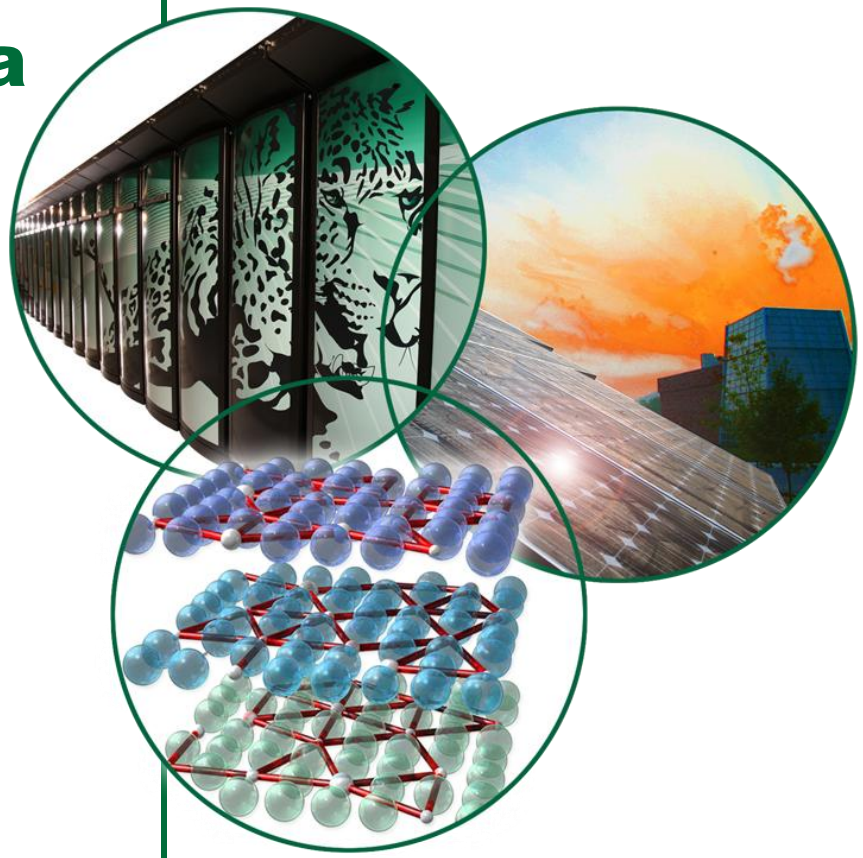
Exploration of High-Dimensional Nuclei Data



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Overview

- **Background information**
  - **Nuclear landscape**
  - **Density functional theory**
- **Methodology**
  - **GGobi**
  - **R**
- **Results**
  - **Neutron quadrupole deformation**
  - **Neutron pairing gap energy**
- **Conclusion**
  - **Correlation**
  - **Universal density functional**
- **Acknowledgments**

Nuclear landscape

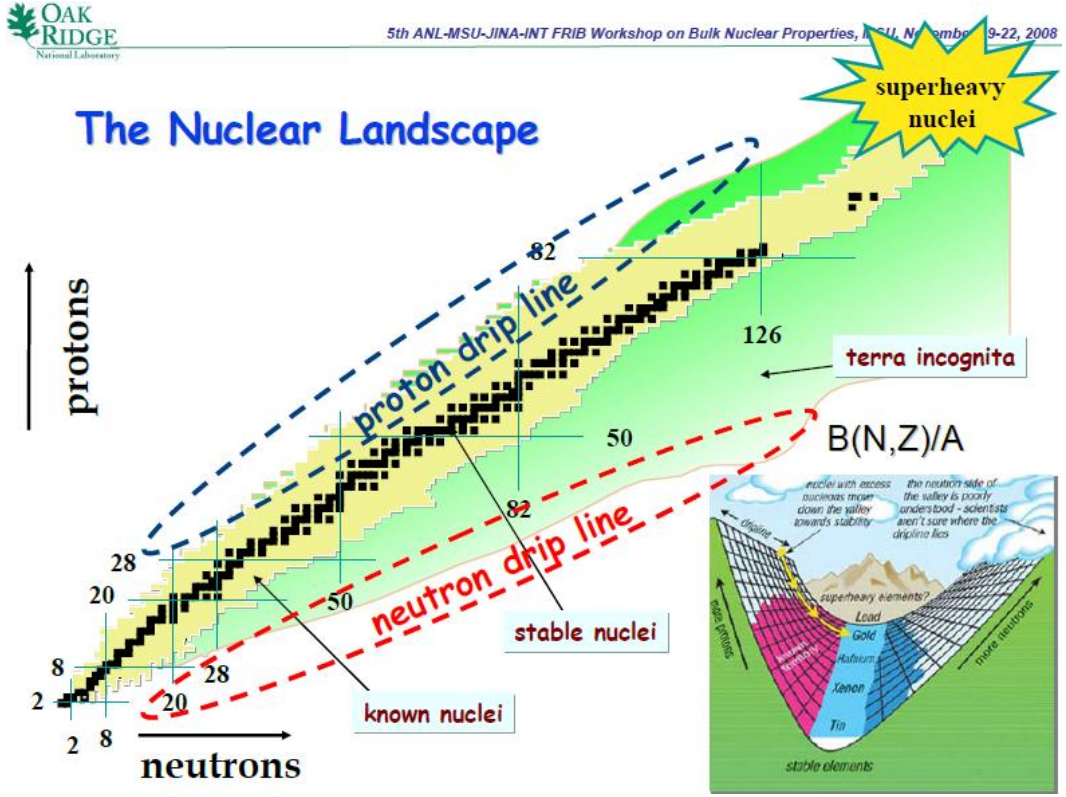
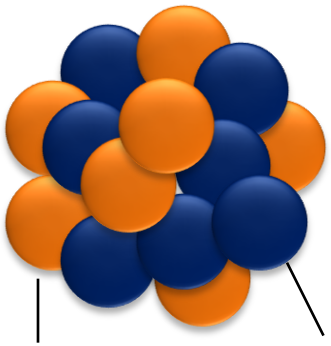


Figure 1: Chart of nuclides. Source: Mario Stoitsov (2008).

