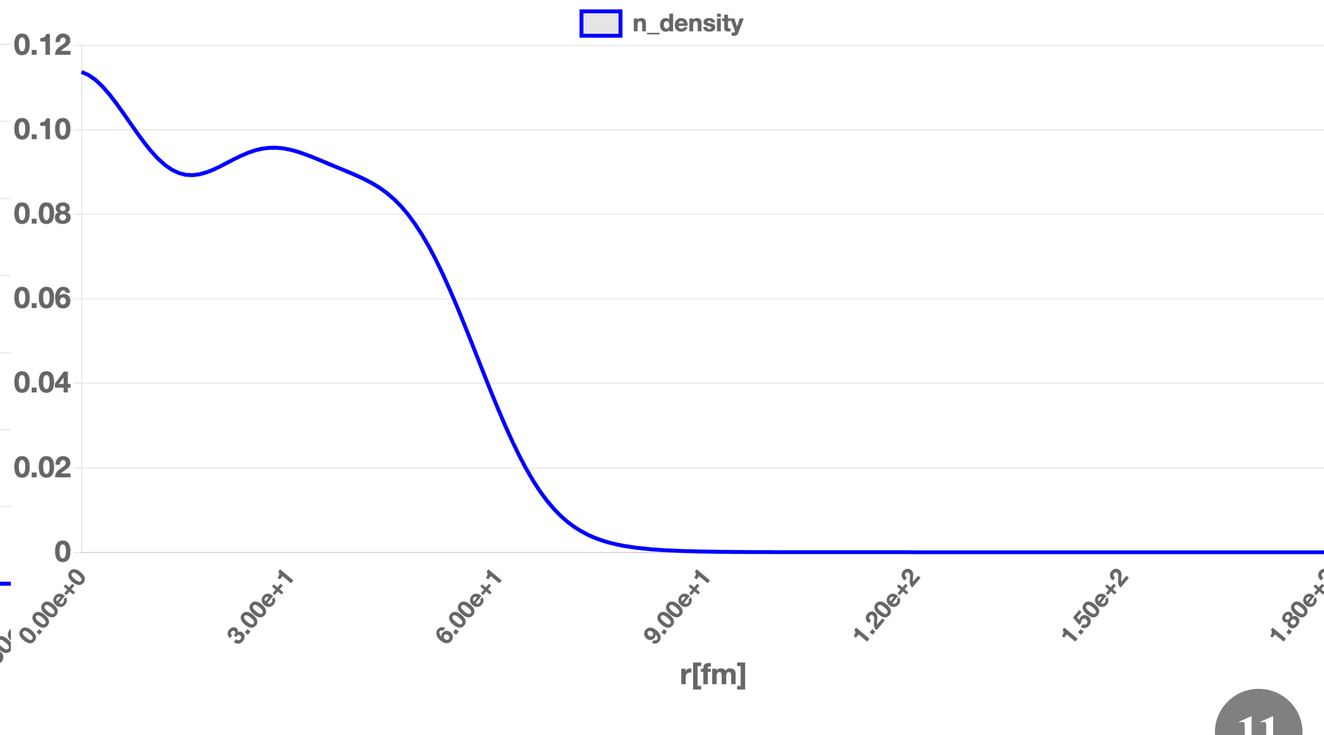
1* Hartree Fock (HF) plus Random Phase Approximation (RPA)

