# Nuclear Density Functional Theory Parameters Correlations

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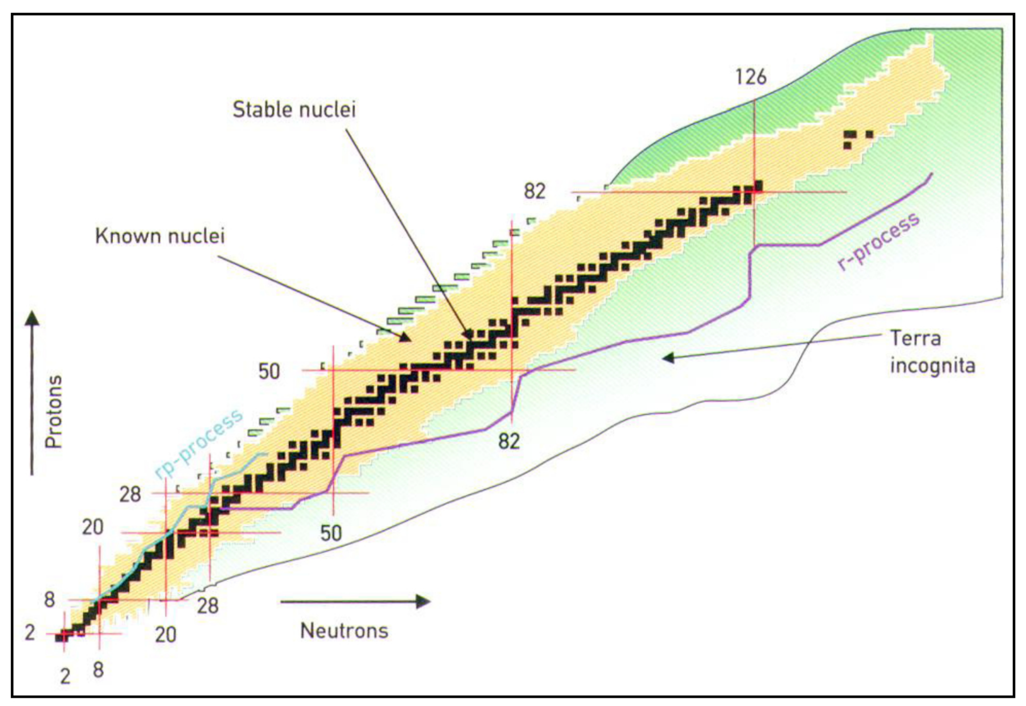
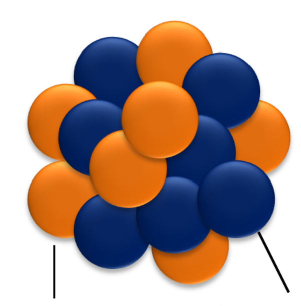
## Nuclear Landscape and DFT

A promising approach to understanding nuclear reactions and obtaining a predictive model lies in density functional theory (DFT). This theory provides the foundation for developing an energy functional which describes and predicts nuclear structure properties across the complete table of nuclides. Developing an optimal nuclear energy density functional (EDF) can render a better understanding of nuclei and how they react.



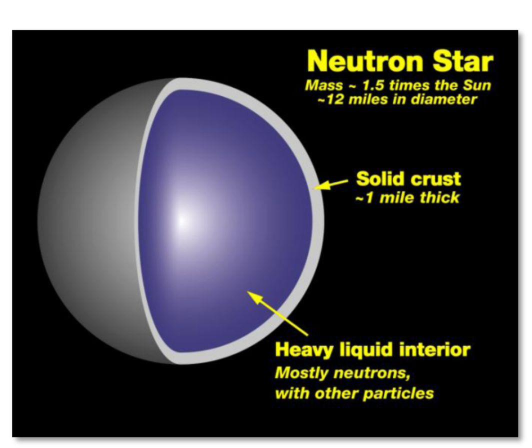




**The atomic nucleus is made up of protons and neutrons.**

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

The nuclear energy functionals currently in use have parameters that are fit to a subset of nuclei and their properties. EDFs rely on parameters that are fitted to experimental data and the use of different experimental data leads to different EDF parameterizations called forces. In a systematic effort to find an optimal EDF, the analysis explores the characteristics and correlations of the different force parameterizations. Specifically, the research investigates how these forces relate to infinite nuclear matter (INM) properties.

INM constitutes a huge number of proton and neutrons interacting by only nuclear forces where the volume and particle number are infinite but the ratio is finite. INM properties are necessary for describing systems such as neutron stars and are considered a useful system because it avoids the complications that arise from having to take into account the properties of a nuclear surface. However, since the surface parameters of finite nuclei are used in the optimization of the forces, it is of interest to see how these parameters indirectly affect the INM properties.




