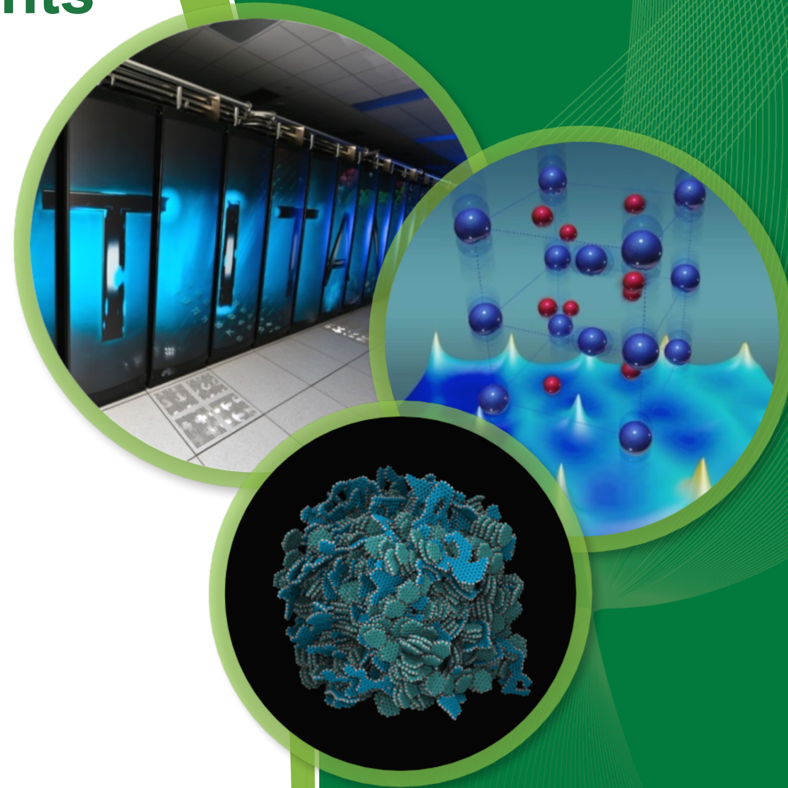
Implementation of Resonance Parameter Sensitivity Coefficients Calculation in CE TSUNAMI-3D