Results page: Density Distribution ^{132}Sn

Proton Density

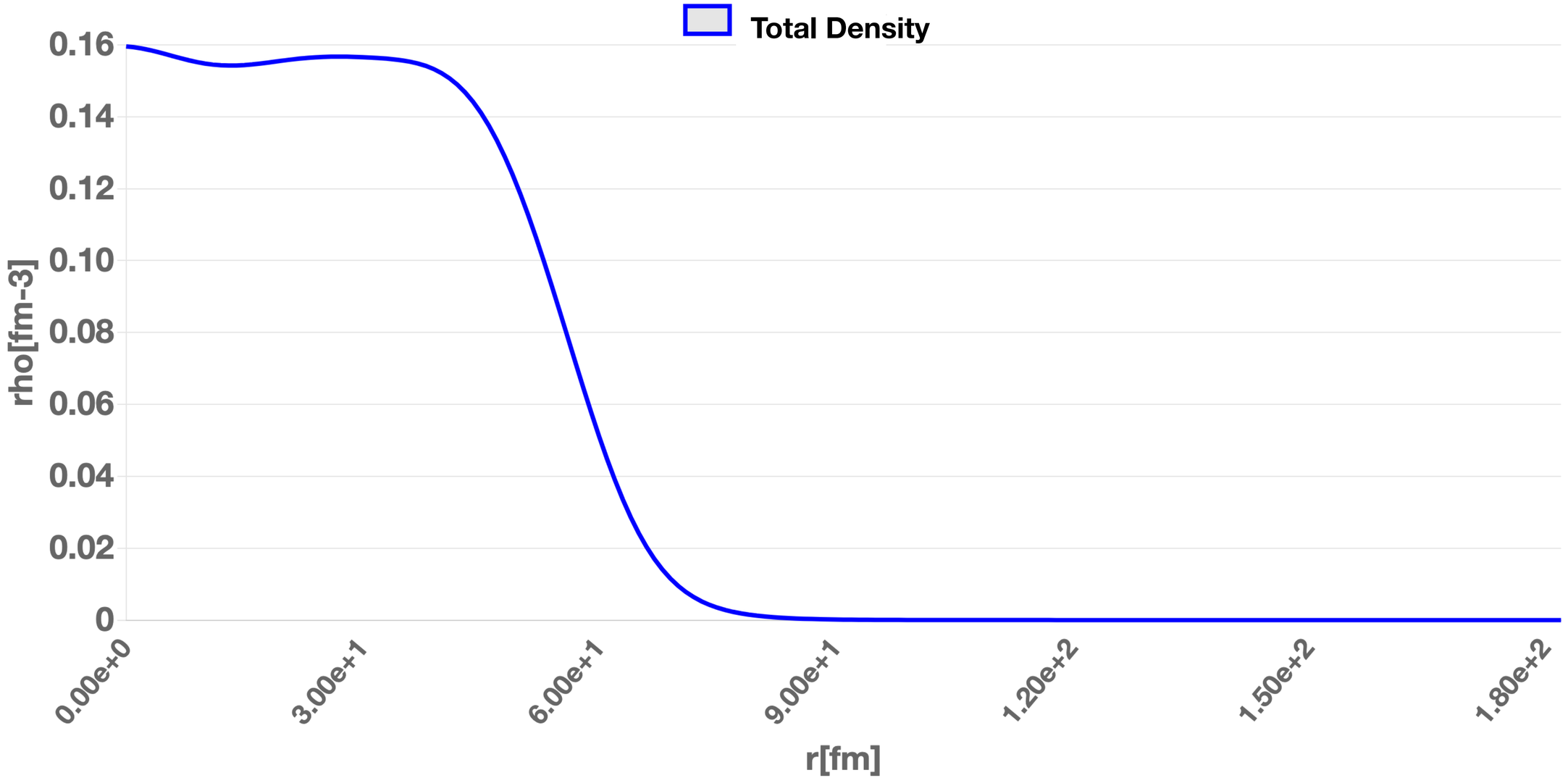


Neutron Density



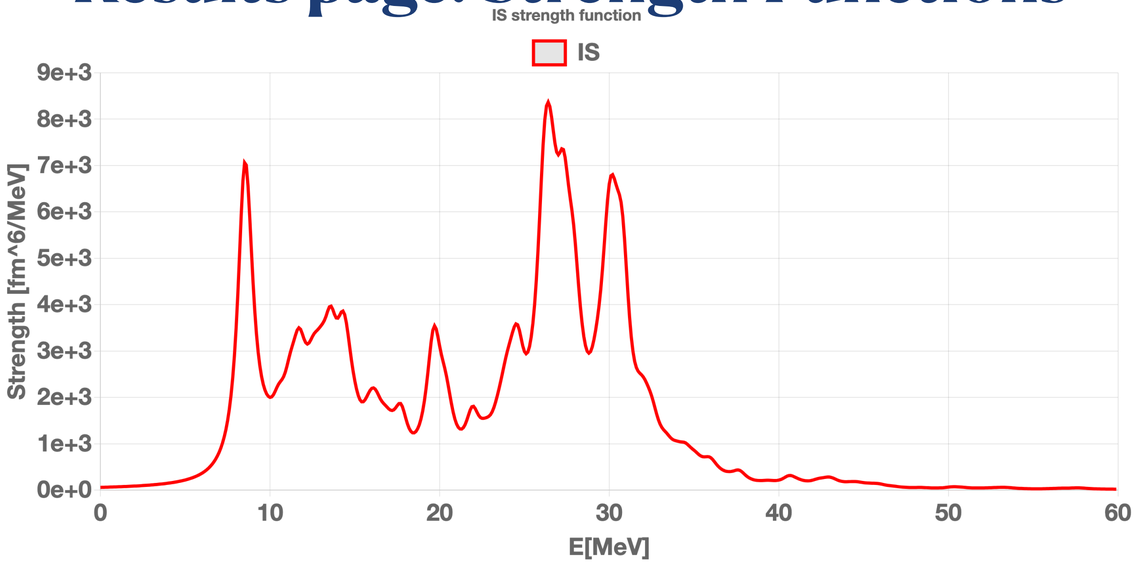
1* Hartree Fock (HF) plus Random Phase Approximation (RPA)

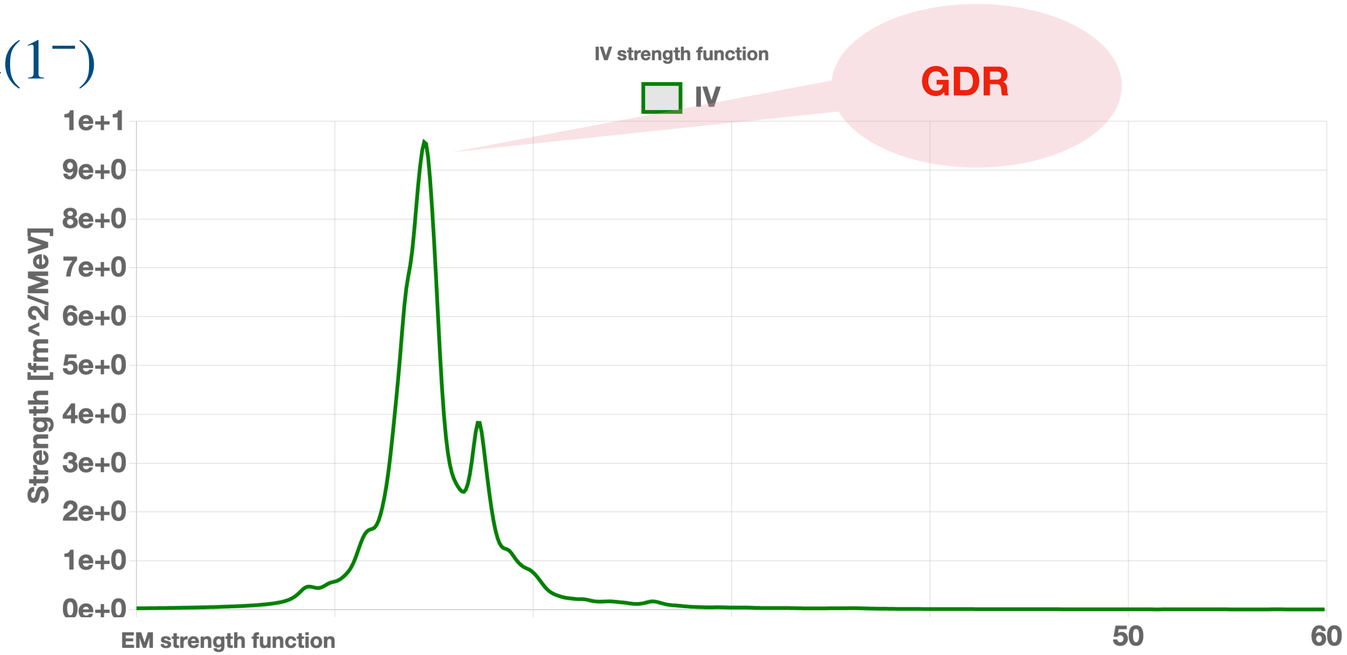
- **Results page: Density Distribution** ^{132}Sn