Figure 2: Atomic nucleus



- **Density functional theory**
  - **Energy of a system**
  - **Density of the bodies**
- **Universal functional**
  - **Nuclei parameters**
  - **Unknown regions**

Ggobi visualization tools

- **Brush**
  - **Parameter**
  - **User defined**
- **2D Tour**
  - **Multiple dimensions**
  - **Variable projections**
- **Sub-sets**
  - **High number of data**
  - **Random selection**
- **Shadow**
  - **Dimming of colors**
  - **Hide data**

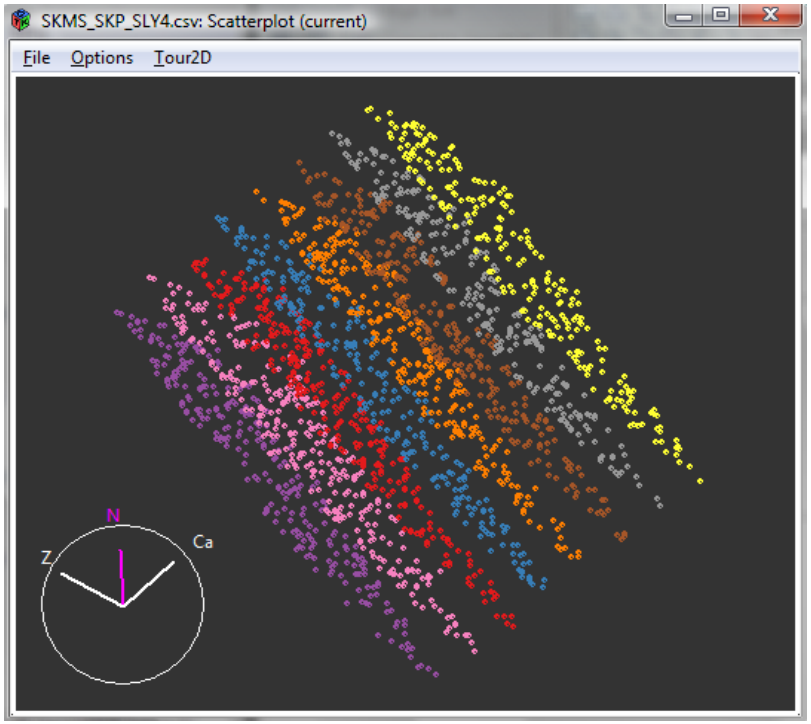
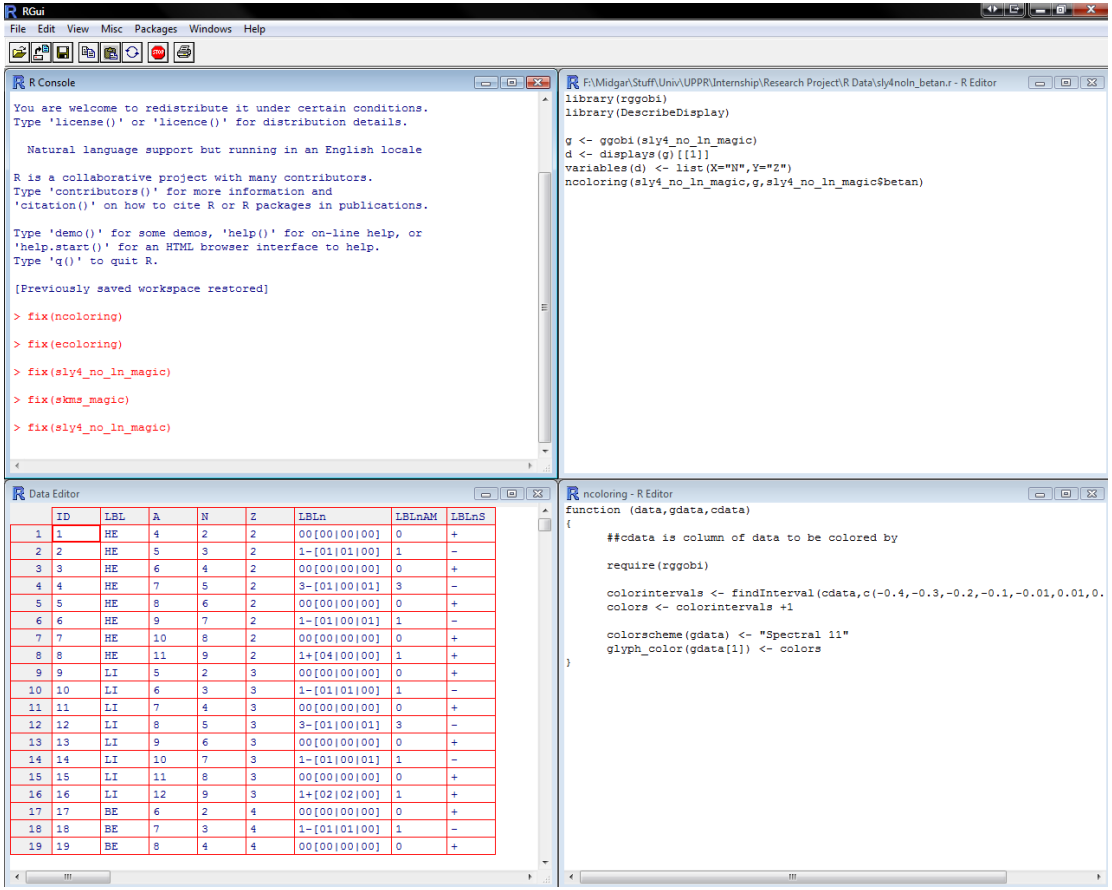


Figure 3: Automatic brushing.

