Exploration of High-Dimensional Nuclei Data

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***Abstract*—Density Functional Theory (DFT) provides the theoretical foundation for a self-consistent mean-field description of the nucleus in terms of one-body densities and currents. The idea is to construct a 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. Extensive computations of ground-state energies and other observable properties of several thousand nuclei are required in order to find a universal functional that covers the entire chart of nuclei. The analysis looks for hidden relationships between observables to determine a functional that can reliably predict nuclear properties in regions where no experimental data exist. Using methods for dimension reduction and visualization tools, it is hypothesized that the deformation of the neutrons is related to other characteristics of the nuclei. The discovered relationships with the deformation of the neutrons take us a step closer toward the universal functional.**

Keywords-Density Functional Theory; Neutron Pairing Gap; Neutron Quadrupole Deformation; Universal Functional

I. INTRODUCTION

The nucleus of an atom is a dense region at the center of an atom that consists of protons and neutrons. Nuclei, the fuel that burns in stars, make up 99.9% of all baryonic matter in the universe [1]. The nuclear forces among protons and neutrons generate a broad range of nuclear phenomena.

Nuclei with ratios of neutron to proton number much larger or much smaller than those found in nature are called exotic or rare and are difficult to produce experimentally. The proposed Facility for Rare-Isotope Beams (FRIB) in the US [2], along with other new generations of rare isotope facilities hold the key to unlock more information about nuclei production.

On the theoretical side, new computational tools are enabling a clearer vision of nuclei with increasing precision. These tools pave the path to move from a qualitative to a quantitative understanding of all nuclei.

The Nuclear Landscape presented in Figure 1 shows the stable nuclei represented by the black squares and known nuclei in the yellow region. Some 270 of the isotopes are stable. About 2000 isotopes have been measured, but a large number, perhaps as many as 4000, have not been studied in experiment [4].

Density Functional Theory (DFT) is a quantum mechanical theory used in physics to investigate the ground state of many-body systems. With this theory, the properties of a system can be determined by using functionals, i.e. functions of another function.

One of the goals of nuclear science is formulating a comprehensive description of all nuclei and their properties. 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.

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.

II. ANALYSIS PROCEDURE

Defining a universal energy functional requires computation of ground-state energies and of other observable properties in the nuclear landscape [5]. For this research, the data utilized is the result of extensive computations on supercomputers. The results of different algorithms to interpret the density functional provided multiple datasets for this work. The SLY4 functional without Lipkin-Nogami (SLY4_NO_LN) dataset was used in order to analyze the different parameters of the nuclei. The dataset was formatted into a comma separated value (CSV) file in order to be used by analysis and visualization programs. Some of the parameters described by the dataset are shown in Table 1.

In order to take a multivariate look at the dataset and its parameters, the program GGobi was utilized. GGobi is an open source visualization program for exploring high-dimensional data. It provides highly dynamic and interactive graphics such as tours, as well as familiar graphics such as

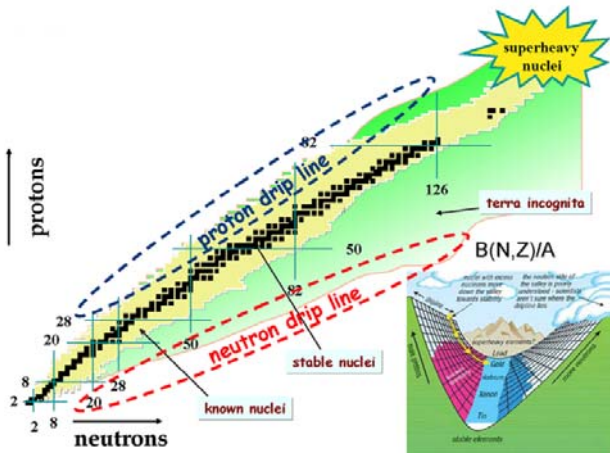

Figure 1. Chart of Nuclides [3].