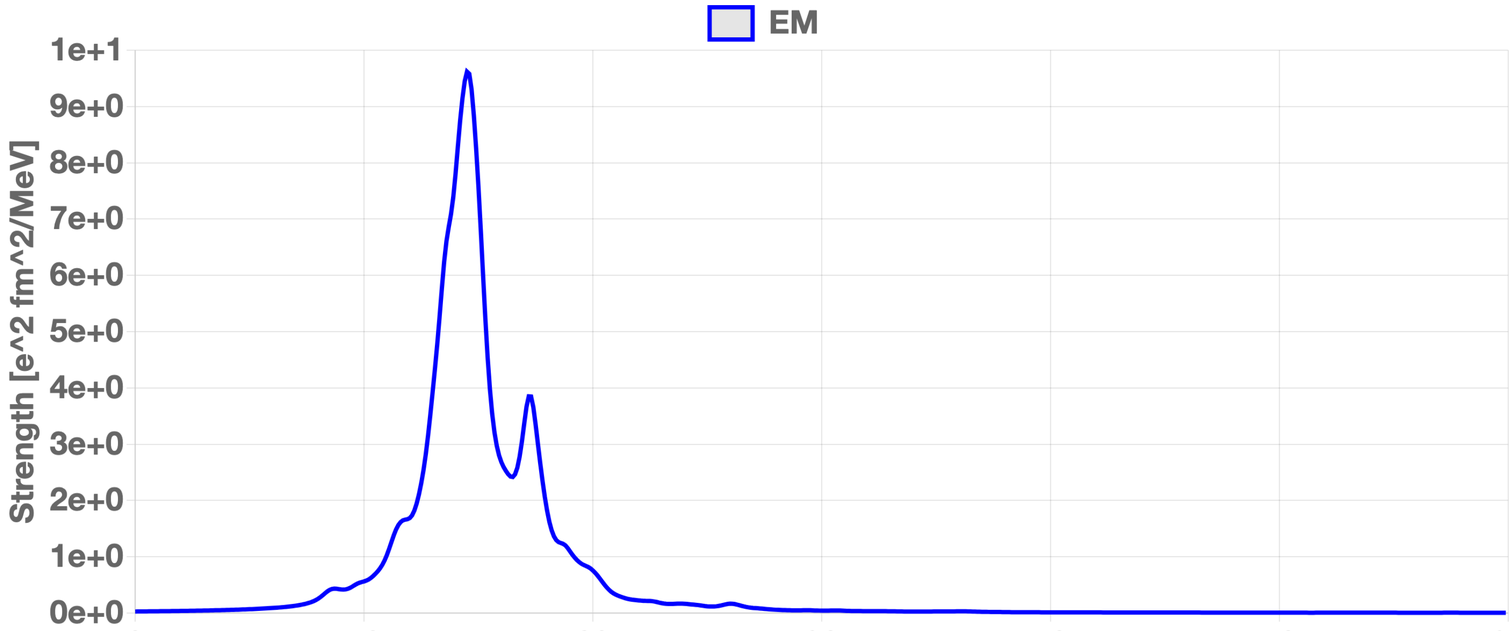
1* Hartree Fock (HF) plus Random Phase Approximation (RPA)

Results page: Strength Functions $^{132}Sn(1^-)$





Computed Strength Functions



2* HF_Bardeen_Cooper_Schrieffer-Quasiparticle RPA (HFBCS-QRPA)

HFBCS-QRPA

- Combines **HF-BCS** for ground state + **QRPA** for excited states.
- Designed for even-even, spherical nuclei, open-shell nuclei.
- Accounts for pairing correlations.
- Inputs and interface similar to HF-RPA, with **additional pairing parameters.**

2* HF_Bardeen_Cooper_Schrieffer-Quasiparticle RPA (HFBCS-QRPA)

Input Interface

Input Parameters for *hfbcs-qrpa* calculation

To perform the hfbcs-qrpa calculation, please enter the parameter values for the system under study

