Atomic Data Calculations and their application in Kilonovae Modeling

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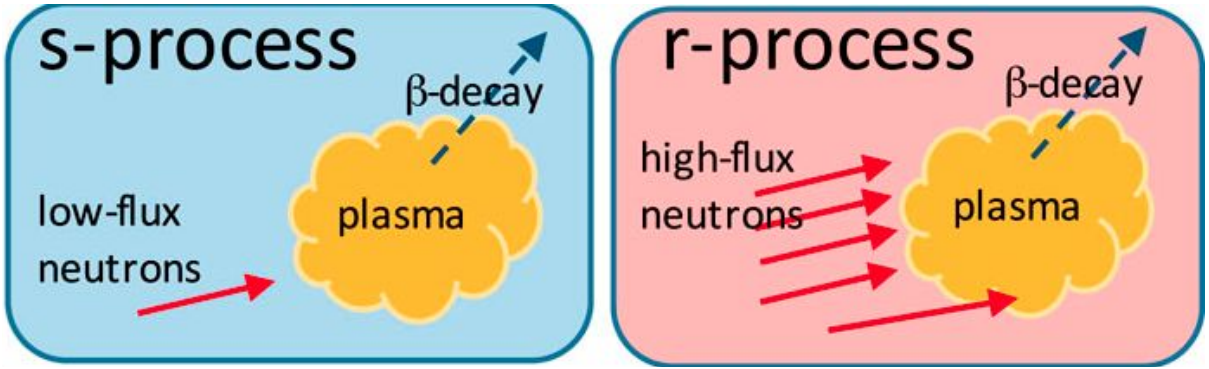
Introduction

- The r and s processes;

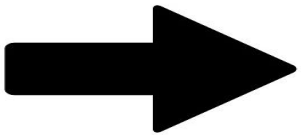


Source: S. N. Chen et al, Extreme brightness laser-based neutron pulses as a pathway for investigating nucleosynthesis in the laboratory, Matter and Radiation at Extremes, 2019

- Atomic data calculations for lanthanides and actinides;

The Atomic Code and the Potential of Interaction

- Why do we use the FAC code?
- The Potential of Interaction, $\mathcal{V}(n_1, n_2, ..., n_k)$, depends on the k weights of the orbitals, n ,considered;



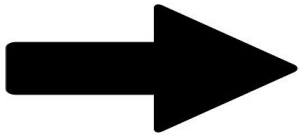
The Problem: find the weights, n , that give the FAC's results for the energy levels as close as possible to NIST's experimental data

My solution:

Function(Input Data)

- It runs FAC with the weight of each orbital given as Input Data;
- It compares the result from the simulation with NIST Data;

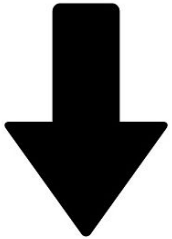
It returns the absolute energy difference between NIST and FAC data;



