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Comparison of different Transport Solution Methodologies for fast Reactors Design and Cross Section Uncertainty Effects

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Summary first hour

- We will examine two problem
 - Takeda 4 benchmark
 - A full 3d fast reactor assembly
- We will analyze the behavior on this benchmark of the following solution algorithms

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- Second order PN
- Second order SN
- -MOC



Takeda 4 Benchmark Description



Takeda 4 Benchmark Description (2)

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- It is a 4 energy group benchmark
- 1/12 core symmetry
- Reference K_{eff} values (Monte Carlo method)
 - Control rod half inserted: 0.98340 ± 0.00039
 - Control rod fully inserted: 0.88001 ± 0.00038
 - Control rod withdrawn: 1.09515 ± 0.00040

Qualitative Considerations

- It is a homogenized problem:
 - Discontinuity in angle should be mild
 - We expect a boundary layer effect surrounding the control rod

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- No void, therefore no problem using second order methods
- Spherical harmonics methods should be more suited for this analysis
- We expect an easier task when control rod is out with respect when in
- It is a relative small reactor with a strong heterogeneity due to the control road therefore diffusion should not be sufficient



Flux Shapes at middle Plane Control Road in (Gr 1, & 2)



- From left to right, flux solution for the 2nd to the 1st energy group
- The fast energy spectrum neutron are generated by fission in the interior part of the core



Flux Shapes at middle Plane Control Road in (Gr 1, & 2)





- From left to right, flux solution for the 4th to the 3rd energy group
- Slower neutron are produced by slowing down in the shield and completely *eat* in the core and control rod position



Space Angle Convergence





What were the Numbers of This Simulation

- 1/12 symmetry
- 6.5 millions of element
- 72 angular directions over 4π
- ~55 trajectory intersecting each region for each fixed direction
- 16*10⁹ total unknowns
- 26 million of scalar unknown
- 552 Gb
- 70 processor
- 6.3 hours

Wrong!!

This is what happen when killing a fly with a tank

A nodal PN second order code would have solved in a couple of minute on one processor



How the PN Second Order Goes?

	Control Rod In		Control	Control Rod Half		Control Rod Out	
	DOF		DOF		DOF		
	19079	24362	19079	24362	19079	24362	
P 1	-0.02840	-0.02720	-0.02583	-0.02464	-0.02180	-0.02072	
P 3	-0.00447	-0.00310	-0.00330	-0.00210	-0.00210	-0.00105	
P 5	-0.00240	-0.00096	-0.00152	-0.00030	-0.00071	0.00033	
P 7	-0.00201	-0.00053	-0.00111	0.00012	-0.00034	0.00071	
P 9	-0.00190	-0.00041	-0.00099	0.00025	-0.00022	0.00084	
P 11	-0.00187		-0.00095		-0.00017		

Number of Unknown

• From this morning we know P9 is equivalent to

(N+1)N/2 = (9+1)9/2 = 45

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... angular moments

- times 4 energy groups
- times 24362 DOF
- Total ~4.3 millions
- There is 3 order of magnitude in the number of unknown
- This is expected since MOC is discontinuous zero order



Fast Reactor Assembly Description



•9 energy group
•No reference value provided
•Only MOC solution

•We used 1/4 symmetry

Number of pins	217
Pin pitch, cm	0.9134
Outer radius of clad (cm)	0.4057
Inner radius of clad (cm)	0.3501
Fuel radius (cm)	0.3501
Assembly pitch (cm)	14.6850
Duct outer Flat-to-Flat Distance (cm)	14.2826
Duct inside flat-to-flat distance (cm)	13.6790
Lower reflector height (cm)	60, (0 <z<60)< td=""></z<60)<>
Active core height (cm)	84.41, (60 <z<144.41)< td=""></z<144.41)<>
Bonded plenum height (cm)	19.76, (144.41 <z<164.17)< td=""></z<164.17)<>
Gas Plenum height (cm)	28, (164.17 <z<192.17)< td=""></z<192.17)<>

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Qualitative Considerations

- It is not a core but if we look to the level of detail description it is a large case
- We may face angular discontinuities
- Sodium is much more transparent that many other material in nuclear reactor cores, we should aspect ray effect



