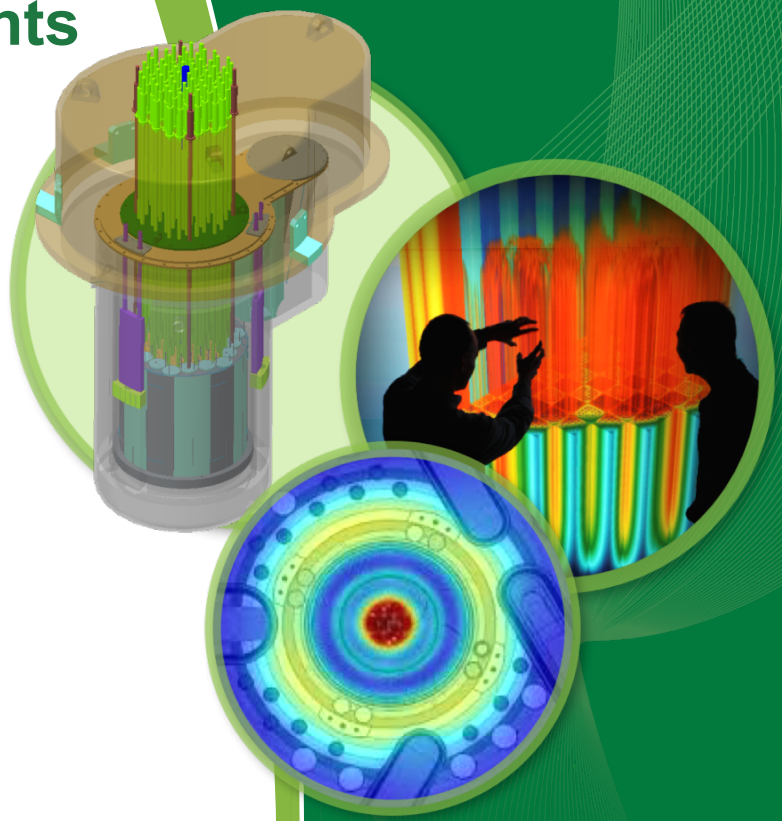
Implementation of Resonance Parameter Sensitivity Coefficients Calculation in CE TSUNAMI-3D

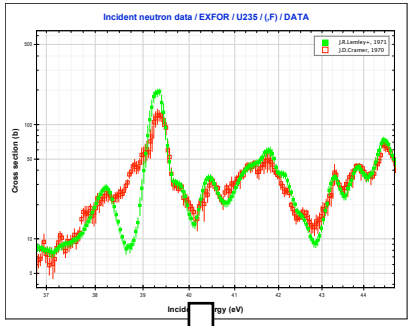


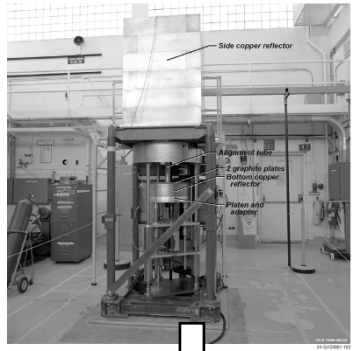
Vladimir Sobes, Chris Perfetti (ORNL)

Abdulla Alhajri (MIT)

Project History

- V. Sobes: PhD dissertation (2013) at MIT developed coupling capability for resonance parameter adjustment based on integral experiments
- Production level code SAMINT, released with SAMMY8.1 nuclear data evaluation code
- Abdulla Alhajri, MIT, PhD candidate summer project with V. Sobes and C. Perfetti at ORNL: Implementation of Resonance Parameter Sensitivity Coefficients Calculation in CE TSUNAMI-3D





SAMMY

ENDF

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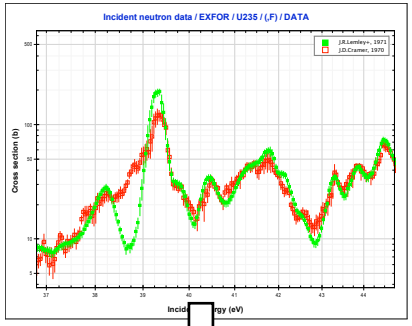

