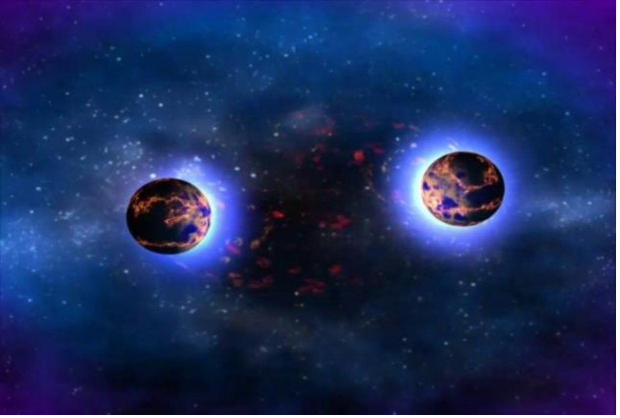

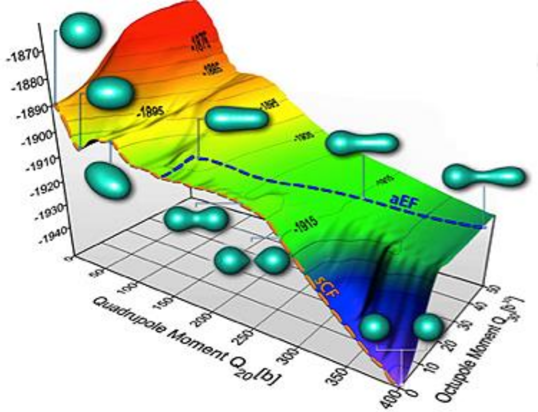

Iterative Gaussian Process Regression for Potential Energy Surfaces

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ISNET-5 Workshop

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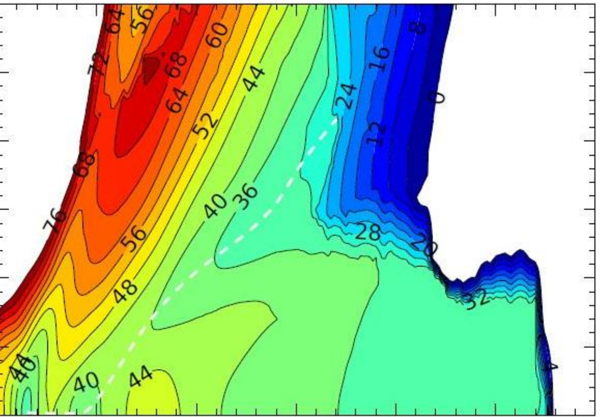
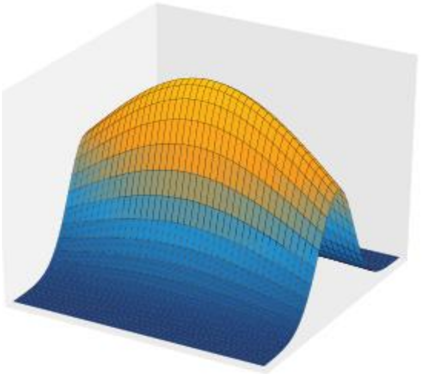