Which Radial Mesh



11022 Elements

21944 Elements



Where we are in Angle-Axial-Radial Meshes

			Number of angular directions		
Axial layer	Radial meshes	Total meshes	18	72	288
25	3507	87675	1.32264	1.30716	1.30883
51	3507	178857	1.34131	1.33590	1.33645
51	11022	562122	1.34232	1.33692	1.33739*
51	21944	1119144	1.34254	1.33713*	
102	11022	1124244	1.34714		
153	11022	1686366	1.34797		



Power Axial Effects





Radial Power Profile Sensitivity to Mesh





Middle Plane Radial Cut Flux Profile for Group 1





Middle Plane Radial Cut Flux Profile for Group 4





Middle Plane Radial Cut Flux Profile for Group 9





Remarks on the Assembly Simulation

- Unfortunately I was not able to recollect the second order study for one pin that we perform with the second order PN so you have just to believe me...
 - surprising the larger difficulty was the modeling of the axial leakage. To correctly catch this effect we had to go up to P25.
 - P27 means 325 angular moment
 - This number looks close to the 288 direction that we used in the for the finest but we were satisfactory close already at 72
- Ray effect exists..



Questions??



Lets' move to Uncertainty from Nuclear Data

- *Few words on the adjoint sensitivity method*
- *Few words on the forward sampling techniques for sensitivity analysis*
- We will perform an interesting exercise
 - We consider the design of a fast reactor
 - Compute the uncertainties on few integral parameters with the adjoint method
 - Compute the uncertainties on few integral parameters with the forward method
 - *Compare the two methods*
- By the way this is a paper that is going to be presented next week at PHYSOR 2010 keep it as a private preview ©

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Definition of Sensitivity Coefficient

- Lets be *Q* any integral parameter characterizing a system (reactor neutronic integral parameter)
- Be σ_j input parameter for the simulation of the system (cross sections)
- Without any assumption on the system a first order approximation of the variation of *Q* could be expressed by

$$\delta Q/Q = \sum_{j} S_{j} \frac{\delta \sigma_{j}}{\sigma_{j}}$$

• Where the sensitivity coefficient S_i are defined by:

$$\mathbf{S}_{j} = \frac{\partial \mathbf{Q}}{\partial \boldsymbol{\sigma}_{j}} \cdot \frac{\boldsymbol{\sigma}_{j}}{\mathbf{Q}}$$

• On a practical not the index i runs over energy, isotope, and reaction type



Total Uncertainty: the Sandwich Formula

Let's try to make an example

- We take an input parameter that has a behavior (for example changing in time) that could be described by a two point gauss evaluation.
- If the system is linear than also the answer would be described by the answer at the two gauss point
- Similarly if the input parameter has a statistical distribution that could be expressed by its average value and its variance
- So the system response to the expected value of the input parameters $\overline{\sigma}_{i}$ gives the expected value of the response \overline{Q}
- The response to a perturbation of the input parameter equal to the square root of the variance $R_{\sigma_j}^2 = (\delta \sigma_j)^2$ gives the square root of the variance of the response R_o^2

Total Uncertainty: the Sandwich Formula (Cont.)

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• In a very simple case we would have:

 $R_{\varrho}^{2} = \left(\delta\sigma_{j}\right)^{2} \left(\mathbf{S}_{j}\right)^{2}$

• Some of the parameters are bounded each other (you can not vary one alone) simply due to physics they express. We account for this using the covariance matrix D

$$D = \begin{bmatrix} E\left[\left(\sigma_{1} - \overline{\sigma}_{1}\right)\left(\sigma_{1} - \overline{\sigma}_{1}\right)\right] & \cdot & E\left[\left(\sigma_{1} - \overline{\sigma}_{1}\right)\left(\sigma_{1} - \overline{\sigma}_{N}\right)\right] \\ \cdot & \cdot & \cdot \\ E\left[\left(\sigma_{1} - \overline{\sigma}_{1}\right)\left(\sigma_{N} - \overline{\sigma}_{N}\right)\right] & \cdot & E\left[\left(\sigma_{N} - \overline{\sigma}_{N}\right)\left(\sigma_{N} - \overline{\sigma}_{N}\right)\right] \end{bmatrix}$$