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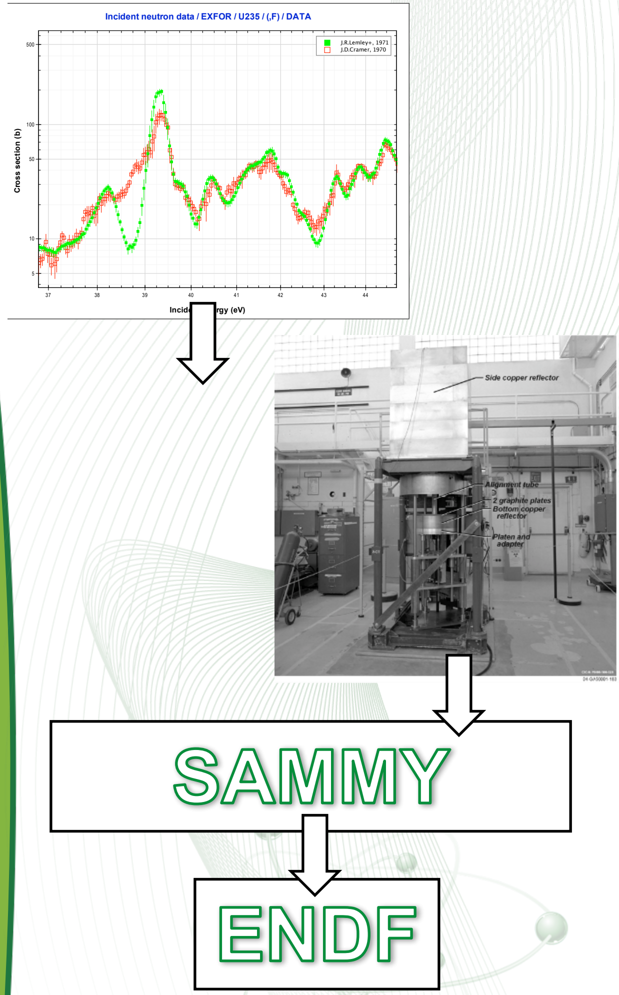
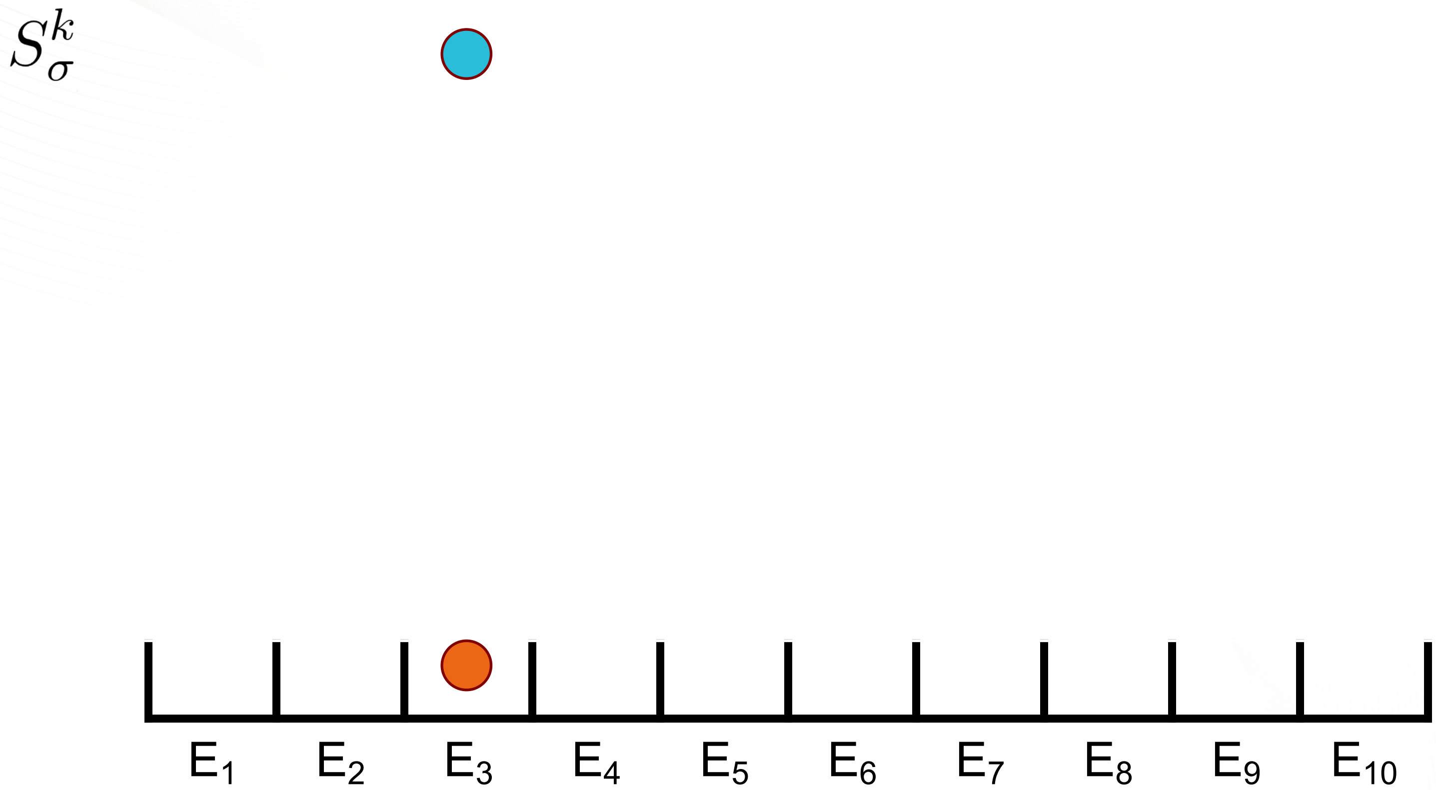
Project History

- V. Sobes Ph.D. dissertation (2013) at MIT developed coupling capability for resonance parameter adjustment based on integral experiments funded by US DOE NCSP.
- Presented at SG-39 December 2015.
- Production level code SAMINT, released with SAMMY8.1 (2016) nuclear data evaluation code.
- Manuele Aufiero, presents CE adjustment capability at SG-39 meeting, May, 2016
- Abdulla Alhajri, MIT, Ph.D. candidate summer project with V. Sobes, C. Perfetti at ORNL: Implementation of Resonance Parameter Sensitivity Coefficients Calculation in CE TSUNAMI-3D