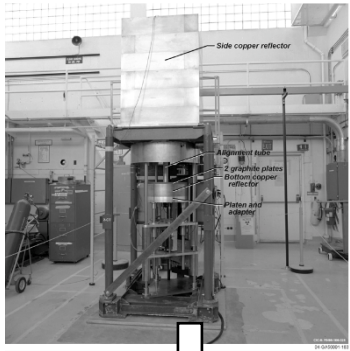

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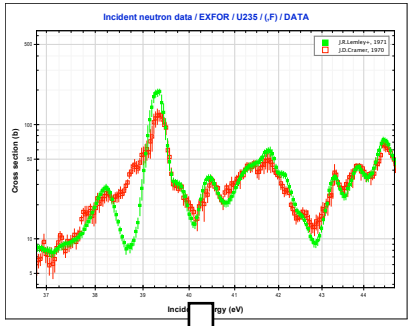
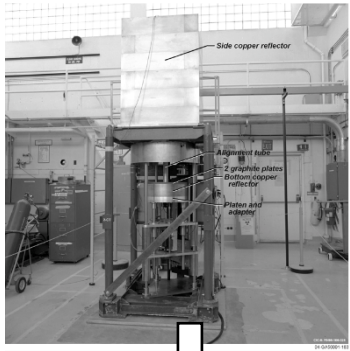


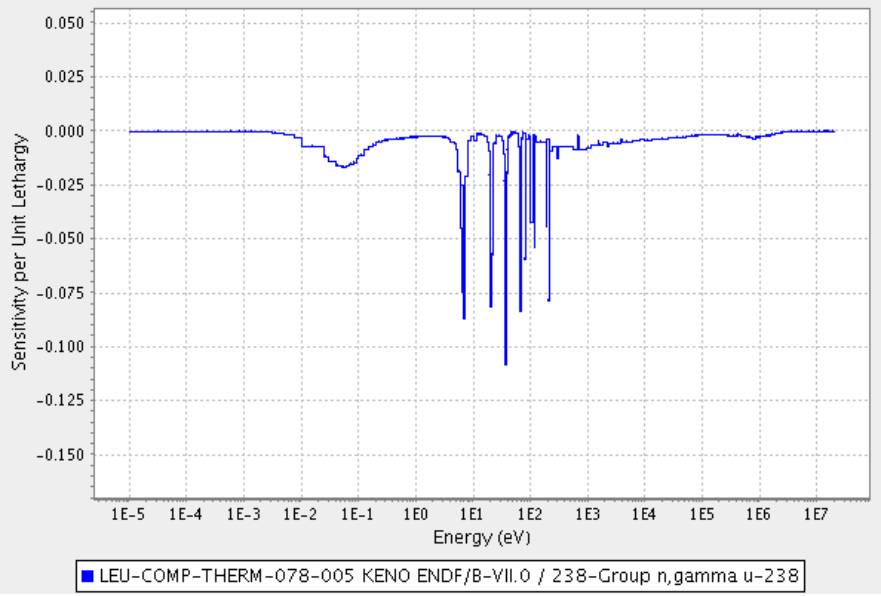


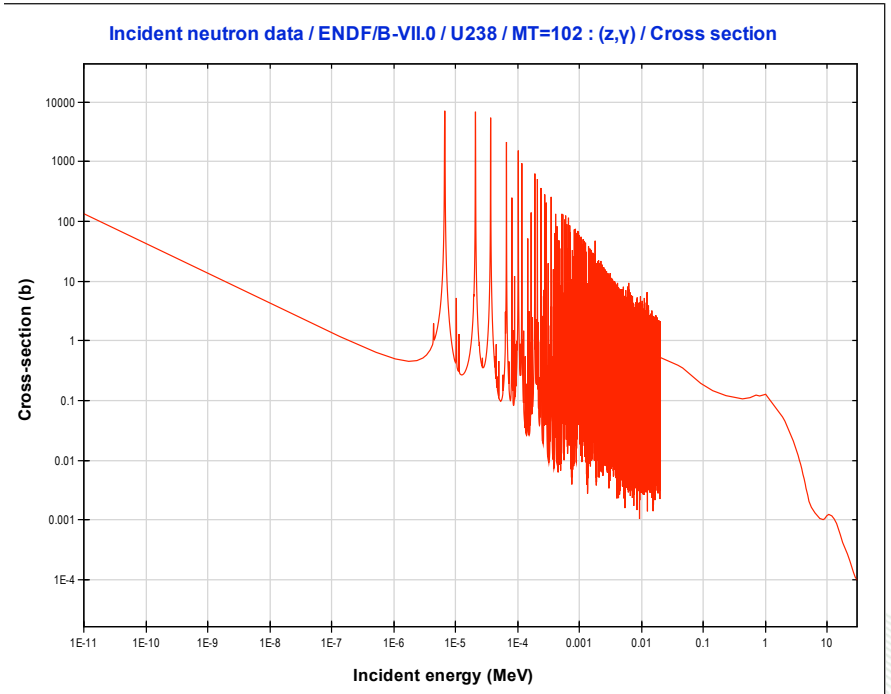
SAMMY

ENDF

Sensitivity Coefficient Calculation in the Resolved Resonance Region

- Calculation of sensitivity coefficients in the resonance region requires many energy bins to *resolve* individual resonances
- For most isotopes, all of the reaction cross sections in the resonance region are defined by resonance parameters
- For SAMINT, it is necessary to generate k_{eff} sensitivities on a dense energy grid and then post-process to get resonance parameter sensitivities
- Instead of *post-processing,* we implement resonance parameter sensitivity calculations *on the fly*