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Total Uncertainty: the Sandwich Formula (Final)

We place together the results so far

$$R_{Q}^{2} = \begin{bmatrix} S_{1} \\ \vdots \\ \vdots \\ S_{N} \end{bmatrix}^{T} \begin{bmatrix} E\left[\left(\sigma_{1} - \overline{\sigma}_{1}\right)\left(\sigma_{1} - \overline{\sigma}_{1}\right)\right] & \vdots & E\left[\left(\sigma_{1} - \overline{\sigma}_{1}\right)\left(\sigma_{1} - \overline{\sigma}_{N}\right)\right] \\ \vdots & \vdots & \vdots & \vdots \\ E\left[\left(\sigma_{1} - \overline{\sigma}_{1}\right)\left(\sigma_{N} - \overline{\sigma}_{N}\right)\right] & \vdots & E\left[\left(\sigma_{N} - \overline{\sigma}_{N}\right)\left(\sigma_{N} - \overline{\sigma}_{N}\right)\right] \end{bmatrix} \begin{bmatrix} S_{1} \\ \vdots \\ \vdots \\ S_{N} \end{bmatrix}$$



Now How to Compute the Sensitivity Coefficient?

- Sensivity Coefficient are computed in general by the Equivalent Generalized Perturbation Theory (GPT), (Gandini 1967)
- First of all a little bit of nomenclature, then a couple of example:

 $\Phi = \int \psi d\Omega$

Scalar flux

 $A\Phi = \frac{F\Phi}{K_{a}}$

Integrated homogenous transport equation

$$A * \Phi * = \frac{F * \Phi *}{K_{\text{eff}}}$$

 $A * \Phi * = F * \Phi * + S *$

Integrated homogeneous adjoin transport equation

Integrated in-homogeneous adjoin transport equation

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Reactivity Coefficient

- Reactivity coefficient are fundamental to reactor control.
- The describe how the reactor reactivity change between two different status
- Examples of reactivity coefficient are: temperature, void, expansion etc.

• Reactivity is defined by:
$$\rho = \frac{K_{eff}}{K_{eff}}$$

- The reactivity delta between two different status is: $\Delta \rho = \frac{1}{K_{\text{off}}} \frac{1}{K_{\text{off}}}$
- Where the K_{aff} satisfy respectively

$$A\Phi = \frac{F\Phi}{K_{_{eff}}} \qquad \qquad A_{_{p}}\Phi_{_{p}} = \frac{F_{_{p}}\Phi_{_{p}}}{K_{_{eff},p}}$$



Reactivity Coefficient Sensitivity Coefficient

- Now the question we want to answer to is: how much would change the reactivity difference between the two status if we would perturb the cross section *i*?
- It is possible to use the GPT theory to get the sensitivity coefficient for reactivity coefficient and has the form:

$$\mathbf{S}_{j} = \frac{\partial(\Delta\rho)}{\partial\sigma_{j}} \cdot \frac{\sigma_{j}}{\Delta\rho} = \frac{1}{\Delta\rho} \left\{ \frac{\left(\Phi_{P}^{*}, \sigma_{J,P} \Phi_{P}\right)}{\left(\Phi_{P}^{*}, F_{P} \Phi_{P}\right)} - \frac{\left(\Phi^{*}, \sigma_{J} \Phi\right)}{\left(\Phi^{*}, F \Phi\right)} \right\}$$

• Where we have used the following adjoint problem definitions:

$$A^{*} \Phi^{*} = \frac{F^{*} \Phi^{*}}{K_{eff}^{*}} \qquad A^{*} \Phi^{*} = \frac{F^{*} \Phi^{*}}{K_{eff}^{*}}$$

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Conclusion on the Adjoint Method

