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Title: Finding Minimum Critical Values with MCNP6

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Finding Minimum Critical Values with MCNP6

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WPNCs SG17
OECD/NEA, Paris, FR
July 6-10, 2026

LA-UR-26-XXXXX

Roadmap

- SG17 Overview
- Finding Critical Values with MCNP6
 - Exploration
 - Optimization
 - Sensitivity Study
 - Final Simulation
- Next Steps



SG17 Overview



Brief Overview of SG17 Exercise

- Materials (19 total)
 - Uranium
 - 4 enrichments (5%, 10%, 20%, 93.5%)
 - Metal, dioxide, fluoride, and nitrate
 - Plutonium metal, dioxide, and nitrate
 - Water (used to moderate fuel and as reflector)
- Geometry and target for minimum critical (or target) value
 - Sphere: minimum mass and volume
 - Infinite cylinder: minimum diameter
 - Infinite slab: minimum thickness
- Goal: Find minimum critical (or target) value of mass, volume, diameter, and thickness at optimal moderation ratio for each fuel type.

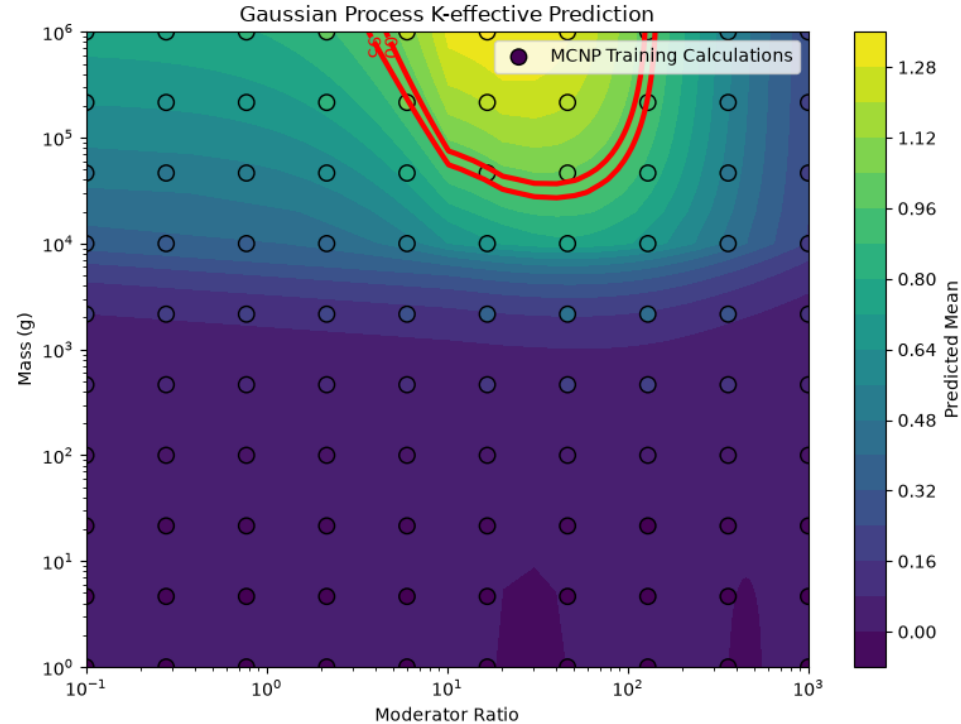


Finding Critical Values with MCNP6



Broad Exploration: Step 1 in Finding Target Values

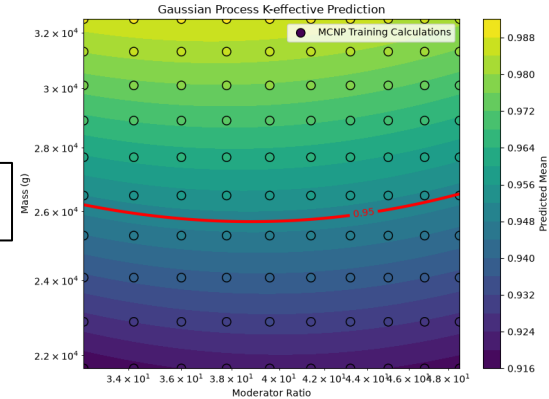
- Gaussian process prediction
 - Using Python scikit-learn
- Use wide search criteria. For example,
 - Mass between 1 and 10^6 g
 - Moderator ratio between 0.1 and 1000
 - Logarithmically spaced 10×10 grid
- Red contours represent target k_{eff} values (1.0 and 0.95)
- Find minimum mass and associated moderator ratio for each target k_{eff}
- Fast MCNP6 calculations (~500 pcm statistical uncertainties)