Example:
$^{120}Sn(2^{+})$

Mass Number: 120

Atomic Number: 50

Skyrme Interaction: SKM*

Spin: 2

Parity : +1

Proton BCS: 0

Neutron BCS: 1

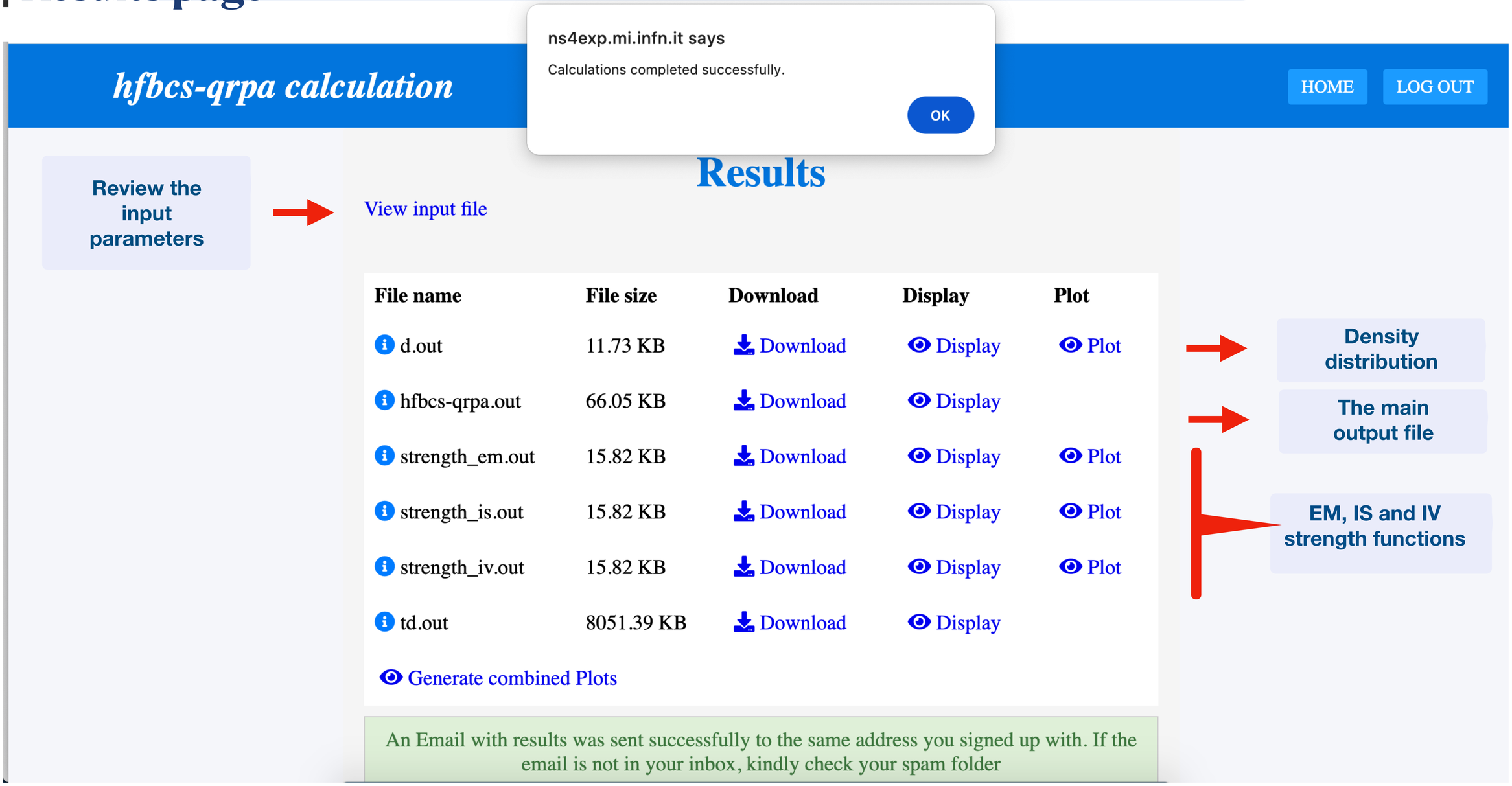
BCS Pairing

Can be modified if needed for specific cases

Default Parameters

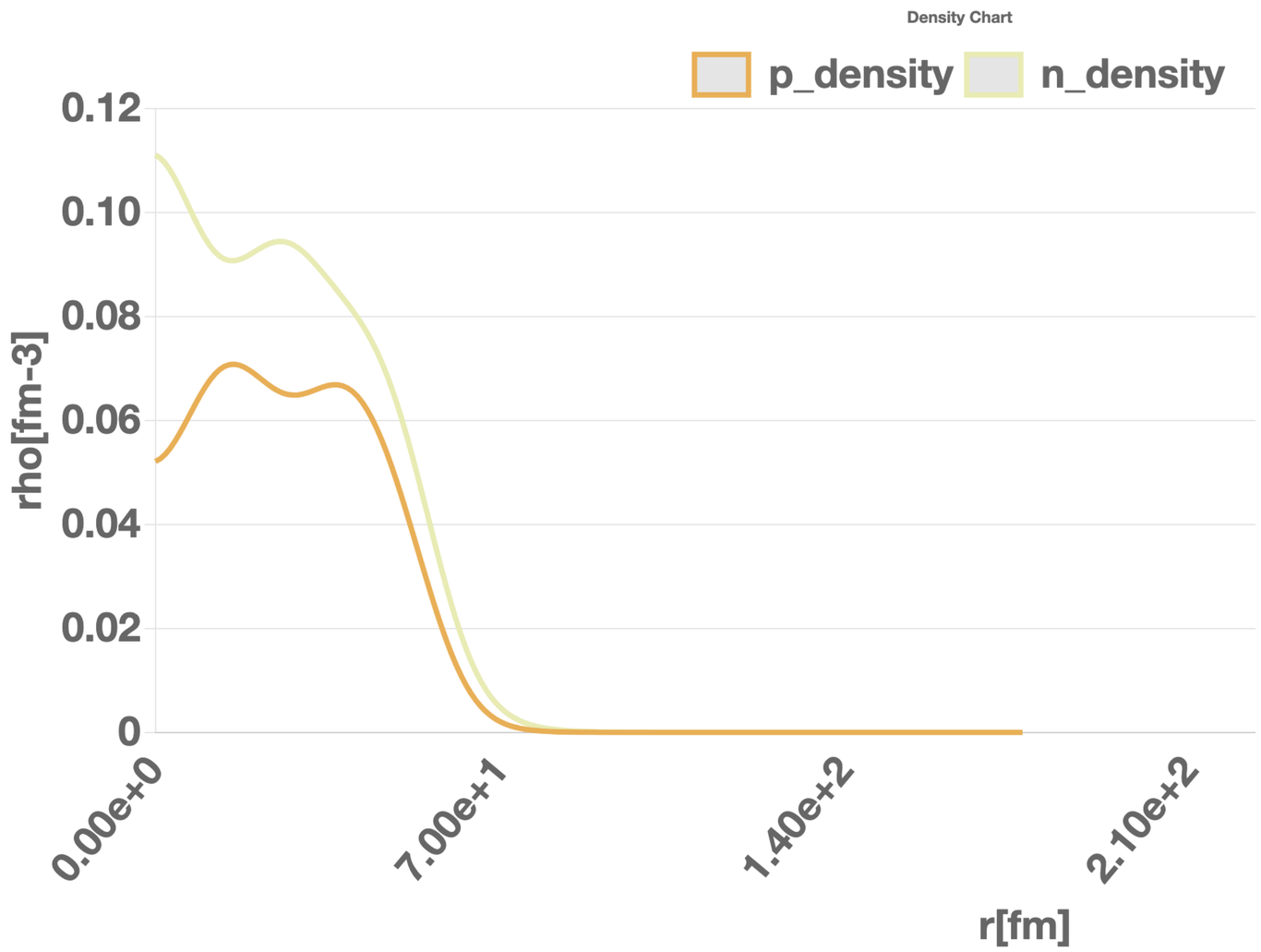
2* HF_Bardeen_Cooper_Schrieffer-Quasiparticle RPA (HFBCS-QRPA)

