Quantifying Uncertainty of Microscopic Nuclear Theories

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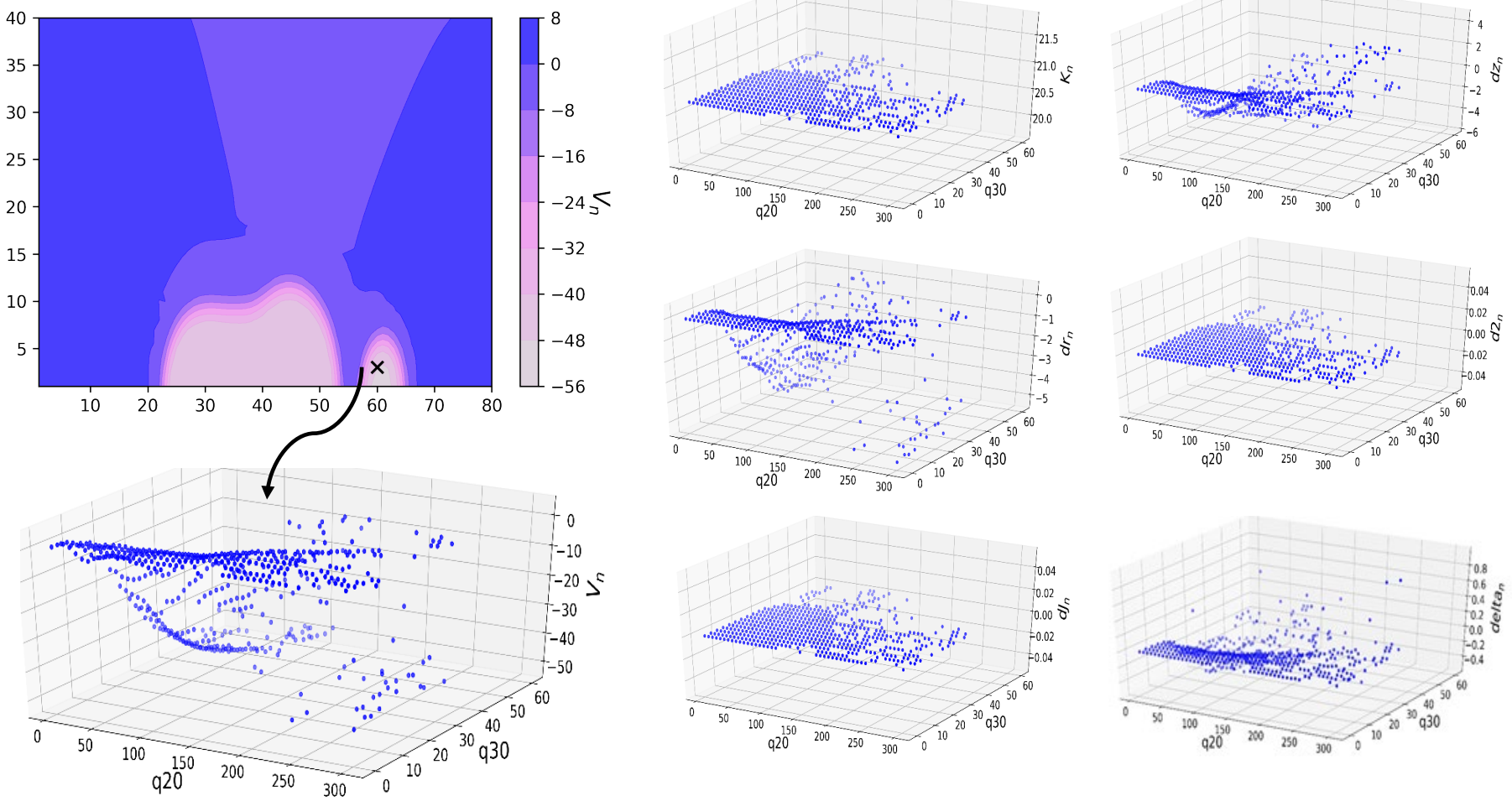
Application: Model Atomic Nuclei Fission

- Nuclear fission discovered in 1939, and we have reactors + weapons so why do we need to model this process?
  - Most data obtained experimentally for very specific cases
  - **Need an accurate and precise theoretical model of fission**
- Use a model called density functional theory to provide robust predictions on how atomic nuclei fission
  - Involves a three step calculation, where the first is to calculate the deformation properties of the nucleus
  - However, very computationally expensive to calculate realistic potential energy surface (PES)

Can we use statistical methods to emulate the potential energy surface?

Data Structure

Dimension: ((80x40), 14, 512)



Preliminary Results

- Use a Gaussian Process with 10-fold cross validation to model the PES
  - Initially ignored the correlation structures, but need to account for them

Parameter	Mean	StnDev	Abs(Max)
V_n	0.081	8.404	39.029
dr_n	-0.002	0.909	5.205
dz_n	0.002	0.755	4.132
$delta_n$	0.003	0.106	0.877
V_p	0.081	9.558	45.040
dr_p	-0.004	0.805	4.217
dz_p	-0.001	0.617	3.425
$delta_p$	-0.003	0.178	1.200

Mean, standard deviation and absolute max of the residuals.