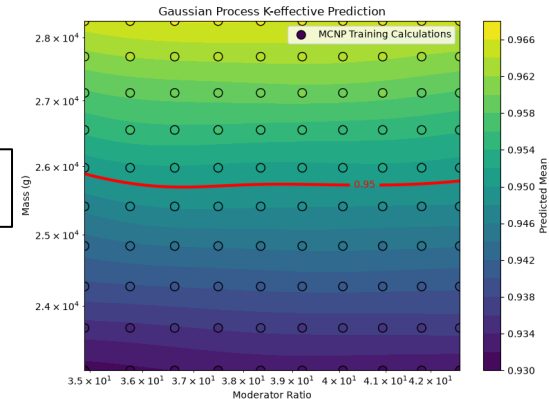
Refined Exploration: Step 2 in Finding Target Values

- Based on previous predicted minimum mass and moderator ratio, narrow the search criteria. For example,
 - Mass and moderation ratio between +/- 20% minimum values
 - Linearly spaced 10x10 grid
 - Iterate (refine range, increase MCNP6 precision)
- Red contours represent target k_{eff}
- Find minimum mass and associated moderator ratio for each target k_{eff}
- Moderate MCNP6 calculations (~100 pcm statistical uncertainties)

Iteration 1



Iteration 2

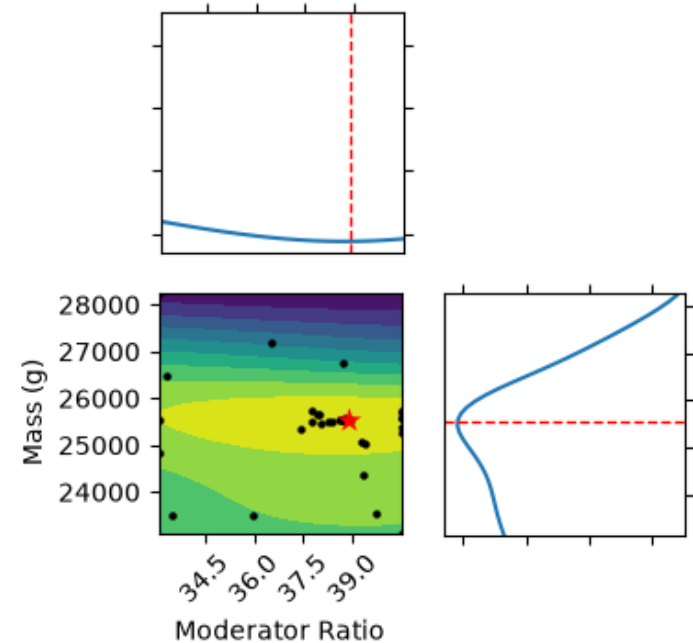


Optimization: Step 3 in Finding Target Values

- Gaussian process optimization
 - Using Python scikit-optimize (gp_minimize)
- Based on previous predicted minimum mass and moderator ratio, narrow optimization search,
 - Mass and moderation ratio between +/- 10% minimum values.
 - Set number of optimizer evaluations (used 50).
 - Minimization function:

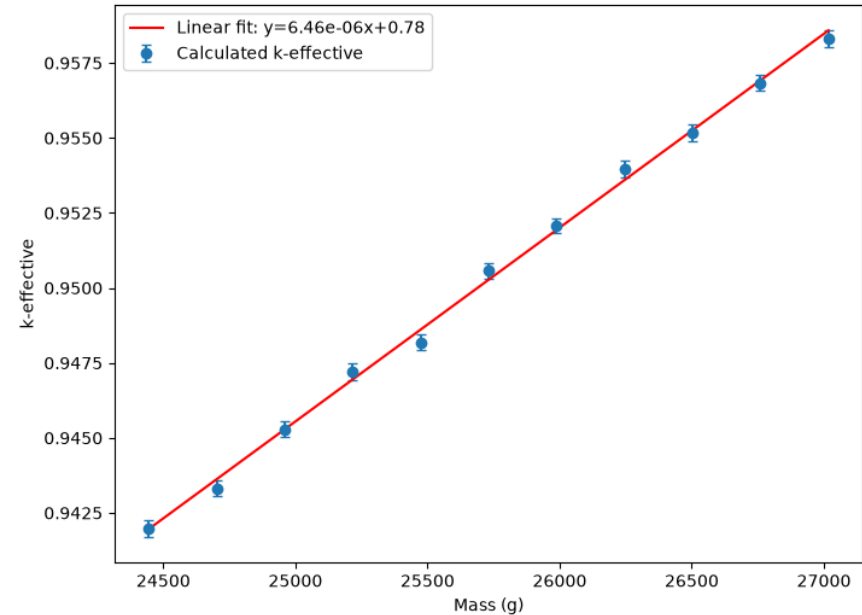
$$\text{Mass} \times (1 + A|k_{\text{calc}} - k_{\text{target}}|)$$

- A is a positive multiplier that enhances the difference in calculation and target k_{eff} (used 10).
- Production MCNP6 calculations (~50 pcm statistical uncertainties).



Sensitivity Study: Step 4 in Finding Target Values

- Using the minimum value found in the optimization process, perform a linear fit to the value. For example,
 - Fix the moderation ratio to the value found in optimization
 - Vary the mass and linearly fit k_{eff} as a function of mass
 - Coefficients translated to $k_{\text{eff}}/\text{mass}$ sensitivity
- Use this linear function to find final minimum mass.
- Production MCNP6 calculations (~50 pcr statistical uncertainties)



Final Calculation: Step 5 in Finding Target Values

- Use final minimum mass and moderation ratio from sensitivity study.
- Run MCNP6 with enough histories to obtain k_{eff} with ~10 pcm statistical uncertainty.
- Initial result from optimizer:

Initial optimized mass (g) = 25537.71
Moderator ratio = 38.86
k-effective = 0.94916 +- 0.00027

- Final result after sensitivity study:

Final optimized mass (g) = 25688.92
Moderator ratio = 38.86
k-effective = 0.95025 +- 0.00010



Next Steps



Next Steps

- “Raw values” for $k_{\text{eff}}=1.0$, 0.95 have been computed with MCNP6.3.1 using ENDF/B-VIII.0.
 - ENDF/B-VII.1 and ENDF/B-VIII.1 may be considered.
- Need to refine the search workflow and algorithms
 - Balance of computational cost and result robustness.
 - Refine the current Gaussian Process implementation.
 - Will look at other prediction/minimization algorithms (e.g., differential evolution).
- Need to compute “best estimate” values by considering calculational bias, nuclear data uncertainties, etc.
 - Likely use benchmarks and covariances from Whisper to identify similar benchmarks.
 - Likely use generalized linear-least squares (GLLS) approach and/or machine learning approach (e.g., Random Forest) for bias estimation.



Questions?



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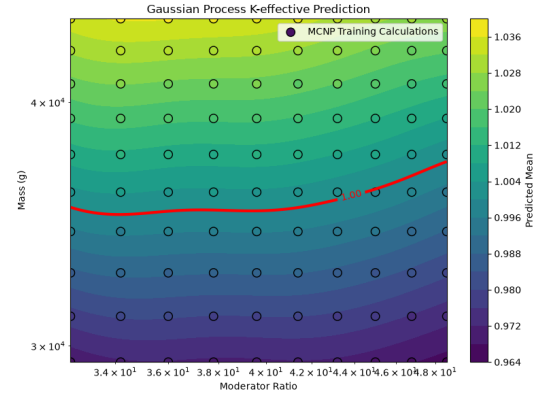
Extra Slides