- If we want to consider the impact of the uncertainty of an array of cross section over a reactivity coefficient we have to:
 - Compute the adjoint and forward solution for the two different states
 - Evaluate the sensitivity coefficient for each cross section
 - Use the sandwich formula

$$A\Phi = \frac{F\Phi}{K_{eff}} \qquad A_{p}\Phi_{p} = \frac{F_{p}\Phi_{p}}{K_{eff,p}} \qquad A^{*}\Phi^{*} = \frac{F^{*}\Phi^{*}}{K^{*}_{eff}} \qquad A^{*}_{p}\Phi^{*}_{p} = \frac{F^{*}_{p}\Phi^{*}_{p}}{K^{*}_{eff,p}}$$
$$S_{j} = \frac{\partial(\Delta\rho)}{\partial\sigma_{j}} \cdot \frac{\sigma_{j}}{\Delta\rho} = \frac{1}{\Delta\rho} \left\{ \frac{\left(\Phi_{p}^{*}, \sigma_{j,p}\Phi_{p}\right)}{\left(\Phi_{p}^{*}, F_{p}\Phi_{p}\right)} - \frac{\left(\Phi^{*}, \sigma_{j}\Phi\right)}{\left(\Phi^{*}, F\Phi\right)} \right\} \qquad j = 1, \dots, N$$
$$R_{\lambda\rho}^{2} = \left[S_{j}\right]^{T} D\left[S_{j}\right]^{T}$$

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The Forward Sampling Method: Latin Hyper Cube

- The Latin Hypercube Sampling is a constrained Monte Carlo method
- Consider in general a response variable Y as a function of variables X₁, X₂, ..., X_k.
- Here Y represents, for example, an integral neutronic parameter and X_i the input cross sections
- Assuming the X_i are characterized by statistical distributions, the goal is to determine through Monte Carlo sampling over X_i, the statistical distribution of Y.
- Each realization of the random variables X_i requires calculation of Y by executing the neutronics simulation.



The Forward Sampling Method: Latin Hyper Cube (cont.)

• The probability distribution of each variable X_i is independently decomposed into *n* equally probably sub-domains and a sample value is selected within each sub-domain.



0.2	0.2	0.2	0.2	0.2
G I	H I	[]	J k	K L

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The Forward Sampling Method: Latin Hyper Cube (cont.)

- To generate a sample of size *n* of $X = (X_1, X_2, ..., X_k)$, the *n* values for X_1 are paired at random without replacement with the *n* values for X_2
- These pairs are then paired with the *n* values for X₃ forming triples, and so on through all *k* variables
- Thus each interval of each variable is used only once and each one-dimensional projection of the k-dimensional sample is a faithful representation of the distribution of X_i
- There is the capability of doing restrict paring to respect the correlation, if present, among the variables (same approximation are involved)

A Picture Will Help

- This is just one of the many LHS realization
- Each realization is constitute by n k-dimensional vectors



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DAKOTA Implementation on ERANOS





The Accuracy Requirements

Parameter	Input data origin (a priori) Input data origin (av. Modeling origin		Total	Uncertainty		
Neutronics						
		Core				
Multiplication factor, K_{eff} ($\Delta k/k$)	1%	0.2%	0.5%	0.5%	0.3%	
Power peak	1%	1%	3%	3%	2%	
Reactivity coefficients: total	7%	5%	15%	15%	7%	
Reactivity coefficients: component	20%	10%	20%	20%	10%	
Control rod worth: Element	5%	4%	6%	7%	5%	
Control rod worth: Total	5%	4%	4%	5%	2%	
Burnup reactivity swing (Δk/k)	0.7%	0.5%	0.5%	0.7%	0.3%	



The Reactor R-Z





The Average Compositions

Isotope	Density at equilibrium cycle (#/cm ³)	Isotope	Density at equilibrium cycle	Isotope	Density at equilibrium cycle (#/cm ³)
U234	1.545E-5	Pu242	2.726E-4	Fission Products	4.126E-4
U235	5.030E-6	Am241	1.069E-4	Fe	2.061E-2
U236	1.119E-5	Am242m	7.408E-5	Cr	2.994E-3
U238	1.697E-3	Am243	9.517E-5	Ni	1.153E-4
Np237	8.626E-5	Cm242	5.827E-6	Mo	2.117E-4
Pu238	1.414E-4	Cm243	5.688E-7	Zr	2.478E-3
Pu239	7.325E-4	Cm244	6.698E-5	Na	1.099E-2
Pu240	8.822E-4	Cm245	1.738E-5	Mn	2.218E-4
Pu241	1.610E-4	Cm246	9.456E-6		