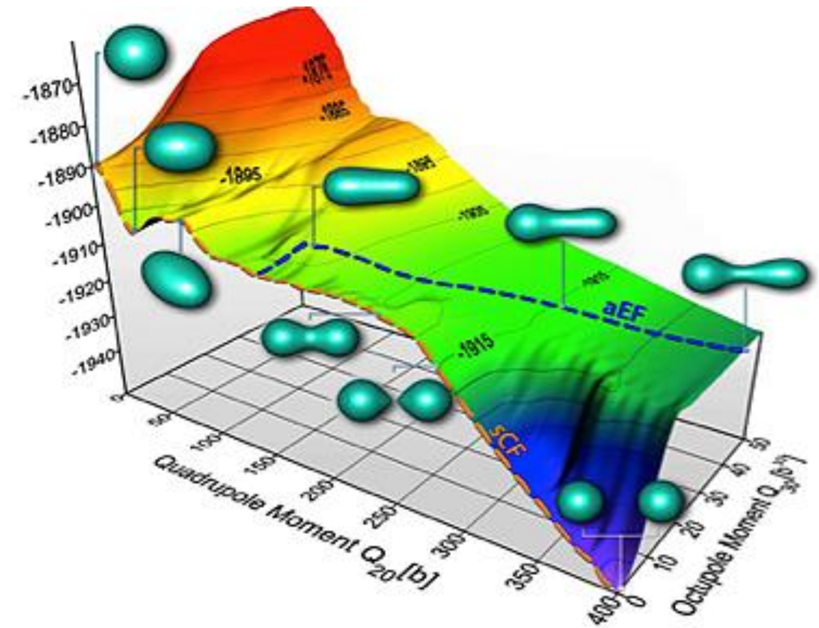


Outline

- Motivation:
  - Calculation of potential energy surfaces (PES)
- Gaussian Process Regression (GPR):
  - Background
  - Motivation - **can we use GPR to reduce the CPU time needed to calculate a PES?**
  - Method; iteration
- Results for PES for fission of ^{240}Pu :
  - 1D
  - 2D
- Future work

Motivation: potential energy surfaces (PES)

- E.g. fission:
  - Nucleus slowly deforms, from roughly spherical shape to 2 distinct nuclei
  - Nucleus has different potential energy for different deformations
  - PES can yield properties like path taken to fission, lifetime, mass distributions of fission fragments
- Computationally expensive NDFT is used - 5-10 CPU hours per calculation
- 1000s of calculations required
- **By how much can we reduce the number of calculations with GPR?**



Calculated PES for fission of ^{258}Fm

Gaussian Process Regression (GPR)

- Regression method from machine learning
- Outputs a model/prediction which is a smooth interpolation of points on a surface
- Predictions at unknown locations on surface are made using **all** calculated points
- Most useful for expensive computer simulations, with smoothly-varying outputs
- Surface *Y(x)* is modelled as the sum of a regression model (comprising *k* regression functions f_j) and a random (Gaussian) process *Z*:

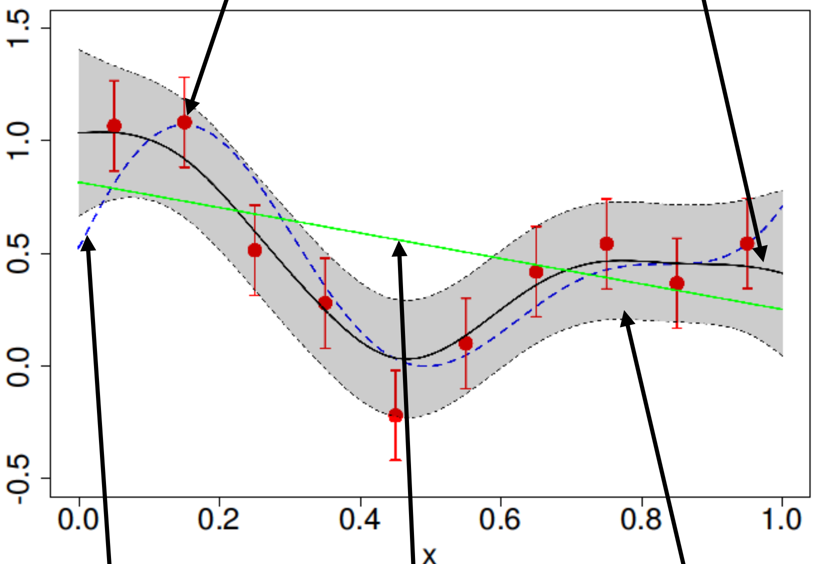
$$Y(x) = \sum_{j=1}^{k} \beta_j f_j(x) + Z(x)$$

