

#### **Quantifying Uncertainty of Microscopic Nuclear Theories**

Michelle Ngo Computing / DSSI Collaborators: Kevin Quinlan, Nicolas Schunck



LLNL-PRES-812946 This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC



# 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?

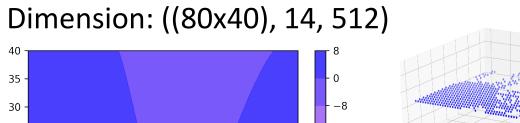


<sup>30</sup> a 30

250

300

### Data Structure



60

70

11 .

10

0

300

80

<sup>40</sup> 20 <sup>30</sup> q30 -16

-32

-40

-48

-56

0

-10 -20 5

-30

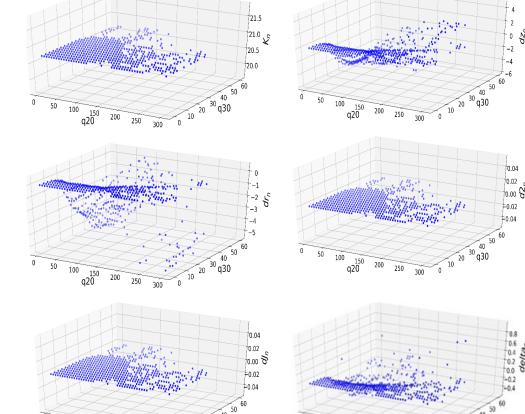
-40

60 50

200 250

300

-24 5



150 q20

200

250

50 100

20

10

30

40

. 50

25 -

20 -

15 -

10 -

5 -

0



a20

## 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

				$V_n$ $dr_n$ $dr_n$
Parameter	Mean	StnDev	Abs(Max)	00 -
$V_n$	0.081	8.404	39.029	$ \begin{array}{c} 40 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 $
$dr_n$	-0.002	0.909	5.205	
$dz_n$	0.002	0.755	4.132	
delta <sub>n</sub>	0.003	0.106	0.877	
$V_p$	0.081	9.558	45.040	$dz_n$ $delta_n$
$dr_p$	-0.004	0.805	4.217	50 - 40 - 3.6 = 50 - 3.0 - 3
$dz_p$	-0.001	0.617	3.425	
$delta_p$	-0.003	0.178	1.200	
ean, standard d	eviation and	absolute ma	ix of the residu	

LLNL-PRES-812946



#### Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence National Security, LLC, and shall not be used for advertising or product endorsement purposes.