- **Variable manipulation**
  - **Limits**
  - **Exclude data**

R data manipulation

- **Import data**
  - **CSV**
  - **Data frames**
- **Edit data**
  - **Add Parameters**
  - **Remove labels**
- **Export data**
- **Scripts**
  - **Color schemes**
  - **Scale values**
  - **Parameters**



	ID	LBL	A	N	Z	LBLn	LBLnAM	LBLnS
1	1	HE	4	2	2	00[00|00|00]	0	+
2	2	HE	5	3	2	1-[01|01|00]	1	-
3	3	HE	6	4	2	00[00|00|00]	0	+
4	4	HE	7	5	2	3-[01|00|01]	3	-
5	5	HE	8	6	2	00[00|00|00]	0	+
6	6	HE	9	7	2	1-[01|00|01]	1	-
7	7	HE	10	8	2	00[00|00|00]	0	+
8	8	HE	11	9	2	1+[04|00|00]	1	+
9	9	LI	5	2	3	00[00|00|00]	0	+
10	10	LI	6	3	3	1-[01|01|00]	1	-
11	11	LI	7	4	3	00[00|00|00]	0	+
12	12	LI	8	5	3	3-[01|00|01]	3	-
13	13	LI	9	6	3	00[00|00|00]	0	+
14	14	LI	10	7	3	1-[01|00|01]	1	-
15	15	LI	11	8	3	00[00|00|00]	0	+
16	16	LI	12	9	3	1+[02|02|00]	1	+
17	17	BE	6	2	4	00[00|00|00]	0	+
18	18	BE	7	3	4	1-[01|01|00]	1	-
19	19	BE	8	4	4	00[00|00|00]	0	+

Figure 4: R environment.

Data visualization

- **Rggobi**
  - **Glyph color**
  - **Glyph size**
  - **Color scheme**
- **Describe display**
  - **Import GGobi plot**
  - **Create R object**

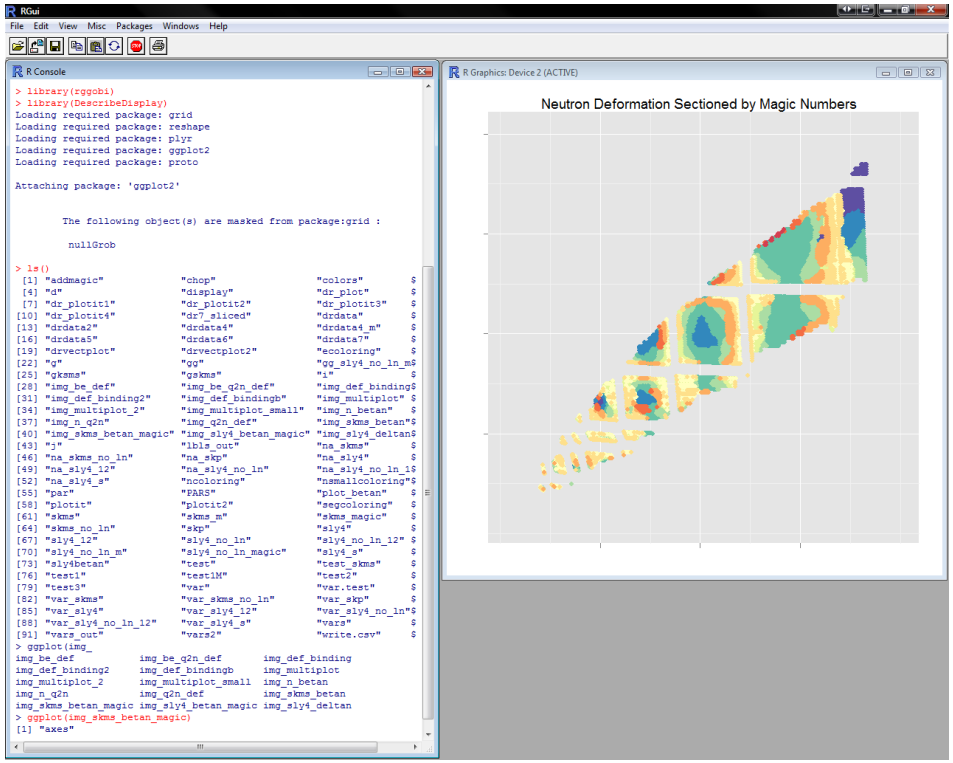


Figure 5: GGobi plots through R.