Results page



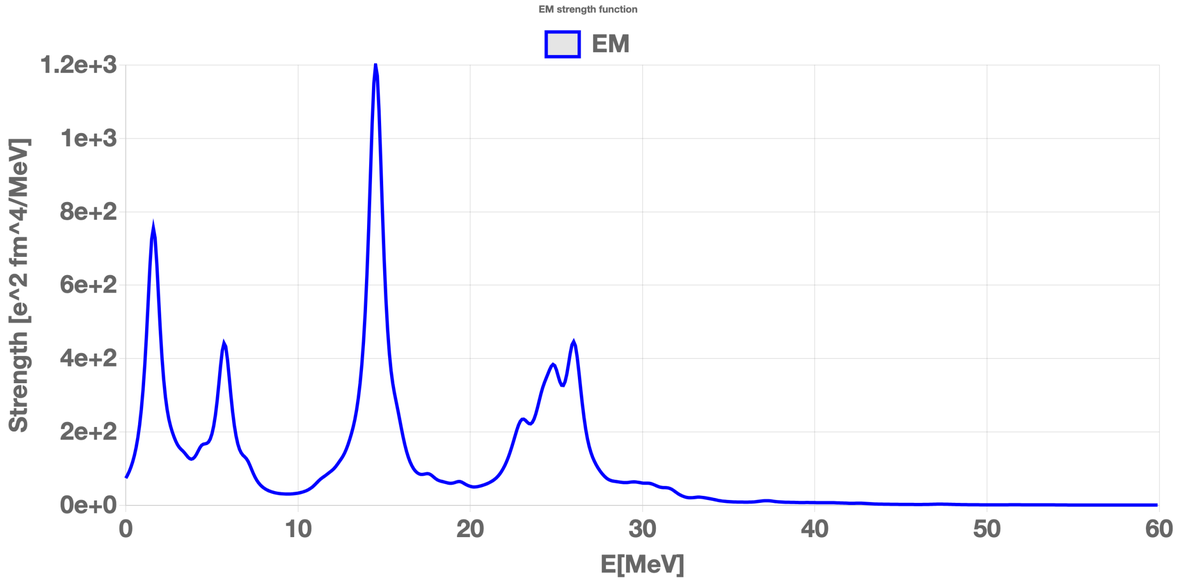
2* HF_Bardeen_Cooper_Schrieffer-Quasiparticle RPA (HFBCS-QRPA)

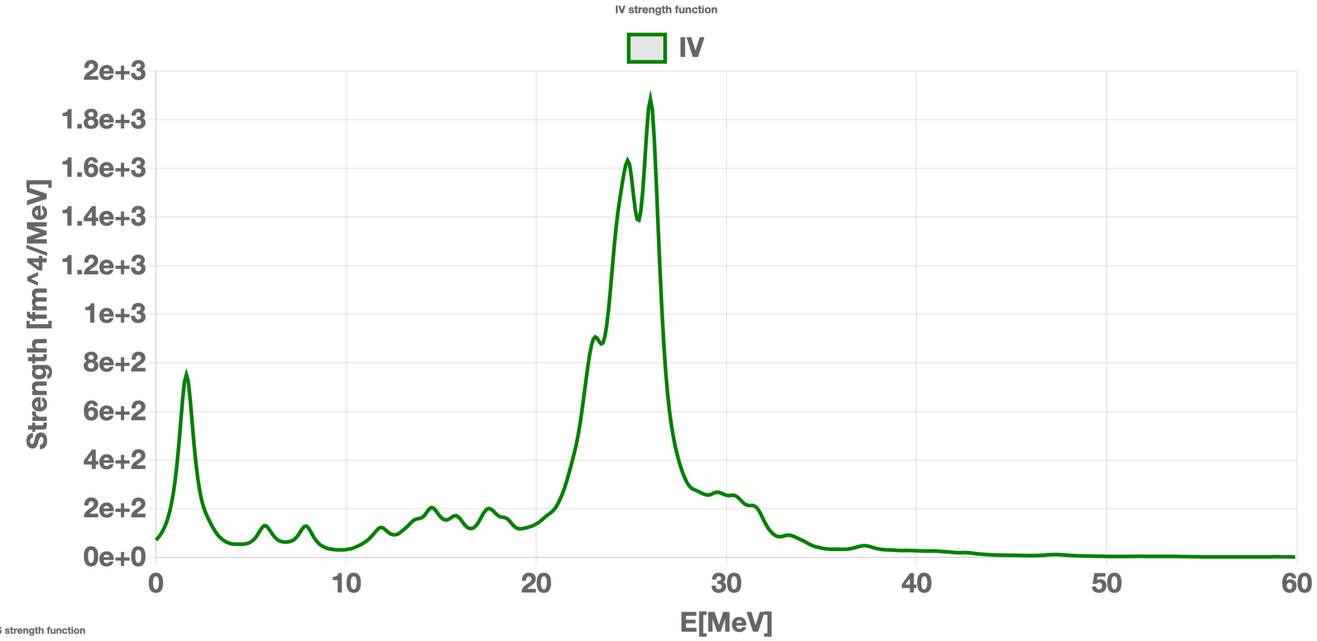
Results page: Density Distribution ^{120}Sn