A	Number of particles (A=N+Z)	DELTAn	Neutron pairing gap
N	Number of neutrons	DELTAp	Proton pairing gap
Z	Number of protons	Rt	Total rms radius
LHLn	Quantum Numbers: neutrons	Rn	Neutron rms radius
LHLp	Quantum Numbers: protons	Rp	Proton rms radius
BEA	Binding energy per particle (BE/A)	Rc	Charge rms radius
BE	Total Binding energy	Ht	Total hexadecapole moment
betat	Total quadrupole deformation	Hn	Neutron hexadecapole moment
betan	Neutron quadrupole deformation	Hp	Proton hexadecapole moment
betap	Proton quadrupole deformation	EKINt	Total kinetic energy
Q2t	Total quadrupole moment	EKINn	Neutron kinetic energy
Q2n	Neutron quadrupole moment	EKINp	Proton kinetic energy
Q2p	Proton quadrupole moment	ESO	Total spin orbit energy
EFn	Neutron Fermi energy	ECDIR	Direct coulomb energy
EFp	Proton Fermi energy	ECEX	Exchange coulomb energy
EPAIRn	Neutron pairing energy	SN	Neutron separation energy
EPAIRp	Proton pairing energy	S2N	Two neutron separation energy

Table 1. Nuclei data parameters

scatter plots, bar charts, and parallel coordinate plots. Plots are interactive and linked with brushing and identification. After learning to use GGobi, the datasets were explored visually using several techniques.

A. Visualization

Brushing in GGobi allows us to color specific points, in this case nuclei, automatically or manually. Automatic Brushing colors a parameter using a specific color scheme and scale. This tool helps identify the changes in the parameters across the nuclear landscape in the dataset.

Different types of graphics are also available in GGobi. The usual scatter plot helps identify quick relationships between two nuclei parameters. Also used was the two dimensional tour. This type of graphic allows the user to see as many dimensions or parameters as needed with a minimum of three. The parameters are shown by using different projection values.

Another GGobi tool used was the subset option. This allows the user project a certain number of randomly selected points in the dataset. Since the dataset analyzed contains approximately 7000 nuclei, when all the points are displayed the computer slows down considerably. By using a randomly sampled subset of the dataset it allows a faster exploration of the data while still showing the original patterns.

Shadowing, part of the GGobi tools, allows the diming of colors on a certain brushed colored field. Once shadowed, the user can exclude that field from the points displayed on the graph. This allows us to take a closer look at specific sections of the graph to see how it behaves. In this case, all nuclei of the selected section can be used without sampling.

Variable manipulation in GGobi shows valuable information about the dataset like the minimum, maximum, mean and median. More importantly it allows us to set limits on certain parameters. With the ability to set limits and shadow certain parts of the graph the user is able to explore the dataset thoroughly.

B. Exploration

Using GGobi and its tools the dataset was explored and familiarized. The next step in the research involved finding a parameter that correlates to the deformation of the neutron quadrupole deformation, which refers to the shape of the nuclei which varies in relation to how close to the magic number the nuclei are. When deformation is less than zero, its shape is prolate, stretched vertically. When deformation is more than zero, its shape is oblate, stretched horizontally

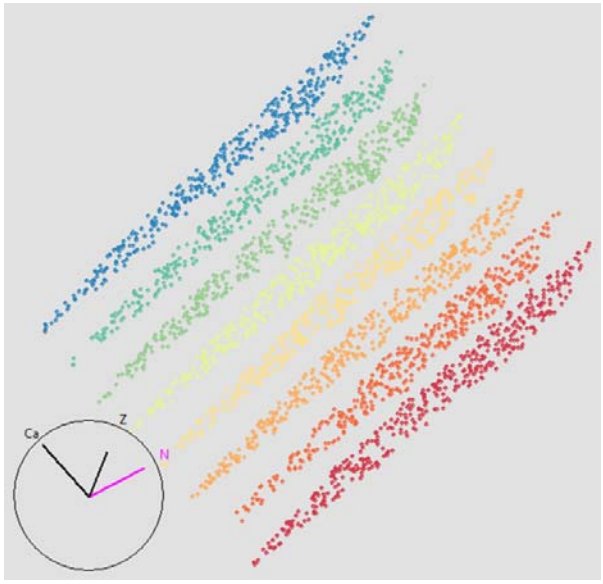

Figure 2. A GGobi Automatic Brushing. Example of automatic brushing on a spectral coloring scale by dataset using GGobi.