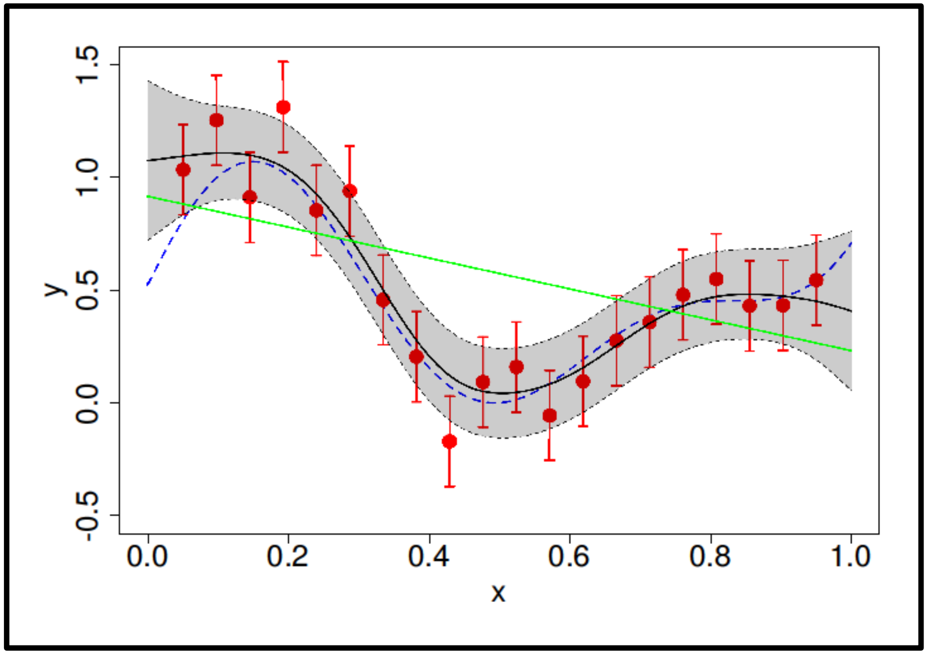
- Used previously in atmospheric chemistry, locating mineral ores, modelling of oceans and diseases, atomic physics

GPR example in 1D

Design points (red) (with error bars)

GPR prediction (black line)





Unknown function/ surface (blue dotted line)

Linear trend line

95% confidence intervals (shaded)

Increase number of design points:

- Increase accuracy of emulation
- Decrease size of confidence intervals

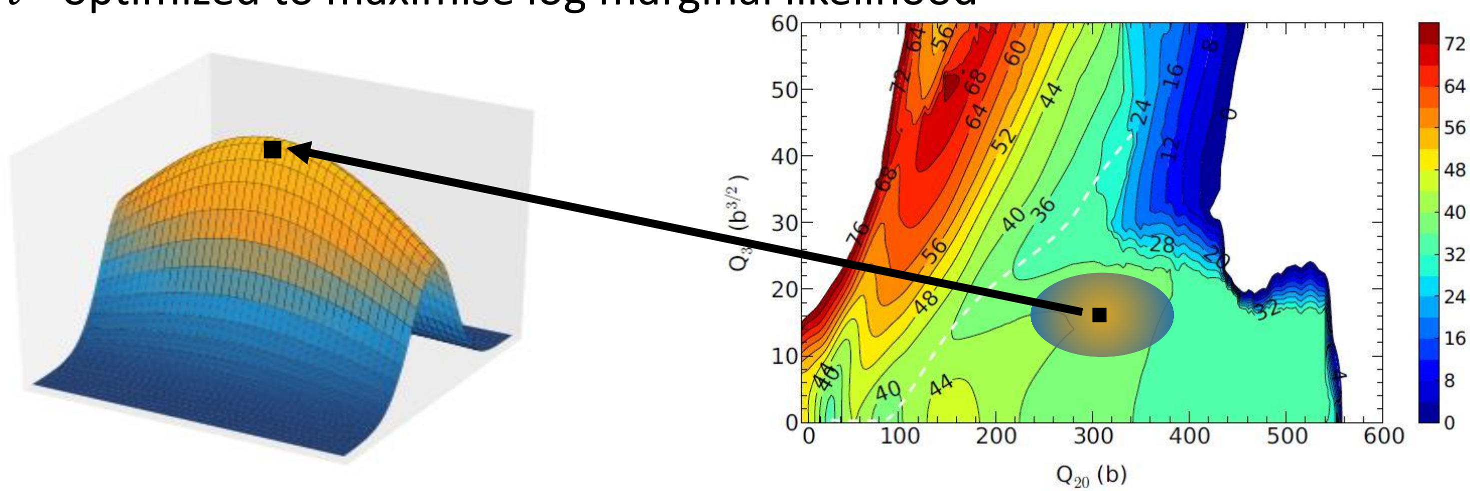
Gaussian Process Regression (GPR) - kernels