The new problem: find the minimum of this Function

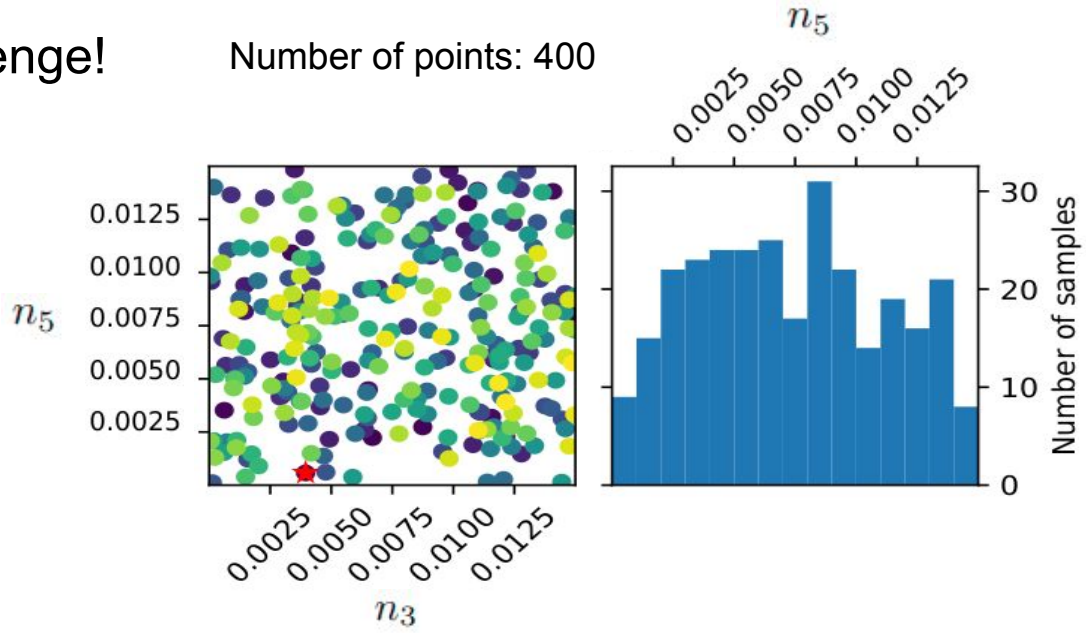
Minimization of the Function

Its minimization is quite a challenge!