High-dimensional exploration

Ggobi 2D Tour

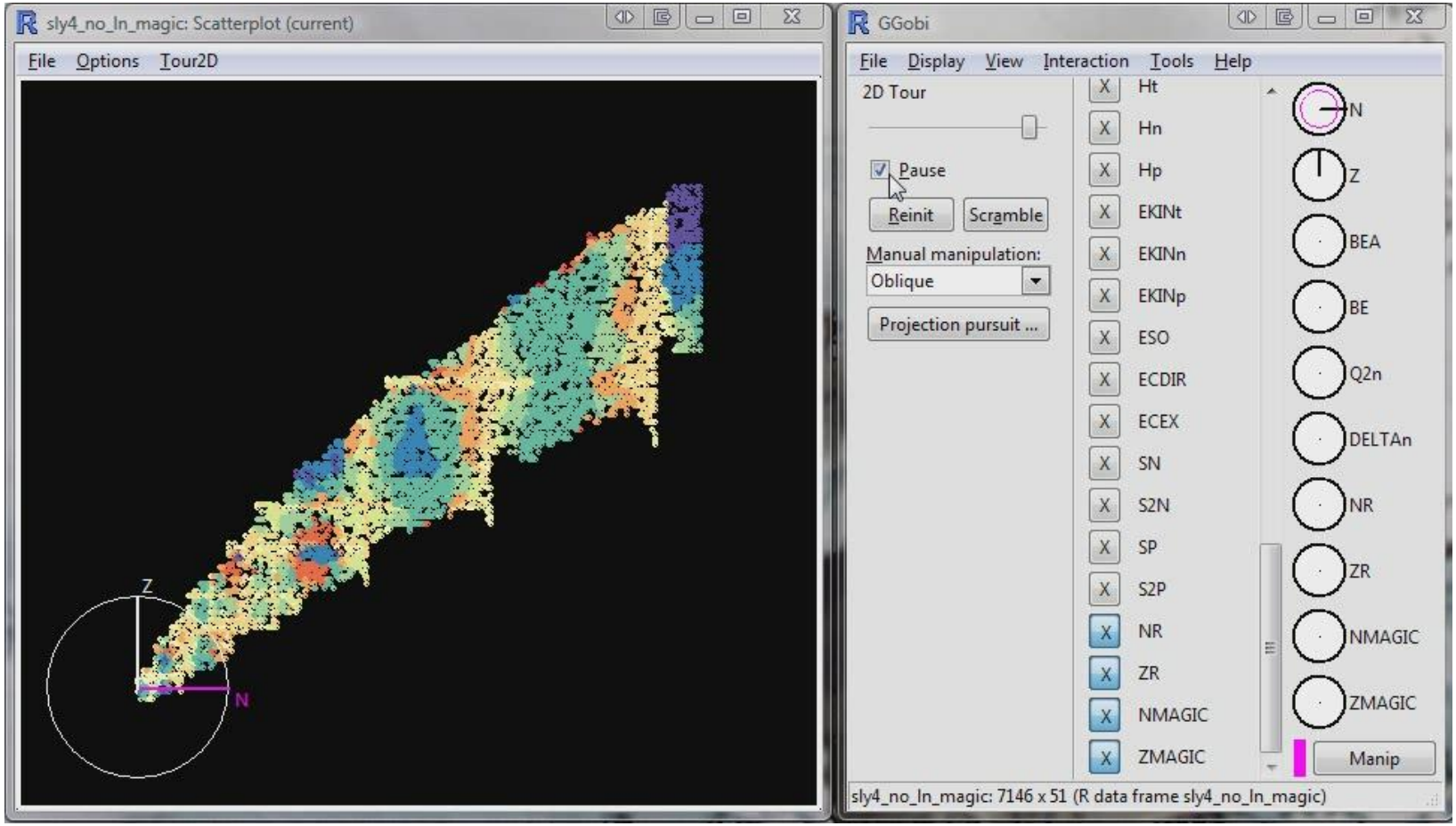
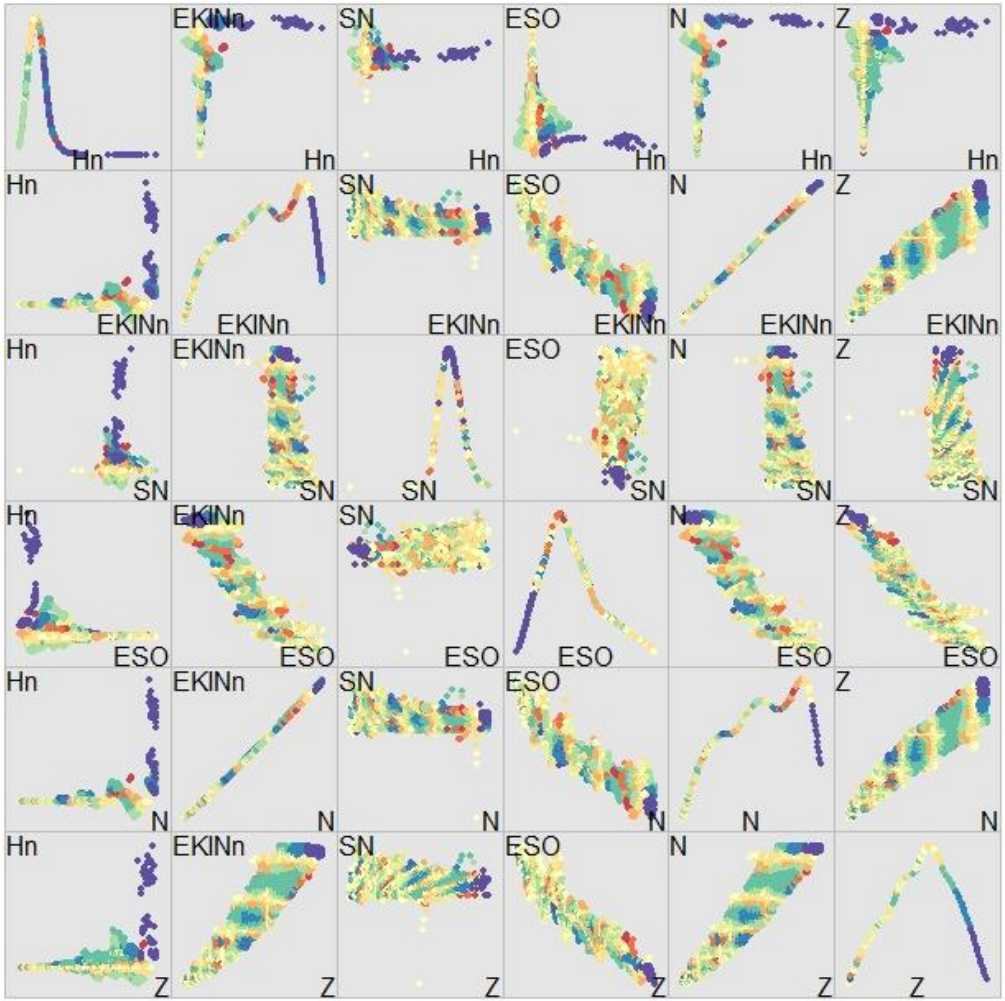


Figure 6: GGobi environment while exploring nuclei data colored by neutron quadrupole deformation.