**A neutron star is a type of remnant that can result from the gravitational collapse of a massive star during a supernova event. Such stars are composed almost entirely of neutrons, which are subatomic particles without electrical charge and with slightly larger mass than protons.**

## Exploration and Analysis

Nuclei data are highly correlated and contain a large number of pairs to analyze. Visualizing their high-dimensional attributes in an ordinary display is difficult and segmentation occurs. The visualization display EVEREST overcomes this through its massive high resolution display capabilities. EVEREST, **E**xploratory **V**isualization **E**nvironment for **RE**search in **S**cience and **T**echnology, is capable of displaying 35 million pixels (11,520 by 3,072 ).

R, a software environment for statistical computing, was used to process the data and create the visualization images.

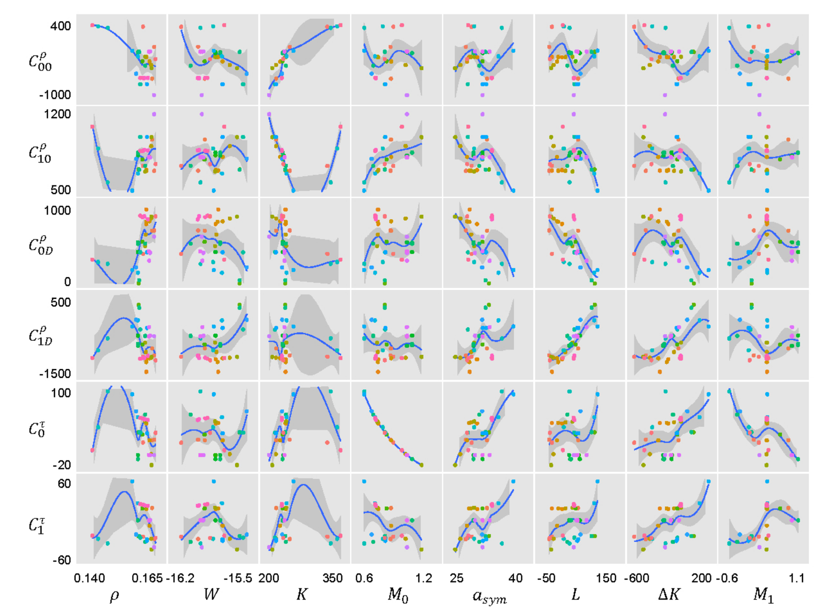


**Figure 2.** *Infinite nuclear matter properties vs. volume parameters. Some correlation is expected. LOESS modeling method is used to generate the regression curve in blue. The shaded regions show the standard error of the LOESS smoothing spline.*

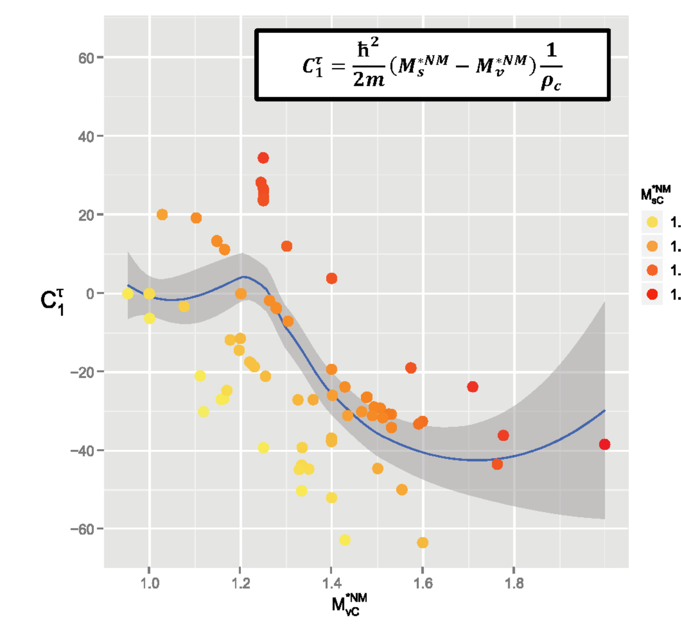


**Figure 3.** *Volume parameter $C_1^\tau$ vs. isovector effective mass. This plot presents an expected correlation between the infinite nuclear matter properties and volume parameters.*

The fitted Skyrme EDF was used to calculate the infinite nuclear matter properties. Theoretically, these properties depend only on volume parameters. The relationships between both the infinite nuclear matter properties and the volume and surface parameters are analyzed through the exploration of nuclei data.

Each point represents a force, that is, a particular set of data fitted to the Skyrme functional. Many different combinations were used, each attempting to model the nuclear landscape. Included in the analysis were a total of 189 forces.