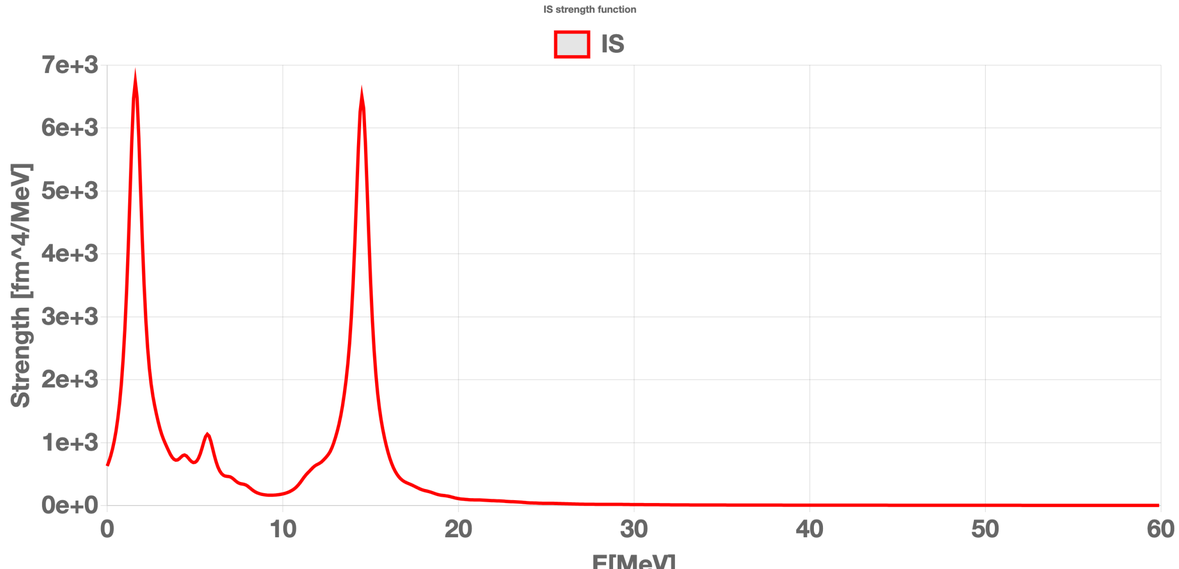


2* HF_Bardeen_Cooper_Schrieffer-Quasiparticle RPA (HFBCS-QRPA)