Multi-plot



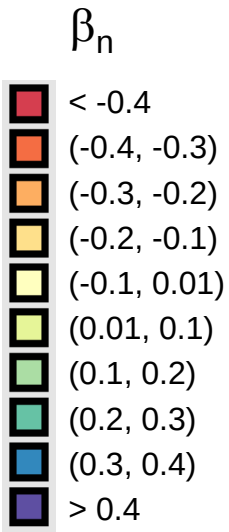


Figure 9: Parameter relationships on deformation.

Multi-plot

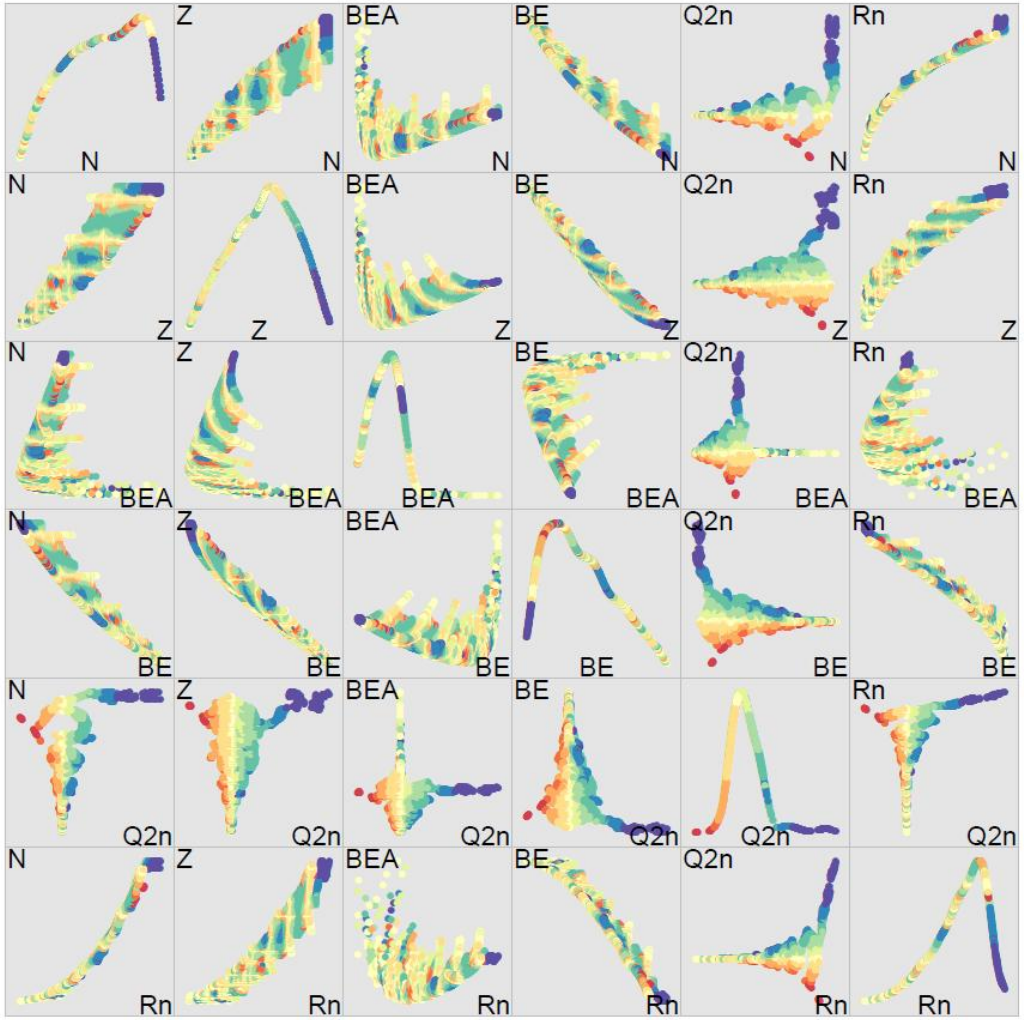
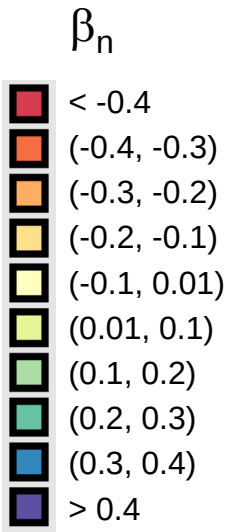


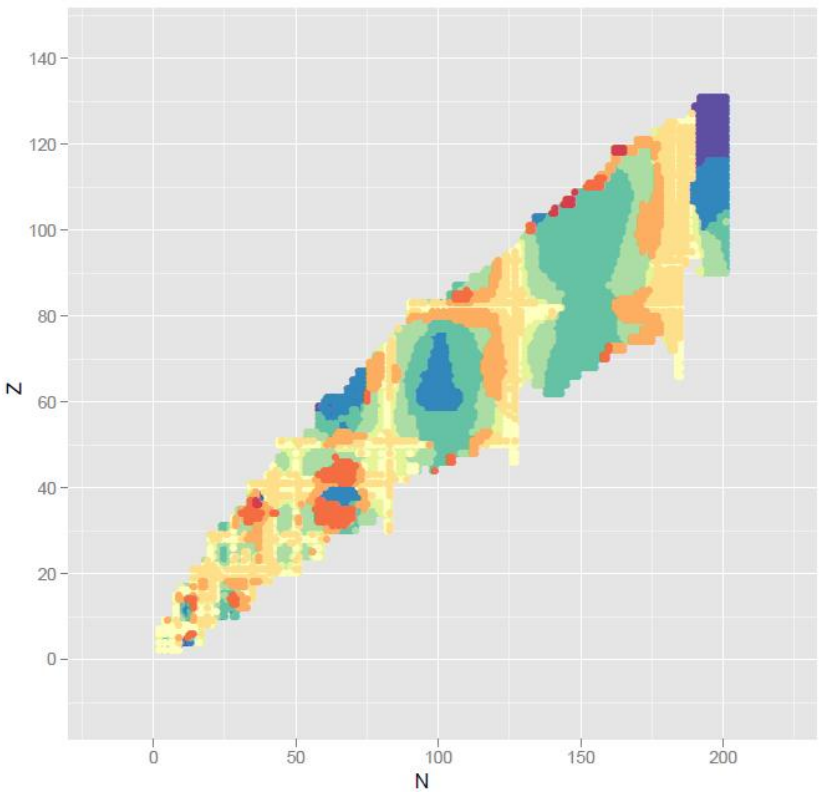
Figure 10: Parameter relationships on deformation.