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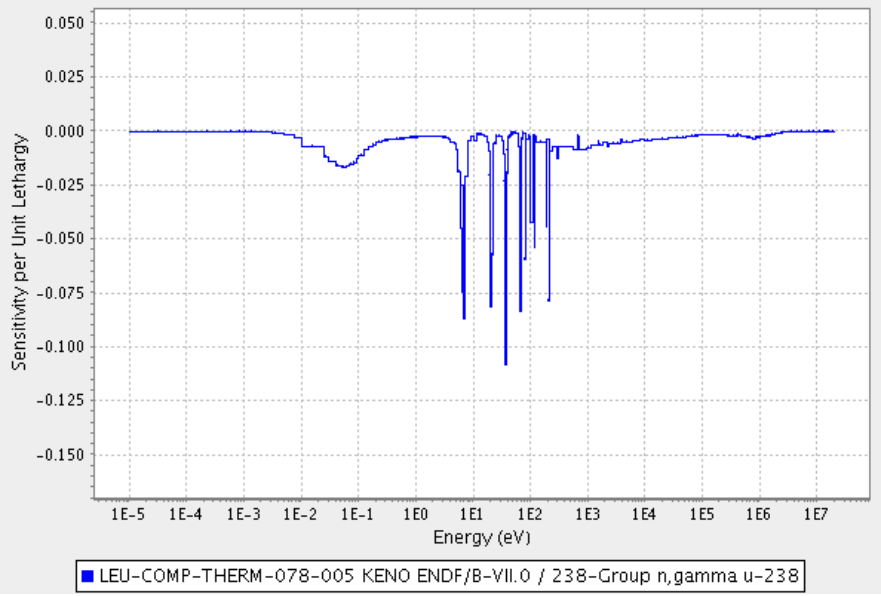