Results page: Strength Functions $^{120}Sn(2^+)$

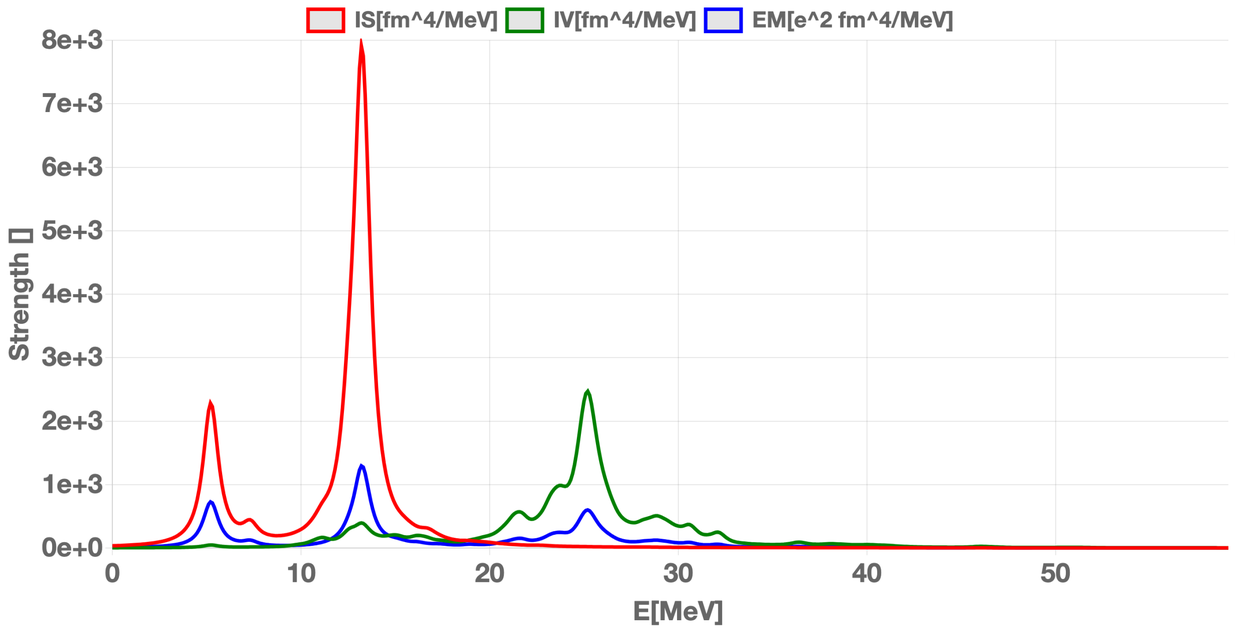




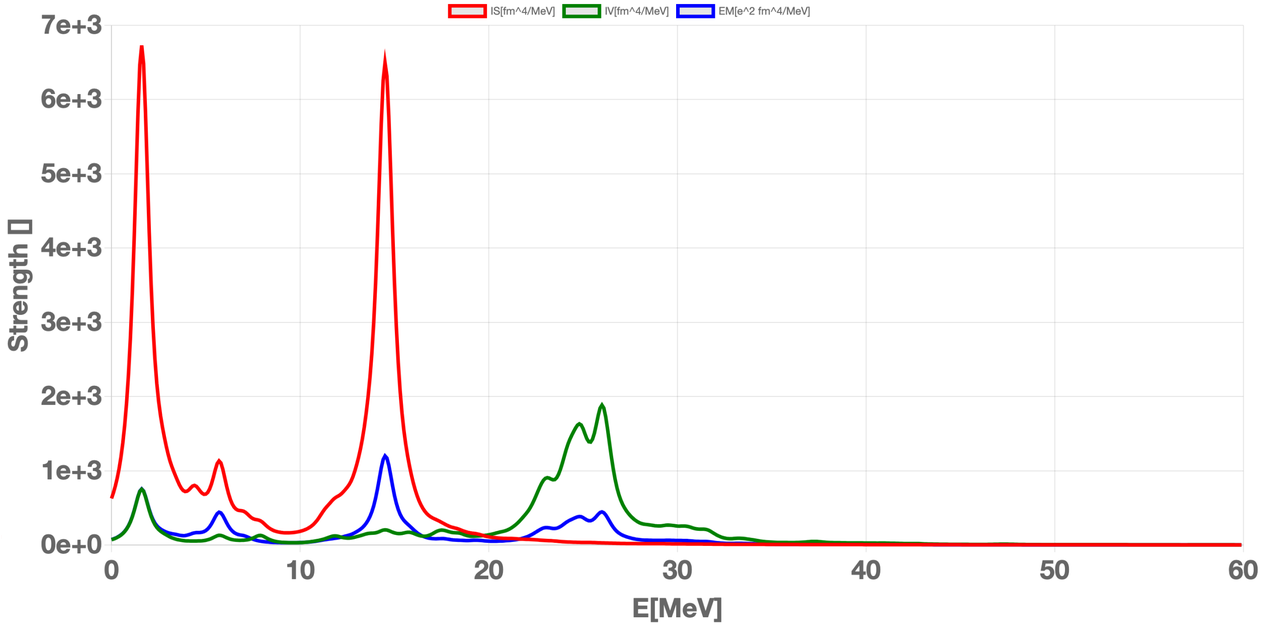


Effect of Pairing: RPA vs QRPA Strength Functions $^{120}Sn(2^+)$

HF-RPA



HFBCS-QRPA



3* KSHELL code

Kshell Code

- Developed by N. Shimizu and collaborators at the University of Tsukuba.
- Performs **nuclear shell model** calculations using two-body interaction.
- Captures detailed nuclear structure:
  - Energy levels.
  - E2/M1 transitions probabilities.
  - Magnetic/Quadrupole moments.

3* KSHELL code

Input Interface

Shell model calculations with KSHELL code

HOME LOG OUT

Selection of the interaction

Please, enter the proton and neutron number for the system under study

Number of Protons: 14

Number of Neutrons: 14

Example: ^{28}Si

Calculate

3* KSHELL code

Input Interface

Result of the interaction:

```
SM calculation for 28Si
number of valence protons 6
number of valence neutrons 6
Core nucleus 160
```

Effective Interactions:

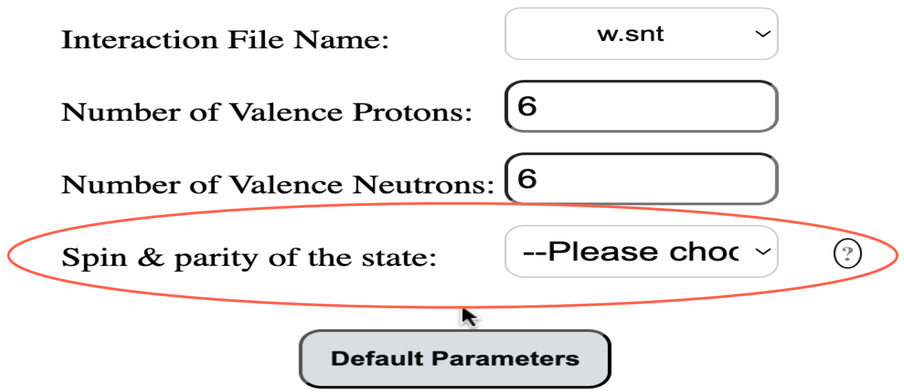
w.snt (Click to view reference) ▼

usda.snt (Click to view reference) ▼

usdb.snt (Click to view reference) ▼

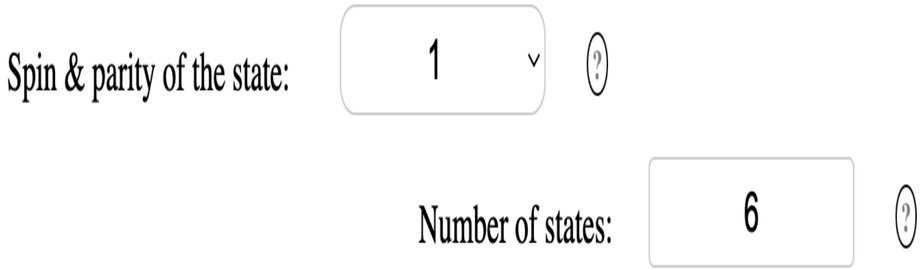
Input Parameters for *KSHELL calculation*

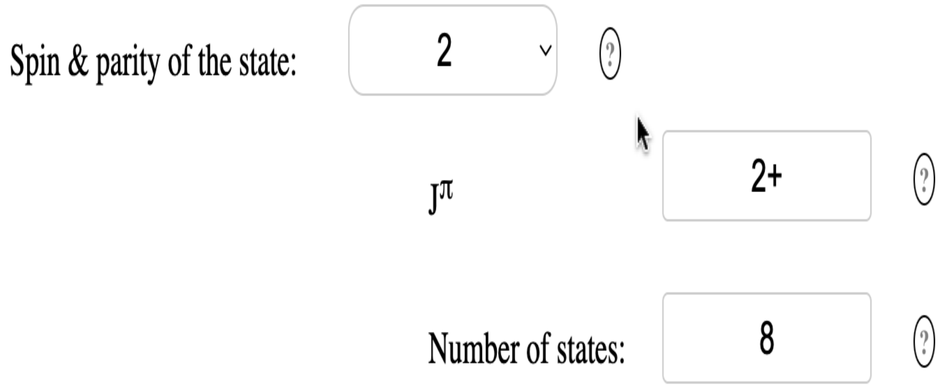
To perform the *KSHELL* calculation, please enter the parameter values for the system under study:



