Exploration of High-Dimensional Nuclei Data

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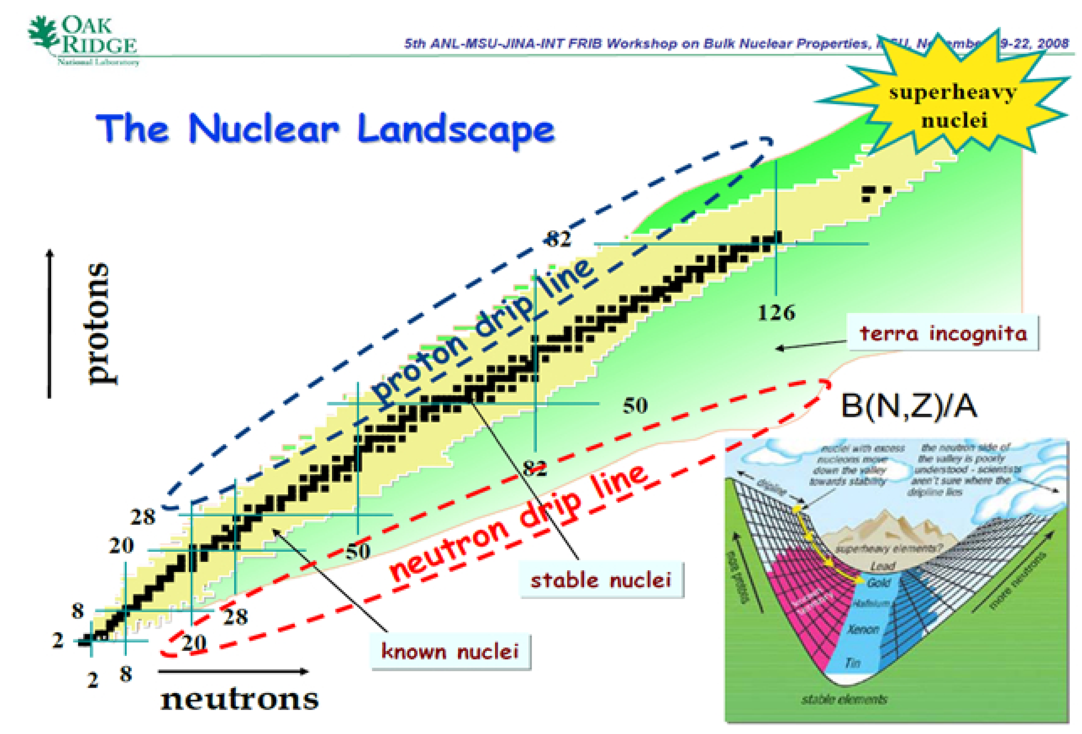
http://wiki.ornl.gov/sites/rams09/f_fuentes_delgado

Introduction

One of the goals of nuclear science is formulating a comprehensive description of all nuclei and their properties. Density Functional Theory (DFT) is an attractive approach due to its broad ranging reach of the entire mass table. DFT provides the theoretical foundation for a self-consistent mean-field description of the nucleus in terms of one-body densities and currents. The task is to construct a universal functional whose input is the proton and neutron densities and currents, and whose output yields the ground-state energy and other properties of the nucleus.



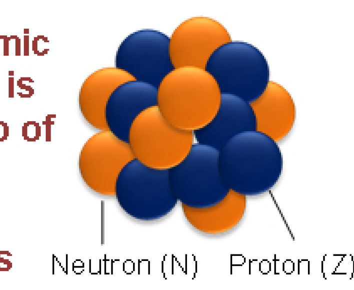


Figure 1. Chart of Nuclides: stable nuclei represented by the black squares and known nuclei in the yellow region [2]. There are ~3,000 known nuclei and roughly 6,000-8,000 yet to be discovered in the *terra incognita*.

Background

Determining the optimal density functional requires extensive computations of properties of several thousand nuclei. Discovering relationships between observables, for thousands of nuclei, over many functionals requires high-level data analysis techniques.