Cross section sensitivity in CE TSUNAMI-3D



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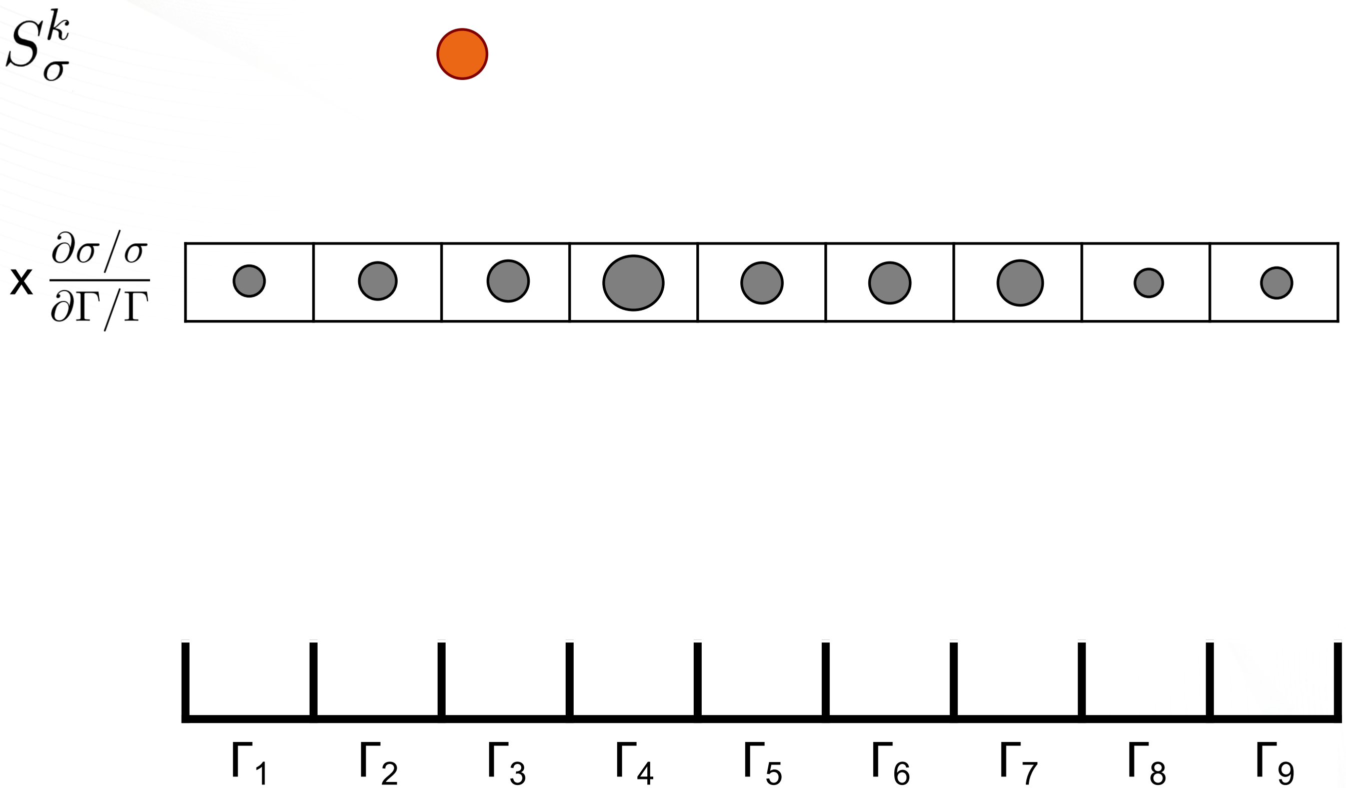
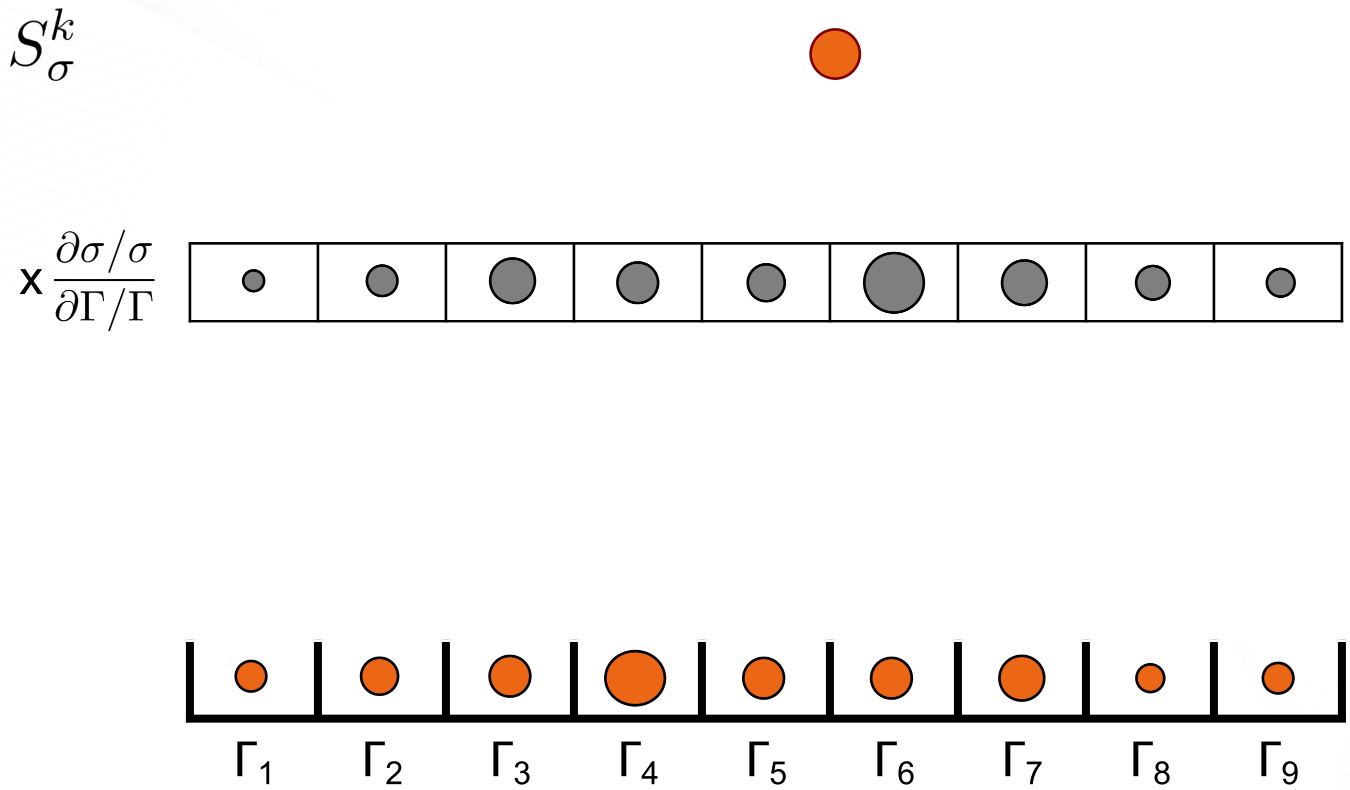
New implementation in CE TSUNAMI-3D