3* KSHELL code

Input Interface: Spin & Parity





Option 1: Automatic selection of lowest-energy states

- Specify the **total number of states** to compute.
- Example inputs:
  - `+10` → First 10 **positive-parity** states
  - `-10` → First 10 **negative-parity** states
  - `10` → First 10 **states of any parity**

☑ Use this when you're interested in the lowest states, regardless of spin

Option 2: Manual selection

- Angular momenta list ($0^+,2^+,4^+$)
- Number of states for each J^π (2,3,6)

☑ Use this when you want specific angular momentum/parity combinations

3* KSHELL code

Input Interface

Default Parameters

Proton effective charge for E2:	1
Neutron effective charge for E2:	0
g_l^p factor for M1:	1,0
g_l^n factor for M1:	0,0
g_s^p factor for M1:	5,586
g_s^n factor for M1:	-3,826
Transition probabilities:	N

By default, electromagnetic transitions are not calculated

3* KSHELL code

Results page

Shell model calculations with KSHELL code

HOME | LOG OUT

Results

File name	File size	Download	Display
save_input_ui.txt	0.07 KB	Download	Display
summary_Si28_w.txt	1.69 KB	Download	Display
log_Si28_w_m0p.txt	20.68 KB	Download	Display
log_Si28_w_tr_m0p_m0p.txt	7.17 KB	Download	Display
w.snt	6.21 KB	Download	Display

Main Output

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

3* KSHELL code

- **KSHELL Output Comparison: Option 1 vs. Option 2 (Energy levels+Transitions)** ^{28}Si

Option 1: Lowest-energy states (6)

Energy levels

N	J prty	N_Jp	T	E(MeV)	Ex(MeV)	log-file
1	0 +	1	0	-135.938	0.000	log_Si28_w_m0p.txt
2	2 +	1	0	-133.950	1.987	log_Si28_w_m0p.txt
3	4 +	1	0	-131.279	4.659	log_Si28_w_m0p.txt
4	0 +	2	0	-130.927	5.011	log_Si28_w_m0p.txt
5	3 +	1	0	-129.771	6.167	log_Si28_w_m0p.txt
6	4 +	2	0	-128.901	7.037	log_Si28_w_m0p.txt

B(E2) (> -0.0 W.u.) mass = 28 1 W.u. = 5.1 e^2 fm^4 e^2 fm^4 (W.u.)

J_i	Ex_i	J_f	Ex_f	dE	B(E2)->	B(E2)<-
2+(1)	1.988	0+(1)	0.000	1.987	25.0(4.9)	124.9(24.7)
4+(1)	4.659	2+(1)	1.988	2.671	35.4(7.0)	63.6(12.6)
0+(2)	5.011	2+(1)	1.988	3.024	21.0(4.2)	4.2(0.8)
3+(1)	6.167	2+(1)	1.988	4.180	0.0(0.0)	0.0(0.0)
3+(1)	6.167	4+(1)	4.659	1.509	2.0(0.4)	1.6(0.3)
4+(2)	7.037	2+(1)	1.988	5.050	2.5(0.5)	4.5(0.9)
4+(2)	7.037	4+(1)	4.659	2.378	1.9(0.4)	1.9(0.4)
4+(2)	7.037	3+(1)	6.167	0.870	24.7(4.9)	31.8(6.3)

Option 2: Fixed J^{π} (2^{+},8)

Energy levels

N	J prty	N_Jp	T	E(MeV)	Ex(MeV)	log-file
1	2 +	1	0	-133.950	0.000	log_Si28_w_j4p.txt
2	2 +	2	0	-128.415	5.535	log_Si28_w_j4p.txt
3	2 +	3	0	-128.032	5.919	log_Si28_w_j4p.txt
4	2 +	4	0	-127.481	6.470	log_Si28_w_j4p.txt
5	2 +	5	0	-127.270	6.681	log_Si28_w_j4p.txt
6	2 +	6	1	-126.492	7.458	log_Si28_w_j4p.txt
7	2 +	7	0	-126.145	7.805	log_Si28_w_j4p.txt
8	2 +	8	0	-125.249	8.702	log_Si28_w_j4p.txt

B(E2) (> -0.0 W.u.) mass = 28 1 W.u. = 5.1 e^2 fm^4 e^2 fm^4 (W.u.)

J_i	Ex_i	J_f	Ex_f	dE	B(E2)->	B(E2)<-
2+(2)	5.535	2+(1)	0.000	5.535	3.4(0.7)	3.4(0.7)
2+(3)	5.918	2+(1)	0.000	5.919	1.7(0.3)	1.7(0.3)
2+(3)	5.918	2+(2)	5.535	0.384	0.3(0.1)	0.3(0.1)
2+(4)	6.469	2+(1)	0.000	6.470	0.3(0.1)	0.3(0.1)
2+(4)	6.469	2+(2)	5.535	0.935	0.2(0.0)	0.2(0.0)
2+(4)	6.469	2+(3)	5.918	0.551	7.8(1.5)	7.8(1.5)
2+(5)	6.680	2+(1)	0.000	6.681	0.0(0.0)	0.0(0.0)
2+(5)	6.680	2+(2)	5.535	1.146	4.2(0.8)	4.2(0.8)
2+(5)	6.680	2+(3)	5.918	0.762	2.2(0.4)	2.2(0.4)
2+(5)	6.680	2+(4)	6.469	0.211	3.7(0.7)	3.7(0.7)
2+(6)	7.458	2+(1)	0.000	7.458	0.5(0.1)	0.5(0.1)
2+(6)	7.458	2+(2)	5.535	1.923	0.8(0.2)	0.8(0.2)

Conclusion

- **Structure4Exp** provides access to three specialized codes for nuclear structure studies:
  - *HF-RPA* for closed-shell systems
  - *HFBCS-QRPA* for open-shell nuclei with pairing
  - *KSHELL* for full shell-model calculations
- The platform is user-friendly and designed to support experimental and theoretical work.
- Structure4Exp bridges the gap between **nuclear theory** and **experimental applications**.

Thank you for your attention