- Gaussian correlation model (covariance kernel), for *d* dimensions:

$$V(\boldsymbol{x}', \boldsymbol{x}) = \sigma^2 \prod_{j=1}^{d} \exp\left(-\frac{(x'_j - x_j)^2}{2\theta_j^2}\right) + \tau^2 \delta_{\mathbf{0}}(\boldsymbol{x}' - \boldsymbol{x})$$

where σ^2 is variance of random process *Z*

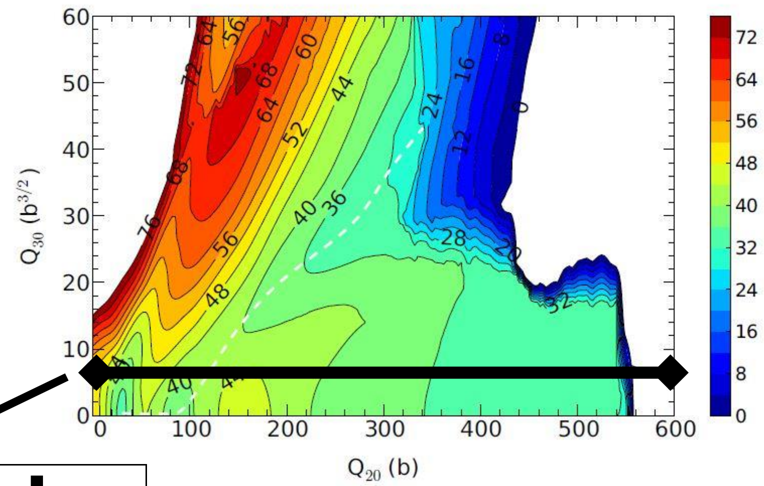
- θ_j are 'characteristic length-scales' → control spatial correlation lengths
- τ^2 is 'nugget variance' → treats numerical instabilities caused by jitters/kinks on surface
- σ^2, θ_j's, τ^2 optimized to maximise log marginal likelihood

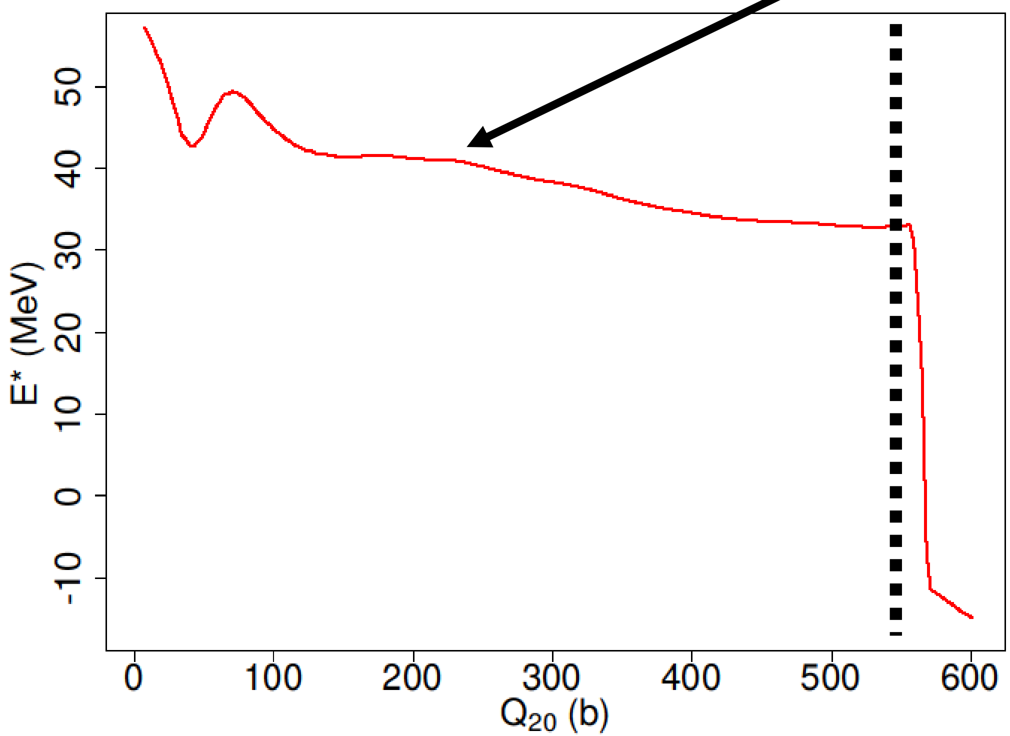


Gaussian Process Regression (GPR) - method

- Use previously calculated surfaces
- Choose a sample of calculated points
- **Normalise the sample**
- Use these 'design points' to emulate surface
- Compare emulated surface with original surface (how accurate was the emulation?)
- Iteration:
  - Add new point at location of max σ from last iteration
  - Re-emulate