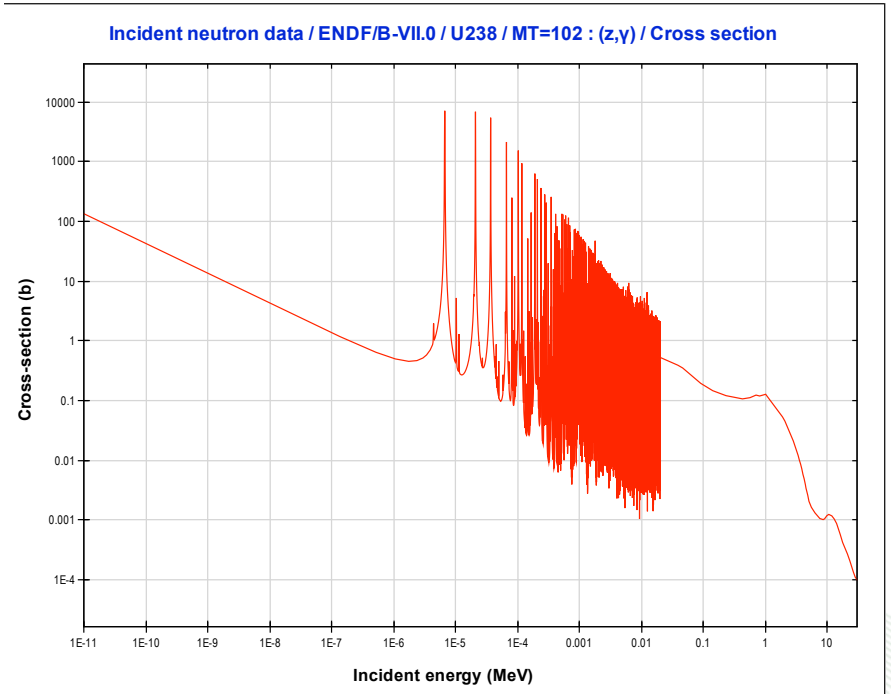

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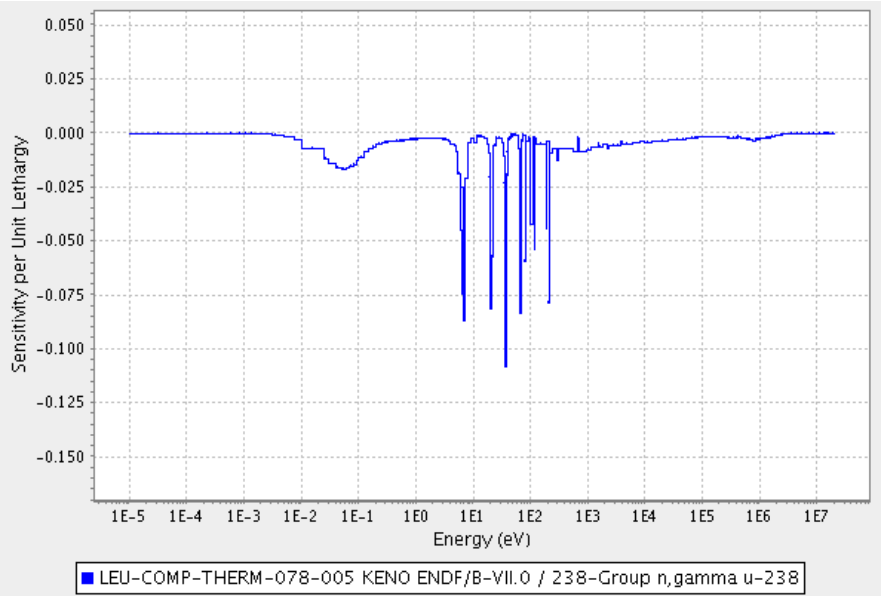