Replaced cross section energy bins with resonance parameter bins

Implemented in CE TSUNAMI-3D



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

Advantages of On-the-fly Calculation: Better Physics

Res. Par. Sensitivity Coefficients in TSUNAMI

- Continuous energy physics
- Calculate resonance parameter derivative on-the-fly
- Constant memory requirement: number of resonance parameters
- Allows for on the fly temperature dependence
- Great for multi-physics coupling

SAMINT Implementation

- Need an ultra-tight grid in energy
- Precompute resonance parameter derivatives and store: costly for multiple isotopes and reactions
- Memory and runtime change with fidelity, number of reactions and isotopes
- Derivatives must be pre-computed and stored at predetermined temperatures

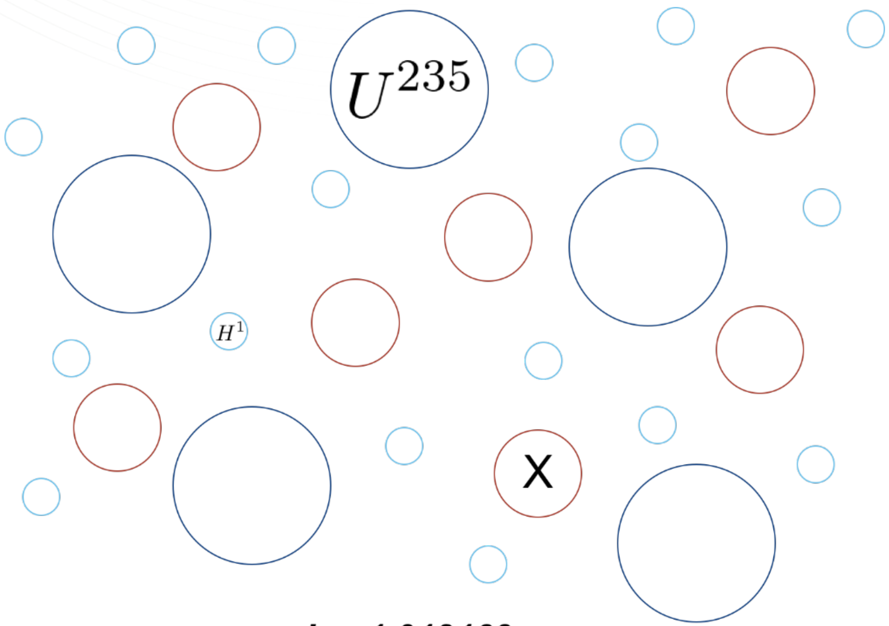
Pole cross section formalism

$$\sigma(E) = \frac{1}{E}\Re\sum_i \frac{r_i}{p_i - \sqrt{E}}$$

Doppler Broadening can now be performed analytically, this is a massive performance advantage!