GPR in 1D

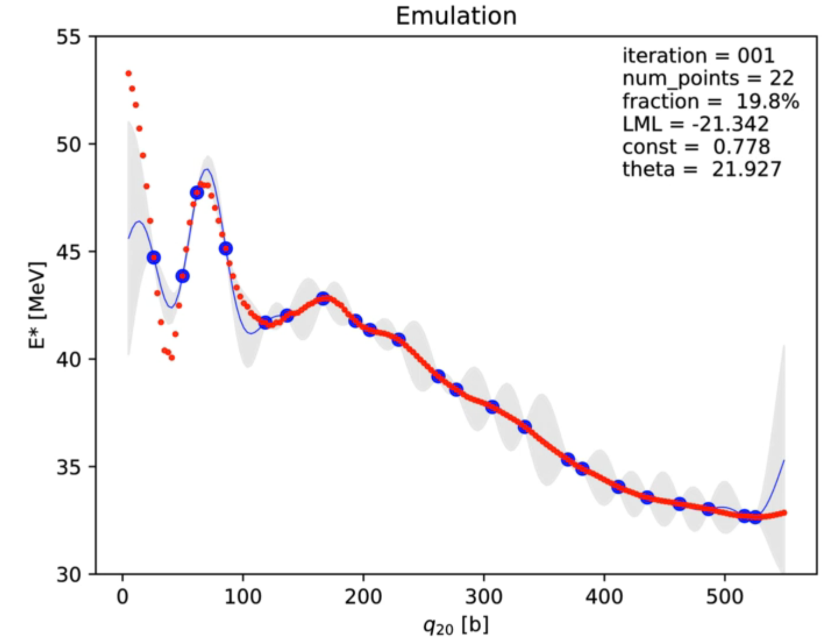




Calculated PES for fission of ^{240}Pu. Plot shows calculated energy (MeV) of nucleus relative to -1840 MeV.

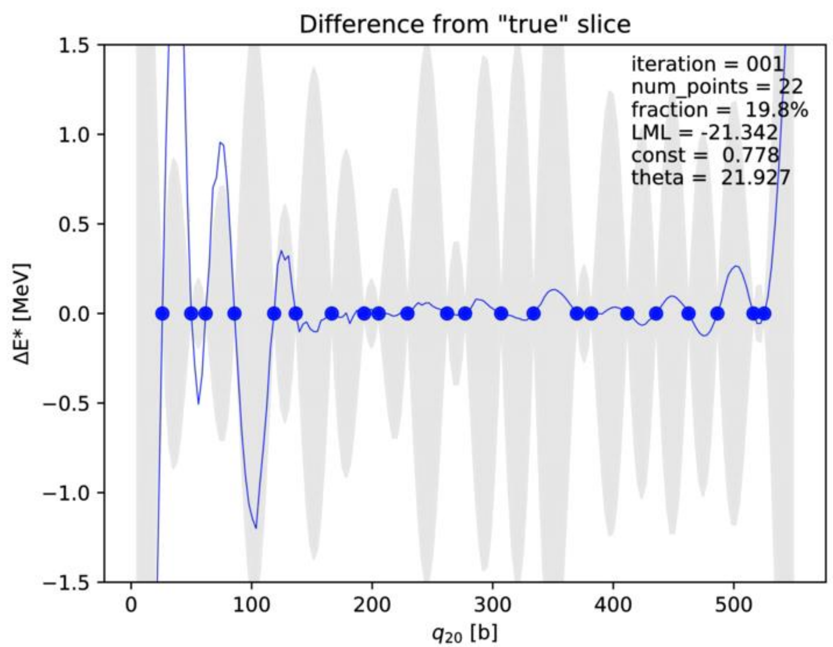
Schunck et al. – Phys. Rev. C **90**, 054305