First the Reference Value (Mean Value)

k _{eff}	Void Reactivity ^(b) (pcm)	Doppler Reactivity ^(b) (pcm)	Control-rod Reactivity ^(b) (pcm)
1.11418	2040.2	280.6 ^(a)	5746.8

(a) temperature from 850 K to 300 K

(b) Note: 1 pcm (percent mille):= $1.0e-5 \Delta k/k$

- R-Z model with 71x81 mesh, S4 angular approximation
- 33 energy group cross sections generated with a 1968 energy group library based on JEFF3.1.
- The cross section covariance data, called AFCI 1.2
- The analysis differentiates six reaction types: fission, capture, nu, (n,xn), elastic, and inelastic.



Keff Uncertainty Comparison: Reference = 1.11418

Isotope	ERANOS K _{eff} Uncertainty (%)	DAKOTA K _{eff} Uncertainty (%)	Absolute Difference in %: ERANOS vs. DAKOTA	Average K _{eff} from DAKOTA LHS Samples
Pu-238	1.32	1.23	0.09	1.11510
Pu-241	1.00	0.98	0.02	1.11406
Pu-240	0.76	0.73	0.03	1.11393
Am-242M	0.66	0.66	0.01	1.11413
Fe-56	0.29	0.52	0.23	1.11383
Pu-242	0.44	0.43	0.01	1.11398
Cm-245	0.42	0.40	0.02	1.11440
Cm-244	0.25	0.23	0.02	1.11377
Pu-239	0.21	0.20	0.01	1.11422
Na-23	0.11	0.11	0.00	1.11417
TOTAL UNCERTAINTY	2.08	2.04	0.04	-



Void Reactivity Uncertainty Comparison: Reference = 2040.2

Isotope	ERANOS Void Reactivity Uncertainty (%)	DAKOTA Void Reactivity Uncertainty (%)	Absolute Difference in %: ERANOS vs. DAKOTA	Average Void Reactivity from DAKOTA LHS Samples (pcm)
Fe-56	4.70	10.01	5.31	2025.0
Pu-238	8.82	8.24	0.58	2036.8
Na-23	4.94	4.94	0.00	2044.2
Pu-241	4.04	3.95	0.09	2039.0
Pu-240	3.74	3.61	0.13	2029.1
Pu-242	3.29	3.20	0.09	2036.6
Am-242M	2.57	2.54	0.04	2041.3
Cm-244	2.27	1.93	0.34	2050.2
Pu-239	1.94	1.78	0.16	2040.8
Fe-54	0.91	1.24	0.33	2043.1
TOTAL UNCERTAINTY	13.48	15.69	2.21	-



Doppler Reactivity Uncertainty Comparison: Reference = 280.6

Isotope	ERANOS Doppler Reactivity Uncertainty (%)	DAKOTA Doppler Reactivity Uncertainty (%)	Absolute Difference in %: ERANOS vs. DAKOTA	Average Doppler Reactivity from Dakota LHS Samples (pcm)
Fe-56	3.71	3.17	0.54	277.5
Pu-238	3.39	3.15	0.24	277.3
Pu-241	2.60	2.53	0.07	277.9
Am-242M	1.71	1.70	0.01	277.7
Pu-240	1.63	1.55	0.07	277.6
Pu-242	1.15	1.13	0.03	277.8
Cm-245	1.01	0.99	0.02	277.6
Cm-244	0.69	0.66	0.03	277.4
Pu-239	0.67	0.58	0.09	277.7
Am-241	0.61	0.57	0.04	277.7
SUM	6.42	5.91	0.50	-