- 7000+ nuclei in the dataset
- 51 parameters/dimensions describing each nuclei

Results

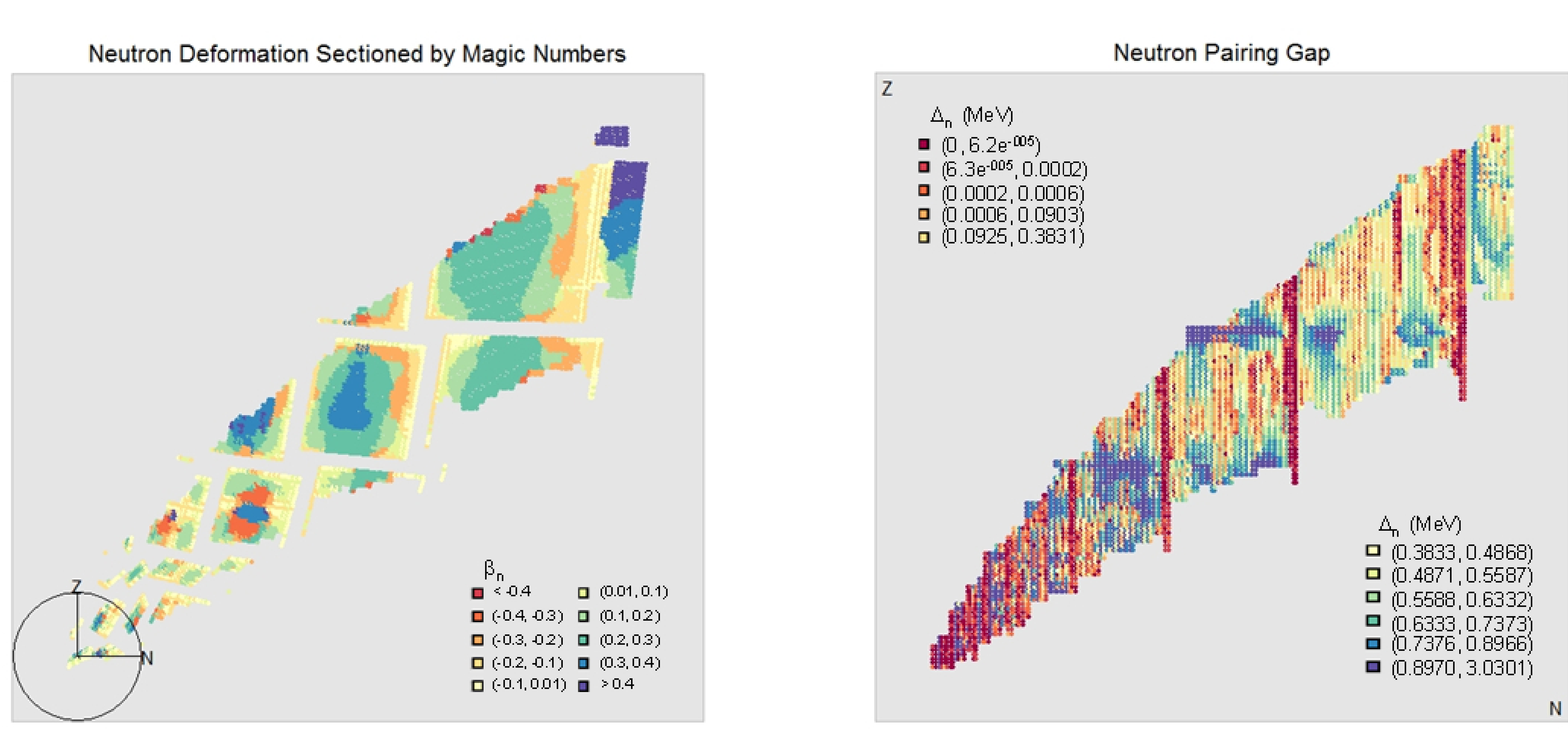


Figure 4. Visualization techniques to find correlations.

Correlation between neutron pairing gap energy and neutron quadruple deformation

- β_n = neutron quadrupole deformation
  $\beta_n < 0$ oblate, $\beta_n > 0$ prolate
  $\beta_n = 0$ sphere
- Δ_n= neutron pairing gap energy
  Coupling energy for an unpaired neutron