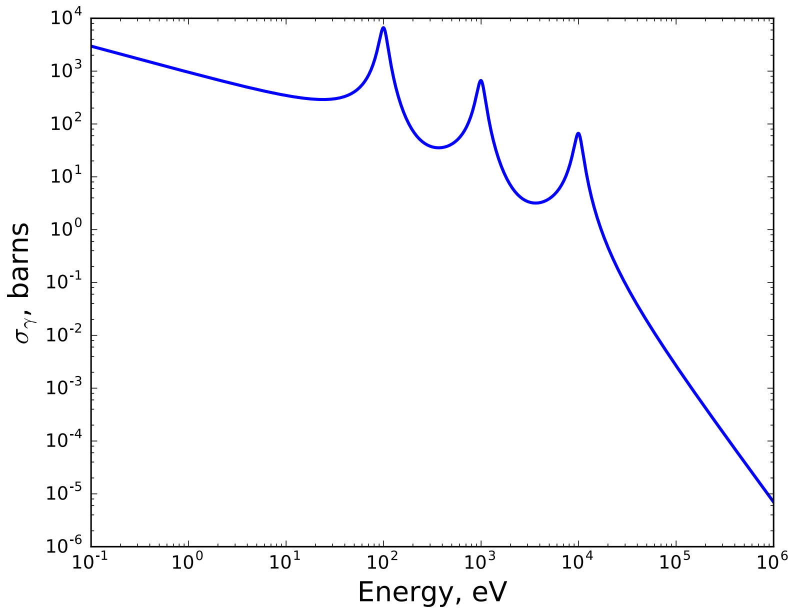
Direct Perturbation Validation

Infinite Homogeneous System



k = 1.013169

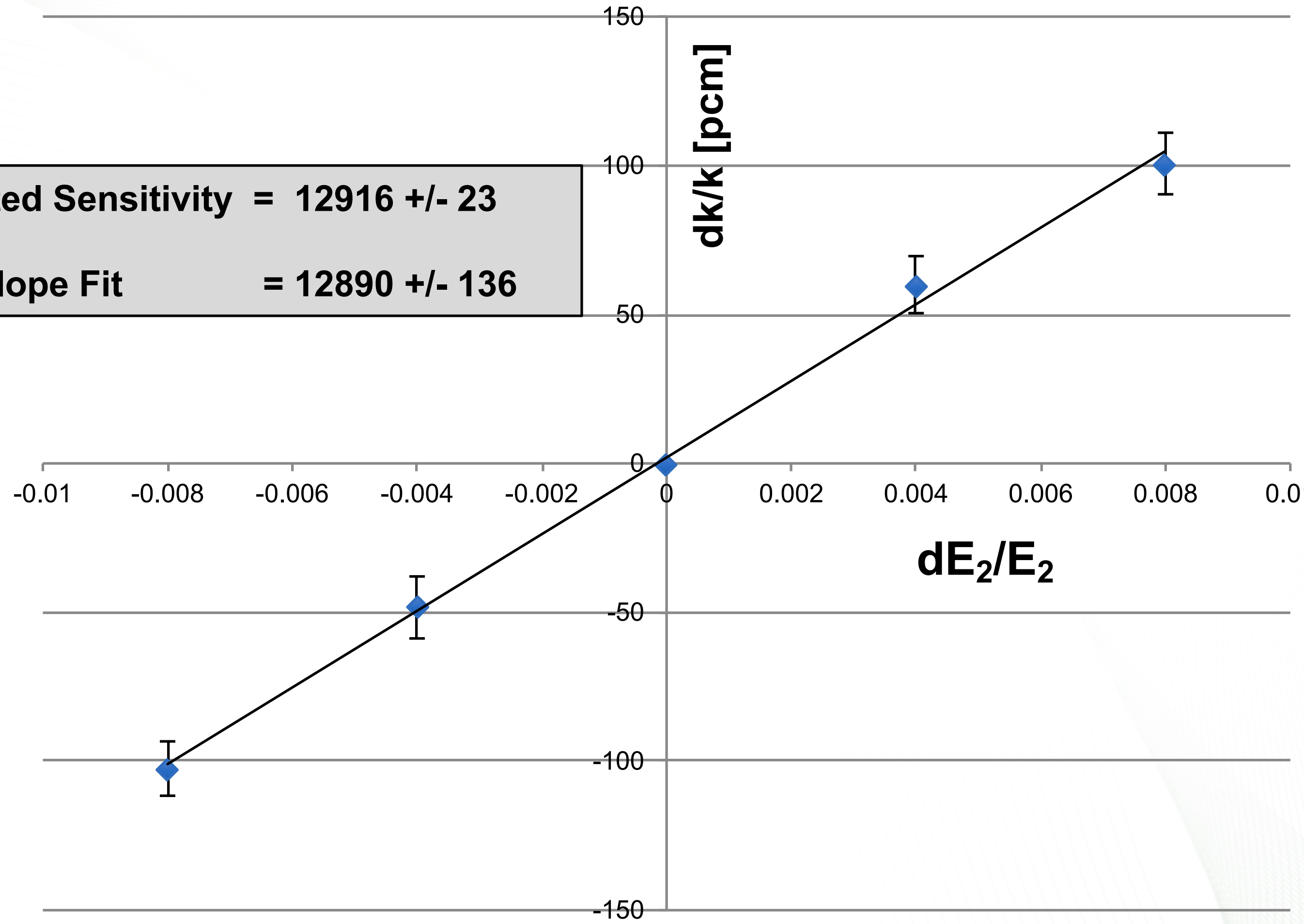
Isotope X



Compute resonance parameter sensitivities for isotope X

Resonance Parameter	Value [eV]	$\dfrac{\partial k / k}{\partial \Gamma / \Gamma}$	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