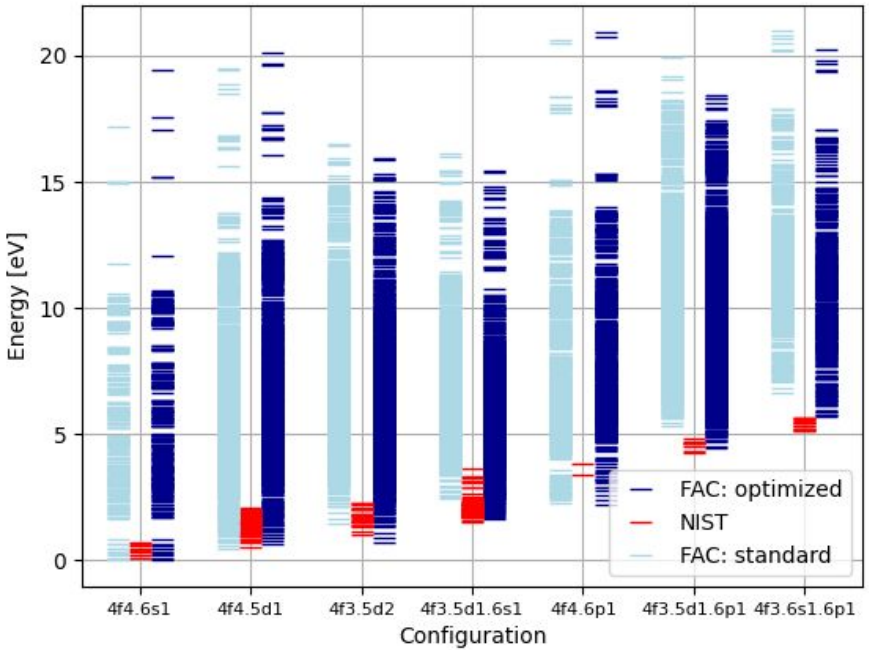


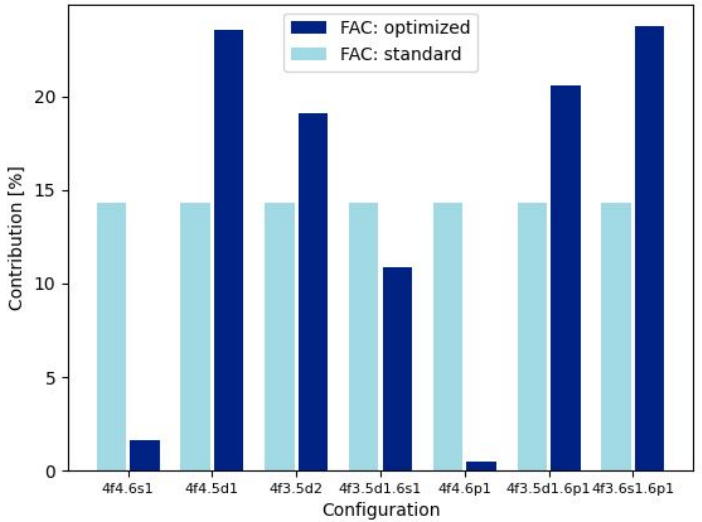
`skopt`.forest_minimize

Number of points: 400

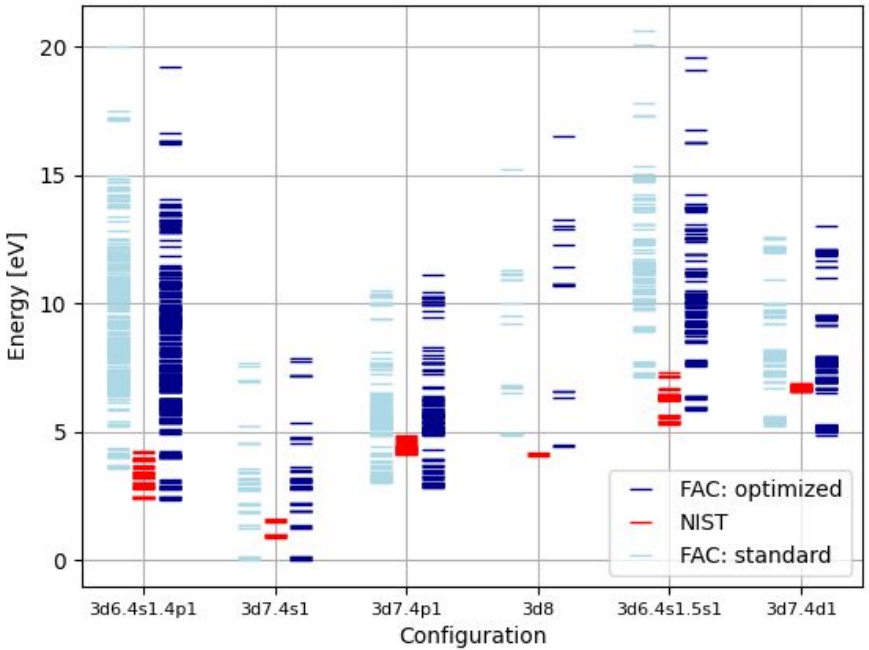


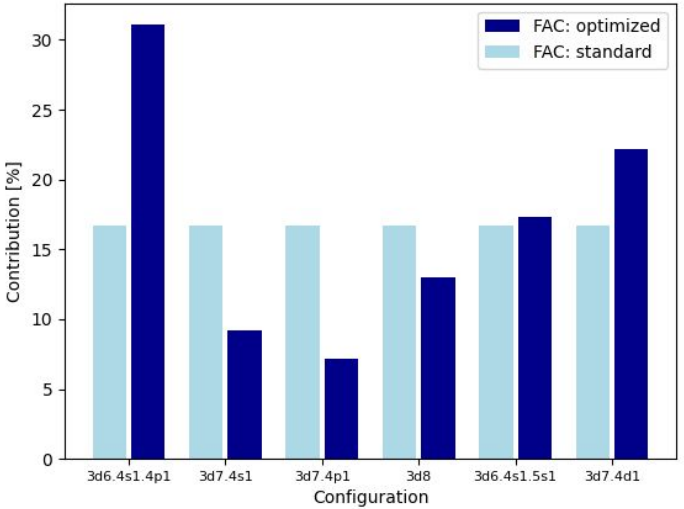
Nd II results:





Fe I results:


Energy [eV]
20
15
10
5
0
3d6.4s1.4p1
3d7.4s1
3d7.4p1
3d8
3d6.4s1.5s1
3d7.4d1
Configuration
FAC: optimized
NIST
FAC: standard


Contribution [%]
30
25
20
15
10
5
0
3d6.4s1.4p1
3d7.4s1
3d7.4p1
3d8
3d6.4s1.5s1
3d7.4d1
Configuration
FAC: optimized
FAC: standard

Conclusion

- There is a significant improvement in the optimized results: 55% in the case of Nd II and 27% in the Fe ‘s case;

- The sequential model-based algorithms are adequate for minimization of the Function;

Thanks for your attention!