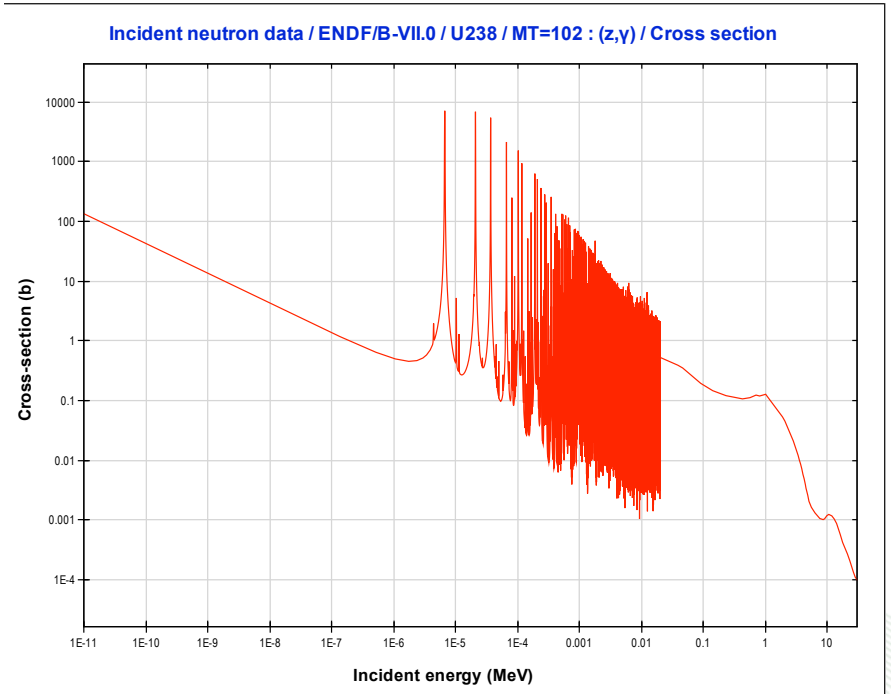

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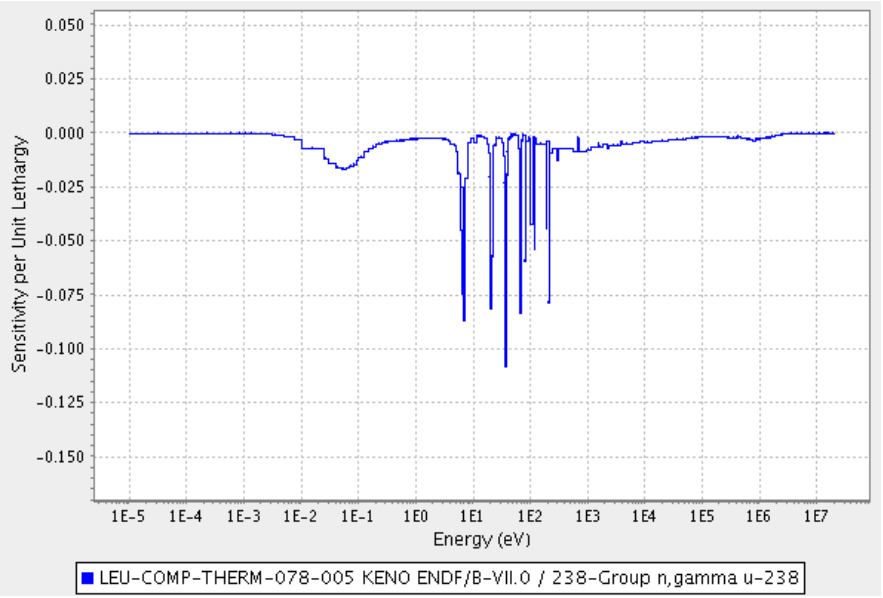
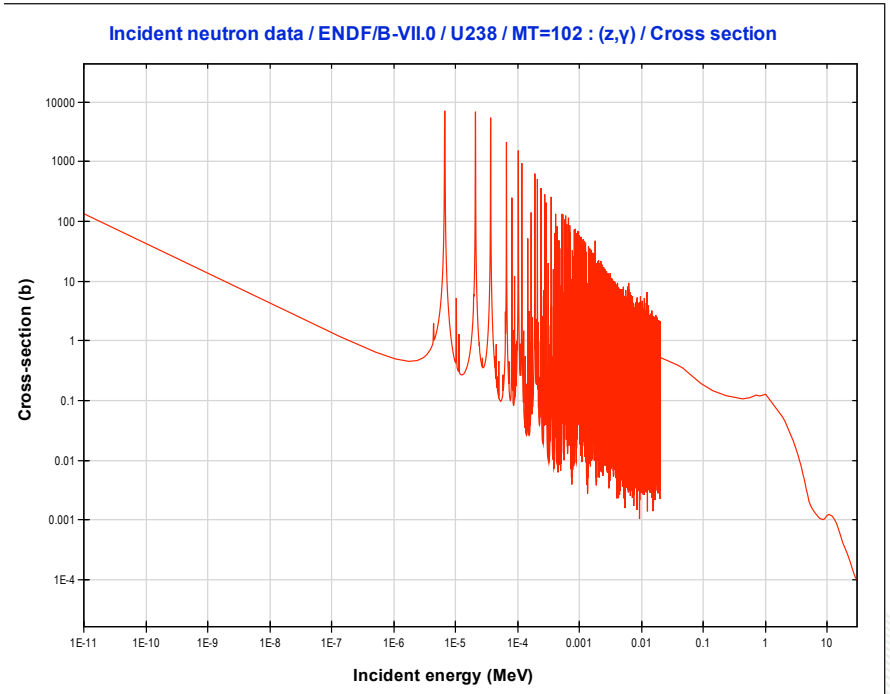
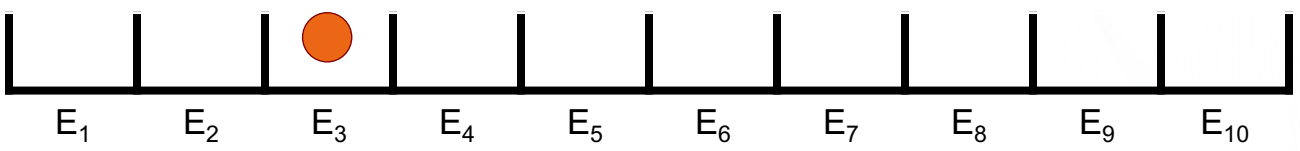




Cross Section Sensitivity in CE TSUNAMI-3D

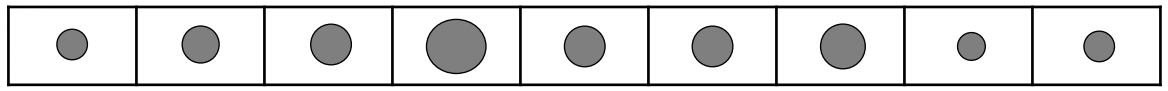
S_{σ}^{k}

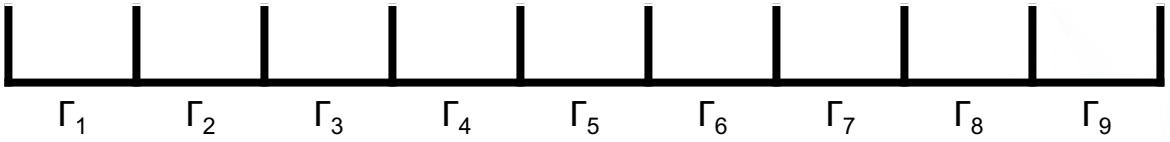


Resonance Parameters Sensitivities in CE TSUNAMI-3D

S_σ^k

x $\frac{\partial\sigma/\sigma}{\partial\Gamma/\Gamma}$





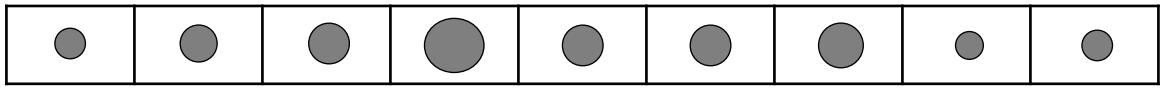
Replaced cross section energy bins with resonance parameter bins