Data exploration:

- **Quick overview**
- **Neutron quadrupole deformation**

Detailed exploration



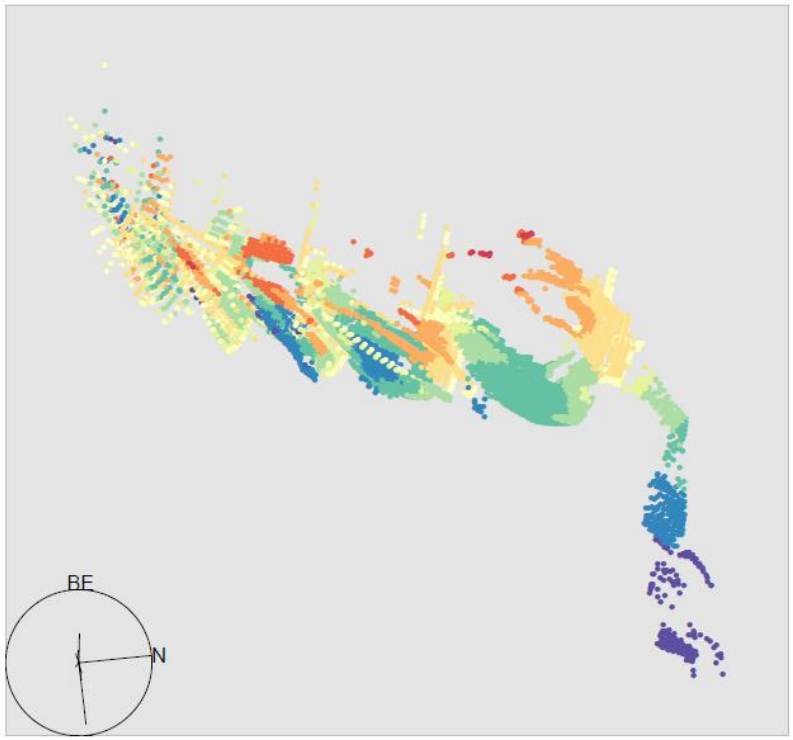
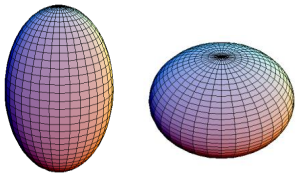


Figure 7: Neutron quadrupole deformation exploration.

β_n

- < -0.4
- (-0.4, -0.3)
- (-0.3, -0.2)
- (-0.2, -0.1)
- (-0.1, 0.01)
- (0.01, 0.1)
- (0.1, 0.2)
- (0.2, 0.3)
- (0.3, 0.4)
- > 0.4

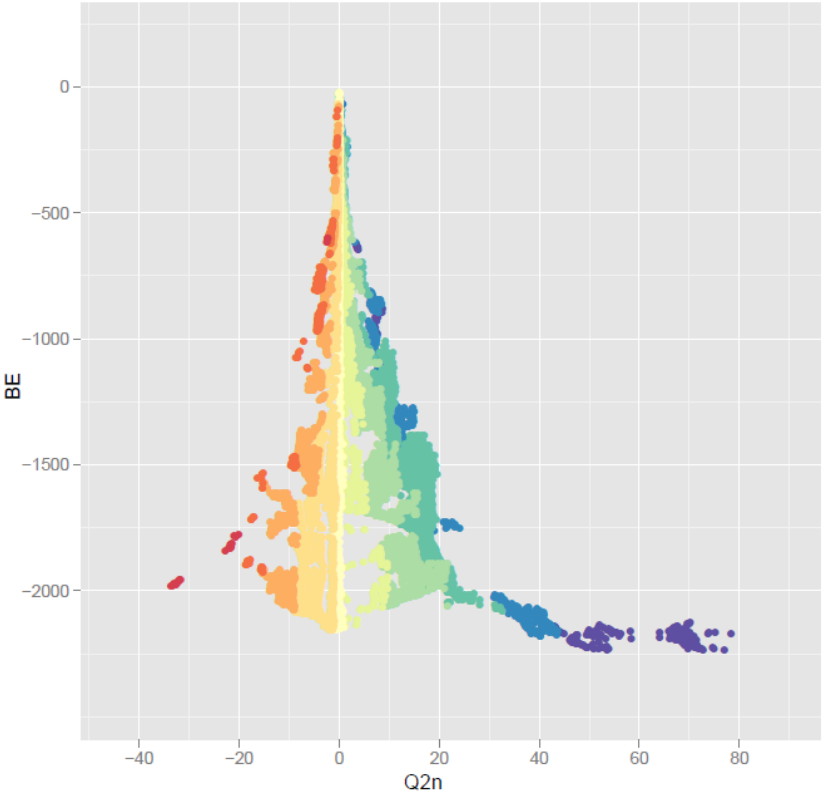
- $\beta_n < 0$ oblate
- $\beta_n > 0$ prolate
- $\beta_n = 0$ sphere