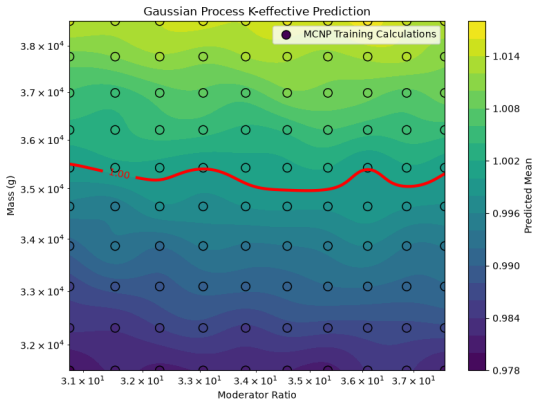
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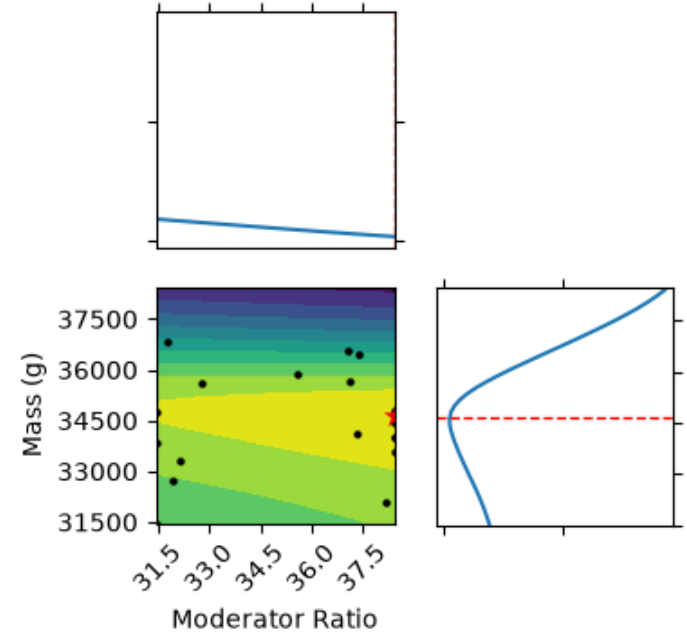


Optimization: Step 3 in Finding Target Values

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 - Minimization criteria:

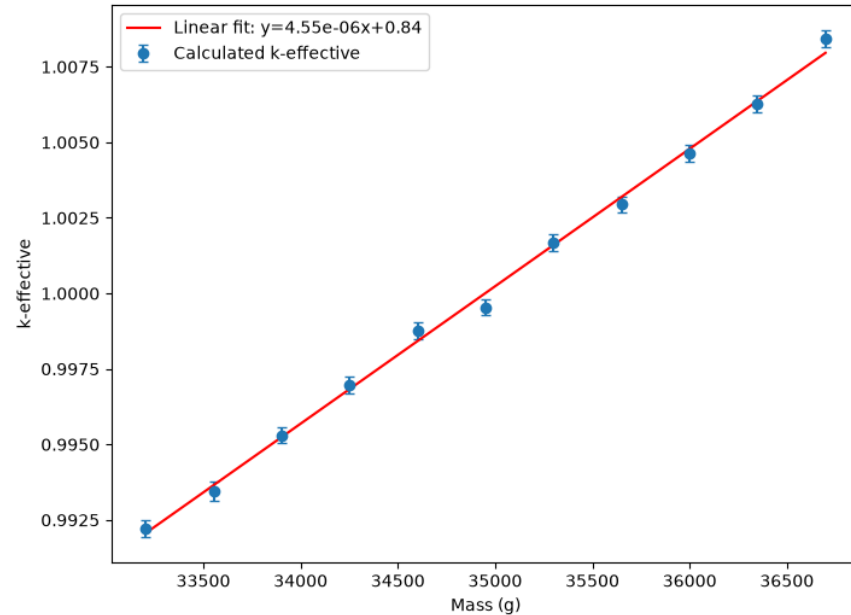
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Sensitivity Study: Step 4 in Finding Target Values

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Final Calculation: Step 5 in Finding Target Values

- Use final minimum mass and moderation ratio from sensitivity study.
- Run MCNP6 with enough histories to obtain k_{eff} with ~ 10 pcm statistical uncertainty.
- Initial result from optimizer:

Initial optimized mass (g) = 34799.92
Moderator ratio = 36.67
k-effective = 0.99950 +- 0.00029

- Final result after sensitivity study:

Final optimized mass (g) = 34948.32
Moderator ratio = 36.67
k-effective = 1.00011 +- 0.00010