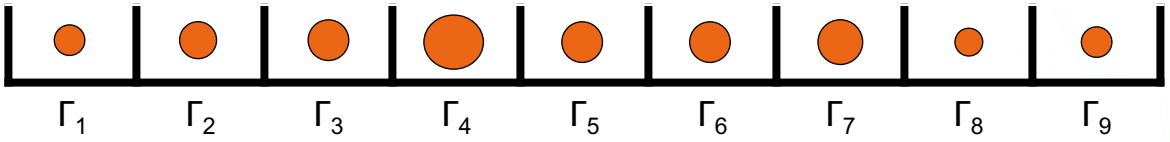
Resonance Parameters Sensitivities in CE TSUNAMI-3D (continued)

$$S_\sigma^k$$

$$S_\Gamma^k = S_\sigma^k \frac{\partial\sigma/\sigma}{\partial\Gamma/\Gamma}$$

x $\frac{\partial\sigma/\sigma}{\partial\Gamma/\Gamma}$





Advantages of On-the-Fly Calculation: Better Physics, Less Memory

Resonance Parameter Sensitivity Coefficients in TSUNAMI

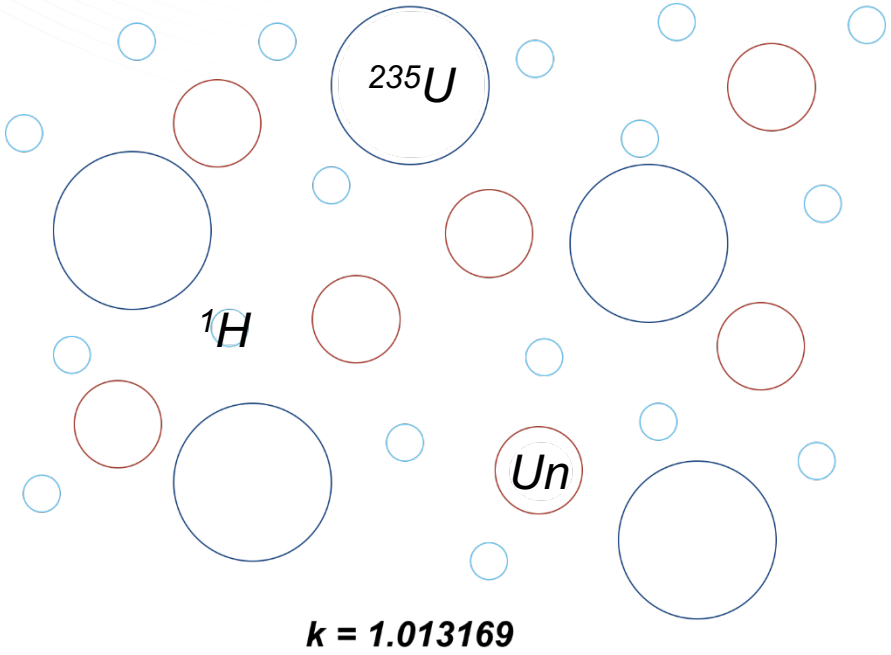
- Continuous energy physics
- Calculate resonance parameter derivative on the fly
- Constant memory requirement: number of resonance parameters

SAMINT Implementation

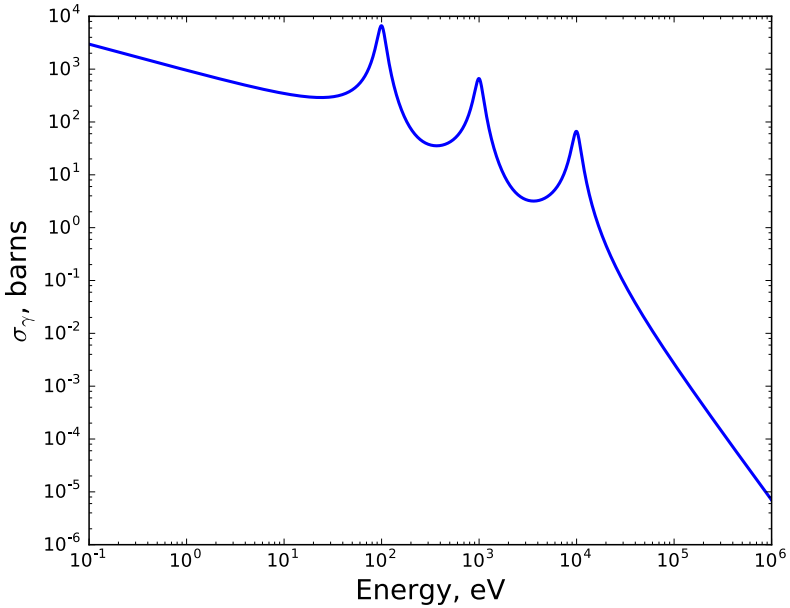
- Need an ultra-tight grid in energy
- Precompute resonance parameter derivatives and save: costly for multiple isotopes and reactions
- Memory and runtime change with fidelity, number of reactions, and isotopes