A B

Deformation shapes:
(A) Prolate, (B) Oblate

Further exploration



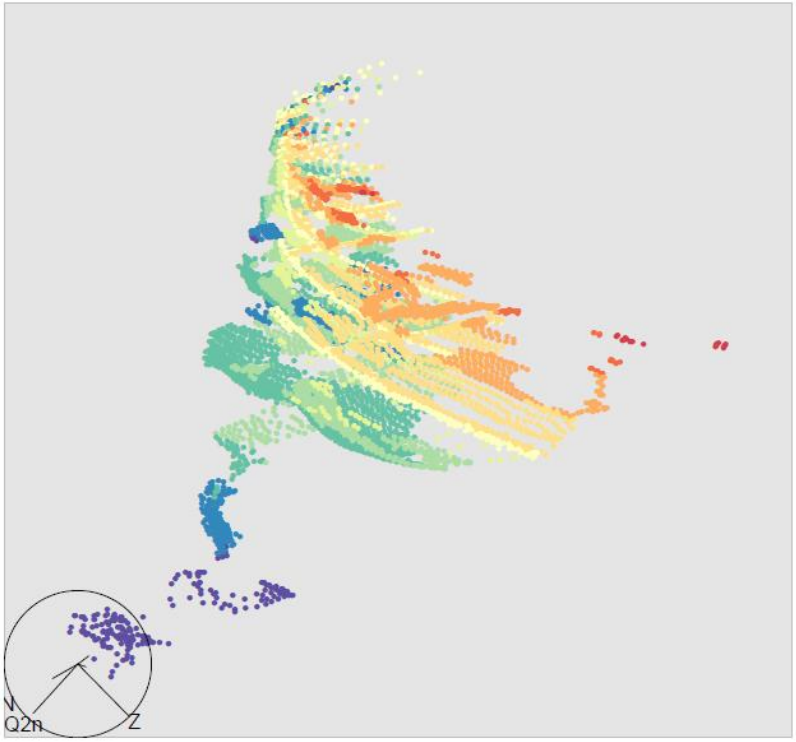
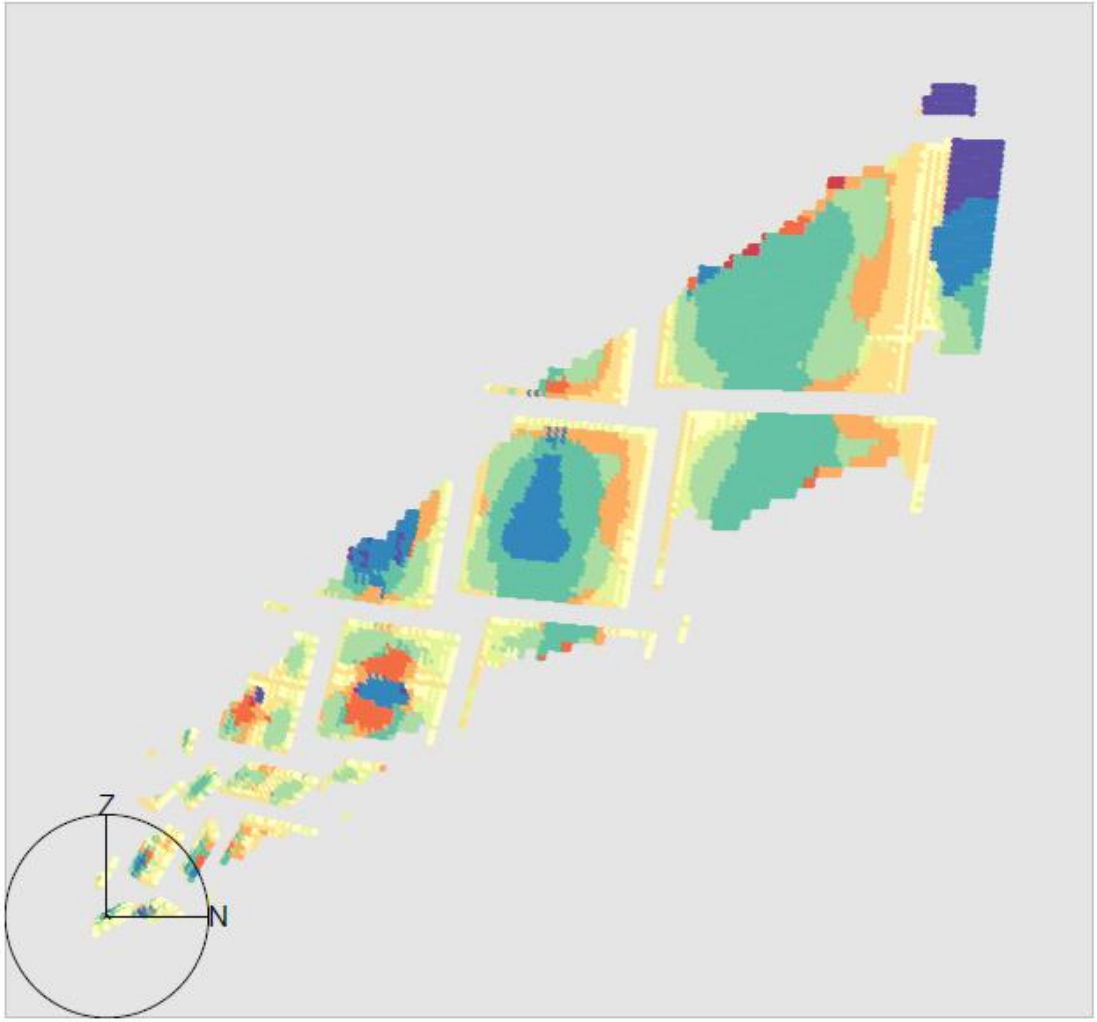


Figure 8: Neutron quadrupole deformation exploration.