Calculated Sensitivity = 12916 +/- 23

Slope Fit = 12890 +/- 136

Compute resonance parameter sensitivities for isotope X

Resonance Parameter	Value [eV]	$\frac{\partial k / k}{\partial \Gamma / \Gamma}$	Uncertainty
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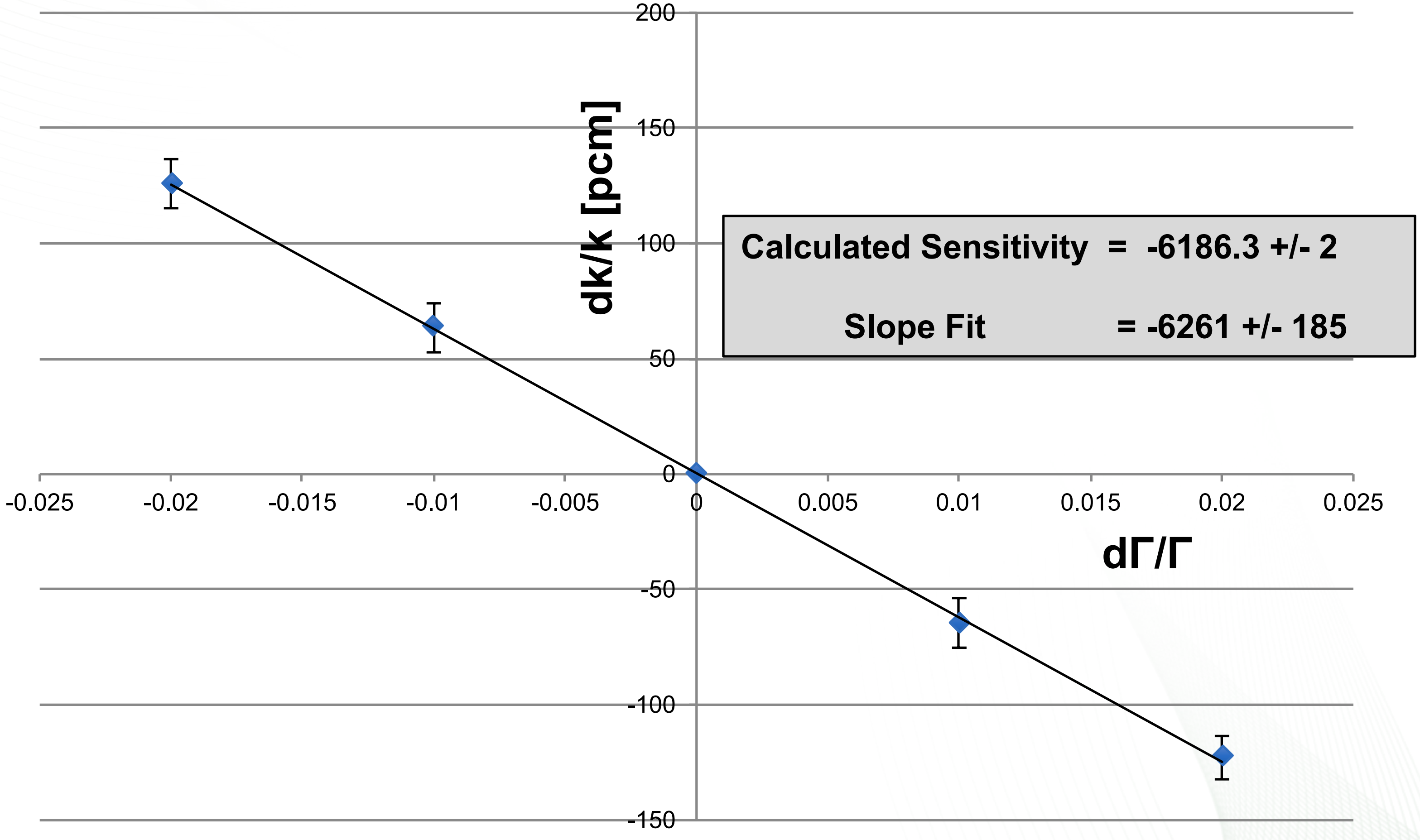