**Figure 4.** *Infinite nuclear matter properties vs. surface parameters. The properties are not explicitly dependent on the parameters.*

$$\mathcal{H}_t(\boldsymbol{r}) = C_t^{\rho}\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + \frac{1}{2}C_t^{J}\boldsymbol{J}_t^2 + C_t^{\nabla J}\rho_t\boldsymbol{\nabla}\cdot\boldsymbol{J}_t$$

$$C_t^{\rho} = C_{t0}^{\rho} + C_{tD}^{\rho}\rho_0^{\gamma}\cdot$$

**In the Skyrme functional approach, energy density can be represented as a sum of kinetic and potential isoscalar (t = 0) and isovector (t = 1) energy terms which contains all together 13 parameters.**

**Surface parameters:** $C_t^{\Delta\rho}, C_t^{\Delta J}, C_t^{J}$

**Volume parameters:** $C_{t0}^{\rho}, C_{tD}^{\rho}, C_t^{\tau}$

## Results and Conclusions

Figure 5 shows an unexpected high correlation coefficient of 0.86 and a near-linear plot behavior in the relationship between the Skyrme surface parameter $C_0^{\Delta\rho}$ and the isoscalar effective mass. The correlation from the plot reveals that infinite nuclear matter properties, calculated using the volume parameters derived from the Skyrme functional, are being indirectly influenced by finite nuclei surface parameters. The reason for this behavior lies in the fitting process used to determine the Skyrme EDF parameters. In order to establish the Skyrme force, finite nuclei surface and volume parameters are fitted into the EDF. Although infinite nuclear matter is not theoretically expected to be influenced by nuclei surface parameters, the current methods for deriving these properties cause hidden correlations.

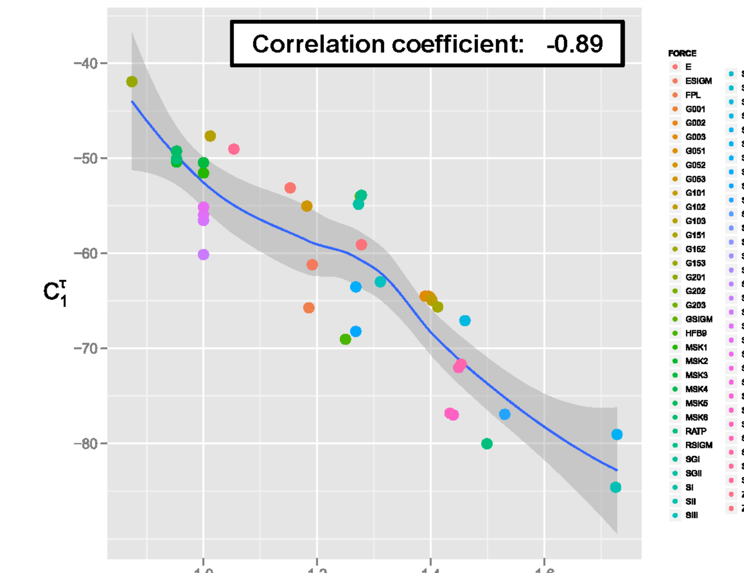



**Figure 5.** *Skyrme surface parameter $C_0^{\Delta\rho}$ vs. isoscalar effective mass.*

This relationship was discovered due to the clear and high resolution display of the **EVEREST** visualization facility. The management of high-dimensional data through the **R** software environment and programming language allowed the interactive processing of plots and the export of images for large-display visualization. The combination of these tools enables a novel perspective for analyzing and exploring nuclei data through a new information layer.

An undetermined property of the force data is responsible for the relationship depicted in Figure 5. Careful consideration of the data properties relative to the near-linear LOESS curve is expected to result in a new correction to the EDF. As a result of this analysis, an extensive literature review will be conducted to extract relevant data attributes. These attributes will then be used to develop an EDF correction, and remove the relationship described above.

## References

M. Kortelainen, T. Lesinski, J. Moré, W. Nazarewicz, J. Sarich, N. Schunck, M. V. Stoitsov, S. Wild, "Nuclear Energy Density Optimization," *arXiv: 1005. 5145v1 [nucl-th]*, May 28, 2010.

M. V. Stoitsov, J. Moré, W. Nazarewicz, J.C. Pei, J. Sarich, N. Schunck, A Staszczak, S. Wild, "Towards the universal nuclear energy density functional," *Journal of Physics: Conference Series Vol.180-1*, SciDAC 2009.

M. Bender, P. Heenen and P. Reinhard, "Self-consistent mean-field models for nuclear structure," *Review of Modern Physics*, Volume 75, January 2003.

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