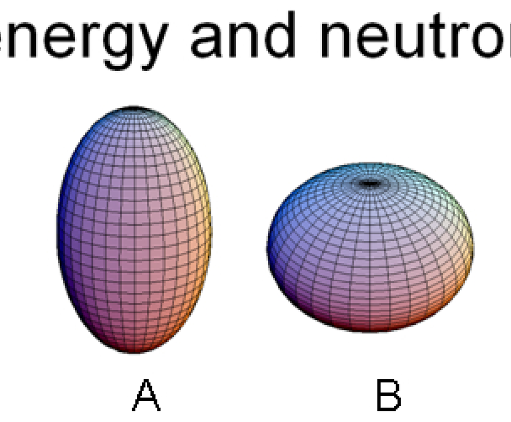


Figure 5. Deformation Shapes: (A) Prolate, (B) Oblate

Methods of Analysis

- Data projected and analyzed using:
  - **GGobi**, open source visualization program for exploring high-dimensional data
  - **R**, software environment for statistical computing
- Relationships between observables hidden in higher dimensions
- Universal functional that can predict nuclear properties

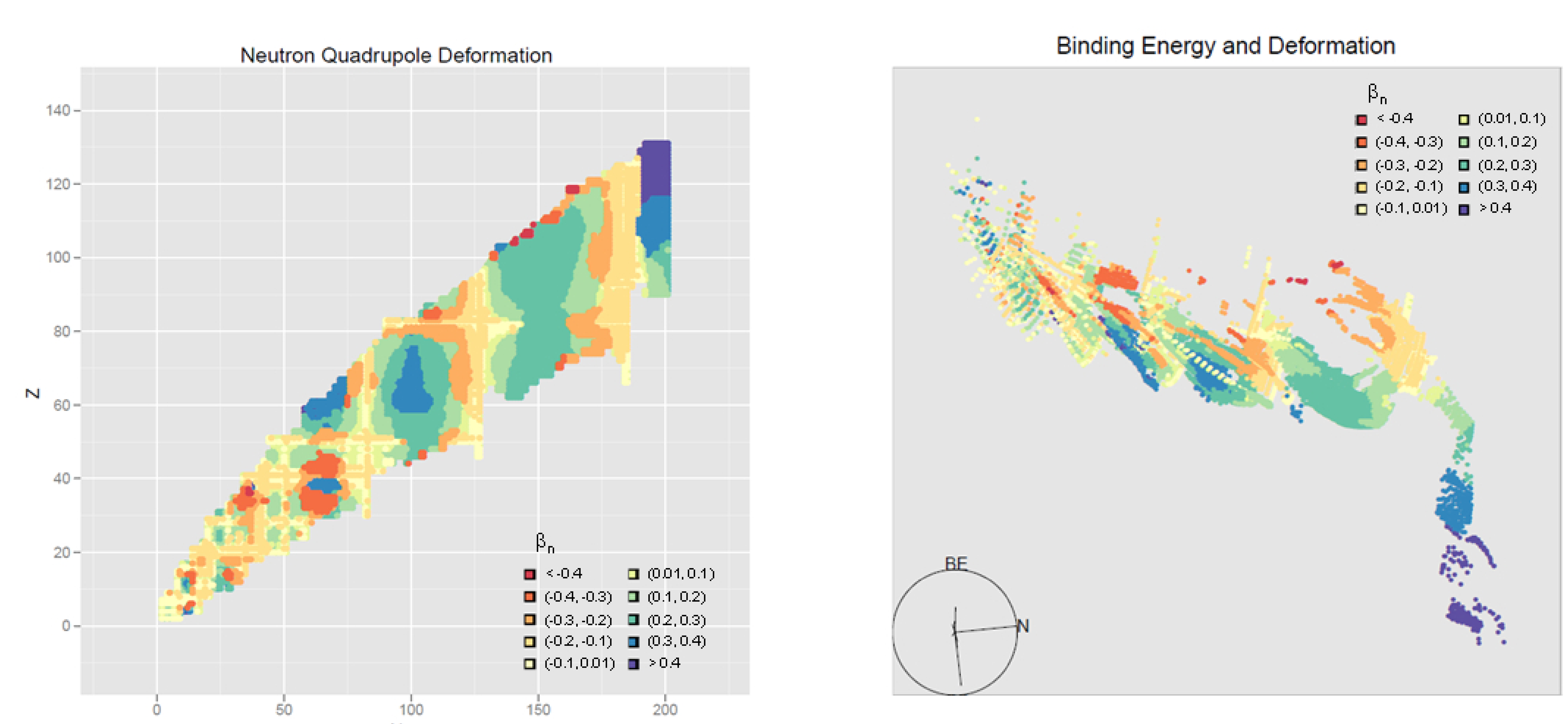


Figure 2. Neutron Deformation colored in different visualization plots.