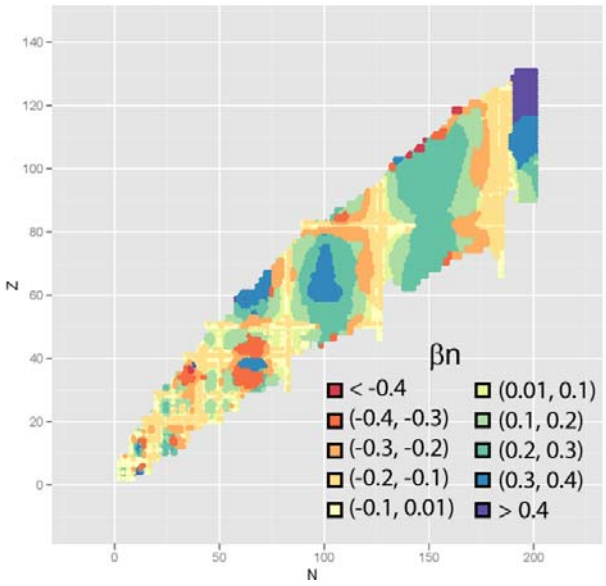

Figure 3. Neutron quadrupole deformation. Neutron vs. Proton scatter plot colored by deformation.

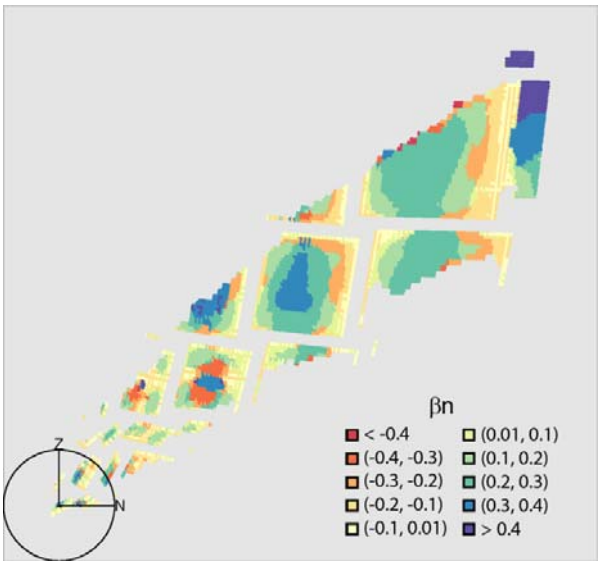

Figure 5. Neutron deformation sections. Neutron vs. Proton graph segmented by magic number region.

and when it is equal to zero it has a sphere shape.

In nuclear physics, the magic number is a number of nucleons (either protons or neutrons) such that they are arranged into complete shells within the atomic nucleus [6]. After visualizing the data with GGobi it was perceived that segmenting the dataset on their magic number regions would be beneficial to finding correlations. In order to section the dataset by magic number regions, four new parameters were introduced: The relative distance to the next magic number for neutrons and protons (NR and ZR) and the group number where the neutrons and protons belong in relation to its magic number (NMAGIC and ZMAGIC). With these new parameters in the dataset the graphs made by GGobi were able to visualize the regions formed by the magic numbers. Blending a small amount of the magic number variable into the projection of Figure 3 results in the pattern shown in Figure 5.