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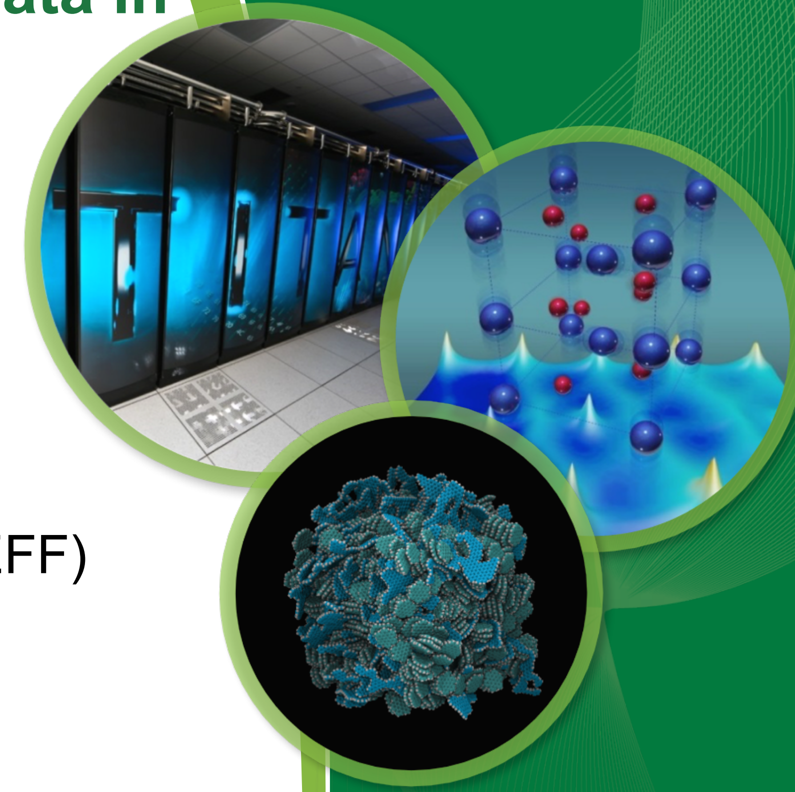
Future work

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

WPEC sub-group proposal: “Investigation of Covariance Data in General Purpose Nuclear Data Libraries”



Subgroup Monitor:

Cyrille de Saint Jean, CEA, France, (JEFF)

Subgroup Coordinator:

Vladimir Sobes, ORNL, USA, (ENDF)

WPEC sub-group proposal

(Cyrille de Saint Jean (CEA, France) and Vladimir Sobes (ORNL, USA))

Title:

Investigation of Covariance Data in General Purpose Nuclear Data Libraries

Justification for a Subgroup

The motivation for the subgroup is to bring together the international covariance community to understand how the covariance data can be so different between the different evaluated nuclear data files, ENDF, JEFF, JENDL, CENDL, etc., while the mean values (cross sections, nu-bar, etc.) are generally very similar. Many questions have emerged from the groups applying covariance data for analysis, such as the Working Party on Nuclear Criticality Safety (WPNCS) Expert Group on Uncertainty Analysis for Criticality Safety Assessment (UACSA), on how the use of different covariance libraries (e.g. ENDF, JEFF, JENDL, etc.) affect uncertainty quantification and similarity assessment. Further, significant differences in covariance libraries lead to differences in the adjustment of parameters for fast reactors, which is an important topic for WPEC sub-group (SG) 39.

The CIELO project, WPEC SG-40, established an international effort of nuclear data evaluators from different nuclear data projects to provide nuclear data evaluations that will be consistently accepted by all major nuclear data projects. This work has certainly driven the progress towards minimizing the disagreement in the mean values (cross sections, nu-bar, etc.) between different nuclear data libraries. However, with that project coming to a close the coming year, there has not yet been a concentrated effort on providing consistent covariance evaluations across the different nuclear data libraries. The maturity of the nuclear data evaluation process is such, at this time, that it is warranted to create an international collaboration on cross section covariance evaluation methodologies.

This sub-group will be tasked with the goal to investigate covariance data for a broad range of system types, not just fast reactors as in the focus of WPEC SG-39. This sub-group will leverage the work of previous sub-groups which investigated the generation of covariance data for in specific physical regions, such as WPEC SG-24 and SG-36, which focused on evaluations of fast neutron region and the resolved resonance region as well as WPEC SG-42 which focused on the evaluation and covariance generation for thermal scattering. This sub-group will focus its attention on providing guidance to the international community on methods for systematic and consistent evaluation of covariance data for the whole energy range, paying special attention to energy domain interface (resolved resonance/unresolved resonance/continuum). The group will also deliver examples of the application of the proposed methodology on a few selected isotopes. The ultimate goal of the subgroup is to provide an overview of the best practices of how to generate more consistent covariance data sets.

Subgroup Monitor:

Cyrille de Saint Jean, CEA, France, (JEFF)

Subgroup Coordinator:

Vladimir Sobes, ORNL, USA, (ENDF)

Subgroup Participants

The persons listed below already expressed some interests in the proposed activities, pending confirmation by the data projects and/or their home institutes.