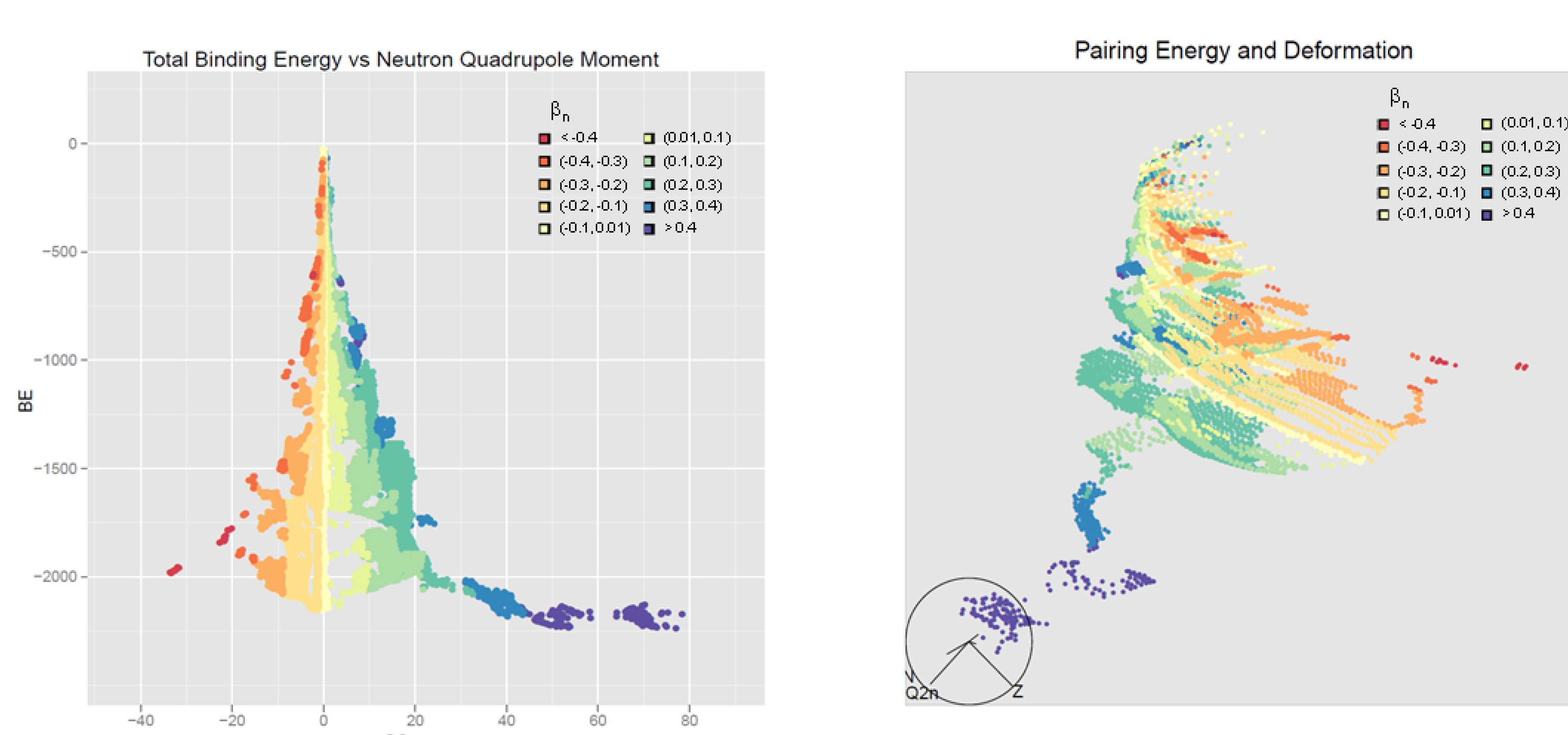


Figure 3. Deformation of the nuclei patterns explored in different parameter combinations.

Conclusion

Using methods for dimension reduction and visualization tools, it is hypothesized that the neutron quadrupole deformation is related to the neutron pairing gap energy. The relationship discovered is a step closer to defining a universal density functional.

References

• D.J. Dean, "Beyond the nuclear shell model," *Physics Today*, pp. 48-53, November 2007.
• M. Stoitsov, "Large-Scale Mass Table Calculations", 5th ANL-MSU-JINA-INT FRIB Workshop on Bulk Nuclear Properties, MSU, November 19-22, 2008.

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