β_n

- < -0.4
- (-0.4, -0.3)
- (-0.3, -0.2)
- (-0.2, -0.1)
- (-0.1, 0.01)
- (0.01, 0.1)
- (0.1, 0.2)
- (0.2, 0.3)
- (0.3, 0.4)
- > 0.4

Magic number sections



β_n

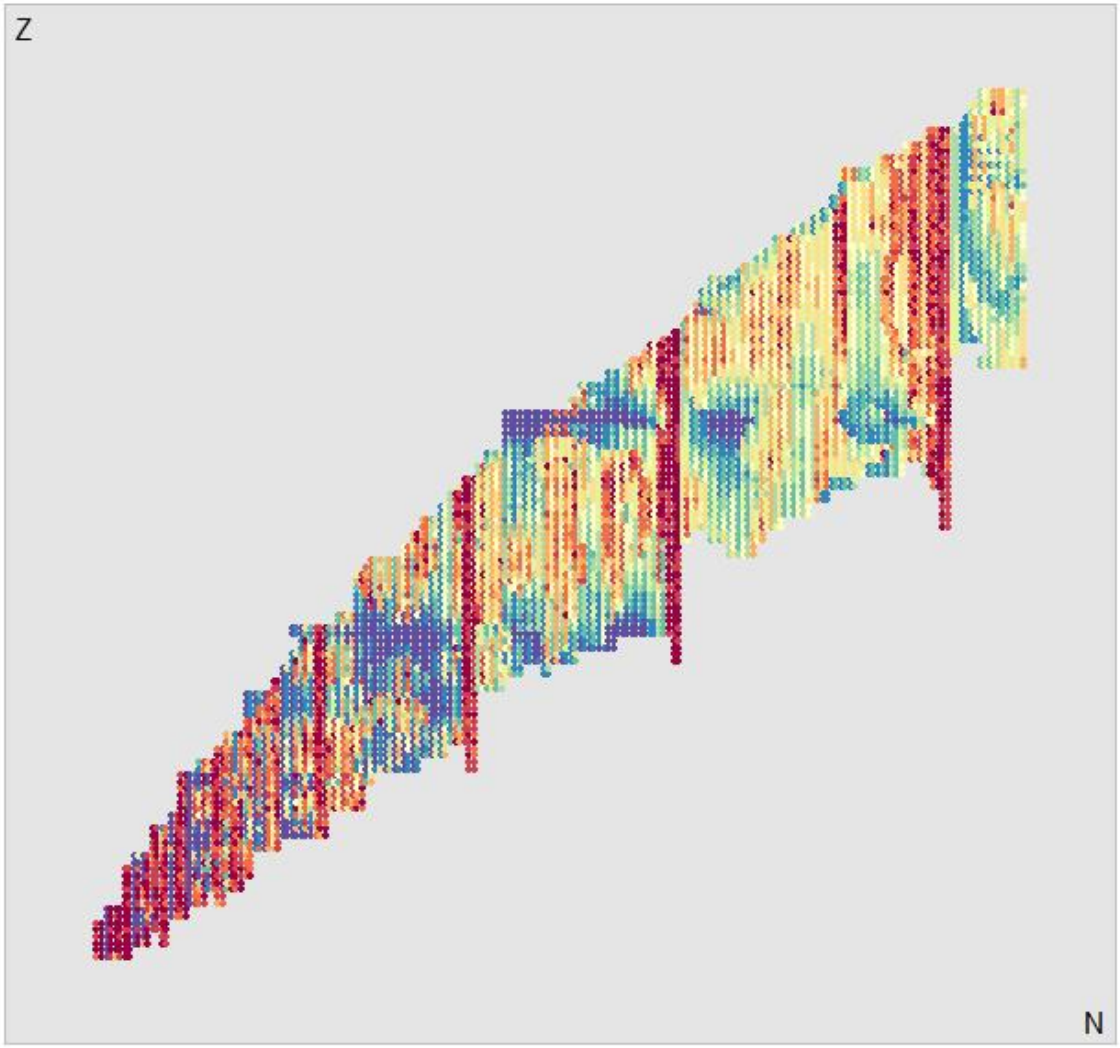
- < -0.4
- (-0.4, -0.3)
- (-0.3, -0.2)
- (-0.2, -0.1)
- (-0.1, 0.01)
- (0.01, 0.1)
- (0.1, 0.2)
- (0.2, 0.3)
- (0.3, 0.4)
- > 0.4

Magic numbers:

- **Arranged into complete shells**
- **Neutron quadrupole deformation by regions**

Figure 11: Neutron deformation segmented by magic numbers.

Pairing gap



Δ_n (MeV)

- (0, 6.2e^{-005})
- (6.3e^{-005}, 0.0002)
- (0.0002, 0.0006)
- (0.0006, 0.0903)
- (0.0925, 0.3831)
- (0.3833, 0.4868)
- (0.4871, 0.5587)
- (0.5588, 0.6332)
- (0.6333, 0.7373)
- (0.7376, 0.8966)
- (0.8970, 3.0301)

Figure 12: Neutron pairing gap energy.

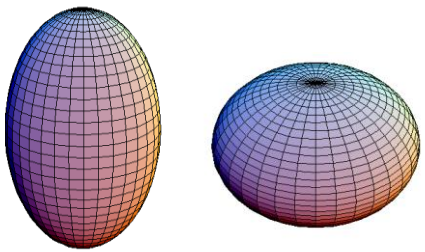
Pairing gap energy:

- **Magic number regions**
- **Phase patterns**

Results

- **Correlation**
  - **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



A B

Deformation shapes:
(A) Prolate, (B) Oblate.

Conclusion

- Relationship
  - Neutron quadrupole deformation
  - Neutron pairing gap energy
- Step closer toward universal density functional

Future work

- Quantify correlation
- Universal functional

Applications

- Stock-pile stewardship
- Fuel-cycle research
- Medical research
- Nuclear reactions

Acknowledgements

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- Rashida Askia
  - Research Alliance in Math and Science program assistant