- Original slice represented by **red points**
- Design points in **blue**
- New points in **green**

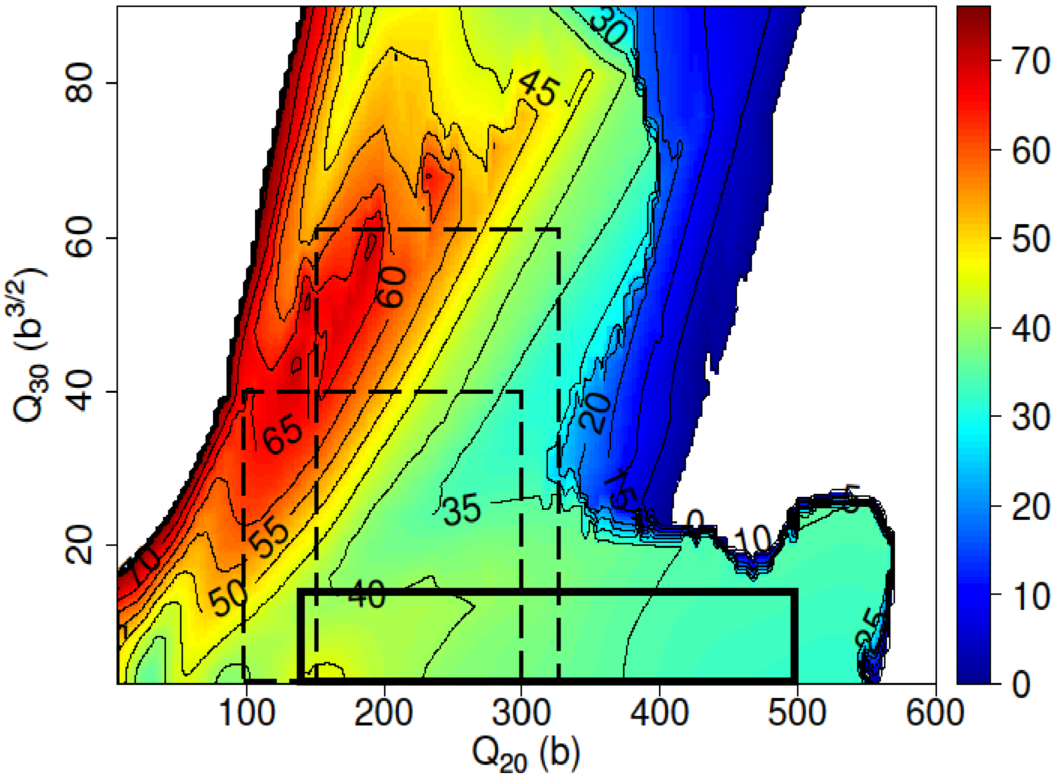


- Occasionally, addition of one new point completely changes the estimation kernel parameters
- When this happens, the prediction changes completely, and the confidence grow suddenly

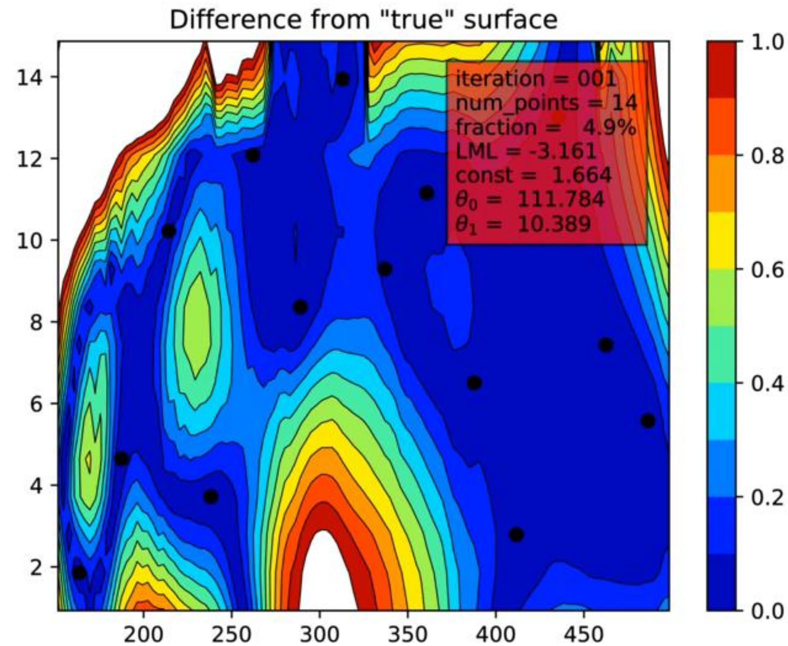
- Blue line gives difference between GPR prediction and original slice →