Rod Worth Reactivity Uncertainty Comparison: Reference = 5746.8

Isotope	ERANOS Control Rod Reactivity Worth Uncertainty (%)	DAKOTA Control Rod Worth Reactivity Uncertainty (%)	Absolute Difference in %: ERANOS vs. DAKOTA	Average Control Rod Reactivity Worth Uncertainty from Dakota LHS Samples (pcm)
Pu-238	2.22	2.07	0.15	5741.5
Pu-241	1.44	1.40	0.03	5748.3
Pu-240	1.03	1.02	0.01	5748.8
Pu-242	0.87	0.85	0.03	5747.8
Am-242M	0.84	0.84	0.00	5746.8
Fe-56	0.47	0.80	0.33	5749.2
Cm-245	0.54	0.52	0.03	5745.5
Cm-244	0.37	0.36	0.02	5744.6
B-10	0.25	0.25	0.00	5746.7
Pu-239	0.24	0.23	0.01	5746.8
SUM	3.20	3.14	0.06	-



Conclusion on the Adjoint Comparison

- The adjoint technique required only four neutronics calculations and the evaluation of scalar products over space, angle, and energy for each uncertainty contribution.
- For this reason it was possible to compute the uncertainty contribution from each cross section with a breakdown according to energy group, reaction type, and isotope



Conclusion on the Forward

- LHS studies were conducted for each isotope, considering joint variation in all reaction type and energy groups simultaneously.
- The six reaction types and 33 energy groups considered led to 198 total input "parameters" to jointly perturb for each isotope
- LHS generated 6000 samples by isotope
- Strong sensitivity of the LHS results towards few bad calculation was also a reason of concern

The two methodology agreed fairly well



Questions??

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Bringing the Sensitivity Analysis One Step Further: Adjustment

- IF we know:
 - Uncertainties of the input parameter of a certain simulation
 - The discrepancy between the measure and the simulation
 - The sensitivity coefficient of the measured value from the uncertain parameter
- Then we can perform an statistical adjustment to select the value of the parameter within their uncertainty range that minimize the error (we choose the most probable set of value for the input that minimize the error)

How We Do It in Practice

- We select an experiment
- We compute the ratio between the computed values and the experimental ones (C/E) using a method virtually exempt from numerical and modeling errors

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- We compute the sensivity coefficient using an adjoint approach with a simplified model (sensitivity coefficient are less sensitive to the modelling)
- We use a statistical adjustment process to select the most likely value of the inputs.
- Next slides shows an ongoing work that apply this framework to the adjustment of the nuclear parameter.



Application to sodium cross sections: JANUS 8

- Deep penetration shielding problems through sodium slabs.
- Consider neutron attenuations within Na tank zone (detectors I6~I11).
- MCNP model is almost as-built configuration.
- ERANOS deterministic model was built by equivalently transforming MCNP model into R-Z model.
- Weight window technique was used for MCNP variance reductions.
- ERANOS calculations use 41-group structure (at this moment ENDF/B-VI) and S4 quadrature.



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3D view of MCNP model for Janus Phase 8 experimental facility in the ASPIS Trolley

EU6



C/E for Au197(n,γ) \rightarrow Au198 reaction rate slope



(Error Bar = $\sim \pm 3.5\%$)

EU7

Sensitivity & Uncertainty on Au197(n, γ) \rightarrow Au198

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Uncertainties from Na23 cross sections



C/E for S32(n,p) \rightarrow P32 Slope



EU9

Sensitivity & Uncertainty on S32(n,p) → P32

Uncertainties from Na23 cross section to S32(n,p) \rightarrow P32

Slope	17/16	I10/I6
Capture	5.3476e-4	3.3676e-3
Elastic	5.0125e-2	8.7948e-1
Inelastic	4.7759e-2	6.8506e-2
N,XN	4.4627e-5	4.3690e-4

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EU10

Summary

• JANUS Phase 8 sodium propagation experiment has been analyzed by MCNP and ERANOS. MCNP model is almost asbuild configuration in Cartesian coordinate, whereas ERANOS model is in R-Z coordinate which is equivalently transformed from MCNP model.

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- Sensitivity coefficient profiles helped for identifying important contributions to the uncertainty of reaction rate slopes.
- In future works:
 - Based on the benchmark results, carry out the consistent data assimilation for Na cross sections and perform calculations with adjusted cross sections.
 - Iron experiments.



Questions??