ENDF	B. Beck (LLNL), C. Mattoon (LLNL), E. Jurgenson (LLNL), M. Zerkle (NNL), D. Barry (NNL), D. Brown (BNL), M. Herman (BNL), D. Smith (ANL, retired), B. Rearden (ORNL), M. Dunn (ORNL), M. Williams (ORNL), D. Wiarda (ORNL), K. Guber (ORNL), P. Talou (LANL), D. Neudecker (LANL), M. White (LANL), M. Chadwick (LANL), G. Palmiotti (INL), Y. Danon (RPI)
JEFF	G. Noguere (CEA), P. Archier (CEA), E. Bauge (CEA), L. Leal (IRSN), S. Pignet (IRSN), S. Evo (IRSN), E. Letang (IRSN), W. Haeck (IRSN), E. Ivanov (IRSN), Dimitri Rochman (PSI), T. Ivanova (NEA), O. Cabellos (NEA), P. Schillebeeckx (JRC), M. Salvatores (Consultant), D.H. Kim (KAERI), R. Mills (NNL), Helmut Leeb (TU Wien, Atominstitut)
JENDL	O. Iwamoto (JAEA), G. Chiba (Hokkaido U.)
BROND	A. Ignatyuk
CENDL	Z. Ge, X. Ruirui
IAEA-NDS	Roberto Capote
Other (non-NEA)	?

Project Definition and proposed activities

The implications for the propagation of nuclear data uncertainty through current modelling and simulation capabilities to the safety of nuclear installations around the world justify the creation of a new sub-group. An international collaboration through a NEA/WPEC subgroup will be essential for leveraging efforts allowing the sharing of information needed for achieving the project goal.

The project will be divided in the following phases:

I) Evaluation of the differences between discrepant covariance data evaluations in different evaluated nuclear data libraries
II) Assessment of the methodologies for generating covariance data utilized by the different nuclear data projects;
III) Documentation and evaluation of the current state-of-the-art methodologies for covariance data generation;
IV) Discussion of the representation and interpretation of nuclear data uncertainty (covariance) in evaluated nuclear data files;
V) Definition of a dedicated benchmark to test various covariance evaluation methodologies: this benchmark will propose a limited set of input data (microscopic/integral measurements) with detailed uncertainties description for one isotope to be defined (e.g. ^{239}Pu,^{235}U,^{238}U).

Relevance to Evaluated Data Files

Recommendations for generating nuclear data covariance evaluations.

Time Schedule and Deliverables

2017-2018: The first period will be devoted to collect and review existing evaluations and to identify the major discrepancies between different projects as well as the major issues driving the discrepancies in the propagated nuclear data uncertainties in applications.

2018-2019: The second period will be devoted to the exploration of systematic and consistent methodologies for generating covariance data.

2019-2020: The third period will address the representation of nuclear of data covariance in evaluated nuclear data files and their interpretation. Of particular interest will be the representation and interpretation of covariance data for non-cross section data (i.e. prompt neutron fission spectra, angular distributions, cross-correlations).

Detailed time schedule (preliminary version)

year	Period	activities
2017	May	Start of SG activities at the NEA: • Review of the motivation by WPNCS UACSA Expert group • Review of the previous work of WPEC SG-36, WPEC SG-39, WPEC SG-42
	May-June	Collect evaluated nuclear data files for discrepant covariance evaluations
	June- Dec.	Status/performance of available data
2018	Jan-May	Begin to put together justification for of existing covariance data
	May	Status of the one-year activity: • Review of the existing differences in the covariance in different evaluated nuclear data libraries • Review of the existing covariance generation methodology
	May-July	Collect justification for of existing covariance data
	July-Dec.	Collate report on current state-of-the-art covariance data generation methodology
2019	May	Status of the two-year activities: • Review of the systematic and consistent covariance generation methodologies • Discuss the representation and interpretation of nuclear data covariance in evaluated nuclear data files
	May-Dec.	Study of the effects of different representation of nuclear data covariance in evaluated nuclear data files
2020	Jan-May	Document the recommendations of the sub-group for covariance data representation in evaluated nuclear data files
	May	Status of the three-years activities • Proposal for a draft version of the final report that includes a review of a systematic and consistent methodologies for covariance evaluation and recommendations for nuclear data covariance storage and interpretation

Justification for a Subgroup

- How can the covariance data be so different while the mean values are generally very similar between different evaluated nuclear data files?
- Different covariance libraries affect uncertainty quantification and similarity assessment.
- CIELO project driven the progress towards minimizing the disagreement in the mean values but no dedicated work towards covariance.
- Previous WPEC Subgroup with specific energy regions/applications: SG-24 (fast energy region), SG-36 (RRR), SG-39, SG-42 (S(α,β)).

<u>This group:</u>

- Methods for systematic and consistent evaluation of covariance data for the entire energy range.
- Deliver examples of the application of the proposed methodology on a few selected isotopes.
- Ultimate goal: provide an overview of the best practices of how to generate more consistent covariance data sets.

Subgroup Participants (Tentative)

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BROND A. Ignatyuk

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Proposed activities

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