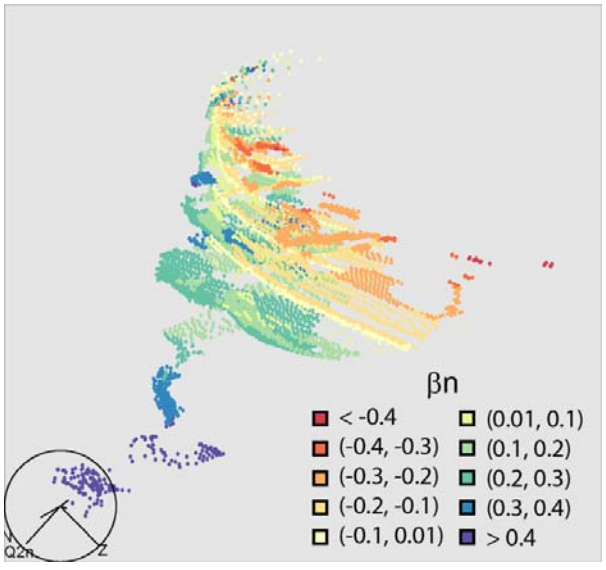

Figure 4. Pairing energy and deformation. Exploring in 2D Tour and coloring by deformation.

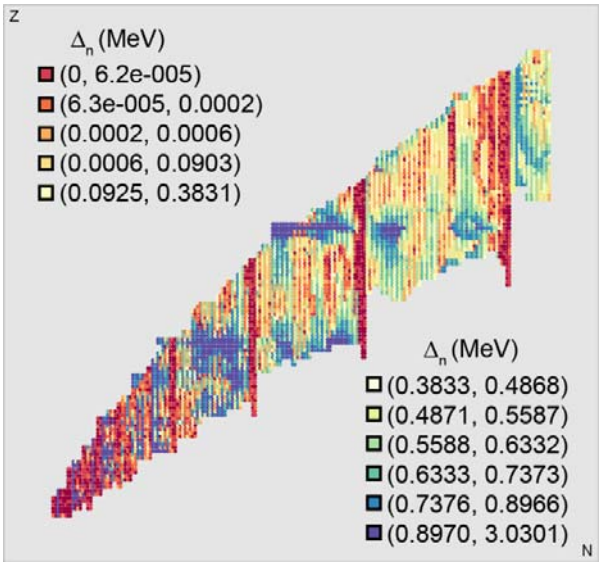

Figure 6. Neutron pairing gap. Neutron vs. Proton colored by the neutron pairing gap energy.

In order to modify and add the new parameters to the dataset, the R environment was used. R is a language and environment for statistical computing and graphics. This language was used in order to modify the datasets as needed, as well as graph plots like histograms and scatter plots for quick reference. The data was imported into R, modified, and exported into a CSV file for future reference.

C. Analysis

In order to combine R and GGobi, the package RGGobi for R was used. This package allows the control of GGobi functions through the R language. Function shortcuts were created to allow quick reproducibility of important coloring scales and plots of interest previously explored.

After thorough exploration an initial correlation was found between the neutron quadrupole deformation and the neutron pairing gap energy, shown in Figure 4. The correlation is in the phase pattern that both follow inside the magic number segmented regions. This is evident in the comparison of Figures 5 and 6.

III. CONCLUSION

Using methods for dimension reduction and visualization, the research was able to explore the nuclei data extensively. Using R, scripts of the coloring functions were prepared in order to easily replicate the important plots and color schemes that were discovered.

It is hypothesized that the neutron quadrupole deformation is related to the neutron pairing gap energy. This relationship was found by visual exploration of the data. For future work, this hypothesis needs to be analyzed and quantified.

The relationship discovered is a step toward defining a universal density functional. This functional will help understanding of the nuclei properties, particularly in the unknown regions of the nuclear landscape.

A more accurate description of nuclear properties can be beneficial in several areas in nuclear physics, for a better understanding of nuclear reactions. Also, the science-based stockpile stewardship will benefit from this knowledge. This will minimize the need to experiment with weapons because of understanding how the reactions of the nuclei in use behave.

Medical advances in radioactive therapy will also be possible through the knowledge of how the therapy tar-get will modify and change its structure thanks to understanding how nuclei behave and what their parameters are. Advanced fuel-cycle research for next generation nuclear reactors will also benefit. The US Department of Energy's Advanced Fuel Cycle Initiative will require wall-to-wall reactor-core simulations that, among other things, will have an impact on reactor safety and the economy.

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