Direct Perturbation Validation

Infinite Homogeneous System



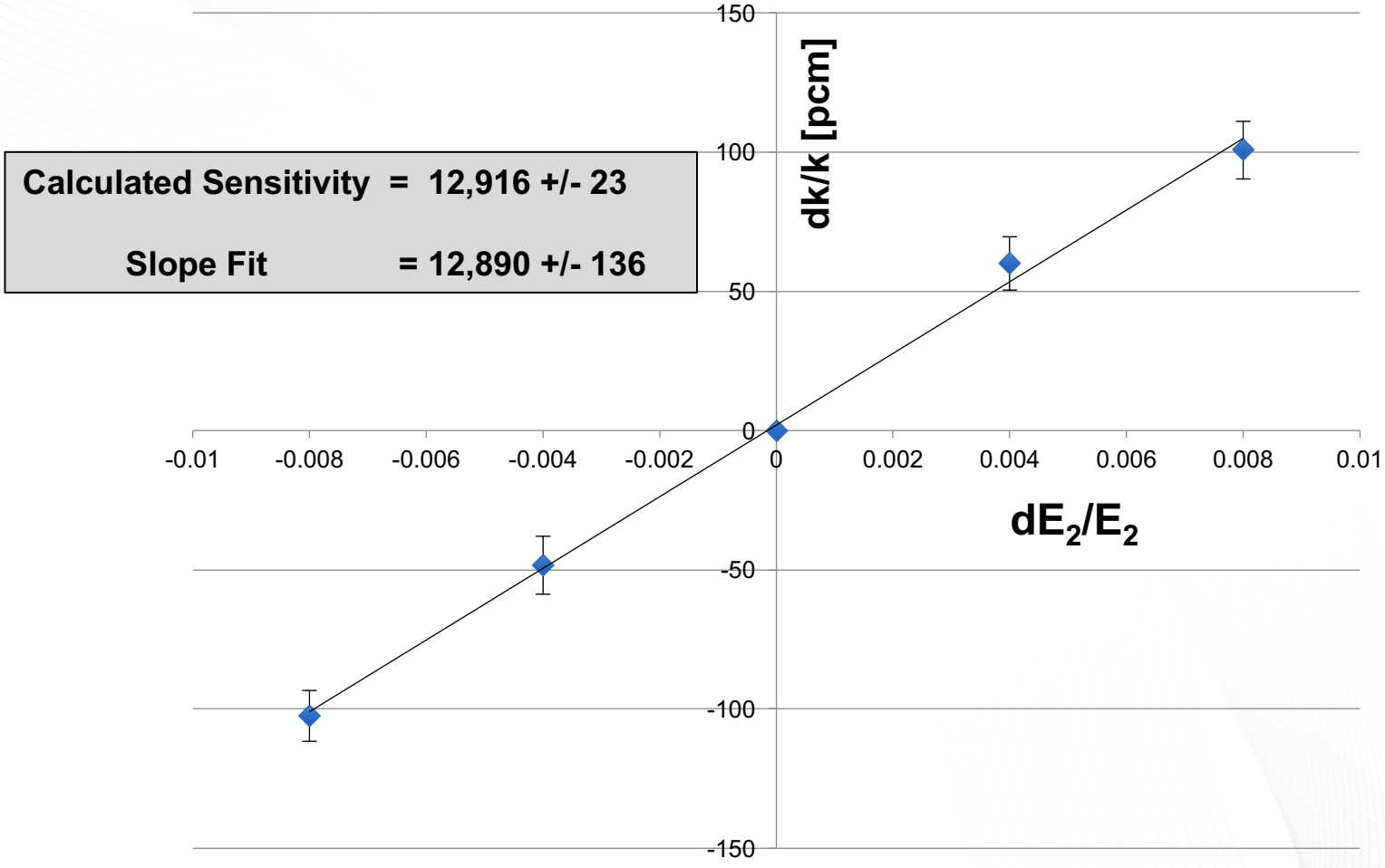
Unobtainium (Un)