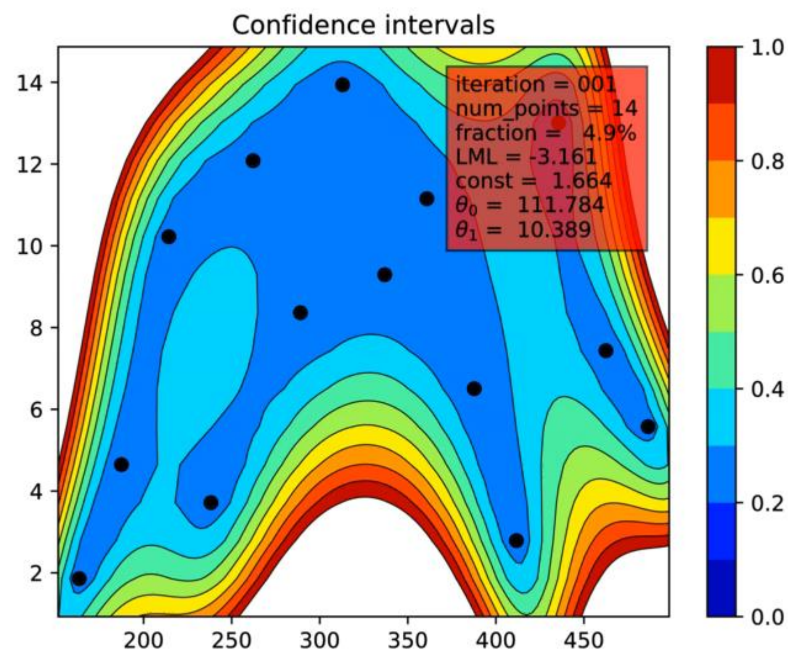


GPR in 2D



Fission barriers (bottom left) and scission 'cliff' (right-hand edge) pose problems


Difference from "true" surface
iteration = 001
num_points = 14
fraction = 4.9%
LML = -3.161
const = 1.664
θ_0 = 111.784
θ_1 = 10.389
14
12
10
8
6
4
2
200
250
300
350
400
450
1.0
0.8
0.6
0.4
0.2
0.0


Confidence intervals
iteration = 001
num_points = 14
fraction = 4.9%
LML = -3.161
const = 1.664
θ_0 = 111.784
θ_1 = 10.389
14
12
10
8
6
4
2
200
250
300
350
400
450
1.0
0.8
0.6
0.4
0.2
0.0

Conclusions and future work

- To successfully perform regression for surface with very different behaviours, need one or both of the following:
    - non-stationary correlation model - θ_j allowed to vary across surface
    - better pre-processing of data, to make it more normally distributed before regression is performed
- Better iteration method:
    - Bias against selection of new points at edges
    - More cautious selection of new points to avoid sudden changes in GPR output
    - Multiple new points at once
    - We know location of fission barriers/ other tricky areas – take advantage of this knowledge
- Compare fission observables from emulated and ‘normal’ surfaces
- Emulating higher dimensional fission surfaces:
    - Ideally need 5D surface for description of fission
    - GPR should provide a better speedup for higher dimensional surfaces

Thank you!

- Acknowledgments:
  - Supervisors: Dr Alessandro Pastore, Dr Christian Aa. Diget
  - Dr Nicolas Schunck (LLNL)
  - Prof Jacek Dobaczewski
- Introduction to Gaussian Process Regression:
  - Sacks et al. “Design and Analysis of Computer Experiments” *Statistical Science* **4**(4), 409-423 (1989)

Design point selection for GPR

- Latin Hypercube Sampling (LHS) provides better coverage of surface