Compute Resonance Parameter Sensitivities for Unobtainium

Resonance Parameter	Value [eV]	$\frac{\partial k/k}{\partial \Gamma/\Gamma}$	Uncertainty
E_1	100	0.034	0.000013
Γ_n^1	10	-0.033	0.000018
Γ_γ^1	10	-0.033	0.000041
E_2	1000	0.129	0.000233
Γ_n^2	100	-0.062	0.000019
Γ_γ^2	100	-0.062	0.000045
E_3	10000	0.093	0.000192
Γ_n^3	1000	-0.031	0.000013
Γ_γ^3	1000	-0.031	0.000026

Direct Perturbation Validation



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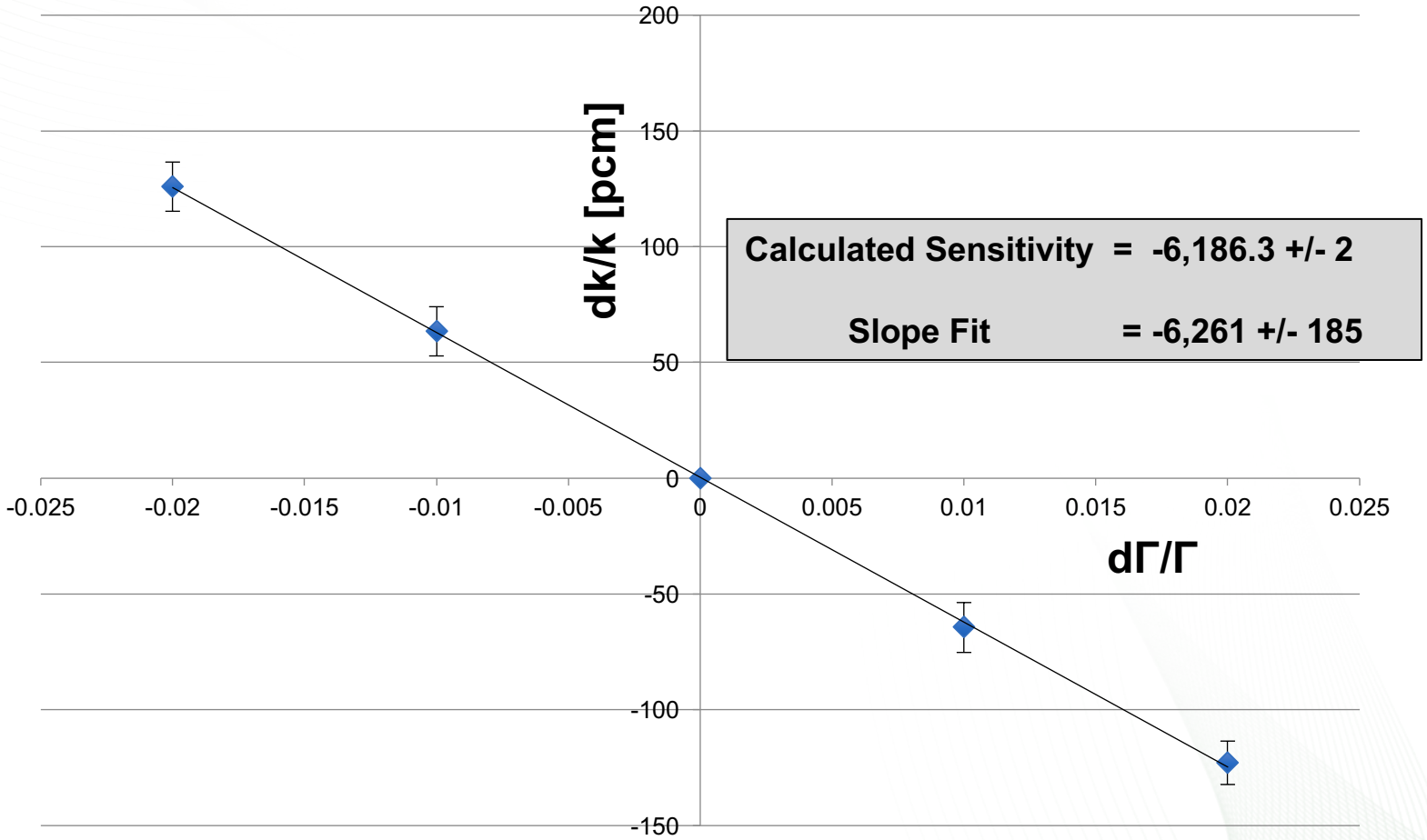

Future work (MIT PhD Thesis)

1. Full implementation in CE TSUNAMI-3D
2. Investigate run time reduction aspirations due to improved Monte Carlo statistics
3. Implement resonance parameter sensitivities through angular distributions
4. Pole cross section formalism implementation